Vortex patterns and infinite degeneracy in the uniformly frustrated XY models and lattice Coulomb gas

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We find analytically and numerically that there exist infinite degeneracies in the ground state vortex configurations of a uniformly frustrated XY model on a square lattice for cases of frustrations $f=1/6$, 1/7, 1/8, and 1/10. More generally, we could also obtain a class of exact solutions for the phase configurations corresponding to the cases of $f=1/q=1/(2m)$ with an integer $m\geqslant 3$ of which the above cases of $m=3$, 4, and 5 correspond to the true ground states. These states are analogous to the staircase solutions originally given by Halsey [Phys. Rev. B **31**, 5728 (1985)], which, however, are relevant in a different regime of the frustration parameter (or vortex density). In these quasistaircase states, all the gauge-invariant phase differences are found to be integer multiples of $\pi/2q$. The supercurrents are conserved at each node in a trivial manner by separate channels. The infinite ground state degeneracy is preserved in the case of an arbitrary screening length for the corresponding lattice Coulomb gas.

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I. INTRODUCTION

Frustration [1,2] provides an important conceptual framework for understanding various equilibrium and nonequilibrium properties of statistical systems with competing interactions. Typically, existence of frustration strongly influences the low temperature properties in such a way that the symmetry of the Hamiltonian is changed and a complex low energy landscape is generated with many metastable states. In these frustrated systems, it is important to identify the ground and low lying excited states in order to understand the thermodynamic properties of the systems.

The uniformly frustrated XY (UFXY) model on a regular planar lattice is one example of the simplest frustrated systems where the strength of frustration can be continuously varied [3]. It provides an excellent theoretical laboratory for studying the commensuration-incommensuration effect and phase transitions as the magnitude of the frustration is varied. One important physical realization can be found in the two-dimensional Josephson junction arrays under a uniform magnetic field [4]. Periodic Josphson junction arrays (JJA) under a uniform magnetic field exhibit very rich phenomena as the strength of the magnetic field is varied. For the simplest case of a JJA on a square lattice or a triangular lattice with nearest neighbor Josephson coupling, an important parameter determining the frustration is the ratio f of the (external) magnetic flux Φ piercing a unit plaquette and the superconducting quantum flux $\Phi_0=hc/2e$.

In terms of the superconducting phases, the Hamiltonian can be written as

$$H(\{\theta\})=-J\sum_{(ij)}\cos(\theta_i-\theta_j-A_{ij}) \qquad (1)$$

where θ_i represents the phase variable of the superconducting order parameter at site i, J is the coupling energy and (ij) denotes nearest neighbor pairs. The bond angle $A_{ij}=(2e/\hbar c)\int_i^j\vec{A}\cdot d\vec{r}$ is proportional to the line integral of the magnetic vector potential $\vec{A}$ along the bond connecting sites i and j. A_{ij} satisfies the constraint $\Sigma_{i,j\in P}A_{ij}=2\pi f$ where the sum is over (i,j) belonging to the unit plaquette P. Since one can map the phase angle θ onto a planar XY spin via $\vec{S}_i\equiv(\cos\theta_i,\sin\theta_i)$, the above model Hamiltonian is also called a uniformly frustrated XY model.

One characteristic feature of the system is a sensitive dependence of physical properties on the rationality of the frustration parameter $f=p/q$ [3,5,6]. In spite of various research efforts during the past two decades or so, understanding of the low temperature behavior is still not complete for general values of the frustration $f=p/q$. Even the ground state configurations are known exactly only for some limited values of f. Via Villain transformation [7], the above UFXY model can be transformed into the two-dimensional lattice coulomb gas (LCG) [8], which is described by the following Hamiltonian,

$$H_{CG}=\frac{1}{2}\sum_{ij} q_iG(r_{ij})q_j \qquad (2)$$

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 $(1-f)$ or $-f$ which also correspond respectively to a vortex and an antivortex in the UFXY model. The lattice Green's function $G(r_{ij})$ solves the equation

$$\left(\Delta^2-\frac{1}{\lambda^2}\right)G(r_{ij})=-2\pi\delta_{r_{ij},0}, \qquad (3)$$

where Δ^2 is the discrete lattice Laplacian and λ is the screening length that, in normal case of no screening, is set to an infinity. For the case of usual Villain transformation of the

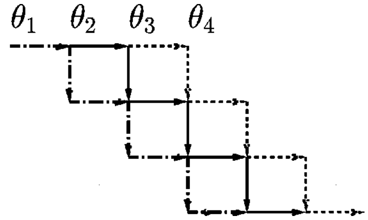

FIG. 1. The quasi-one-dimensional staircase state: gauge-invariant phase differences along a given staircase are constant.

UF*XY* model, we have $\lambda=\infty$. On a square lattice with periodic boundary conditions, $G(r)$ is given by

$$G(\vec{r})=\frac{\pi}{N}\sum_{k\neq 0}\frac{e^{i\mathbf{k}\cdot r}-1}{2-\cos k_x-\cos k_y+1/\lambda^2}, \qquad (4)$$

where $\mathbf{k}$ are the allowed wave vectors with $k_\mu=(2\pi n_\mu/L)$, with $n_\mu=0,1,\ldots,L-1$ and $N=L^2$ with linear dimension L. In the case of infinite screening length, for large separation r, one gets $G(\vec{r})\simeq-\ln r$.

In the case of UF*XY* model on a square lattice, the first systematic solutions were proposed by Halsey, which are called staircase states [9]. These states turn out to be the true ground state for some limited values of f with simple rational forms such as $f=1/2$, 1/3, 2/5, 3/7, 3/8, etc. The staircase states are characterized by quasi-one-dimensional current distribution where constant currents flow along the diagonal staircases (Fig. 1). The phase configurations exhibit periodicity with $q\times q$ unit cells.

In this work, we present another class of analytic solutions that are analogous to the staircase states of Halsey. We may call these states as *quasistaircase states*. These are solutions for the cases of the frustration parameter f in the form of $f=1/q$ with an even integer $q=2m$ and $m\geqslant 3$. We note again that the staircase states of Halsey are relevant in the dense frustration regime e.g., $1/3\leqslant f\leqslant 1/2$. On the other hand, the quasistaircase states that will be presented here are relevant in the lower vortex density regime $f<=1/6$. We find that for the special cases of $f=1/6$, 1/8 and 1/10, these analytic quasistaircase states correspond to the true ground states. We could slightly extend the above solutions to the cases of odd denominators $q=2m+1$, $m\geqslant 3$ and found numerically that at least for $f=1/7$ the ground state configuration can be represented by these solutions [10].

It is also found that, in contrast to the case of the staircase states, quasistaircase states exhibit infinite nontrivial degeneracies in the vortex configurations [11]. These states consist of parallel arrays of diagonal stripes that are half filled with positive vortices. In between these half-filled diagonals, there exist diagonals that are empty (in other words, filled with negative vortices (Figs. 4–6). Except for the half-filled diagonals, all the gauge-invariant phase configurations follow the staircase form where, for each diagonal staircase, a given single current flows from end to end. We can compare this situation with of the Halsey's staircase states where, for all of the diagonal staircases, unique (depending on the staircase) constant currents are flowing.

The existence of the half-filled diagonals together with that of the constant current staircase are the essential features that enable the infinitely degenerate vortex configurations. We also find that the gauge-invariant phase differences are all integer multiples of $\pi/2q$, i.e., they may be called rational states (or phase configurations). Due to the property of channel-wise conservation of the supercurrents, the gauge-invariant phase configurations also satisfy exactly the linearized (Gaussian) versions of the current conservation equation modulo 2π. We also find that the same infinite degeneracy holds in the corresponding LCG for an arbitrary value of the screening length λ, which probably comes from the above-mentioned Gaussian nature and rational property of the solutions in the UF*XY* model.

II. STAIRCASE STATES AND QUASISTAIRCASE STATES

Let us first work in the LCG picture of the vortices with the energy function given in Eq. (1). Since the vortex charges are constrained to lie on the lattice sites only, the continuum Abrikosov (triangular) configuration should be deformed to accomodate the lattice constraints. Simplest cases correspond to those where the ordered vortex structure forms a Bravais lattice. Suppose that $\vec{a}$ and $\vec{b}$ are the two (simple) unit Bravais vectors out of which we can form the whole sites of the vortices. That is, $\vec{r}_{n_1,n_2}=n_1\vec{a}+n_2\vec{b}$, n_1, $n_2=0,\pm 1,\pm 2,\ldots$. Now if we put $\vec{a}=(a_1,a_2)$ and $\vec{b}=(b_1,b_2)$, these components a_1, a_2, b_1, b_2 all take integer values in units of the lattice constant. We can see that the first condition to satisfy for the simple cases of $f=1/q$ is (due to the vortex density condition) the following [12,13]:

$$f^{-1}=q=|\vec{a}\times\vec{b}|=|a_1b_2-a_2b_1|. \qquad (5)$$

Since the underlying lattice has a square geometry, we expect that the vortex lattice with highest symmetry would also exhibit a square lattice configuration. In those cases of square vortex lattices, we have $|\vec{a}|=|\vec{b}|$ and $\vec{a}\perp\vec{b}$, i.e., $a_1^2+a_2^2=b_1^2+b_2^2$ and $a_1b_1+a_2b_2=0$. Combining the above relations, we can easily see that $a_1=b_2$, $a_2=-b_1$. Therefore, we get

$$f^{-1}=q=a_1^2+a_2^2=b_1^2+b_2^2. \qquad (6)$$

The simplest solution to the above relation is $q=2$, $f=1/2$ with $a_1=a_2=-b_1=b_2=1$, which corresponds to the checkerboard vortex pattern. The next simplest case corresponds to $q=5$, $f=1/5$ with $\vec{a}=(2,1)$ and $\vec{b}=(-1,2)$. Further possible solutions include, for $q=8$, $f=1/8$ with $\vec{a}=(2,2)$ and $\vec{b}=(-2,2)$ and also, for $q=18$, $f=1/18$ with $\vec{a}=(3,3)$ and $\vec{b}=(-3,3)$.

By relaxing the squareness constraint on the vortex lattice structure, we can find all possible Bravais lattice configurations for an arbitrary case of $f=1/q$. However, each of these configurations is only one of the many possible solutions. Whether or not these solutions (configurations) correspond to the real ground state configurations should be determined by either numerical means or analytic arguments. The only sys-

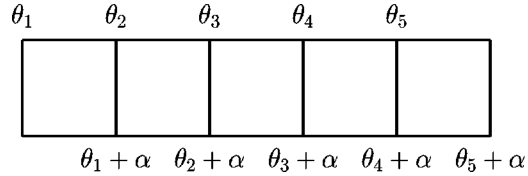

FIG. 2. The phase angles in the quasi-one-dimensional staircase state. The twist angle α determines the net current flow along the staircase direction.

tematic solutions are the staircase states given by Halsey [9] that turn out to be the true ground states only for some limited values of f in the dense regime $1/3 \leqslant f \leqslant 1/2$.

A. Staircase states

Here, we briefly review Halsey's staircase states. Halsey's staircase states are characterized by quasi-one-dimensional distribution of supercurrents such that, along a given diagonal staircase, a constant supercurrent flows. In other words, the gauge-invariant phase differences are constant along a given staircase. For concreteness, we work in a Landau gauge for the magnetic vector potential $\vec{A}(\vec{r})$ with $A_x=0$, $A_y=B_0x$. and $\Phi_0 \equiv B_0 a^2 = f\Phi_0 = (p/q)\Phi_0$. Thus we have

$$A_{ij}=\frac{2e}{\hbar c}\int_i^j \vec{A}\cdot d\vec{r}=\frac{2\pi}{\Phi_0}B_0 a^2 x_i = 2\pi f x_i \tag{7}$$

for (ij) along the y direction $(x_i \equiv x/a = 0, 1, 2, \ldots)$, while $A_{ij}=0$ for bonds (ij) along the x direction. We put the gauge-invariant phase differences along the horizontal bonds (i.e., bonds along the x direction) as $\phi_1, \phi_2, \ldots, \phi_q$ as in the Fig. 1, where

$$\phi_i \equiv \theta_i - \theta_{i-1}, \tag{8}$$

θ_i being the phase variable at site i.

We require an ansatz (staircase ansatz) that the configuration of supercurrents be quasi-one-dimensional along a diagonal direction that can be realized as in Fig. 2 with the introduction of a uniform phase twist α along a diagonal direction. Now, by combining the current conservation for each node and the vorticity constraints, we get

$$\sin(\theta_i - \theta_{i+1}) = \sin[\theta_{i+1} - (\theta_i + \alpha) + 2\pi f(i+1)], \tag{9}$$

which gives

$$\theta_i - \theta_{i+1} = [\theta_{i+1} - (\theta_i+\alpha) + 2\pi f(i+1)] + 2\pi n \tag{10}$$

with $n=0, \pm 1, \pm 2, \ldots$, leading to

$$(\theta_i - \theta_{i-1}) = \frac{\alpha}{2} - \pi f i + \pi n. \tag{11}$$

For each real value of the angle α in the above equation, we get a staircase state. However the state with vanishing net current corresponds to the ground state configuration with minimum energy. This condition of energy minimum gives $\alpha/2 = \pi/2q$ for $q=$ even and $\alpha/2=0$ for $q=$ odd [9]. The resulting staircase state is characterized by quasi-one-dimensional vortex configuration where all the plaquettes on a given diagonal are occupied with the same vorticity. It can be shown that for a given value of $f=p/q$, the configuration of vorticity along the direction perpendicular to the staircase becomes equivalent to those states given by Hubbard [14] and also by Pokrovsky and Uimin [15] derived from the representation of continued fraction.

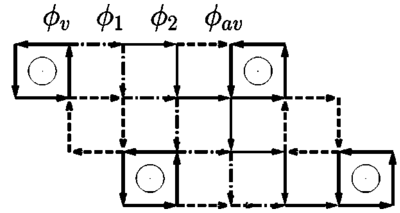

FIG. 3. The configuration of gauge-invariant phase differences in the quasistaircase state for $f=1/8$. Four independent gauge-invariant phase differences are shown with the corresponding bonds denoted by different line types. The plaquettes with positive vortices are denoted by circles.

B. Quasistaircase states

Now one can ask whether analogous solutions can be possible for the case of $f=1/q$ with $q>3$, namely, in the intermediate to low vortex density regime, such that Bravais (lattice) configuration corresponds to the ground states. To begin with, consider the cases of q an even number, that is, $q=2m$, m a positive integer. In the case of the staircase solutions, diagonal stripes are either fully filled with positive vortices or else fully empty (i.e., fully filled with negative vortices). We will show here that we can slightly modify the staircase states in such a way that the diagonal vortex stripes are replaced by half-filled diagonals of vortices placed at regular intervals. Suppose that the periodicity of the (vortex) diagonals is equal to m, then the vortex density becomes $f=1/q=1/(2m)$ because vortices are located every other plaquettes along the half-filled (vortex) diagonals. There are two questions to answer concerning this half-filled diagonal states. First is whether one can find an analytic or semianalytic solution for this class of states.

If the answer is yes, then the second question would be whether there exist cases when these solutions become (stable) ground states. We find that the answers to these questions are in the affirmative. Especially to the second question, we find that there are some cases where the quasistaircase states form the ground states. Furthermore, these states are shown to exhibit infinite degeneracies.

As shown in Fig. 3 we put an ansatz phase configuration such that the bonds on the diagonal staircases have constant supercurrents (or gauge-invariant phase differences), except those on the staircases enveloping the half-filled vortex diagonals. At each node, four bonds meet and currents are conserved trivially in separate channels (in the sense that we can separate the four bonds into two separate channels, each of which consists of two bonds such that the current along each channel is conserved. Now we denote the gauge-invariant phase differences surrounding the vortex plaquette as ϕ_v. Similarly, ϕ_{av} represents the phase differences per bond around the antivortex on the partially filled diagonal.

Now the remaining variables are the gauge-invariant phase differences along the diagonal staircases denoted by $\phi_1, \phi_2, \ldots, \phi_{m-2}$. The definition for these phase differences is such that positive phase differences denote positive currents in the direction of positive x axis. That is, we have, for example, $\phi_i \equiv \theta_i - \theta_{i+1}$ along the horizontal bonds on the top layer where θ_i is the phase variable at site i. From the vorticity condition of $\Sigma_{(ij)\in P}(\delta\theta - 2\pi A_{ij}) = 1-f \ (-f)$ for a positive vortex (a negative vortex), we find that $\phi_v = -\pi(q-1)/2q$ and $\phi_{av} = -(\pi/2q)$ satisfies the frustration constraints. Now we can also see that from vorticity constraints, we get

$$\frac{2\pi}{q} = \frac{(q-1)\pi}{2q} - \frac{\pi}{2q} + 2\phi_1. \tag{12}$$

Furthermore, ϕ_i and ϕ_{i+1} are related by $2\phi_{i+1} - 2\phi_i = 4\pi/2q$ or, $\phi_{i+1} = \phi_i + \pi/q$ from which we get

$$\phi_j = \frac{\pi(6-q)}{4q} + \frac{\pi(j-1)}{q}, \quad j = 1,2, \ldots, m-2. \tag{13}$$

We could numerically confirm that these states correspond to the real ground states for the cases of $f=1/6$, 1/8, 1/10. By summing the gauge-invariant phase differences along the horizontal axis, we get (in the Landau gauge)

$$\theta(0,j) - \theta(q,j) = 2(\phi_v + \phi_{av}) + 2\sum_{i=1}^{m-2} \phi_i = -\pi. \tag{14}$$

That is, the phase configuration is periodic with the period $2q$ lattice spacings along the horizontal axis. Similarly along the vertical axis, we get (taking the Landau gauge into consideration) $\theta(i,q) - \theta(i,0) = 0$ or $\pi(\text{mod}2\pi)$ for $q = 6+4n$ and $q = 8+4n$ (n a non-negative integer) respectively. Therefore, we conclude that for the case of $f=1/6$ and 1/10, the ground state configuration is $2q \times q$ periodic in phase configuration, while that of $f=1/8$ is $2q \times 2q$ periodic. We could confirm this expectation numerically. The energy (per site) for these states are

$$E_q = \frac{-4J}{q}\left[\cos\left(\frac{q-1}{2q}\pi\right) + \cos\left(\frac{\pi}{2q}\right) + \sum_{i=1}^{m-2} \cos\phi_i\right]$$
$$= \frac{-4J}{q}\left[\cos\left(\frac{q-1}{2q}\pi\right) + \cos\left(\frac{\pi}{2q}\right) + \frac{\sin\left[\pi\frac{(q-4)}{4q}\right]}{\sin\left(\frac{\pi}{2q}\right)}\right]. \tag{15}$$

Now, we also find that there exist a class of infinite number of states that are degenerate with the above staircase states, which can be described as follows. First cut in half the square lattice of the system across a diagonal that borders any one of the half-filled diagonals. Then, we can easily see that we can take one of the two regions and perform parallel transport of that region by one diagonal displacement. That is, all the gauge-invariant phase differences on one side being transported by one diagonal displacement which also results in a new configuration with the vortices on the transported side are correspondingly displaced exactly by one diagonal lattice constant. We can see that the total energy is simply conserved in this process. This is because, by the obvious definition of parallel phase transport, the change in energy can occur only along the interface region separating the two sides and the interfacial bonds simply change the direction of the current flow hence with no change in the total the energy.

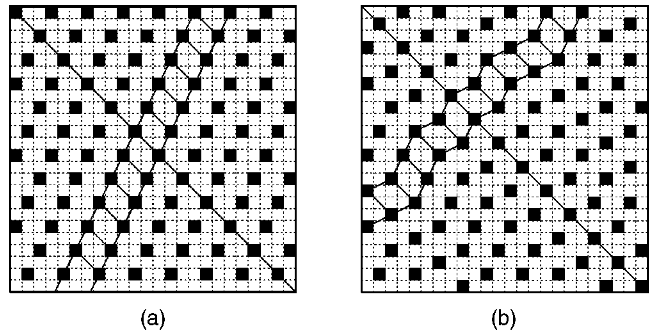

FIG. 4. (a) Bravais and (b) non-Bravais ground state vortex configurations (filled squares represent positive vortices) for $f = 1/6$. Solid lines are only guides to the spatial regularity of the vortex configurations.

Figure 4 shows the degenerate vortex configurations for the quasistaircase states of $f=1/6$, where Fig. 4(a) represents the Bravais vortex lattice and Fig. 4(b) is an example out of infinitely many non-Bravais states. The energy per site [see Eq. (15)] is $E(f=1/6) = -(2/3)J(1+\sqrt{3/2})$. The case of $f = 1/8$ is shown in Fig. 5. Here we find that there exist two kinds of Bravais states [Figs. 5(a) and 5(b)], one with square shaped vortex lattice and the other with oblique vortex lattice. Also shown is the case of $f=1/10$ in Fig. 6.

III. NUMERICAL RESULTS AND DISCUSSIONS

We performed Monte Carlo annealing simulations of both the UF*XY* model and the LCG Hamiltonian. For the cases of $f=1/8$ and 1/10, we could always obtain one of the degenerate vortex configurations corresponding to the quasistaircase states as the lowest energy states. We could also confirm that the gauge-invariant phase configuration showed perfect agreement with our analytical solutions for these cases. On the other hand, for the case of $f=1/6$, Monte Carlo annealing could not find any of the degenerate ordered configurations given above. Beginning with disordered initial states, we always ended up with some disordered metastable configuration, the energy of which is higher than (the predicted) degenerate configurations given above. This is probably related to the characteristic glassy behavior of the system at $f=1/6$ (see Ref. [16]). In order to numerically find the true ground state in this case, we relied on a global optimization method called the conformational space annealing method [17,18]. By using this method, we could identify the true ground state configuration for $f=1/6$, which agrees with the analytic solution of the quasistaircase state.

One thing to note is that, even though our proof of infinite

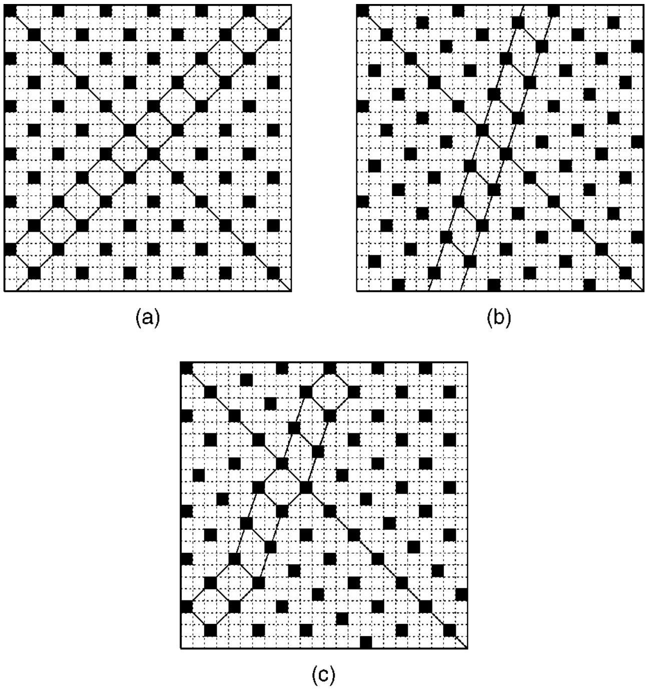

FIG. 5. Bravais ground states with (a) square and (b) parallelepiped patterns as well as (c) non-Bravais ground state for $f=1/8$. Solid lines are only guides to the spatial regularity of the vortex configurations.

degeneracy of quasistaircase states is based on the phase configuration of UFXY model, exactly the same degeneracy is found to be valid *numerically* in the corresponding LCG with the same value of f. Not just that, we could also confirm that the same degeneracy holds for the general case of an arbitrary screening length λ. This nontrivial result can probably be understood by noting that for q an even positive integer, the gauge-invariant phase differences of the quasistaircase states take integer multiples of $\pi/2q$ and also that these phases satisfy simple Gaussian equations [19].

Next, we turn to the cases of $f=1/q$ with odd integers $q \geqslant 7$. We first present the result of annealing simulations of LCG with $f=1/7$. Here we find that the ground state vortex configurations for $f=1/7$ consist of alternatingly 1/6-like and 1/8-like diagonal vortex configurations (Fig. 7). We also find

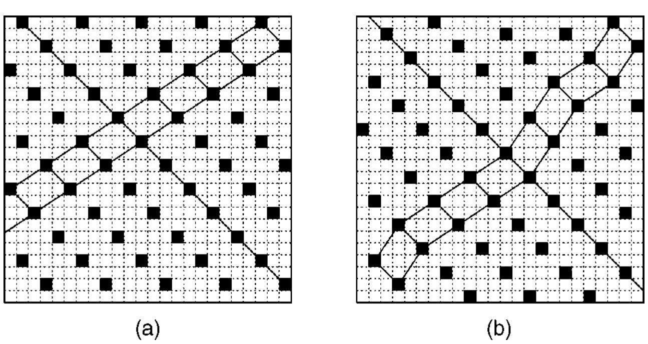

FIG. 6. The ground state vortex configurations for $f=1/10$. (a) Bravais state and (b) a non-Bravais state. Solid lines are only guides to the spatial regularity of the vortex configurations.

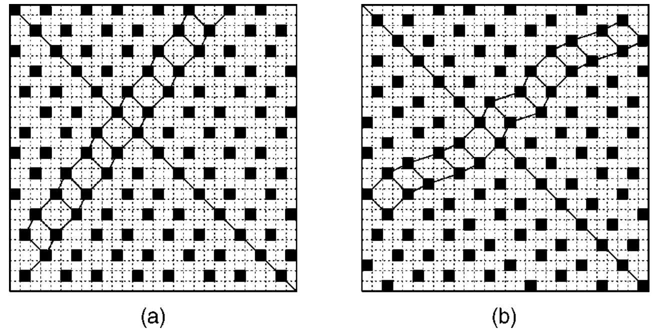

FIG. 7. The ground state vortex configuration for $f=1/7$ (a) Bravais; (b) non-Bravais states. Solid lines are only guides to the spatial regularity of the vortex configurations.

that there exist infinite degeneracies here (also shown in Fig. 7). The infinite degeneracy can also be understood [10] in the corresponding frustrated XY model in terms of diagonal staircases in a manner analogous to the cases of $f=1/6$, 1/8, and 1/10, but involves a more intricate combination of the phase configurations of $f=1/6$ and $f=1/8$, which we do not present here.

Next, we look into the case of $f=1/9$ by means of LCG methods and find that the lowest energy states have non-Bravais vortex configurations as in Fig. 8(a) that has an energy slightly below the Bravais state configuration of Fig. 8(b). In this case, however, there exists no infinite degeneracy in the vortex configurations.

Now, we investigate the nature of phase transitions in these systems. Since, in most cases, these systems are expected to undergo first order transitions, we apply the standard histogram methods [20]. Existence of first order transition near a specific temperature can be identified by double peaks in the energy histograms. The transition temperature can be determined as the temperature for which the areas under the two peaks are equal to each other (in the thermodynamic limit). We briefly mentioned above that simple Monte Carlo annealing simulations could not find any of the ground state configurations in the case of $f=1/6$. An interesting result in connection with this fact is that, for this case, we cannot discern a clear signature of first order transition in the energy histogram as the system size increases [21] (Fig.

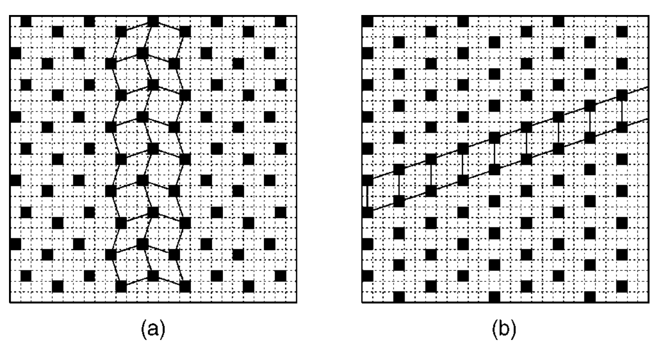

FIG. 8. Low energy vortex configurations for $f=1/9$ (a) non-Bravais and (b) Bravais states, among which the former corresponds to the ground state. Solid lines are only guides to the spatial regularity of the vortex configurations.

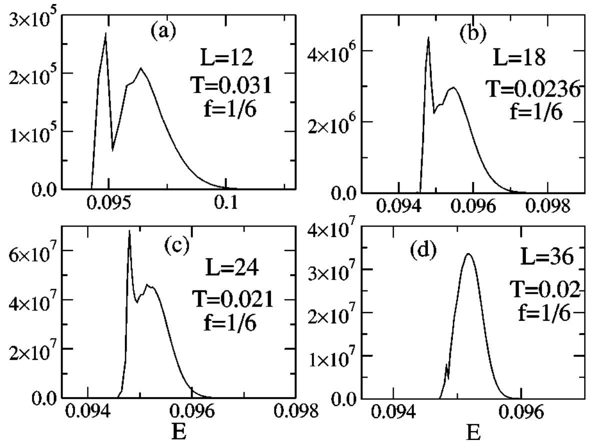

FIG. 9. The energy histogram for $f=1/6$ with (a) $L=6$, (b) $L=12$, (c) $L=24$, and (d) $L=36$. The energy E (horizontal axis) is in dimensionless units where the units of charges are simply put equal to unity [see Eq. (2) in the text].

9), which signals a sort of glassy features in this system as the temperature is lowered. On the other hand, for the case of $f=1/8$ (Fig. 10), 1/10 (data not shown), we clearly see a first order transition nature in the histogram of the energy.

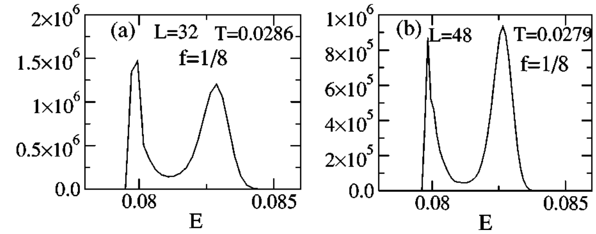

FIG. 10. The energy histogram for $f=1/8$ with (a) $L=32$ and (b) $L=48$. The energy E (horizontal axis) is in dimensionless units as in Fig. 9.

In summary, we showed that there exist infinite ground state degeneracies for selected values of f in the uniformly frustrated XY model and LCG on a square lattice. This happens especially for the values of $f=1/q$ with $q=6,7,8,10$. We showed that these states, in the phase representation of the UFXY model, can be described analytically as quasistaircase states.

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