Finding local minimum states of Josephson-junction arrays in a magnetic field

Mohammad R. Kolahchi
Atomic Energy Organization of Iran, Center for Theoretical Physics and Mathematics, P.O. Box 11365-8486, Tehran, Iran
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We conjecture that certain shift maps generate the local-minima phase structure of Josephson-junction arrays in a magnetic field. We propose a method of constructing the local minima. The classification scheme of the ground states is greatly simplified. [S0163-1829(97)04925-4]

Study of the ground states of Josephson-junction networks not only has aesthetic appeal, but also implications for its phase-transition properties. An array of Josephson junctions in a magnetic field perpendicular to its plane is the physical realization of the frustrated XY model, and is described by[1]

$$H=-J\sum_{\langle ij\rangle}\cos(\theta_i-\theta_j-2\pi f_{ij}). \tag{1}$$

Superconducting islands occupy the sites of the (square) array. In the classical regime, the physical state of an island is described by a phase. Nearest-neighbor islands, $\langle ij\rangle$, are coupled via the Josephson effect with the coupling strength, J, which is taken to be positive in Eq. (1). f_{ij} is the ratio of the line integral of the vector potential along the bond ij, to the flux quantum, Φ_0, where $\Phi_0=hc/2e$.[2] In terms of the flux Φ, through a unit cell of the square lattice, $f_{ij}=\eta_{ij}\Phi/\Phi_0$; with η_{ij} being an integer giving the x or y coordinate of the ij bond, depending on the choice of gauge. It is seen that when $f=\Phi/\Phi_0$ is an integer, the extra phase is a multiple of 2π—for all bonds. Therefore alignment of phases produces the ground state, and each bond is at its lowest possible energy. At noninteger values of f, it is not possible for every bond to be at its lowest energy state. In this sense the system is said to be frustrated, and the measure of frustration f is called the frustration factor. Due to the symmetries of the Hamiltonian, the model need only be considered for values of f in the range [0,1/2]. When $f=1/2$, the system is said to be maximally frustrated. A useful, though approximate way of representing the distribution of bond energies is to define the circulation of a cell[3]

$$\begin{matrix} l-k \\ |\quad | \\ i-j \end{matrix}\qquad S_i=I_{ij}+I_{jk}-I_{lk}-I_{il}. \tag{2}$$

The circulation or vorticity of a cell is the superconducting current circulating around it. The ground-state phase configuration is then transformed into a pattern, which is called the ground-state vortex lattice. Figure 1(a), shows the vortex lattice of the $f=1/4$ ground state, due to Teitel and Jayaprakash (TJ).[4]

Laboratory experiments[5] and computer simulations,[3,4] along with theoretical considerations,[6–8] indicate that for rational frustration factors $f=p/q$, the basic unit of the ground-state formation is a square having q cells on its edge. There are also cases where this basic unit is larger and has $2q$ cells to an edge. From these studies f takes on another meaning; it represents the ratio of the cells having large circulation to the total number of cells in the basic unit. A large circulation cell, usually called a vortex, is actually a high-energy cell, if the sum of bond energies is considered. The ground state is an orderly arrangement of few high-energy cells amongst many low-energy cells.

Here we study the minimum set of phases required to generate the ground state, hence the relation among the phases that compose the minimum energy vortex lattice. We conjecture that local minima of Eq. (1), could be generated from a minimal set via a kind of shift map. The manifest order of the ground-state vortex lattice, as well as other local minima, is encoded in phase correlations (‘‘symmetries’’) of a structure having a much smaller size than the basic unit.

We start by constructing a local minimum of $f=6/13$; the choice is made due to the difficulty of obtaining it using the standard methods. It is known that its ground state belongs to the class of vacancy vortex lattices. The idea of a vacancy lattice and the discovery of its generic structure is due to Straley.[9] When the density of vortices is near its maximum value, i.e., $f=1/2$, the system seems to prefer an orderly arrangement of ‘‘holes’’ against a checkerboard background. The vorticity of a hole or vacancy is what is expected of the negative vortex cell, however the four neighboring cells,

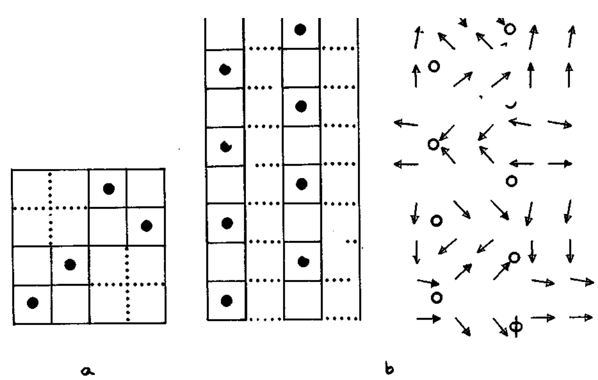

FIG. 1. Ground-state vortex lattice unit cells for $f=1/4$: (a) TJ ground state, (b) KSB (Korshunov-Straley-Barnett) ground state; broken lines indicate bonds carrying zero current. In (b) the phase configuration is also shown, $\tan\phi=-\sqrt{2}$. To find the configuration degenerate with it, start with $\theta_{1,1}=\theta_{2,1}=0$, $\theta_{3,1}=\theta_{4,1}=-\phi$, and $\alpha=3\pi/4$.

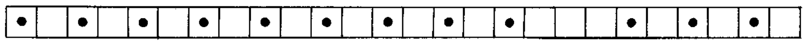

FIG. 2. This one-dimensional vortex lattice is used to generate the 6/13 vacancy vortex lattice of the ground state, $n=5$ and $\alpha=0$.

which also have negative vorticity, are of slightly less circulation. Except for such places, there is a checkerboard pattern. To fit such a pattern, the structure must be of even edge. For the present case, the density is 1/26 less than the maximum. This is exactly the density of vacancies in the 26×26 lattice.

Now, consider a lattice that has 26 cells in the form of a ladder. We intend to minimize the energy of this lattice when $f=6/13$. The boundary conditions we require are, periodic along the ladder, and open along the rungs. We use Landau gauge, so that only vertical bonds (i.e., the rungs of the ladder) carry the vector potential. The usual way of finding the ground state is application of the Metropolis Monte Carlo algorithm; we, however, equip the algorithm with the constraint

$$\theta_{\{i+n\},j+1}=\theta_{i,j}\,. \tag{3}$$

In Eq. (3), and in what follows, i denotes across and j denotes up; also, $\{i+n\}=(i+n)\mathrm{mod}q$. Hence, we have established a one-to-one relation between the top row and the bottom row of phases (for a ladder $j=1$). Using $n=5$, the resulting vortex lattice is given in Fig. 2.

The idea of constructing the whole vortex lattice is taken from the phenomenon of crystal growth. A crystal is grown from what is called the seed. The seed crystal is a minimum energy, minimum instruction set structure which has singled out certain symmetries for the growth of the large crystal. We intend to ''grow'' the 6/13 minimum energy vortex lattice using the lattice of Fig. 2 as its seed. The vortex lattice is grown one row at a time, keeping close to the minimum of the assembly at each stage. We call the one-dimensional (1D) vortex lattice of Fig. 2 a generating lattice.

Let us see the ''symmetry'' in the generating lattice. To do this, consider three rows of phases built according to

$$\theta_{\{i+n\},2}=\theta_{i,1}+\alpha, \tag{4a}$$

$$\theta_{\{i+n\},3}=\theta_{i,2}+\alpha-2\pi f n, \tag{4b}$$

where α is an arbitrary constant. The above relations are written in the Landau gauge. The term involving f in Eq. (4b), guarantees that first row of vertical bonds shares gauge-invariant phase differences with the second row of vertical bonds shifted n units to the right (Fig. 3). Due to the Landau gauge, the same statement is easily seen to hold for the three rows of horizontal bonds. Hence, if Eq. (4a) has resulted in a vortex lattice (similar to that of Fig. 2), then the same vortex lattice is formed by the second and third rows of phases, only shifted n units to the right, as shown in Fig. 3.

The basic idea of constructing the complete vortex lattice, is to use the vortex translation operations of Eq. (4) to shift the vortex lattice of a row by n units in the row above it. In the sense that the generating lattice could be any of the rows of the whole lattice, we see that the symmetry of the generating lattice of Fig. 2, with $n=5$, is to form a complete lattice with the property that each row of vortices is repeated in the row above it, only shifted 5 units to the right. The translation operation is generalized into the main result

$$\theta_{\{i+n\},j+1}=\theta_{i,j}+\alpha-(j-1)2\pi f n,\quad j=1,2,\ldots\,. \tag{5}$$

After construction of the vortex lattice, in our case when a 26×26 cell structure is formed, we quench it using the usual Metropolis Monte Carlo (MC) routine. The final product has energy of about $-1.3054J$ per site, and its structure is similar to that of $f=5/11$ given in Ref. 9. With $n=19$, the generating lattice looks the same as Fig. 2, but has a different phase configuration; the vacancies end up closer together on average, and energy per site is slightly higher, $-1.3031J$.

The remarkable finding of our study is that the phase correlation imposed in the beginning, is preserved after the vortex lattice is quenched. This is the important result of this study.

We can offer a heuristic argument for this result. With a constraint such as Eq. (3), it is no longer true that energy minimization corresponds to current conservation at each site. However, energetically each site is at a local minimum relative to its nearest neighbors. The shift map defined by Eq. (5) has the property of replicating a site along with its neighbors, and maintaining the corresponding bond currents. The product is a configuration of phases where each phase is inside a local potential well, but not at its bottom; because Kirchoff's current law does not yet hold at each site. Only after the system is quenched do we have a local minimum state. The experiments show that quenching at $T=0.01$ J/k reduces energy per site by about $0.11J$ to $0.28J$, indicating that the constructed vortex lattice had been in a metastable state, with its true temperature close to the quenching temperature. Therefore, only specially ordered arrangements of vortices constitute the states of local minima. In other words, only stable commensurate configurations are important, which could lend support to the TJ conjecture.[4]

When $n=1$, the vortex lattices are called staircase states, and there is a rigorous mathematical proof for the above finding due to Halsey.[7] The $f=1/4$ staircase state, constructed by the plan described is given in Fig. 4; its energy is about $-1.306(3)J$ per site. Halsey's analysis gives $-1.30656J$. The discrepancy is small enough to be confident that more MC steps and lower temperatures will result in more significant figures.

The constant α in the shift map, Eq. (5), serves the same purpose as α in Halsey's analysis, i.e., α is set by energy minimization; in our case by the quenching process. In general, quenching does not preserve the shift map (5), even though the phase configuration could still be approximately obeyed, and the vortex lattice preserved.[10] Our studies lead us to conjecture that: ground states fall in the class of local

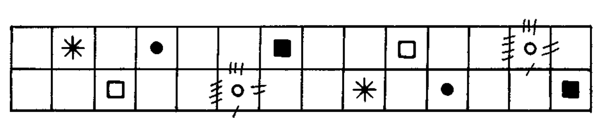

FIG. 3. The first row of vortices is shifted by seven units in the row above, by using the vortex shift maps of Eq. (4). Bonds carrying same current are shown for one of the vortices; $n=7$.

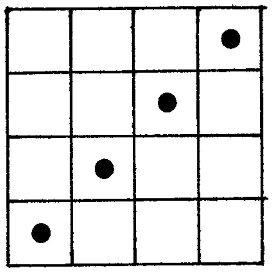

FIG. 4. The Halsey staircase local minimum for $f=1/4$; $n=1$.

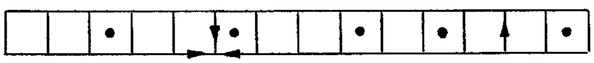

FIG. 5. If the stack of shifted 1D vortex lattices is to leave the phase configuration intact, as energy is minimized in the quenching process, each site must be in its local minimum before quenching. Therefore currents into each site of the complete vortex lattice must sum to zero, to begin with. This implies that the generator should obey Eq. (6). Here, the currents that participate in that equation are indicated for one of the sites. Compare with Fig. 3.

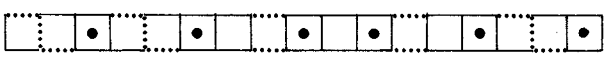

FIG. 6. The 1D generator vortex lattice of $f=6/17$. The ground-state vortex lattice is given in Fig. 7 of Ref. 3, $n=13$, energy per site is $-1.2902J$. Broken lines show bonds with zero gauge-invariant phase differences.

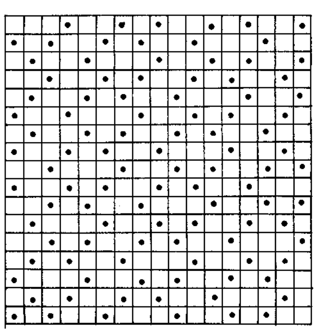

FIG. 7. A local minimum of $f=6/17$, $n=6$, energy per site is $-1.2634J$.

minimum vortex configurations which preserve the shift map. Then the generating lattice must have the property (see Fig. 5)

$$\sum I_{(i,1)}=I_{\{i+n\}}, \quad i=1,\ldots,q, \tag{6}$$

stating that, the net current into the site $(i,1)$ must equal the current in the vertical bond $(\{i+n\},1)-(\{i+n\},2)$. So to form local minimum configurations (instead of q^2 phases), one needs the parameters of the shift map, α and n, and the starting q phases obtained by Eqs. (6).[11]

For $q\times q$ periodicity, we must have

$$q\alpha-[(1/2)(q-1)q]2\pi fn=2\pi m, \tag{7}$$

where m is an integer. Then it easily follows that for q being even, when n is odd, $q\alpha=(2k+1)\pi$, $k=0,1,2,\ldots$, and when n is even, $q\alpha=2k\pi$. For q being odd, $q\alpha=2k\pi$. It also can be shown that different values of k do not amount to new configurations, but to a shift in the j coordinate. Hence, for $n=1$ we get $\alpha=\pi/q$ when q is even, and $\alpha=0$ when q is odd; results obtained by Halsey.[7]

Straley and Barnett[3] have found that for several f values, the ground state has a larger than $q\times q$ unit cell. Of those f values, we have studied $f=1/4$, 1/6, 3/10, 3/14, 5/16, 5/18. We find that in each case the phase configuration rotates by $\pi/2$ or $3\pi/2$ after $q/2$ shifts, at which point the vortex configuration repeats, i.e., the basic unit of formation in each case is $q\times 2q$. We also find that in each case $n=2$.[12] A relation similar to Eq. (7) gives $\alpha=\pi/q$ or $3\pi/q$. Now, considering consecutive-row phase rotation, $\theta_{\{i+n\},j+1}-\theta_{i,j}$, we note that each choice of α has its own set of phase rotations for various j. The conclusion is that such $q\times 2q$ states are doubly degenerate. In Fig. 1(b) we have shown the $\alpha=\pi/4$ phase configuration for $f=1/4$ Korshunov-Straley-Barnett ground state. The exact energy per site of the $f=1/4$ ground state is $-(3+\sqrt{3})J/2\sqrt{3}$.

The generator of $f=6/17$ ground state, having $n=13$, is given in Fig. 6. As Eq. (6) implies, it is as if we had taken such a structure, with its phase configuration, out of the ground-state vortex lattice. The complete vortex lattice of the ground state is shown in Fig. 7 of Ref. 3; we find its energy to be $-1.2902J$ per site. A local minimum of $f=6/17$ is given in Fig. 7; $n=6$.

We should emphasize that there are other ground states (or local minima) which do not belong to the 1D generator class. For instance, the TJ ground state of $f=1/4$ [Fig. 1(a)], the 5/14 ground state,[3] or the 7/15 vacancy lattice ground state.[9] In such cases more complicated generators are needed (e.g., a two-row vortex lattice as the generator of the TJ $f=1/4$ ground state).

In summary, we have helped to reveal the phase structure of the local minima of the frustrated XY models with rational frustration. Our study should be useful in developing a pinning potential model for the vortex lattice of Josephson-junction arrays in a magnetic field.

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[1] There is vast literature on the subject, see for example, Physica B **222** (1996).

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[10] This is directly related to the question of why ground states (or local minimum states) almost always have $q\times q$ unit cells. For example, a 7×14 vortex lattice of $f=5/14$, suffers from a strain due to the boundary condition imposed on it. The phase configuration cannot follow the shift map exactly and minimize energy at the same time; vortices remain in their places. A 2×14 lattice of $f=5/14$ (Fig. 3), on the other hand, is kept together solely by boundary condition effects.

[11] The tendency of the one row lattice to form a lattice according to f, as a function of n is an open question. For a given q there are $q/2$ (for even q) or $(q-1)/2$ (for odd q) distinct n values. (n and $q-n$ give mirror image vortex lattices.) In practice it is easier to use the shift-map-equipped MC algorithm on the one row lattice followed by quenching of the constructed vortex lattice, rather than actually solving Eqs. (6). For a given n there could be more than one solution. It could be that a given n produces a vortex lattice, that when shifted, results in a configuration with nearest-neighbor vortices. These are high-energy states. The choices for n giving low-lying states are few.

[12] In general, if a $q\times q'$ unit cell is to be found, both the vortex configuration and the phase configuration must repeat after q' shifts. In the vacancy lattices of the type discussed here, the phase periodicity is q, but the vortex periodicity is $2q$. Equation (7) gives the condition for phase periodicity; for vortex periodicity we need $\{m+nq'\}=m$, where m is an integer not greater than q. For example, $f=5/14$ with $q'=2$ and $n=7$, has $\alpha=\pi/2$ and a 22212 generator (numbers give vortex spacings); its energy per site is $-1.254J$. For having $q\times 2q$ periodicity, as described in the text, i.e., with $q/2$ vortex periodicity, even n would do. For $f=5/18$ and $n=4$ the energy per site is $-1.280J$; the generator has 21514 structure. When $n=2$, the energy is $-1.335J$, and the structure becomes 32332. It remains to be explained why $n=2$ results in the ground state in $q\times 2q$ lattices.