Fractional vortices in the XY model with $\pi$ bonds

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We define a new set of excitations in the XY model which we call “fractional vortices”. In the frustrated XY model containing $\pi$ bonds, we make the ansatz that the ground state configurations can be characterized by pairs of oppositely charged fractional vortices. For a chain of $\pi$ bonds, the ground state energy and the phase configurations calculated on the basis of this ansatz agree well with the results from direct numerical simulations. Finally, we discuss the possible connection of these results to some recent experiments by Kirtley et al [Phys. Rev. B 51, R12057 (1995)] on high-$T_c$ superconductors where fractional flux trapping was observed along certain grain boundaries.

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I. INTRODUCTION

The classical XY Hamiltonian is one of the most studied models in statistical physics. In its usual, unfrustrated form, it is written

$$ H = \sum_{\langle ij \rangle} J_{ij} [1 - \cos(\phi_i - \phi_j)], \quad (1) $$

where $\phi_i$ is a phase variable on the $i$th site ($0 \leq \phi < 2\pi$), the sum runs over distinct pairs $\langle ij \rangle$, and $J_{ij}$ is the energy of the coupling between sites $i$ and $j$. In the ferromagnetic, nearest-neighbor case, $J_{ij}$ vanishes except between nearest-neighbor sites and all the $J_{ij}$’s are equal to a single positive constant $J$. In this case, for spatial dimensionality $d \geq 3$, there is a phase transition to a ferromagnetic state at a critical temperature, with conventional critical phenomena. If $d = 2$, there is instead the Kosterlitz-Thouless-Berezinskii phase transition, in which pairs of opposite-charge integer vortices unbind at a finite temperature $T_{KTB}$. The classical XY model has been found to describe a wide variety of systems with complex scalar order parameters, including bulk superconductors in $d = 3$, superconducting films, Josephson junction arrays in $d = 2$, and superfluid He$_4$ films.

Recently, the XY model with anti ferromagnetic bonds i.e., with bond strengths $J_{ij} < 0$ (also called $\pi$ bonds), has received much attention in particular due to its possible relevance to high-$T_c$ superconductors and other experimental systems. Specifically, if we consider the grain boundary between two high-$T_c$ superconductors with suitable misorientation of the crystalline axes, then the resulting Josephson coupling across the boundary can have the coupling energy $J_{ij} < 0$. This is a consequence of the $d_4^{2g}$ symmetry of the order parameter in many high-$T_c$ materials. Such grain-boundary interfaces have lately been studied in a variety of experiments and in several geometries. These experiments have led to interesting results, such as the observation of the trapping of half-integer and also other fractional flux quantum. These results can be explained using models involving $\pi$ bond and $\delta$ bond. Similar models involving $\pi$ bonds have also been developed to explain such phenomena as the paramagnetic Meissner effect, also observed in samples of high-$T_c$ superconductors.

A key concept in understanding the effects of $\pi$ bonds is “frustration.” Consider, for example, the XY model on a square lattice with only the nearest-neighbor couplings nonvanishing. If a plaquette has an odd number of bonds, that plaquette is frustrated, in the sense that no choice of angles in the four grains making up the plaquette can simultaneously minimize all the bond energies. Thus, a single $\pi$ bond will cause the two plaquettes adjoining that $\pi$ bond to become frustrated. In a line of $\pi$ bonds, only the two plaquettes at the end of the line will become frustrated. Because of the frustrated plaquettes, it is non-trivial to find the ground state of the XY-model with $\pi$ bonds. In this paper, we will show, both numerically and by analytical arguments, that these ground states are characterized by certain spatial phase configurations which we call fractional vortices. We will also derive an expression for the interaction energy of two fractional vortices in the XY model.

The rest of the paper is organized as follows. In Section II, we define the fractional vortices and calculate the interaction energy of a bound pair of fractional vortices for the XY model. In Section III, we study the ground state of XY-lattices containing a single $\pi$ bond, two $\pi$ bonds, and a string of $\pi$ bonds. In each case, using a variational ansatz for the ground-state configuration, we find that there is a critical $\pi$ bond strength, above which the ground state contains pairs of oppositely charged fractional vortices. To check these results, we directly calculate the ground-state energy of these lattices using a numerical relaxation technique based on the equations of motion for overdamped Josephson junctions. We find that both the ground-state energy and the critical $\pi$ bond...
strength, predicted by the variational approach, are in
excellent agreement with the numerical results. Finally,
in Section IV, we discuss the possible relevance of these
numerical results to experiments carried out in systems
containing $\pi$ junctions, such as high-$T_c$ superconductors
containing grain boundaries and tricrystals, as recently studied by Kirtley et al.\textsuperscript{[3-5]}

II. FRACTIONAL VORTICES IN THE
UNFRUSTRATED XY MODEL

Consider the Hamiltonian \( H \) for an XY model defined
on a square lattice with \( N \times N \) sites. If all the nearest
neighbor couplings are equal, this may be written

\[
H = J \sum_{\langle ij \rangle} [1 - \cos(\phi_i - \phi_j)].
\]  

(2)

Hereafter, we shall use units such that \( J = 1 \). The phase
angle, \( \phi_i \), at point \((x_i, y_i)\) due to a fractional vortex of
charge \( q \) at point \((x_0, y_0)\) is defined to be

\[
\phi_i(x_0, y_0, q) = q \times \tan^{-1}(\frac{y_i - y_0}{x_i - x_0}).
\]  

(3)

For \( q = 1 \), we recover the standard configuration for an
integer vortex. This definition can be seen as a generalization
of the concept of half-vortices introduced by Villain\textsuperscript{[2]}
for the same model. Note that, while for the integer vortex the bond angles change continuously, the
fractional vortex case is characterized by a branch cut, across which the bond angles are discontinuous.

This singularity leads to several other distinctions be
tween integer and fractional vortices. For example, the
energy associated with a single integer vortex is propor
tional to \( \ln(N) \). In the thermodynamic limit, this is a
weak divergence which makes the KT vortex-antivortex unbinding transition possible. By contrast, the energy of
an unbound fractional vortex is \( \propto N \), since the number of
bonds along the branch cut is \( \propto N \). Thus, it is energetically
unfavorable at all temperatures to create isolated fractional vortices. But a bound pair of fractional vortices with charges \( q \) and \(-q\) is much less expensive energetically, because then the branch cut is restricted to the line joining the two charges: the total energy should be proportional to the separation of the fractional vortices.

For fixed \( q \) and large enough separations, this energy is always larger than that of a pair of oppositely charged integer vortices, whose energy varies as the logarithm of their separation. Nevertheless, for fixed separation, it is always possible to find a non-integer \( q \) such that that the energy of the fractional vortex pair is less than the corresponding energy for the integer vortices. In the following, we derive expressions for the energy of a bound pair of fractional vortices in the XY model, and compare them to numerical results obtained by calculating the energy explicitly for these configurations.

We first consider a bound pair of integer vortices of
charge \( \pm 1 \) located at \((x_0, y_0)\) and \((x_1, y_1)\). The standard
KT expression for the energy of the pair is obtained by
approximating the Hamiltonian as

\[
H \sim \frac{1}{2} \sum_{\langle ij \rangle} (\phi_i - \phi_j)^2.
\]  

(4)

For the phase configuration, we use \( \phi_i = \phi_i(x_0, y_0, +1) + \phi_i(x_1, y_1, -1) \), where \( x_1 - x_0 = n \) and \( y_1 - y_0 = 0 \) (in units of the lattice constant \( a \)). Substituting this configuration into \( H \) gives the Kosterlitz-Thouless formula for the interaction energy, \( E_{KT} \), of two oppositely charged integer vortices:

\[
E_{KT}(n) = 2\pi \left[ \ln n + \frac{\pi}{2} \right].
\]  

(5)

In Fig. 1, we compare this expression to the energy of a pair of oppositely charged integer vortices, computed using the same phase configuration but the exact \( H \). The discrepancy arises from the expansion of the cosine factor, which is inaccurate for the bonds closest to the vortices. This inaccuracy is remedied by adding a core correction iteratively, i.e., by calculating the contribution from the bonds on the perimeter of the plaquettes surrounding the vortices exactly, rather than by a quadratic expansion. For large \( n \), the core-correction energy, \( E_c(n) \), is approximately given by

\[
E_c(n) = \pi^2 - 8 + \frac{12 - \pi^2}{2n^2} + \frac{8 + \pi^2}{16n^4}.
\]  

(6)

As can be seen from Fig. 1, the numerically calculated
energy is well approximated by \( E_{KT}(n) + E_c(n) \).
angles in region A are not small for arbitrary quadratic expansion. This is necessary, because the bond arising from the bonds along the branch cut. Note that to the total energy of a bound pair of integer vortices, as just discussed. The phase configuration, the vortices are separated by three plaquettes.

Using the quadratic approximation, the corresponding energy contributions to \( E(q,n) \) coming from these two groups of bonds. Thus \( E(q,n) = E_A(q,n) + E_B(q,n) \). To obtain \( E(q,n) \) we proceed as follows:

1. We calculate \( E_A(1,n) \), using the quadratic expansion for the cosine. \( E_A(1,n) \) is simply the contribution to the total energy of a bound pair of integer vortices arising from the bonds along the branch cut. Note that there are \( n \) bonds in region \( A \). Once \( E_A(1,n) \) is known, we get \( E_B(1,n) = E_{KT}(n) - E_A(1,n) \).

2. We obtain \( E_B(q,n) \) by noting that, in the quadratic approximation, \( E_B(q,n) = q^2 E_B(1,n) \).

3. Finally, we determine \( E_A(q,n) \) by directly evaluating it using the full expression for the cosine, not the quadratic expansion. This is necessary, because the bond angles in region \( A \) are not small for arbitrary \( q \).

We now use the outlined procedure to obtain \( E(q,n) \).

**Step 1:** Let \( \theta_{i,A}(1,n) = \phi_{iu} - \phi_{il} \) denote the \( i^{th} \) bond angle (cf. Fig. 2) in region \( A \) for \( q = 1 \). For the two-vortex configuration, \( \theta_{i,A}(1,n) \) is given by

\[
\theta_{i,A}(1,n) = 2 \left[ \tan^{-1} \left( \frac{1}{2i-1} \right) + \tan^{-1} \left( \frac{1}{2n-2i+1} \right) \right] \tag{7}
\]

Using the quadratic approximation, the corresponding energy contribution \( E_A(1,n) \) is given by

\[
E_A(1,n) = \frac{1}{2} \sum_{i=1}^{n} \theta_{i,A}^2(1,n). \tag{8}
\]

Using the approximation: 
\[
\tan^{-1} \left[ 1/((2i-1)) \right] \sim 1/(2i-1) \quad \text{for} \quad i \geq 2,
\]

we find

\[
E_A(1,n) = \frac{\pi^2}{2} + \left( \frac{\pi}{2} + \frac{2}{2n-1} \right)^2 + \frac{2}{n} [\gamma + 2 \ln 2 - 2 - 2n] + \frac{2}{n} \psi \left( n - \frac{1}{2} \right) - \psi' \left( n - \frac{1}{2} \right)
\]

where \( \psi(x) \) and \( \psi'(x) \) are the Digamma function and its derivative, \( \gamma \) is Euler’s constant, and \( E_{KT}(n) \) is given by Eq. (5).

**Step 2.** Using the results of step 1 and Eq. (3), we get

\[
E_B(q,n) = q^2 \left[ 2 \pi \ln n + \pi^2 - E_A(1,n) \right]. \tag{10}
\]

**Step 3.** The next step is to calculate \( E_A(q,n) \). Bond angles in region \( A \) are given by

\[
\theta_{i,A}(q,n) = q [2 \pi - \theta_{i,A}(1,n)]. \tag{11}
\]

Correspondingly, the energy \( E_A(q,n) \) is given by

\[
E_A(q,n) = \sum_{i=1}^{n} (1 - \cos [\theta_{i,A}(q,n)]). \tag{12}
\]

Since the bond angle \( \theta_{i,A}(q,n) \) is not small for an arbitrary \( q \), we cannot expand the cosine term only to second order. But for any \( q \), the difference \( \theta_{i,A}(q,n) - \theta_{n/2,A}(q,n) \) is a small parameter for any \( i \geq 2 \). Expanding the cosine term in Eq. (12) to second order in this parameter, we obtain an expression for \( E_A(q,n) \). This expression can be summed, and eventually gives

\[
E_A(q,n) = (n-2) \left[ 1 - \cos \alpha_n \right] + \frac{8q^2}{n^2} \cos \alpha_n + \frac{4q}{n} \sin \alpha_n
\]

\[
+ 2 \left( 1 - \cos \left[ 2 \pi + \frac{2}{n-1} \right] \right) - \frac{4q^2}{n} \cos \alpha_n + q \sin \alpha_n
\]

\[
\times \sum_{m=2}^{n-1} \theta_{m,A}(1,n) + \frac{q^2}{2} \cos \alpha_n \sum_{m=2}^{n-1} \theta_{m,A}^2(1,n), \tag{13}
\]

where

\[
\sum_{m=2}^{n-1} \theta_{m,A}(1,n) = 2 \gamma - 4 + 4 \ln 2 + 2 \psi \left( n - \frac{1}{2} \right), \tag{14}
\]

\[
\sum_{m=2}^{n-1} \theta_{m,A}^2(1,n) = \pi^2 + \frac{4}{n} \left( \gamma + 2 \ln 2 - 2 - 2n \right) + \frac{4}{n} \psi \left( n - \frac{1}{2} \right) - 2 \psi' \left( n - \frac{1}{2} \right) \tag{15}
\]

\[
\alpha_n = q \left( 2 \pi - \frac{4}{n} \right). \tag{16}
\]
Adding up the contribution from the two regions, we finally get the required expression for the energy of a bound pair of fractional vortices. As noted earlier, the core corrections must be included to attain high numerical accuracy. In the present case, it is sufficient to include these corrections only for the bonds labeled $C_1$ and $C_2$ in Fig. 2 using the procedure outlined earlier. This approximation is equivalent to extending region A to include bonds $C_1$ and $C_2$. Correspondingly, the core-corrected total energy is given by

$$E(q, n) = E_A(q, n) + E_B(q, n) - q^2 \theta_c^2 + 2 \left[1 - \cos(q \theta_c)\right]$$

(17)

where

$$\theta_c = \frac{\pi}{2} - \frac{2}{2n + 1}. \quad (18)$$

Expressions (17) and (18) are compared to the results of numerical computation in Figs. 3(a) and 3(b); agreement between the two is excellent. On the basis of this agreement, which is equally good for all values of $q$ and $n$ which we have considered, we present this result as a good analytical expression for the interaction energy between two fractional vortices in the unfrustrated XY model on a square lattice. This result is a generalization of the integer vortex excitations proposed by Kosterlitz and Thouless.

For large $n$, we can further simplify the above expression by dropping terms of $O(1/n)$ and smaller in Eq. (17) to get

$$E(q, n) = (n - 2)[1 - \cos(2\pi q)] + 2 \ln n \left[\pi q^2 - q \sin(2\pi q)\right]$$

$$+ \frac{3}{4} \pi^2 q^2 + 2 \left[1 - \cos\left(\frac{3\pi q}{2}\right)\right]. \quad (19)$$

III. FRACTIONAL VORTICES IN THE XY MODEL WITH $\pi$ BONDS

The fractional vortex configurations introduced in the previous section provide a natural way of characterizing the ground state of the XY model containing $\pi$ bonds. In this section, we implement this description by making a variational guess for the ground-state configuration using fractional vortices. We then compare our variational results with those obtained by numerically relaxing to the ground-state configuration, and find excellent agreement. In the following subsections, we will focus on obtaining the critical bond strength, $\lambda_c$, above which the ferromagnetic ground-state solution becomes unstable, and the ground-state configuration contains bound pairs of fractional vortices. For the case of one and two $\pi$ bonds, we also compare our results to those from previous studies by Vannimenus et al. Note that in these calculations, in which the goal is to calculate the threshold bond strength above which the ferromagnetic ground state becomes unstable rather than the absolute energies as a function of $\lambda$, it is unnecessary to include the core corrections. Hence, $\lambda_c$ can be calculated analytically as demonstrated below. The ground-state configuration and energy for $\lambda > \lambda_c$ do need the core corrections for greatest accuracy. We obtain them numerically using our variational guess and discuss them in the subsequent section.

A. One $\pi$ bond

We first consider the case of a single $\pi$ bond i.e, a single antiferromagnetic bond in a host of ferromagnetic bonds.
FIG. 4. Schematic plot of three configurations, each containing π bonds (full lines), which are (a) parallel and adjacent, (b) parallel and non-adjacent, and (c) perpendicular and non-adjacent. Also shown are the corresponding locations of the fractional vortex charges for the variational configurations.

As before, we take the bond strength of the ferromagnetic bonds to equal unity, and we denoted the strength of the antiferromagnetic bond by \( \lambda \) (\( \lambda \geq 0 \)). The problem is to obtain the ground-state configuration and energy for arbitrary strength, \( \lambda \), of the π bond.

To solve this problem, we make a variational guess for the ground-state configuration: it is the phase configuration corresponding to a bound pair of fractional vortices of strength \( \pm q \), located at the centers of the two plaquettes adjacent to the π bond. The charge, \( q \), is a variational parameter with respect to which the ground-state energy is minimized for a given \( \lambda \).

The total energy of this configuration discussed above is readily obtained using the procedure of the previous section, suitably corrected for the fact that we have a π bond instead of a ferromagnetic bond. The angle difference across the π bond is given by \( \theta_\pi = q\pi \). Then, using Eqs. (8) and (10), we get

\[
E_B(q) = \frac{1}{2}q^2 \pi^2 ,
\]  
(20)

while from Eq. (12) we find

\[
E_A(q) = 1 + \lambda \cos(q\pi) .
\]  
(21)

Adding these two terms gives the total energy of the configuration. Minimizing this energy with respect to \( q \) yields the condition

\[
q\pi = \lambda \sin(q\pi) .
\]  
(22)

For \( \lambda \leq 1 \), the ground-state configuration corresponds to \( q = 0 \): all the phases are perfectly aligned. For \( \lambda > 1 \), the ground-state configuration corresponds to a bound pair of fractional vortices with charges \( \pm q \) obtained by solving Eq. (22). Thus, the ferromagnetic ground state is unstable above a critical bond-strength value \( \lambda_c = 1 \).

The same value has been obtained previously by workers using different approaches.

B. Two π bonds

We now consider the case of two parallel, adjacent π bonds. As before, our variational guess for the ground state is the configuration corresponding to a bound pair of fractional vortices; we take these to be located as shown in Fig. 4(a). The corresponding total energy is again calculated using the procedure outlined in Section II. Using Eqs. (8) and (10), the energy contribution \( E_B(q) \) is

\[
E_B(q) = q^2 \left\{ 2\pi \ln 2 + \pi^2 - \left[ \frac{\pi}{2} + 2 \tan^{-1}(1/3) \right]^2 \right\} .
\]  
(23)

Using Eq. (12), we get

\[
E_A(q) = 2 + 2\lambda \cos \left\{ 2q \left[ 3\pi/4 - \tan^{-1}(1/3) \right] \right\} .
\]  
(24)

Adding these two contributions gives the total energy, which is to be minimized with respect to \( q \) for a given \( \lambda \). This procedure gives the critical value \( \lambda_c = 0.563 \), which is in good agreement with the exact value \( \lambda_c = \pi/2 - 1 \), obtained by Vannimenus et al.

Next, we consider the case of two parallel, but non-adjacent π bonds, as shown in Fig. 4(b). Taking the bond centers to have the coordinates \((0,0)\) and \((m,n)\),
we calculate the energy using the variational procedure described above with vortex charges as shown. For large separation between the bonds (\(\sqrt{m^2 + n^2} \gg 1\)), this procedure gives

\[
E_B(q) = q^2 \left[ 2\pi^2 - 2\alpha_{mn} - (\pi - \alpha_{mn})^2 \right]
\]

(25)

and

\[
E_A(q) = 2 + 2\lambda \cos [q(\pi + \alpha_{mn})],
\]

(26)

where

\[
\alpha_{mn} = \frac{m^2 - n^2}{(m^2 + n^2)^2}.
\]

(27)

Minimizing the total energy gives the critical bond strength as

\[
\lambda_c = \frac{1 - 2\alpha_{mn}/\pi}{1 + 2\alpha_{mn}/\pi}.
\]

(28)

Similarly, for two non-adjacent perpendicular \(\pi\) bonds [Fig. 4(c)], we find

\[
E_B(q) = q^2 \left[ 2\pi^2 - 2\beta_{mn} - (\pi - \beta_{mn})^2 \right]
\]

(29)

and

\[
E_A(q) = 2 + 2\lambda \cos [q(\pi + \beta_{mn})],
\]

(30)

where

\[
\beta_{mn} = \frac{2mn}{(m^2 + n^2)^2}.
\]

(31)

In this case, the critical bond strength is

\[
\lambda_c = \frac{1 - \beta_{mn}/\pi}{1 + \beta_{mn}/\pi}.
\]

(32)

These results are identical to those obtained previously by Vannimenus et al, using a different approach. The agreement lends support to our hypothesis that the ground-state configuration of such systems can be characterized by a set of fractional vortices (in the cases considered here, a set of only two oppositely charged fractional vortices). Besides having the merit of simplicity, our approach also easily yields the ground-state configuration and energy for arbitrary \(\lambda\). Moreover, our procedure can be used to obtain the ground-state even when the separation between the bonds is not large. In particular, for two parallel bonds such that \(m = n = 1\), our variational procedure yields the surprising result that \(\lambda_c = 1\) for this configuration. The same result was obtained in a numerical study done by Gawiec et al. Finally, our variational ansatz can readily be generalized to longer \(\pi\) bond chains, as we shall see in the next section.

C. Chains of \(\pi\) bonds

Next, we consider chains of \(\pi\) bonds of length \(n \geq 3\). In this case, we make the variational ansatz that the ground state consists of \(n/2\) or \((n + 1)/2\) pairs of oppositely charged fractional vortices for even or odd \(n\), arranged as shown in Fig. 5. As before, we proceed by calculating the contribution to the total energy from regions A and B. However, the procedure outlined in Section II has to be generalized to include many pairs of fractional vortices. Since the details are significantly different from that outlined in section II, we briefly describe the generalized procedure below.

(1) We consider the case in which all charges have magnitude unity. The total energy of this configuration is given simply by the KT expression

\[
E_{KT} = -2\pi \sum_{j<k} q_j q_k \ln(n_{jk}) + \pi^2 \sum_j q_j^2,
\]

(33)
contribution from bonds in region B is still given by Eq. (35). Correspondingly, the energy fraction of charges, the bond angle differences in region B are fractional ($|q| < 1$). The bonds can still be divided into classes A and B as discussed earlier. In the case of fractional charges, the bond angle differences in region B are still given by Eq. (35). Correspondingly, the energy contribution from each bond angle difference $\theta_b$, and summing those contributions to give

$$E_{KT} = \frac{1}{2} \sum_b (\theta_b)^2. \quad (34)$$

The bond angle $\theta_b$ is, in turn, decomposed as

$$\theta_b = \sum_k q_k \theta_{k,b}, \quad (35)$$

where $k$ labels the position of the charges and $\theta_{k,b}$ is the contribution to $\theta_b$ from a charge of unit magnitude at $k$.

(2) Next, we consider the case in which the charges are fractional ($|q| < 1$). The bonds can still be divided into classes A and B as discussed earlier. In the case of fractional charges, the bond angle differences in region B are still given by Eq. (35). Correspondingly, the energy contribution from bonds in region B is

$$E_B = \frac{1}{2} \sum_b \theta_b^2$$

$$= \frac{1}{2} \sum_{b}^{A+B} \theta_b^2 - \sum_{b}^{A} \theta_b^2, \quad (36)$$

where $\sum_{b}^{B}$ and $\sum_{b}^{A}$ denote sums over all bonds in region B and in region A.

where $n_{jk}$ is the distance between the charges $q_j$ and $q_k$, and the second sum runs over all the individual charges, each of which has magnitude unity. This result is obtained by using a small-angle expansion for the contribution from each bond angle difference $\theta_b$, and summing those contributions to give

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$$= \frac{1}{2} \sum_{b}^{A+B} \theta_b^2 - \sum_{b}^{A} \theta_b^2, \quad (36)$$

where $\sum_{b}^{B}$ and $\sum_{b}^{A}$ denote sums over all bonds in region B and in region A.

where $n_{jk}$ is the distance between the charges $q_j$ and $q_k$, and the second sum runs over all the individual charges, each of which has magnitude unity. This result is obtained by using a small-angle expansion for the contribution from each bond angle difference $\theta_b$, and summing those contributions to give

$$E_{KT} = \frac{1}{2} \sum_b (\theta_b)^2. \quad (34)$$

The bond angle $\theta_b$ is, in turn, decomposed as

$$\theta_b = \sum_k q_k \theta_{k,b}, \quad (35)$$

where $k$ labels the position of the charges and $\theta_{k,b}$ is the contribution to $\theta_b$ from a charge of unit magnitude at $k$.

(2) Next, we consider the case in which the charges are fractional ($|q| < 1$). The bonds can still be divided into classes A and B as discussed earlier. In the case of fractional charges, the bond angle differences in region B are still given by Eq. (35). Correspondingly, the energy contribution from bonds in region B is

$$E_B = \frac{1}{2} \sum_b \theta_b^2$$

$$= \frac{1}{2} \sum_{b}^{A+B} \theta_b^2 - \sum_{b}^{A} \theta_b^2, \quad (36)$$

where $\sum_{b}^{B}$ and $\sum_{b}^{A}$ denote sums over all bonds in region B and in region A.
the center i.e., as \(i \) increases from 1 to \(m\). The inset shows the variation of \(\theta_i\) with chain length for \(\lambda = 1\). Note that with this choice of \(\lambda\), the bond angles saturate quickly; they are roughly constant over the “interior bonds,” such that \(i \geq 3\). Furthermore, this constant value (approximately by the central bond angle) approaches \(\pi\) as the chain length \(n\) increases.

Fig. 8 shows how the bond angles, \(\theta_i\), vary with bond strength, \(\lambda\), for a fixed chain length (\(n = 20\)). As already seen in the previous figure, \(\theta_i\) rapidly tends to saturate towards its central value with increasing \(i\). Moreover, the central bond angle quickly increases from 0 to \(\pi\) as \(\lambda\) increases for \(\lambda > \lambda_c\). Thus, we can ‘tune’ the central bond angle to any desired fraction of \(\pi\) by appropriately adjusting \(\lambda\).

Although the underlying variables are the \(\theta_i\)’s, it is of interest to mention corresponding trends in the fractional charges. For small \(\lambda\), these charges decrease monotonically with increasing \(i\), so that the largest charges reside at the ends of the chain. For larger \(\lambda\), charges comparable in magnitude to those at the ends appear away from the ends.

D. Numerical Check of Variational Procedure.

To check our variational approach, we have carried out an independent minimization to calculate the ground-state energy of the system containing \(\pi\) bonds, without making any assumptions about the presence or absence of fractional vortices. To carry out this minimization, we imagine that the \(ij^{th}\) bond is actually an overdamped Josephson junction connecting nodes \(i\) and \(j\). The current flowing through that bond from node \(i\) to node \(j\) is then

\[
I_{ij} = I_{c,ij} \sin(\phi_i - \phi_j) + \frac{\hbar}{2eR_{ij}} \frac{d}{dt}(\theta_i - \theta_j),
\]

and the sum of these currents must equal the total external current, \(I_{i}^{ext}\), fed into node \(i\):

\[
\sum_b I_{ij} = I_{i}^{ext}.
\]

where \(I_{c,ij}\) is the critical current of the junction between grains \(i\) and \(j\), and \(R_{ij}\) is the corresponding shunt resistance. These equations can be put into dimensionless form using the definitions \(i_{ij} ≡ I_{ij}/I_c\) and \(g_{ij} ≡ R/R_{ij}\), where \(I_c\) and \(R\) are a convenient normalizing critical current and shunt resistance, and introducing the natural time unit \(\tau ≡ \hbar/(2eR I_c)\). Combining these equations yields a set of coupled ordinary differential equations which is easily reduced to matrix form and solved numerically, as described by many previous investigators.

For our work, we employed a fourth-fifth order Runge-Kutta integration with variable time step.

For present purposes, we are interested, not in examining the dynamical properties of arrays with \(\pi\) bonds, but rather in finding the minimum-energy configuration of such arrays. To that end, we have simply iterated this set of coupled equations of motion, with no external current, allowing the phases to evolve until they reach a time-independent configuration. As has been shown by previous workers, this configuration will correspond to a local minimum-energy state of the corresponding Hamiltonian

\[
H = -\sum_{(ij)}(\hbar I_{c,ij}/2e) \cos(\phi_i - \phi_j).
\]

We then compare the resulting configuration and energy with those predicted by the fractional vortex variational ansatz for the ground state.

FIG. 9. Bond angle, \(\theta\), as function of bond strength \(\lambda\) for a single \(\pi\) bond obtained using (a) fractional-charge variational ansatz (*), and (b) numerical simulations (solid line).

FIG. 10. Total energy as function of \(\lambda\) for a single \(\pi\) bond obtained using (a) variational ansatz (*), and (b) numerical simulations (solid line).
To make the comparison as straightforward as possible, we made the simplifying assumption $R_{ij} = R$ for all Josephson junctions, whether 0 or $\pi$. We took $i_{c,ij} = 1$ for all normal junctions, and $i_{c,ij} = -\lambda$ for all $\pi$ junctions. Since no external current is to be applied to the system, we carry out these calculations using square arrays of junctions with periodic boundary conditions in both directions.

Each simulation begins with phases randomized at each grain. The system is then relaxed according to the Eqs. (37) and (38) for an interval of $50 - 100\tau$. We then evaluate the final energy, as well as the phase difference, $\theta_{ij}$, across each $\pi$ junction. Once equilibrium is reached for a given $\lambda$, we increment or decrement $\lambda$, and the system is allowed to relax again without re-randomizing the phases. Even quite large arrays ($50 \times 50$ plaquettes) relax quite quickly using this procedure, except near the critical point, but care must be taken to avoid taking data from simulations in which the system is trapped in a metastable state. We have used arrays ranging from $10 \times 10$ plaquettes to $50 \times 50$, and occasionally as large as $70 \times 70$ to examine convergence of equilibrium values.

Figs. 9 and 10 show the the exact ground-state energy and corresponding $q$ for the case of a single $\pi$ bond in a host of normal bonds, as calculated by this numerical procedure. The results are also compared to the total energy obtained from a ground-state configuration corresponding to a pair of bound fractional vortices of charge $\pm q$, calculated numerically. As shown in the figures, the agreement is excellent, thereby indicating that the ground-state energy is indeed well characterized by a bound pair of fractional vortices.

Figs. 11 and 12 show a similar comparison for the case of two $\pi$ bonds. Once again, the results obtained numerically from the RSJ equations for both the total energy and the bond angle across the $\pi$ bonds, are in excellent agreement with those found from the fractional vortex ansatz, suggesting that the ground state, in the case of two $\pi$ bonds, is again well characterized, over a range of $\lambda$, by a pair of oppositely charged fractional vortices.

Finally, we briefly discuss the accuracy of our variational approximation for the “wave function,” i.e., the phase distribution in the ground state. As is well known, a variational wave function may give an excellent value for the ground state energy, but a less accurate picture of the ground state configuration. In particular, our variational approach ignores the spin-wave degrees of freedom in characterising the ground state of the frustrated XY model, but it is possible that they may be required to get an accurate description of the phase distribution. To test the accuracy of our variational phase distribution, we have compared it to the exact (numerical) phase distribution in the ground state in several cases. The difference between the two configurations is shown graphically in Fig. 13 for the case of two $\pi$ bonds. As can be seen, the difference between the variational and exact wave functions is almost always less than 2-3% of the bond angle at the $\pi$ junction. We have looked at the results for one and two $\pi$ bonds for varying bond strengths, and in all cases considered the discrepancy is small. Thus, we conclude that the phase distribution as well as the energy is well approximated by our variational ground state involving only fractional vortices.

IV. SUMMARY AND POSSIBLE SIGNIFICANCE

The original motivation for this work was to study $\pi$ bonds in relation to the experiments of Kirtley et al. on $\pi$-grain boundaries in high-$T_c$ superconductors.
plained by the fact that one of the grain boundaries can be taken to be a π-boundary. In the second class of experiments, a triangular (or a hexagonal) single-crystal superconductor was inserted into a single crystal superconducting host of the same material, but with crystal axes misoriented with respect to those of the inclusion. In these systems, Kirtley et al. have found evidence of fractional (not half-integer) flux entrainment. These results have been interpreted as evidence that the superconducting order parameter violates time-reversal symmetry, either in the bulk or at an interface. Indeed, recent experiments have reported fractional flux entrainment even in the absence of π-grain boundaries, possibly supporting the existence of an order parameter which violates time-reversal symmetry.

If, in the triangular inclusion, only one of the three boundaries is a π-boundary, the two "zero" boundaries will have little effect on the arrangement of the order parameter phases, and can reasonably be ignored. Similarly, in the tricrystal, if only one of the three grain boundaries is a π-boundary, this boundary would correspond to a semi-infinite chain of π bonds, while the other two "zero" boundaries can again be ignored in the model. Thus, a finite chain of π bonds may be suitable for modeling the triangular inclusions, and the extrapolation for long chain lengths is relevant for the tricrystal experiments.

Next, we speculate about the relationship of our results to the observed trapping of non-half-integers of flux in triangular inclusions. The trapped flux is usually related to the phase difference across the grain boundary by the following argument, which we restate to apply to our geometry. Consider a closed integration contour C (of radius $r \gg a$) centered at one end of the grain boundary, and passing through the grain boundary. We wish to consider the flux enclosed by this loop. The path is taken to be deep inside the grains, so that the Meissner effect dictates that the supercurrent density $j = 0$. Since $j \propto \nabla \phi - (2\pi/\Phi_0)A$, where $\phi$ is the phase of the superconducting wave function, $\Phi_0 = hc/(2e)$ is the superconducting flux quantum, and A is the vector potential, it follows that

$$\nabla \phi = \frac{2\pi}{\Phi_0}A. \quad (39)$$

Now let $C = C^1 + C^2$, where $C^1$ is the part of the contour not including the grain boundary. In the approximation that $C^2$ can be taken to be infinitesimally short, the integral $\int_{C^2} A \cdot dl \sim 0$. In addition, we have $\int_{C^2} \nabla \phi \cdot dl = \Delta \phi$, the phase discontinuity across the grain boundary. But also $\phi$ must be continuous around $C$, modulo $2\pi$. Combining all these conditions with Eq. (39), we find that

$$\Delta \phi = 2\pi n - \frac{2\pi}{\Phi_0} \Phi, \quad (40)$$

where $n$ is an integer and $\Phi$ is the flux enclosed by the entire contour. Thus, the flux enclosed by $C$ is related
to the phase defect across the $\pi$ junction in the loop. In particular, if $\Delta \phi$ is a non-half-integer fraction of $2\pi$ in the ground state, then the flux enclosed will also correspondingly be fractional. Hence, a non-half-integer fractional flux is correlated with a phase jump across the perimeter of the SQUID, which are either $\pi$ bonds in the grain boundary, or lie along the extension of the grain boundary along the $\pm x$ direction. (a) $n = 20$, $\lambda = 0.25$. (b) $n = 40$, $\lambda = 0.25$ (full curve) and 1.0 (dashed curve).

In order to make a reasonable connection to the experimental geometry, we estimate the lattice spacing $a$ in our model using

$$E_J = I_c \Phi_0/c = a^2 J_c \Phi_0/c,$$

where $E_J$ is the Josephson coupling energy between adjacent grains, $I_c$ is the associated intergranular critical current, $J_c$ is the macroscopic critical current density set by the Josephson effect coupling, and $a$ is the lattice spacing of the granular array.

Using the experimental estimates for $E_J$ and $J_c$ (see Ref. 13), we estimate $a = 1.1 \mu m$, which is in agreement with the typical value for these materials. Since the triangular insertions are roughly $20 \mu m$ in length (for each side), we have looked at the results for a $\pi$ bond chain of $n = 20$ lattice spacings, with the SQUID diameter also taken to correspond to the experimental diameter. In Fig. 14(a), we show $\Delta$ as calculated for a $\pi$ bond chain of length $n = 20$ and strength $\lambda = 0.25$, and a SQUID of diameter $d = 10$. In Fig. 14(b), we show the same for a chain of length $n = 40$. We note that for a fixed bond strength, $\Delta$ becomes more concentrated near the chain ends with increasing chain length $n$. Furthermore, we can also make $\Delta$ more localized near the chain ends by increasing $\lambda$, as shown in Fig. 14(b).

The profile of $\Delta$, shown in Fig. 14(a), strikingly resembles the flux profile measured in Ref. 13 across one side of a triangular insertion. In view of this similarity,
it would be interesting to see if the changes we see with bond strength and chain length are also found experimentally. (Experimentally, the strength of the bonds can be changed by varying the misorientation angles of the inclusions.) If inductive effects do not change the qualitative picture presented above, then these experiments would provide evidence supporting the interpretation of the grain boundary as a string of \( \pi \) bonds.

We also comment on the fact that Kirtley et al. were able to reproduce their measured flux configuration with a certain arrangement of fractional magnetic charges. Our picture suggests one way of understanding why this modeling works. The key is that the flux distribution is closely related to the gauge-invariant phase jump \( (\Delta \gamma_{ij}) \) across the boundary, given by

\[
\Delta \gamma_{ij} = \Delta \phi_{ij} - (2\pi/\Phi_0) A_{ij},
\]

where \( i, j \) label sites connected by a bond across the grain boundary, and \( \Delta A_{ij} \) and \( \Delta \phi_{ij} \) are the corresponding discontinuities in the vector potential and the phase across that bond. A nonzero \( \Delta \gamma_{ij} \) can therefore be attributed either to a nonzero \( \Delta \phi_{ij} \) or a nonzero \( \Delta A_{ij} \) (or a combination of both). In our calculations, we have assumed a nonzero \( \Delta \phi_{ij} \) and take \( \Delta A_{ij} = 0 \) across the branch cut. The opposite choice \( (\Delta A_{ij} \neq 0, \Delta \phi_{ij} = 0) \) corresponds to a fractional magnetic monopole, since the vector potential of a magnetic monopole changes discontinuously across a branch cut. Since the physical quantity is the gauge-invariant phase difference, these pictures are equivalent.

In summary, we have introduced a set of “fractional vortex” excitations in the XY model, and have derived an expression for the interaction energy of a bound pair of fractional vortices. Furthermore, we have studied the ground state of the XY model on a two-dimensional lattice containing \( \pi \) bonds. For strings of \( \pi \) bonds of any length, we find that there exists a minimum bond strength, above which the ground state can be characterized by pair(s) of oppositely charged fractional vortices. We have verified this ansatz by carrying out independent numerical simulations for the ground-state configuration of this system. Finally, we have discussed the possible connection between these calculations and the trapped fractional flux quanta, which are observed near grain boundaries in high-\( T_c \) superconductors.

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