Phase transitions in the one-dimensional frustrated quantum *XY* model and Josephson-junction ladders

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A one-dimensional quantum version of the frustrated *XY* (planar rotor) model is considered which can be physically realized as a ladder of Josephson junctions at half a flux quantum per plaquette. This system undergoes a superconductor to insulator transition at zero temperature as a function of charging energy. The critical behavior 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. Depending on the ratio between the interchain and intrachain couplings the system can have single or double transitions which is consistent with the prediction that its critical behavior should be described by the two-dimensional classical *XY*-Ising model.

The two-dimensional frustrated classical *XY* model has attracted considerable attention recently.[1–8] It can be related to Josephson-junction arrays in a magnetic field, where it is expected to describe the finite-temperature superconductor to normal transition in arrays with half a flux quantum per plaquette.[9] At low temperatures where capacitive effects dominate, the array undergoes a superconductor to insulator transition as a function of charging energy.[10–13] These charging effects arise from the small capacitance of the grains making up the array and leads to strong quantum fluctuations of the phase of the superconducting order parameter. The critical behavior is now described by a two-dimensional frustrated quantum *XY* model with a Hamiltonian[12]

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

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.[14] In a square lattice this can be satisfied, for example, by ferromagnetic horizontal rows and alternating ferromagnetic and antiferromagnetic columns of bonds. 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.

In this work we consider a one-dimensional frustrated quantum *XY* (1D FQ*XY*) model[15] which can be regarded as the simplest 1D version of the model (1) consisting just of a single column of frustrated plaquettes as indicated in Fig. 1. This can be physically realized as a periodic Josephson-junction ladder at half a flux quantum per plaquette.[16,17] In the classical limit ($E_c=0$), the ground state of the 1D FQ*XY* model has a discrete Z_2 symmetry associated with an antiferromagnetic pattern of plaquette chiralities $\chi_p=\pm1$, as indicated in Fig. 1, measuring the two opposite directions of the supercurrent circulating in each plaquette. For small 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.

Within a path-integral approach,[16] it can be shown that the effective action describing quantum fluctuations in the

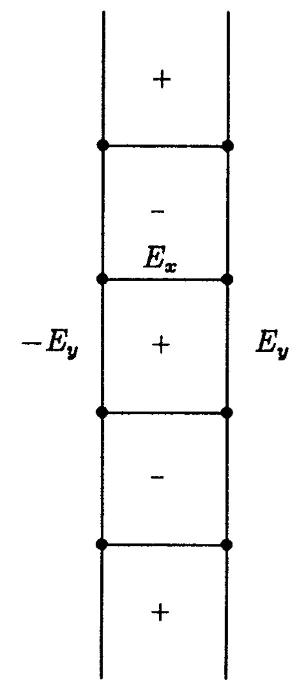

FIG. 1. Schematic representation of the one-dimensional frustrated quantum *XY* model with inter- (E_x) and intrachain ($\pm E_y$) coupling constants. The antiferromagnetic ordering of chiralities $\chi_p=\pm1$ is also indicated.

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1D FQXY model leads to two coupled XY models in two (space-time) dimensions which is expected to have a critical behavior in the universality class of the 2D XY-Ising model[18] defined by the classical Hamiltonian

$$\beta H = -\sum_{\langle rr' \rangle} [A(1+\sigma_r \sigma_{r'} \cos(\theta_r - \theta_{r'}) + C\sigma_r \sigma_{r'})] . \tag{2}$$

The phase diagram of this model consists of three branches, in the ferromagnetic region. One of them corresponds to single transitions with simultaneous loss of XY and Ising order. Further away from the branch point, this line of single transitions becomes first order. The other two lines correspond to separate XY and Ising transitions. The 1D FQXY model is represented by a particular path through this phase diagram which will depend on the ratio E_x/E_y between the interchain and intrachain couplings of the model. In this work we describe the results of a finite-size scaling analysis of extensive calculations on the 1D FQXY model[15,19] which shows that, in fact, the XY and Ising-like excitations of the quantum model decouple for large interchain couplings, giving rise to pure Ising model critical behavior for the chirality order parameter. As a consequence, the universality class of the superconductor–insulator transition in the related Josephson-junction ladder should then depend on the ratio between interchain and intrachain Josephson couplings.

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.[20] 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 one obtains a classical partition function where the parameter $\alpha=(E_y/E_c)^{1/2}$ plays the role of an inverse temperature in the 2D classical model. The scaling behavior of the energy gap for kink excitations (chiral domain walls) of the 1D FQXY corresponds to the interface free energy of an infinite strip in this classical model. 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 $\langle \chi_p \chi_{p'} \rangle = |p-p'|^{-\eta}$ with a critical exponent η. The free energy per unit length $f(\alpha)$ of the Hamiltonian on the infinite strip can be obtained from the largest eigenvalue λ_0 of the transfer matrix between different time slices as $f=-\ln \lambda_0$. To obtain λ_0, we used a Monte Carlo transfer-matrix method[21] which has been shown to lead to accurate estimates of the largest eigenvalue even for models with continuous symmetry. The implementation of this method is similar to the case of the 2D frustrated classical XY model[8] and further details can be found in that work.

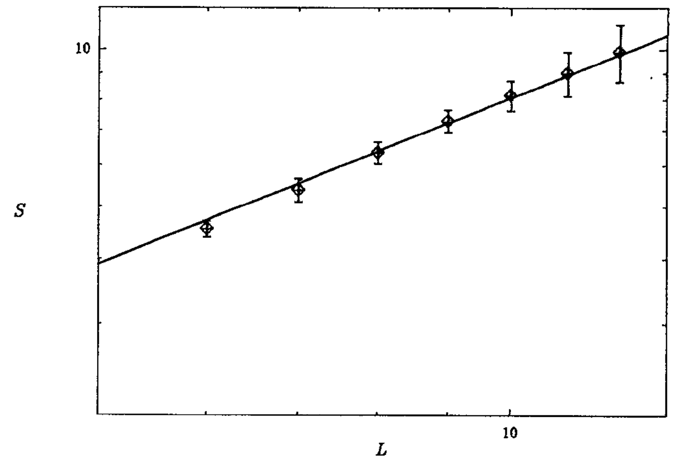

FIG. 2. $S=\partial\Delta F(\alpha,L)/\partial\alpha$ evaluated near the critical coupling α_c. The slope of the straight line gives an estimate of $1/\nu$.

The interfacial free energy for domain walls can be obtained from the differences between the free energies for the infinite strip with and without a wall. To obtain the critical exponents and critical coupling we employ the finite-size scaling $\Delta F(\alpha,L)=A(L^{1/\nu}\delta\alpha)$ where A is a scaling function and $\delta\alpha=\alpha-\alpha_c$. In a linear approximation for the argument of A, we have

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

which can be used to determine the critical coupling α_c and the exponent ν independently.[16] The change from an increasing trend with L to a decreasing trend provides and estimate of α_c. Once the critical coupling is known, the correlation function exponent η can be obtained from the universal amplitude a in Eq. (3) through a result from conformal invariance,[22] $a=\pi\eta$. 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 seen that a log–log plot of S vs L gives an estimate of $1/\nu$ without requiring a precise determination of α_c. In Fig. 2 we show this kind of plot for $E_x/E_y=3$ from where we get the estimate $\nu=1.05(6)$. Of course, this is only valid in the linear approximation of Eq. (3). To ensure that higher-order terms can safely be neglected, the data for $\Delta F(\alpha,L)$ must be obtained in a sufficiently small range near α_c. We also checked, using a more general finite-size scaling analysis,[8] that allowing for higher-order terms gives results agreeing within the errors. The results for the critical coupling α_c and critical exponents ν and η for two different values of the ratio $E_x/E_y=1$ and 3 are indicated in Table I.

For equal couplings $E_x=E_y$, the results for the critical exponents η and ν differ significantly from pure 2D Ising

TABLE I. Critical couplings $[\alpha_c=(E_y/E_c)^{1/2}]$ and critical exponents (ν,η), obtained from finite-size scaling analysis of interfacial free energies for two values of the ratio between interchain and intrachain couplings (E_x/E_y).

E_x/E_y	α_c	ν	η
1	1.04(1)	0.81(4)	0.47(4)
3	1.16(2)	1.05(6)	0.27(3)

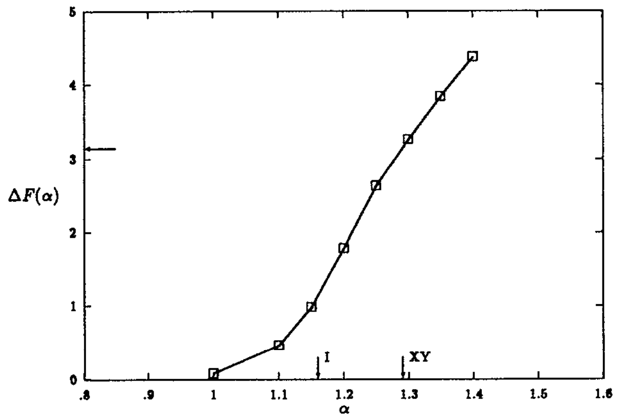

FIG. 3. Behavior of the interfacial free energy $\Delta F = L^2 \Delta f$ for a system of size $L=12$ resulting from an imposed phase twist of π. Vertical arrows indicate the locations of the Ising and XY transitions and the horizontal arrow the value $\Delta F = \pi$ from where the XY transition is located.

exponents ($\nu=1$, $\eta=0.25$). This result points to a single transition scenario. In fact, they are consistent with a point along the line of single transitions in the XY-Ising model.[18] It is interesting to note that this result is also consistent with similar calculations for the 2D frustrated classical XY model.[8] In general, the critical behavior of a d dimensional quantum model is in the same universality class of the $d+1$ dimensional classical version. However, the 1D FQXY model, apparently, is not the Hamiltonian limit of the 2D classical model. Yet, their critical behavior appears to be in the same universality class.

For the case of unequal couplings $E_x/E_y=3$, the results indicated in Table I are in good agreement with pure 2D Ising values. From the relation between the 1D FQXY model and the 2D XY-Ising model this then implies that the XY and Ising-like excitations have decouple in this region of parameters. To show that in fact one has two decoupled and, at the same time, separated transitions we show in Fig. 3 the results for the helicity modulus which measures the response of the system to an imposed twist. The helicity modulus is related to the free-energy differences ΔF between strips with and without any 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 transition should be in the universality class of the 2D classical XY model, where one knows that the transition is associated with a universal jump of $2/\pi$ in the helicity modulus.[23] The critical coupling can be estimated as the value of α at which $\Delta F = \pi$ which gives $\alpha_c=1.29$. This is to be compared with the critical coupling for the destruction of chiral order in Table I, $\alpha_c=1.16$. This clearly indicates the transitions are well separated and thus one expects they are decoupled. 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 transitions 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[24] 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 intrachain couplings.

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