Nambu monopoles interacting with lattice defects in two-dimensional artificial square spin ice

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The interactions between an excitation (similar to a pair of Nambu monopoles) and a lattice defect are studied in an artificial two-dimensional square spin ice. This is done by considering a square array of islands containing only one island different from all others. This difference is incorporated in the magnetic moment (spin) of the "imperfect" island and several cases are studied, including the special situation in which this distinct spin is zero (vacancy). We have shown that the two extreme points of a malformed island behave like two opposite magnetic charges. Then, the effective interaction between a pair of Nambu monopoles with the deformed island is a problem involving four magnetic charges (two pairs of opposite poles) and a string. We also sketch the configuration of the field lines of these four charges to confirm this picture. The influence of the string on this interaction decays rapidly with the string distance from the defect.

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I. INTRODUCTION

Artificial spin ices[1] are systems composed by an array of lithographically defined two-dimensional ($2d$) ferromagnetic nanostructures with single-domain elements (elongate permalloy nanoparticles, in general) where the island net magnetic moment is assumed to be well approximated by an Ising-like spin (for a regime out of the Ising behavior in a single elliptic island, see Ref. 2). They can be organized in diverse types of geometries with lattices like the square[1], brickwork[3], honeycomb or kagome[4,5], triangular[6] etc. Recently, these artificial materials have been object of intense experimental and theoretical investigations[1,3–17] associated mainly with the appearance of collective excitations that behave like magnetic monopoles.

The theoretical and experimental studies concerning the physical properties of the ground state and excitations of the artificial square spin ices have deserved a great deal of attention in the last years[7,9–12,17]. In this system, there are four Ising spins at each vertex and they can be distributed in sixteen configurations grouped in four different topologies (see Fig. 1). It is relatively well established that its ground state has a configuration that obeys the ice rule (two spins point inward while the other two point outward in each vertex but, following only topology T_1 as shown in Fig. 1). In addition, the elementary excitations are quasi-particles akin to opposite magnetic monopoles connected by an energetic string[9–12,17] (this string is an oriented line of dipoles passing by vertices that obey the ice rule but, sustaining only topology T_2). The string energy is associated to the fact that the ice rule is not degenerate in two dimensions since topology T_2 has more energy than topology T_1[1]. These monopoles can be then referred to as Nambu monopoles due to their similarities with the monopoles studied by Nambu in the 1970's (considering a modified Dirac monopole theory[18]). Indeed, the forces that bind "monopoles" and "anti-monopoles" in a $2d$ artificial square spin ice are of two kinds[9,10]. One is the tension b of an energetic string; the other is the Coulomb force q/R^2, where q measures the strength of the interaction and R is the distance between the poles. Then, differently from the three-dimensional crystalline spin ices[19] in which the string is observable but does not have energy, in the $2d$ case, there is an oriented and energetic one-dimensional string of dipoles that terminates in the monopoles with opposite charges. This string costs an energy equal to bX where X is the string length. Thus, the interaction potential between two opposite charges is generally given by $V_N(R,X) = q(\phi)/R + b(\phi)X + c$, where ϕ is the angle that the line joining the monopoles makes with the x-axis of the array (there is a small anisotropy in the interaction[10]). Numerically, the theoretical values[10,11] for the constants arising in the potential $V_N(R,X)$ are $q(0) \approx -3.88\,Da$, $b(0) \approx 9.8\,D/a$ while $q(\pi/3) \approx -4.1\,Da$, $b(0) \approx 10.1\,D/a$, where $D = \mu_0\mu^2/4\pi a^3$ is the coupling constant for the dipolar interaction among the islands and a is the lattice spacing. The constant $c \approx 23\,D$, associated with the pair creation energy $(E_c \approx 29\,D)$[10,11], is independent of ϕ. The modulus of the magnetic charge is, therefore, given by $|Q_M(\phi)| = \sqrt{(4\pi|q(\phi)|/\mu_0)}$.

Although the fabrication of these systems is relatively easy, the limitations of the lithographic techniques are a significant barrier for building "perfect" arrays, with identical islands disposed at all lattice sites. Indeed, a large number of samples are made, for example, with malformed islands (see for example Ref. 20). On the other hand, defects can also be introduced intentionally into the system (for instance, by removing an island from the array or making, by design, some islands with holes[21,22]). Then, as it happens with natural materials, lattice defects could also play an important role in the properties of these artificial frustrated compounds. Our primary

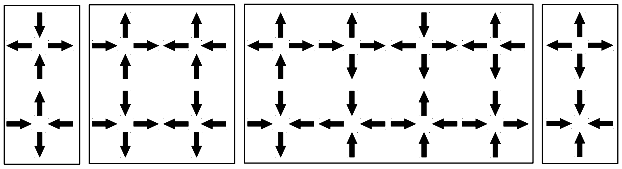


Figure 1. The four topologies for the vertices in an artificial square spin ice. The energy of these topologies increases from left to right. Topologies T_1 and T_2 obey the ice rule (two-in/two-out) but, they are not degenerate. Topology T_3 exhibits the configurations with three-in/ one-out or one-out/ three-in while in the topology T_4, one has four-in or four-out. Topology T_1 gives the ground state. Topology T_2 is associated with the string-like excitations and the last two are associated with magnetic monopoles-like excitations.

aim in this paper is to study the effects that a single malformed island causes on the elementary excitations of the artificial square spin ices. Our results show that the malformed island induces magnetic charges on adjacent vertices, giving in this way further and strong support to the magnetic monopole picture for the excitations of the artificial square spin ice. This picture is also corroborated by the determination of the magnetic field lines produced by excitations. Our results also suggest that by changing the shape and size of some islands of the system it may be possible to tailor design systems with desired properties.

II. DEFORMED ARTIFICIAL SQUARE ICE

Defects may be either naturally present in the system (due to the limitations of experimental techniques) or intentionally introduced in the artificial arrays. For example, one could remove an island ("spin") from a $2d$ square lattice. Thus, it is important to study the effects of these defects on the properties of the system. Here, we will consider an arrangement of dipoles similar to that accomplished in Ref. 1; however, at a particular site (denoted by site l) the island is deformed and may be larger or smaller than the other ones. In our calculations, such island deformation is incorporated in its magnetic moment which is proportional to the island volume (the spin or magnetic moment $\vec{S}_l$ is considered to be proportional to the island's volume). In our approach, the magnetic moment of each island is replaced by a unity Ising-like point dipole at its center ($|\vec{S}_i| = 1$) which is restricted to point along the x or y direction depending on its position for all islands, except for the deformed one, site l, whose magnitude is chosen in the interval $0 \leq |\vec{S}_l| \leq 2$. Note that the special limiting case of a missing island ($\vec{S}_l = 0$) is included in our range. In this way, the system is described by the following Hamiltonian[9,10]:

$$H = Da^3 \sum_{i \neq j} \left[\frac{\vec{S}_i \cdot \vec{S}_j}{|\vec{r}_{ij}|^3} - 3\frac{(\vec{S}_i \cdot \vec{r}_{ij})(\vec{S}_j \cdot \vec{r}_{ij})}{|\vec{r}_{ij}|^5} \right], \quad (1)$$

where $\vec{r}_{ij}$ is the vector that connects sites i and j, $D = \mu_0\mu^2/4\pi a^3$ is the coupling constant for the dipolar interactions. In all calculations periodic boundary conditions were implemented by means of the Ewald Summation[23,24].

In the system with a single defect, like a deformed island, we have observed, by using a simulated annealing process (see Refs. 9 and 10) that, the ground state is the same as that of a perfect array (all vertices obeying the ice rule). However, at the two particular adjacent vertices shared by the malformed island, there is a nonzero net magnetic moment due to the unbalance caused by the defect, since its spin is smaller (or greater) than the other three normal spins that complete the vertex (see Fig. 2). Therefore, although this ground state is neutral, in the sense that it is composed by T_1 vertices only, it should exhibit, in principle, a pair of opposite net magnetic charges separated by a distance of the order of the lattice spacing. To better understand this picture one may think that an augment in the magnitude of the spin, for example, was caused by the inclusion of another (smaller) spin in the vertex, which is located at the same place and that points in the same direction of the increased one. In this case one has five spins instead of four at the adjacent vertices shared by this island, and thus there is no way to achieve neutrality in the vertex that contains the defect. Since vertices that do not satisfy the ice rule are viewed as magnetic monopoles it is likely that these deformed vertices can also be viewed as monopoles. One may also easily arrive at the same conclusion by using a dumbbell picture as the used by Castelnovo et al.[19]. There is thus a pair of magnetic charges of magnitude Q_D, whose value depends on the unbalance at the vertices shared by the deformed island.

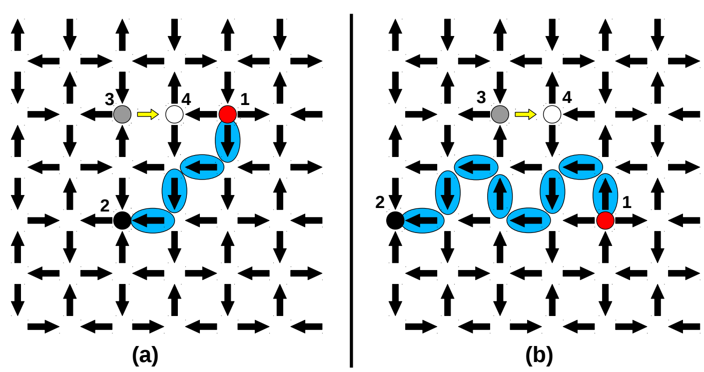


Figure 2. (Color online) Particular configuration of excitations in a lattice with a malformed island (yellow arrow between numbers 3 and 4). We use two basic shortest strings in the separation process of the magnetic charges: pictures (a) and (b)exhibit strings I and II, respectively. The black circle is the positive charge while the red circle is the negative charge.

III. RESULTS

In order to verify these assumptions, we consider now an elementary excitation in the system. It is a single pair of Nambu monopoles and its associated string placed around this static lattice defect as illustrated in Fig. 2. We have analyzed the two particular string shapes shown in Fig. 2; other string shapes were also studied given similar results. In Fig. 2, numbers 1 and 2 indicate the positions of the Nambu monopoles, with charges $-Q_M$ and Q_M respectively, while numbers 3 and 4 indicate the extremes of the lattice defect, which are represented by a small yellow arrow (at these points, as discussed above, two hypothetical opposite magnetic charges $-Q_D$ and Q_D are positioned). Also, the two string shapes considered are referred to as strings I and II as shown in Fig. 2 in (a) and (b) respectively. In our calculations, the Nambu pair size R (the smallest distance of separation between the two charges) is varied but only the position of charge 1 will be shifted for convenience; position 2 is kept fixed while positions 3 and 4 cannot change naturally, since we are considering a static defect. Considering a suitable choice of the origin at position 2, we get $|\vec{r}_1| = R$. Then, in principle, we now have four poles in the array: two hypothetical coming from the static lattice defect and two from the induced excitation (Nambu pair).

Firstly, we would like to know the effects of this defect on the interaction potential between the monopoles 1 and 2, $V_D(R)$. The potential $V_D(R)$ can be easily obtained by calculating the system's energy for each configuration and subtracting the ground-state energy (see Refs. 9 and 10). To extract the effects of the deformed island on the interaction energy we look for the the difference $\Delta = V_D(R) - V_N(R)$, where $V_D(R)$ is the potential obtained for the system with the deformed island and $V_N(R)$ is the potential obtained for a perfect system, where $|\vec{S}_l| = 1$. Since $V_N(R)$ contains the interactions between the monopoles 1 and 2 and the string energy, Δ gives the interaction between the deformed island and the monopoles 1 and 2 as well as the interaction between the deformed island and the string. In this way we can write a general analytic expression for Δ by considering the Coulombian interaction energy between four charges (1 and 2 with magnitude Q_M and the hypothetical 3 and 4 with magnitude Q_D) added by the interaction between the defect and the string. The interaction between charges and strings and also between strings may be very complicated to explicitly write. Thus, for the moment, we are including in the general expression for Δ an *ad hoc* term, such that Δ reads:

$$\begin{aligned} \Delta &= K_1 \left[\frac{1}{|\vec{r}_{13}|} - \frac{1}{|\vec{r}_{14}|} + \frac{1}{|\vec{r}_{24}|} - \frac{1}{|\vec{r}_{23}|} \right] \\ &\quad + K_2 \theta \left(\vec{R}_d \cdot \frac{\vec{r}_1}{|\vec{r}_1|} - |\vec{r}_1| \right) , \end{aligned} \tag{2}$$

where

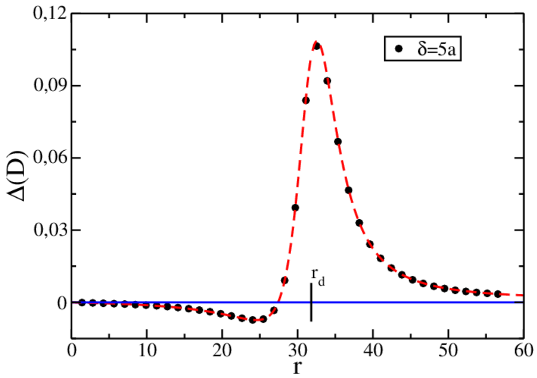
$$K_1 = \frac{\mu_0}{4\pi} Q_D Q_M \tag{3}$$

and K_2 are constants that must be determined, $\theta(x)$ is the step function ($\theta(x) = 0$ for $x < 0$ and $\theta(x) = 1$ for $x > 0$), $\vec{r}_{ij}$ is the distance between vertices i and j, $\vec{r}_1$ is the position of charge 1 and $\vec{R}_d$ is the position of the deformed island. The first term of equation 2 is simply the Coulombian interaction energy between the four charges (we remark that the interaction between charges 1 and 2 is not present in Δ as well as the interaction between the defects 3 and 4). The second term represents the *ad hoc* interaction of the string with the defect and will be discussed later.

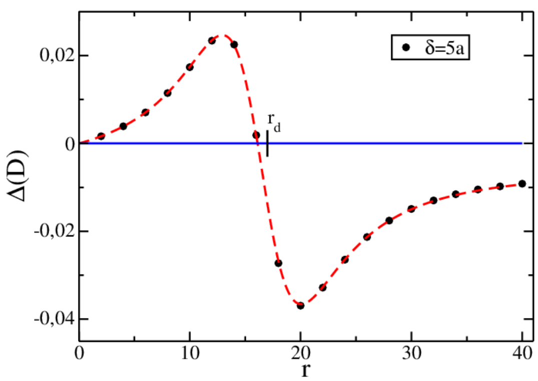
Fig. 3 shows the potential Δ as a function of the distance between the Nambu monopoles 1 and 2 ($r = R/a$) for strings I and II, using $|\vec{S}_l| = 0$, i.e., considering a missing island in the system. The results presented here are for a lattice with size equal to $80a$ (with 12,800 spins). In this figure the smallest distance between the defect and the string is $\delta = 5a$ (δ is measured as the distance between the line that connects the monopoles 1 and 2 and the deformed island; note however that for the string shapes used here this distance is exactly the smallest distance between the string and the deformed island). Since δ is relatively large we may consider that the defect does not effectively interacts with the string, so that the constant K_2 may be set to zero. The dashed red line in Fig. 3 is a nonlinear curve fitting made by using Eq.(2) with $K_2 = 0$. It can be easily seen that the Coulombian interaction between the Nambu monopoles (charges 1 and 2) and the defect charges (3 and 4) correctly describes the data. Similar results are obtained for $0 \leq |\vec{S}_l| \leq 2$ and for any value of $\delta \geq 2$.

These results show that either, the vacancy or even a malformed island, behave simply like a pair of opposite monopoles separated by a lattice spacing a as suspected above. The maximum and minimum of the data in Fig. 3 can be easily understood by considering the repulsion and attraction between the mobile Nambu monopole 1 and the defect charges 3 and 4. Indeed, the potential changes from repulsive to attractive, or vice-versa, as the monopole 1 passes through the defect charges. The repulsion or attraction occurs if the monopole 1 is closest to a defect charge of the same or opposite sign. Another characteristic of this interaction concerns the presence of the string. Since K_2 was set to zero to fit the data, one could conclude that the string connecting the Nambu monopoles does not cause any effect on the interaction if its distance from the defect is relatively large. This is really the situation as we explain latter.

Figure 4 shows the fitted values (K_1) as a function of S_l, obtained for type I string (the same result was also obtained for type II string). The red dashed line is a linear regression. For $S_l = 0$, our results show that $K_1 \approx 2\,Da$. Besides, using the fact that K_1 is given in units of Da, it is easy to show that $Q_D = \dfrac{\mu}{a}\dfrac{k_1}{q_m}$ and since



(a)String I.



(b)String II.

Figure 3. (Color online) Data for Δ as a function of $r = R/a$, considering string type I and II, for the situation in which the smallest distance δ between position 1 and the defect is larger than one spacing lattice. The magnitude of dipole moment is $|\vec{S_l}| = 0$. The simulation data Δ are the points and represent the case with $\delta = 5a$. The dashed lines are the fittings for expression 2.

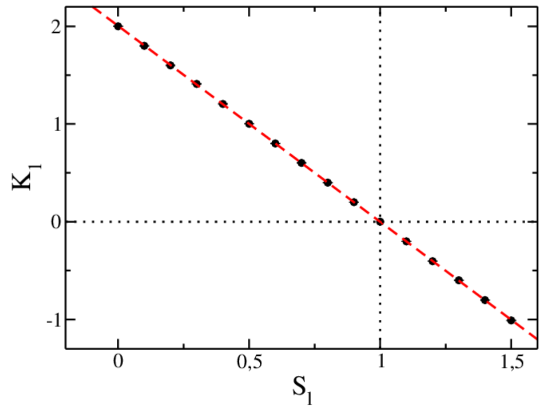


Figure 4. (Color online) Data for K_1 as a function of the size of the malformed island. Observe the linear behavior of K_1 as S_l is increased.

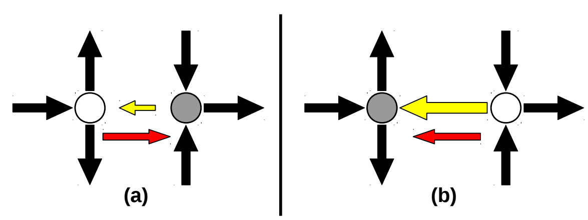
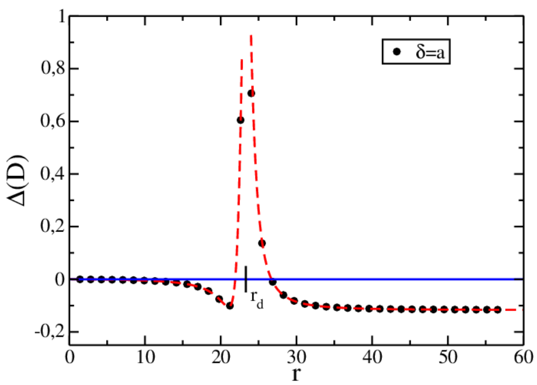


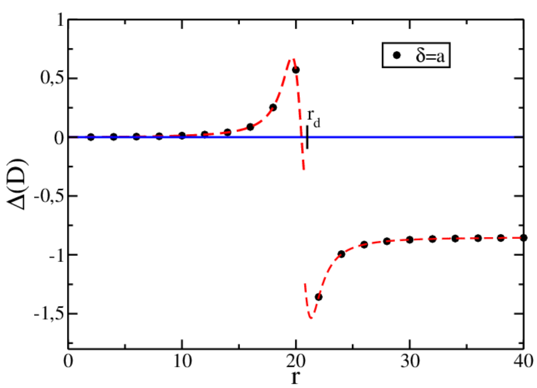
Figure 5. (Color online) Ground state configuration of the system around the malformed island for (a) S_l smaller (b) S_l greater than other islands. The white circle represents the negative charge induced by the lattice defect while, the gray circle represents the positive charge.

$q_m \approx 2$, $Q_D \approx 1 \approx Q_M/2$. It leads to $|Q_D| \approx |Q_M|/2$, which should be expected since the defect topology is an arrangement with configuration 2-in/1-out and vice-versa. The magnitude of K_1 decreases with increasing S_l, vanishing, as expected, when $S_l = 1$ (which is the case of a "perfect array"). For $S_l > 1$, the sign of K_1 changes, indicating that there is a switch in the position of the positive and negative charges produced by the defect, as shown in figure 5. In this figure, the white and gray circles represent the negative and positive charges induced by the lattice defect. In fact, the switch of the position of the induced charges can be easily seen by observing the change in the net magnetic moment (red arrow) on the vertices that form the lattice defect when S_l is smaller or greater than the other islands. Therefore, the effect of varying S_l from values smaller than 1 to values larger than 1 is the same as that of inverting the effective magnetic moment of an island from x to $2 - x$ $(0 \leq x \leq 1)$; hence, the characteristic effect of a vacancy is essentially the same as that caused by a defect island with a spin whose magnitude is twice ($S_l = 2$) the magnitude of the spin of the normal islands (for defects with $S_l = 0$ and $S_l = 2$, the magnetic moment has the same modulus but it points in opposite directions).

On the other hand, if the "moving" Nambu monopole 1 passes around the lattice defect at a distance smaller than $2a$ (on the order of $1a$), a substantial difference in the interaction potential can be noted, as shown in Fig. 6, which is obtained for string shapes I and II near a vacancy ($\delta = 1a$). For large values of r we can see that Δ goes to a constant value, while in Fig. 3 it goes to zero. This difference is attributed to the interaction between the string and defect. Indeed, the string may be viewed as a sequence of magnetic quadrupoles, whose magnetic field decays very quickly, and then, it is expected to interact only with very close objects. In this way, we may see that when all parts of the string are far from the defect there is no contribution from its interaction with the defect to the total energy; on the other hand, if a segment of the string is close enough to the defect (distance smaller than 2 lattice spacings), only the small segment that is close enough to the defect interacts with it. This explain the *ad hoc* term included in Eq. 2. When the "distance" between the defect and the "moving" monopole $\left(r_d - r_1, \text{ where } r_d = \vec{R}_d \cdot \frac{\vec{r}_1}{|\vec{r}_1|}\right)$ is negative, the string has not crossed the defect yet, and thus it is not close enough to contribute to the total energy. On the other hand, for $r_d > 0$ there is a segment of the string at a distance δ from the defect and for $\delta < 2a$ this segment contributes with a constant value K_2 to the total energy. In Fig. 6, the dashed red line was obtained by doing a nonlinear curve fitting according to general Eq. 2, in such a way that for $r < r_d$, K_2 was set to zero and then, keeping fixed K_1 the remaining points ($r > r_d$) were fitted for arbitrary K_2. In Fig. 7 we show the results for the constant K_2 as a function of δ. As can be seen K_2 has a significant value only for $\delta < 3$.



(a)String I.



(b)String II.

Figure 6. (Color online) Data for Δ as a function of $r = R/a$, considering strings I and II, for $\delta = 1a$ and $S_l = 0$. The simulation data for Δ are the black points and the red dashed line is the fitting for the expression 2.

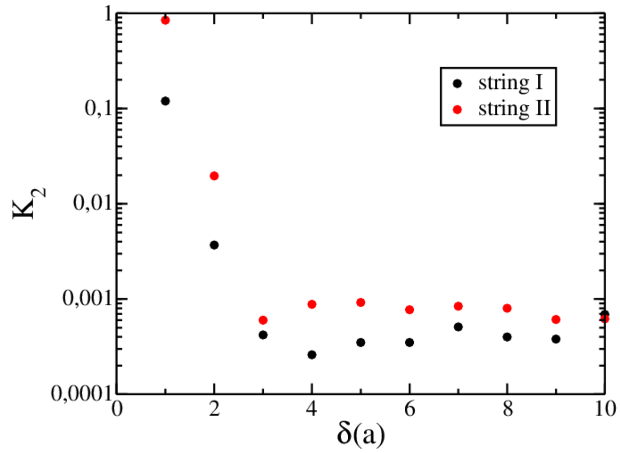


Figure 7. (Color online) The interaction constant between string and defect, K_2, as a function of the distance between the defect and the string, δ.

IV. MAGNETIC FIELD LINES

The above results give a strong support to the monopole-like picture for the excitations and defects of the artificial square spin ice as presented on Ref. 9. To give further support to this scenario we have also analyzed the magnetic field lines for this configuration of charges. We start our analysis by presenting in Fig. 8 a color map of the magnetic field intensity of a perfect system at its ground-state, where all islands have the same spin value. It is easy to see that the field is null at the center of the plaquettes as well as at the center of the vertices. This fact allows us to obtain the field produced by the excitations alone by simply inverting spins (creating excitations) and thus by calculating the resulting magnetic field at the center of the plaquettes and at the center of the vertices. In Fig. 9, we show the stream lines of the aforementioned field for a configuration were the red spins were flipped. We notice that the magnetic field lines far from the flipped spins are very similar to the field lines of a pair of electric charges, while in the space between them the magnetic field follows the string. It became clear then that the string carries the magnetic flux back from one charge to the other. In Fig. 10 (b) we show the stream lines of a configuration containing a vacancy and a pair of magnetic monopoles and its associated string while, for effect of comparison, in Fig. 10 (a) we show the electric field produced by two unity charges located at the same position of the Nambu monopoles and a pair of one half charges located at the same position of the vertices shared by the deformed island. Apart from the region where the string is present, the similarities between these two figures is remarkable. Although very simple, this analysis gives further evidences for the monopole-like behavior of excitations and defects in the artificial square spin ice.

V. CONCLUSION AND PROSPECTS

We have studied the problem concerning the interaction between two magnetic monopoles (and the energetic string connecting them) with a lattice defect present in the square spin ice array. We notice an interesting resemblance between the single defect and a static pair of monopoles separated by one lattice spacing. The

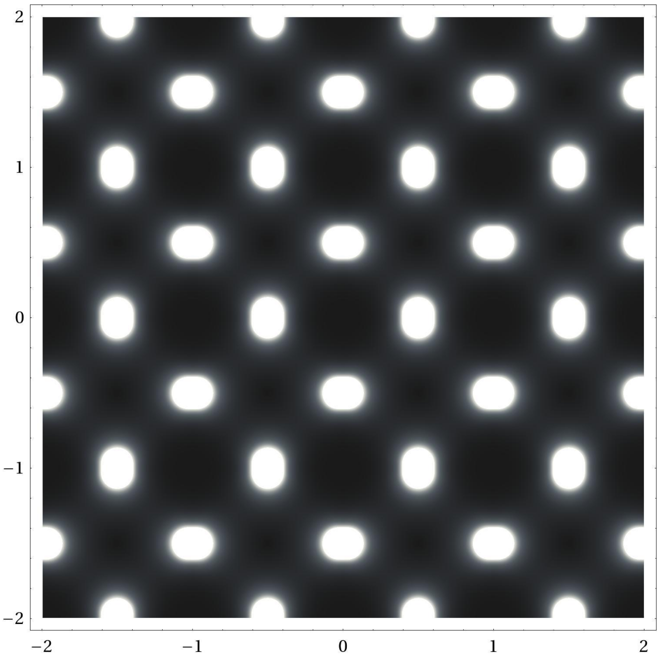


Figure 8. (Color online) Magnetic field intensity of the system's ground state. At the center of the plaquettes and at the centers of the vertices, the field goes to zero (black regions). These points were used to obtain the magnetic field produced by the excitations.

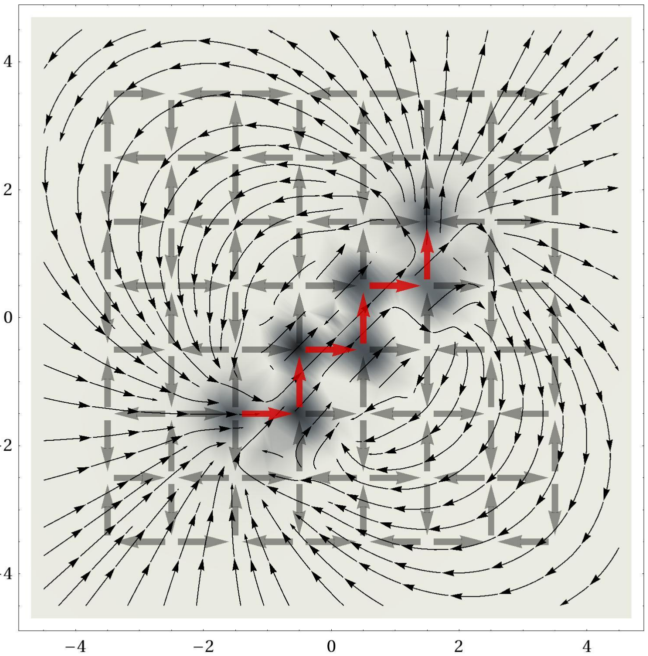


Figure 9. (Color online) This figure exhibts the stream lines of a pair of Nambu monopoles and its string (red spins). Only a small portion of the system is shown for clarifying.

strength of the magnetic charges of this small defect was obtained as a function of the magnetic moment of the malformed island (Fig. 4). Defects with $S_l = 0$ (vacancy) and $S_l = 2$ (double spin) produce the same effects in the lattice, since they have the same magnetic charges (placed in opposite positions). There is also a short range interaction between the string and the lattice defect, which can be attractive or repulsive, depending on the orientation and local shape of the string. Our results are a first step in direction to understanding how lattice defects could change the thermodynamics of artificial spin ices[17]. For instance, considering an array with a finite density ϱ of defects, it should be important to know how the properties of the system change as ϱ increases and how it could affect the formation of the ground state experimentally (a problem usually found in experiments with artificial square ices[1,11]). In general, we expect that the presence of a finite density of these lattice defects will distort deeply the path of the strings and even, they could break or join some different strings. A more detailed study of these questions is in progress at the moment.

A simple way to model unintentional defects in the system is to supposing that the islands have a gaussian size distribution around a given mean value. In a model of point dipoles this would be achieved by considering a gaussian distribution of the spin's magnitude. In this case, one may expect that, for a small variance of the size distribution, the same ground state of the perfect system would be achieved. However, for a large variance or for a system where the defects are not randomly distributed, we may expect some differences in the ground state. For instance, one may expect the formation of an ordered arrangement of charges (like a crystal of charges) similar to what happens in a kagome lattice[25]. The control of some defects (for example, inducing stronger or smaller variances of the size distribution) may thus be used to facilitate the experimental achievement of the system's ground-state.

Another interesting point is the possibility to construct tailor designed systems to achieve some desired property. Since the presence of a defective island can be interpreted in terms of the induced charges at the vertices shared by it, one can think in designing, for example, a magnetic capacitor-like system. This would be constructed by designing a system were all spins in a stripe immersed in a square system have islands smaller than the other ones, for example, in such a way that, in the edges of this stripe, there will be residual charges as far as an ice-like state is achieved. The presence of these residual charges may significantly change the behavior of other excitations inside this capacitor. A more detailed analysis of this hypothesis is under consideration.

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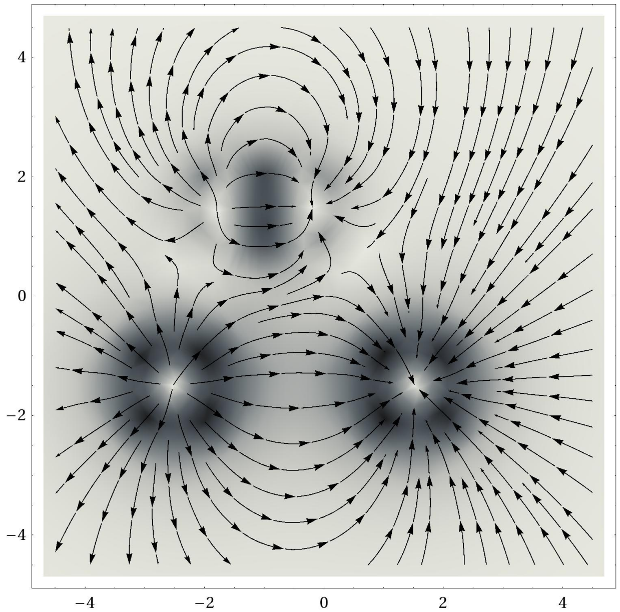
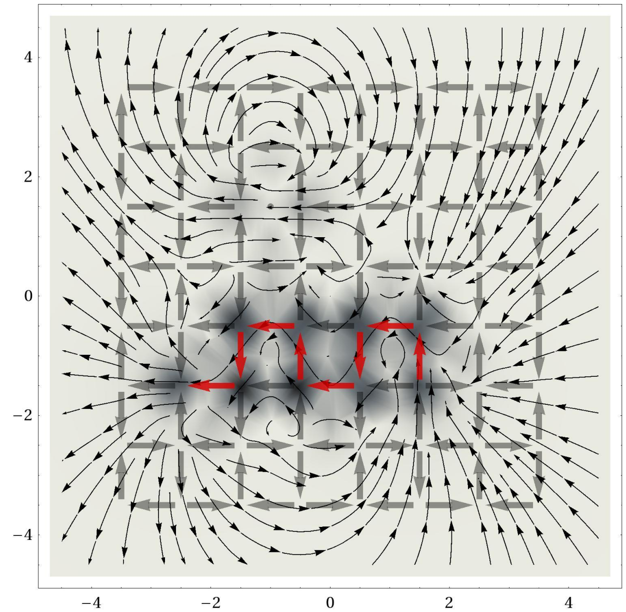


(a)Electric charges.



(b)Nambu monopoles connected by a type II string and a vacancy.

Figure 10. (Color online) (a) Electric field lines produced by four electric charges: two of unity magnitude representing the Nambu monopoles and two of one half magnitude representing the vacancy's charge. (b) Stream lines of the spin configuration. The red spins were flipped to produce the Nambu monopoles and its string. Only a small portion of the system is shown. The vacancy is placed approximately at (-1,2).

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