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ABSTRACT

A generalization of the one-dimensional frustrated quantum XY model is considered in which the inter and intra-chain coupling constants of the two infinite XY (planar rotor) chains have different strengths. The model can describe the superconductor-insulator transition due to charging effects in a ladder of Josephson junctions in a magnetic field with half a flux quantum per plaquette. From a fluctuation-effective action, this transition is expected to be in the universality class of the two-dimensional classical XY-Ising model. The critical behaviour is studied using a Monte Carlo transfer matrix applied to the path-integral representation of the model and a finite-size-scaling analysis of data on small system sizes. It is found that, unlike the previous studied case of equal inter and intra-chain coupling constants, the XY and Ising-like excitations of the quantum model decouple for large interchain coupling, giving rise to pure Ising model critical behaviour for the chirality order parameter in good agreement with the results for the XY-Ising model.

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The one-dimensional frustrated quantum XY model (1D FQXY) has been introduced as a model for studying charging effects in a ladder of Josephson junctions in a magnetic field corresponding to half a flux quantum per unit cell [1]. These charging effects arise from the small capacitance of the grains making up the ladder and leads to strong quantum fluctuations of the phase of the superconducting order parameter. As a result of the competition between the charging energy and the Josephson coupling between the superconducting grains, the one-dimensional array undergoes a superconductor to insulator transition at zero temperature for decreasing capacitance [2, 3, 4]. The universality class of this transition is currently a problem of great interest specially in relation to experiments on two-dimensional superconducting films and Josephson-junction arrays [2, 3, 5, 6, 7]. For a chain of Josephson junctions this critical behavior has been identified with that of the well known classical two-dimensional XY model [8]. However, while for the case of two coupled chains forming a ladder, in the absence of a magnetic field, this critical behavior can be shown to remain unchanged, in the presence of a magnetic field the behavior is more complicated[1, 9]. In particular, at half flux quantum per plaquette, corresponding to the 1D FQXY model [10] we study here, the critical behavior is expected to be described by the 2D classical XY-Ising model [1, 11]. The existence of both XY and Ising-like excitations in this case result from the frustration induced by the magnetic field and are associated with the continuous $U(1)$ symmetry of the phases of the superconducting order parameter and the plaquette chiralities which measures the direction of circulating currents in the Josephson-junction ladder.

The 1D FQXY model is defined by the Hamiltonian [1]

$$H = -\frac{E_c}{2}\sum_r \left(\frac{d}{d\theta_r}\right)^2 - \sum_{<rr'>} E_{rr'} \cos(\theta_r - \theta_{r'}) \qquad (1)$$

and consists of a one-dimensional chain of frustrated plaquettes as indicated in Fig. 1. The first term in Eq. (1) describes quantum fluctuations induced by the charging energy $E_c = 4e^2/C$ of a non-neutral superconducting grain located at site r, where e is the electronic charge and C is the effective capacitance of the grain. The second term is the usual Josephson-junction coupling between nearest-neighbor grains. θ_r represents the phase of the superconducting order parameter and the couplings $E_{rr'}$ satisfy the Villain's 'odd rule' in which the number of negative bonds in an elementary cell is odd [12]. This rule is a direct consequence of the constraint that, for the half flux case, the line integral of the vector potential due to the applied magnetic field should be equal to π in units of the flux quantum [13]. In the classical limit ($E_c = 0$), the ground state of Eq. (1) has a discrete Z_2 symmetry associated with an antiferromagnetic pattern of plaquette chiralities $\chi_p = \pm 1$ measuring the two opposite directions of the super-current circulating in each plaquette. In a previous work [1], a particular case of the 1D FQXY model, i.e., $E_y = E_x$, has been studied in some detail and it has been found that in fact its critical behavior is consistent with the results for the 2D classical

XY-Ising model [11]. From the critical exponents associated to the chirality order parameter the critical behavior has been identified as the one along the line of single transitions where both phase coherence and chiral order are lost simultaneously. However, the XY-Ising model has in addition to this transition line, two other branches corresponding to separate XY and Ising critical behavior which join the line of single transition at a bifurcation point located at some place in the phase diagram. The 1D FQXY model studied previously corresponds to a particular path through this phase diagram: the one located in the region of single transitions.

In this work we consider a generalized version of the 1D FQXY model in which the inter (E_x) and intra-chain (E_y) couplings constants have different strengths. In terms of a fluctuation-effective action which is obtained from an imaginary-time path integral representation of Eq. (1), the ratio between the couplings constants E_x/E_y can be used to tune the system through the bifurcation point in the XY-Ising model [1]. In particular, for $E_x >> E_y$ the 1D FQXY model is expected to have two separate transitions. In this work we find that in fact for $E_x/E_y \sim 2$ the single transition found previously does decouple into two separated transitions. Using a Monte Carlo transfer matrix technique [15] applied to the path-integral representation of the model we study the critical behavior of the chirality order parameter at a particular value of this ratio, $E_x/E_y = 3$. We find, from a finite-size scaling analysis of extensive calculations on small system sizes, that the critical exponents are consistent with pure Ising model critical behavior as expected from the results for the XY-Ising model.

To study the critical behavior of the 1D FQXY model, we find it convenient to use an imaginary-time path-integral formulation of the model [14]. In this formulation, the one-dimensional quantum problem maps into a 2D classical statistical mechanics problem where the ground state energy of the quantum model of finite size L corresponds to the reduced free energy per unit length of the classical model defined on an infinite strip of width L along the imaginary time direction, where the time axis τ is discretized in slices $\Delta\tau$. After scaling the time slices appropriately in order to get a space-time isotropic model, the resulting classical partition function is given by $Z = tr e^{-H}$ where the reduced classical Hamiltonian is defined as

$$H = -\alpha \sum_{\tau,j} [\cos(\theta_{\tau,j} - \theta_{\tau,j+1}) + \cos(\theta_{\tau,j} - \theta_{\tau+1,j}) - \cos(\phi_{\tau,j} - \phi_{\tau,j+1}) + \cos(\phi_{\tau,j} - \phi_{\tau+1,j}) + \frac{E_x}{E_y} \cos(\theta_{\tau,j} - \phi_{\tau,j})] \quad (2)$$

In the above equation, θ and ϕ denote the phases on the left and right columns in Fig. 1, and $\alpha = (E_y/E_c)^{1/2}$ plays the role of an inverse temperature in the 2D classical model.

One can now carry out a detailed study of the scaling behavior of the energy gap for kink excitations (chiral domain walls) of the 1D FQXY model by noting that this corresponds to the interface free energy of an infinite strip in the model of Eq. (2). For large α (small charging energy E_c), there is a gap

for creation of kinks in the antiferromagnetic pattern of χ_p and the ground state has long-range chiral order. At some critical value of α, chiral order is destroyed by kink excitations, with an energy gap vanishing as $|\alpha - \alpha_c|^{\nu}$, which defines the correlation length exponent ν. Right at this critical point, the correlation function decays as a power law $< \chi_p \chi_{p'} > = |p - p'|^{-\eta}$ with a critical exponent η. However to proceed further, one has to be able to calculate the free energy per unit length $f(\alpha)$ of the Hamiltonian on the infinite strip, which is usually obtained from the largest eigenvalue λ_o of the transfer matrix between different time slices as $f = -\ln \lambda_o$. Here, the major difficulty in performing this type of calculation comes from the continuous degrees of freedom of the model which prevents an exact diagonalization of the transfer matrix. This can be overcome by using a Monte Carlo transfer-matrix method [15] which has been shown to lead to accurate estimates of the largest eigenvalue even for this type of problems. Here we just summarize the main steps. The method is a stochastic implementation of the well-known power method to obtain the dominant eigenvalue of a matrix. First helical boundary conditions are implemented, in order to get a sparse matrix. Then, a sequency of random walkers R_i, $1 \leq i \leq r$, representing the configurations of a column with L spins in the infinite strip is introduced with corresponding weights w_i. The number of walkers r is maintained within a few percent of a target value r_o by adjusting the weights properly. A matrix multiplication can be regarded as a transition process with a probability density defined from the elements of the transfer matrix. In the procedure, a Monte Carlo (MC) step consists of a complete sweep over all random walkers and after a large number of MC steps an estimate of the largest eigenvalue can be obtained from the ratio between the total weights $\sum_i w_i$ of two successive MC steps. The implementation and some of the difficulties of the method are similar to the case of the two-dimensional frustrated classical XY model [16] and the reader should refer to that work for further details. For the calculations discussed in this work, typically $r_a = 20000$ random walkers and 80000 MC steps were used which correspond to 1.5×10^8 attempts per (θ, ϕ) pair.

The interfacial energy for domain walls in the model of Eq. (2) can be obtained from the differences between the free energies for the infinite strip with and without a wall. However, because of the antiferromagnetic pattern of the chiralities $\chi_p = \pm 1$, only strips with an odd number of sites L will have a domain wall. Since one is required to obtain the free energy differences at the same value of L, we need to resort to an interpolation scheme for successive odd or even L to determine the interfacial free energy. Results for the interfacial free energy, defined as $\Delta F(\alpha, L) = L^2 \Delta f(\alpha, L)$, near the transition point α_c, for $6 < L < 14$, are indicated in Fig. 2 for a particular value of the ratio $E_x/E_y = 3$. As in the previous work [1], to obtain the critical exponents and critical temperature we now employ the finite-size scaling

$$\Delta F(\alpha, L) = A(L^{1/\nu}\delta\alpha) \tag{3}$$

where A is a scaling function and $\delta = \alpha - \alpha_c$. In a linear approximation for the argument of A, we have

$$\Delta F(\alpha, L) = a + bL^{1/\nu}\delta\alpha \tag{4}$$

which can be used to determine the critical coupling α_c and the exponent ν independently. The change from an increasing trend with L to a decreasing trend provides and estimate of α_c, which from Fig. 2 gives $\alpha_c = 1.16(2)$. Once the critical coupling is known, the correlation function exponent η can obtained from the universal amplitude a in Eq. (4) through a result from conformal invariance [17], $a = \pi\eta$, from which we estimate $\eta = 0.24(2)$. To estimate the correlation length exponent ν we first obtain the derivative $S = \partial\Delta F/\partial\alpha$ near α_c, then it can easily be seeing that a log-log plot of S vs L gives an estimate of $1/\nu$ without requiring a precise determination of α_c. Of course, this is only valid for the linear approximation of Eq. (4). Assuming the data is in fact in this regime we obtain the result for S as indicated in Fig. 3 and get the estimate $\nu = 1.05(6)$. The results for the critical exponents ν and η are good agreement with pure 2D Ising values $\nu = 1$ and $\eta = 0.25$ indicating pure Ising behavior. Moreover, this implies from the relation between the 1D FQXY model and the 2D classical XY-Ising [11] that the XY and Ising-like excitations have decoupled in this region.

To show that in fact one has two decoupled and at the time separated transitions we now consider the results for the helicity modulus which measures the response of the system to an imposed phase twist. In the incoherent phase this quantity should vanishes while it should be finite in the coherent phase. The helicity modulus is related to the free-energy differences ΔF between strips with and without and additional phase mismatch of π along the strip and is given by $\gamma = 2\Delta F/\pi^2$ for large system sizes. If the model is decoupled then the coherent to incoherent (or superconductor-insulator) transition should be in the universality class of the 2D XY model, where one knows that the transition is associated with a universal jump of 2π in the helicity modulus [18]. Finite-size effects smooth out this behavior as indicated in Fig 4 but the critical coupling can be estimated as the value of α at which $\Delta F = \pi$. This criteria leads to the estimate $\alpha_c = 1.29$ which is to be compared with the critical coupling for the destruction of chiral order found above, $\alpha_c = 1.16$. This clearly indicates the transitions are well separated and thus one expects they are decoupled. In contrast, for the case of equal inter and intra-chain coupling constants studied previously these estimates were found to be in fact consistent with each other [1]. We have also performed less detailed calculations at other values of the ratio E_x/E_y from which we can estimate that the Ising and XY transition merge into a single transition roughly at $E_x/E_y \sim 2$. Since, the superconductor to insulator transition is to be identified with the loss of phase coherence [8] we reach the interesting

result that in the 1D FQXY, or alternatively, a Josephson-junction ladder, the universality class of the superconductor-insulator transition depends on the ratio between inter and intra-chain couplings.

In conclusion, we have studied a generalized version of the one-dimensional frustrated quantum XY model which consisted in allowing for different strengths for the inter and intra-chain couplings constants. The model can be physically realized as a one-dimensional array of Josephson junctions in the form of a ladder and in the presence of an external magnetic field corresponding to a half flux quantum per plaquette. It is found that, unlike the previous studied case of equal inter and intra-chain couplings, the XY and Ising-like excitations decouple giving rise to pure Ising behavior for chirality order parameter and a superconductor-insulator transition in universality class of the XY model. Since these arrays can currently be fabricated in any desired geometry and with well-controlled parameters it is hoped that these results will serve to motivate experiments in these systems.

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Figure Captions

1. Schematic representation of the one-dimensional frustrated quantum XY model with inter (E_x) and intra-chain ($\pm E_y$) coupling constants. The antiferromagnetic ordering of chiralities $\chi_p = \pm 1$ is also indicated.

2. Finite-size scaling of the interfacial free energy $\Delta F(\alpha, L) = L^2 \Delta f(\alpha, L)$ for kink (chiral) excitations.

3. $S = \partial \Delta F(\alpha, L)/\partial \alpha$ evaluated near the critical coupling α_c. The slope of the straight line gives an estimate of $1/\nu$.

4. Behavior of the interfacial free energy $\Delta F = L^2 \Delta f$ for a system of size $L = 12$ resulting from an imposed phase twist of π. Vertical arrows indicate the locations of the Ising and XY transitions and the horizontal arrow the value $\Delta F = \pi$ from where the XY transition is located. The Ising transition is located from the finite-size scaling of the chiral order parameter (Fig. 2) as discussed in the text.

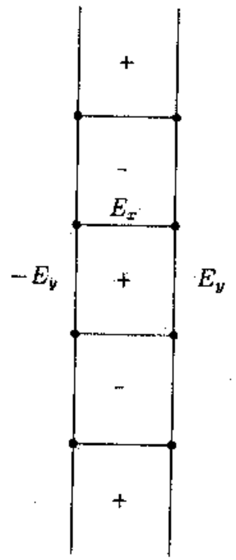

Fig. 1

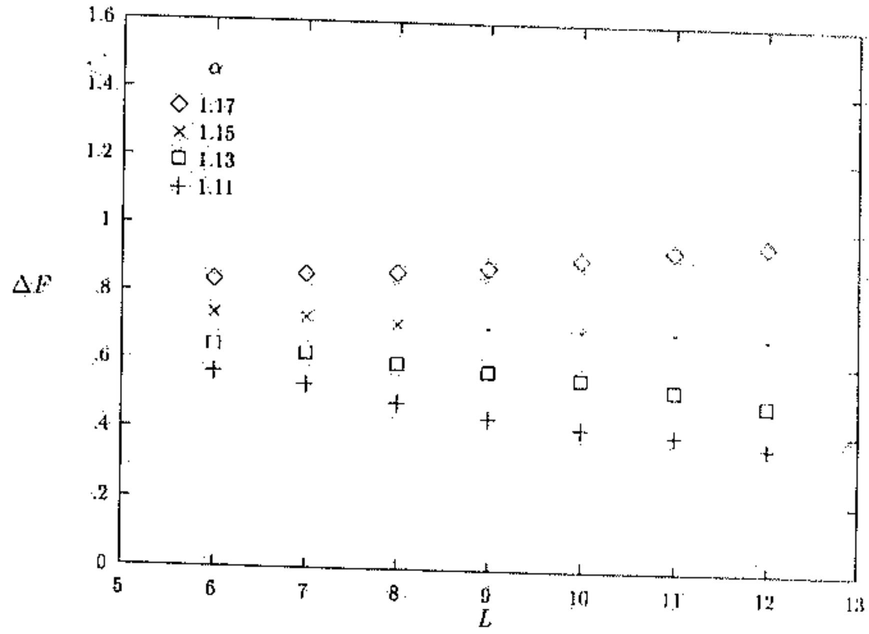

Fig.2

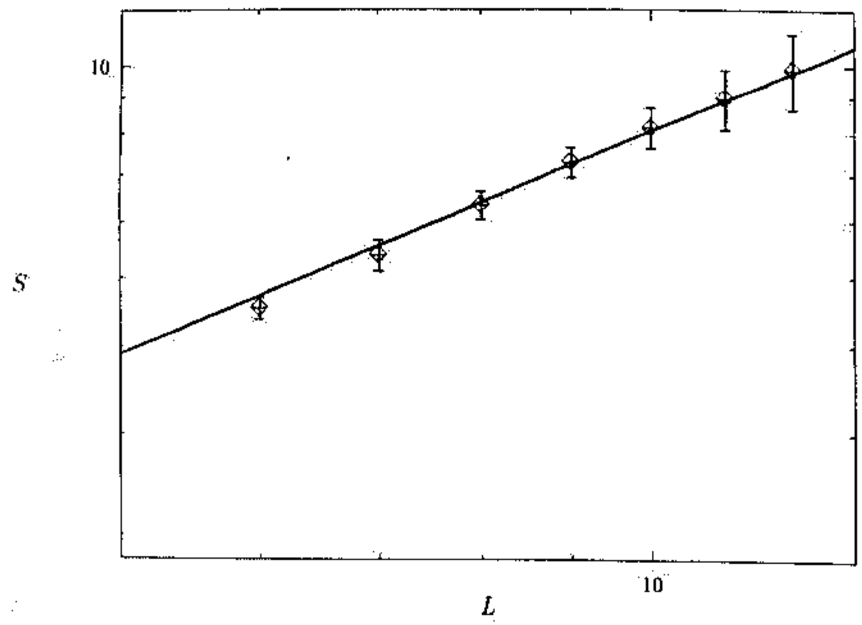

Fig.3

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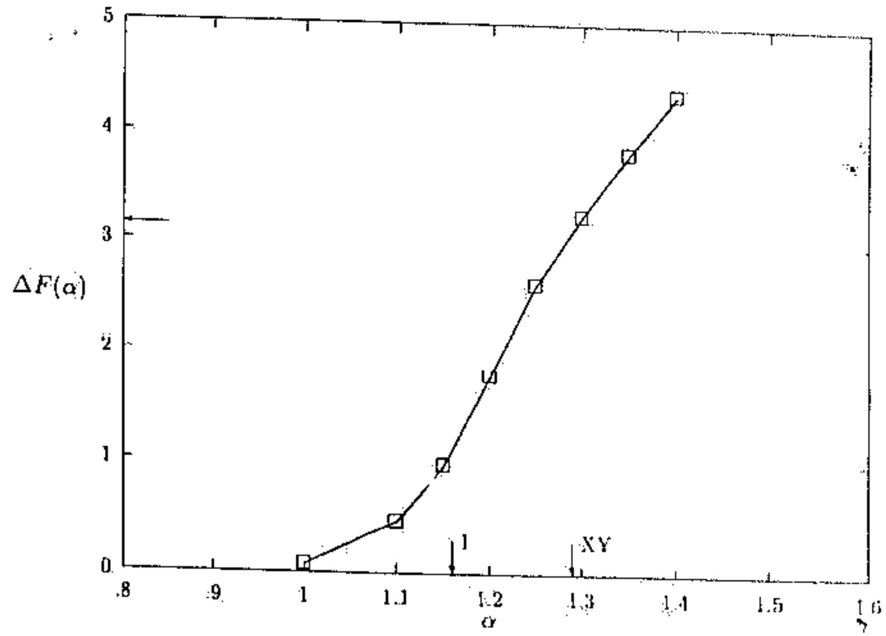

Fig. 4

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