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# Critical behavior of a one-dimensional frustrated quantum $XY$ model

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A one-dimensional quantum version of the frustrated $XY$ model is introduced which can be physically realized as a ladder of Josephson junctions at half of a flux quantum per plaquette. From a fluctuation effective action, the zero-temperature (superconductor-insulator) transition is predicted to be in the universality class of the two-dimensional classical $XY$-Ising model. A Monte Carlo transfer matrix is used to calculate critical exponents and central charge. A finite-size-scaling analysis of extensive calculations on small system sizes supports the prediction. The same critical behavior has recently been found for the two-dimensional classical version. Together, the results strongly support an $XY$-Ising-like critical behavior for these systems.

The two-dimensional frustrated classical $XY$ (2D F$CXY$) model[1] has attracted much attention in the last few years. Most of the studies have been mainly motivated by its relevance for the finite-temperature superconductor-normal transition in arrays of Josephson junctions at half of a flux quantum per plaquette.[2-11] Precisely at the same value of field, but at sufficiently low temperatures where capacitive effects dominate, the array undergoes a superconductor-insulator transition[12,13] as a function of the charging energy. The critical behavior is now described by a 2D frustrated quantum $XY$ (FQ$XY$) model with a Hamiltonian[13]

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

The first term describes quantum fluctuations induced by a finite charging energy of the superconducting grains located at site $r$ and the second term is the Josephson-junction coupling between them. $\theta_r$ represents the phase of the superconducting order parameter.[14] As a consequence of the half flux quantum per plaquette constraint, $E_{rr'}=\pm E_J$ satisfy the Villain's "odd rule" in which the number of bonds with negative sign in any elementary plaquette is odd. In a square lattice this can be satisfied, for example, by ferromagnetic horizontal rows and alternating ferromagnetic and antiferromagnetic columns of bonds.

In this work we consider the simplest one-dimensional version of the FQ$XY$ model (1) consisting just of a single column of frustrated plaquettes as indicated in Fig. 1. This will correspond to a periodic Josephson-junction ladder at half flux quanta per plaquette.[15,16] In the classical limit ($E_c=0$), the ground state is similar to the two-dimensional case.[1-5] The difference is that now each site has only three neighbors instead of four and will give rise to slightly different phase configurations. In addition to a global continuous U(1) symmetry, the ground state has a discrete $Z_2$ symmetry associated with an antiferromagnetic pattern of plaquette chiralities $\chi_p=\pm 1$. The chiral (Ising-like) order parameter is defined as a direct sum around each elementary plaquette as

$$\chi_p=(1/\gamma_0)\sum_{\langle rr'\rangle}E_{rr'}\sin(\theta_r-\theta_{r'})\,,$$

where $\gamma_0$ is a suitable normalization constant, and correspond to the direction of circulating currents in the Josephson-junction ladder. For small $E_c$, there is a gap for creation of kinks in the antiferromagnetic pattern of $\chi_p$ and the ground state has long-range chiral order. At some critical value of the ratio $\alpha=(E_J/E_c)^{1/2}$, chiral order is destroyed by kink excitations, with the energy gap vanishing as $|\alpha-\alpha_c|^{\nu}$, which defines the correlation length exponent $\nu$. At this critical value, the correlation function decays as a power law $\langle\chi_p\chi_{p'}\rangle=|p-p'|^{-\eta}$ with an exponent $\eta$. On the other hand, quasi-long-range order in phase will also be destroyed for increasing $E_c$, due to phase-slip (space-time vortices) processes.[17,18] However, similar to the two-dimensional classical case,[4,5] these exci-

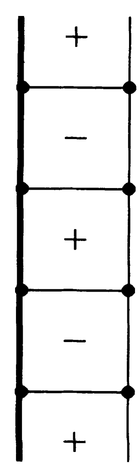


FIG. 1. Schematic of the one-dimensional frustrated quantum $XY$ model. Thin (thick) lines denote $E_J$ ($-E_J$) neighbor couplings. In the classical limit, $E_c=0$, the ground state is an antiferromagnetic pattern of chiralities $\chi_p=\pm 1$, as indicated.

 

tations are strongly coupled since it can be shown that a kink also induces fractional phase slips. Instead of separate phase transitions, it is then also possible to have just a single transition. A fully quantum-mechanical analysis of these excitations would be of some interest and may give some insight into the nature of the phase transition, but we will not pursue this any further here. Instead, we will study this transition by numerical methods.

In a recent paper,[16] an imaginary-time effective action describing quantum fluctuations in a Josephson-junction ladder at $f=p/q$ flux quanta per plaquette was studied. At $f=\frac{1}{2}$, corresponding to the 1D FQ$XY$ model studied here, it leads to two coupled $XY$ models in two (space-time) dimensions, with a coupling term of the form $\cos[2(\theta_1-\theta_2)]$. This is expected to have a critical behavior in the universality class of the 2D $XY$-Ising model defined by the classical Hamiltonian[7,9] ($\sigma=\pm 1$)

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

The phase diagram of this model consists of three branches, in the ferromagnetic region, joining at $C^*\approx 0$. One of them ($C<C^*$) corresponds to single transitions with a simultaneous loss of $XY$ and Ising order. Along this line, the critical behavior is nonuniversal with $\nu\approx 0.85$ and $\eta$ increasing from $\frac{1}{4}$ to $\approx 0.5$ in a small portion of the line. The central charge $c$ is found to be in the range $1.5<c<2$. Further away from the branch point, this line of single transitions becomes first order. The other two lines, in the region $C>C^*$, corresponds to separate $XY$ and Ising transitions. The 1D FQ$XY$ model studied in this paper is represented by a particular path in this model and it would be of interest to find out to which transitions it corresponds.

We have determined the critical exponents $\nu$ and $\eta$, associated with chiral order of the 1D FQ$XY$ model, from a finite-size-scaling analysis of the kink energy gap, using a Monte Carlo transfer matrix[19,20] in the path-integral representation of the model. From extensive numerical calculations on small system sizes, $L=6$ to 14, we find $\nu=0.81(4)$ and $\eta=0.47(4)$. We have also estimated the central charge at the transition and found $c=1.67(4)$. These results are consistent with the corresponding values along the line of single transitions in the $XY$-Ising model[9] and support the above prediction. Recently, similar result has also been found for the 2D FC$XY$ model.[8,10] So, the critical behavior of both models is apparently described by the same model. This is an interesting, and somewhat unexpected possibility, as the 1D FQ$XY$ model is not just a trivial Hamiltonian version of the transfer matrix[21] of the 2D FC$XY$ model. They might, however, be related in a more subtle way as this result suggests.

To study the critical behavior we employ an imaginary-time path-integral formulation of the model.[17,21] For this, the time axis $\tau$ is discretized in slices $\Delta\tau$. This maps the 1D quantum problem onto a 2D classical statistical mechanics problem. In this formulation, the ground-state energy of the 1D quantum model of finite size $L$ corresponds to the reduced free energy per unit length of a classical model defined on an infinite strip along the $\tau$ direction of width $L$. Following the standard procedure, after scaling the time slices appropriately in order to get an isotropic model, we obtain a classical partition function $Z=\mathrm{tr}\,e^{-H}$ with

$$\begin{aligned}H=-\alpha\sum_{\tau,j}[&\cos(\theta_{\tau,j}-\theta_{\tau,j+1})+\cos(\theta_{\tau,j}-\theta_{\tau+1,j})\\&-\cos(\phi_{\tau,j}-\phi_{\tau,j+1})+\cos(\phi_{\tau,j}-\phi_{\tau+1,j})\\&+\cos(\theta_{\tau,j}-\phi_{\tau,j})]\,,\end{aligned} \tag{3}$$

where, for convenience, we denoted by $\theta$ and $\phi$ the phases on the left and right columns in Fig. 1, and $\alpha=(E_J/E_c)^{1/2}$ plays the role of an inverse temperature in the 2D classical model.

The free energy of (3), defined on the infinite strip, can be obtained from the largest eigenvalue $\lambda_0$ of the transfer matrix as $-\ln\lambda_0$. A kink in the 1D quantum model corresponds to a domain wall along the strip. The corresponding energy gap can be obtained from the free-energy differences of the infinite strip with and without a wall. However, because of the continuous degree of freedom in (3), diagonalization of the transfer matrix cannot be done exactly. Recently, Nightingale and Blöte[19] have developed a Monte Carlo transfer-matrix method which can be used to obtain accurate estimates of the largest eigenvalue even for this case. The method is a stochastic implementation of the well-known power method to obtain the dominant eigenvalue of a matrix. Using helical boundary conditions in order to get a sparse transfer matrix, that is the same for every site addition, a sequency of random walkers $R_i$, $1\le i\le r$, representing the configuration of a column in the infinity strip, is then introduced with corresponding weights $w_i$. The number of walkers $r$ is maintained within a few percent of a target value $r_0$ by adjusting the weights properly. The probability density for a transition process is defined from the matrix elements of the transfer matrix. A Monte Carlo step consists of a complete sweep over all random walkers. The method has been discussed in detail in Ref. 20. To apply the method to our case, we rewrite the transfer matrix to add a pair $(\theta_{\tau,j},\phi_{\tau,j})$ as a product of matrices which add these variables successively. We performed extensively calculations using, typically, $r_0=15000$ random walkers and 30000 Monte Carlo steps which correspond to $4.5\times 10^8$ attempts per $(\theta,\phi)$ pair.

Because of the antiferromagnetic pattern of $\chi_p$, strips with an odd number of sites $L$ will have a domain wall along the infinity direction. To obtain the corresponding interfacial free energy, we performed calculations of the free energy per site $f(\alpha,L)$ of the strip as a function of $L$. By numerically interpolating between successive odd and even $L$, we determine $\Delta F(\alpha,L)=L^2\Delta f(\alpha,L)$, from the free-energy differences at the same $L$. Results of these calculations near the transition point $\alpha_c$ for $6<L<14$, are indicated in Fig. 2. From finite-size scaling one has the relation

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

where $A$ is a scaling function and $\delta=\alpha-\alpha_c$. For sufficiently small $|\delta|$, it has a linear expansion

$$\Delta F(\alpha,L)=a+b\delta L^{1/\nu}\,. \tag{5}$$

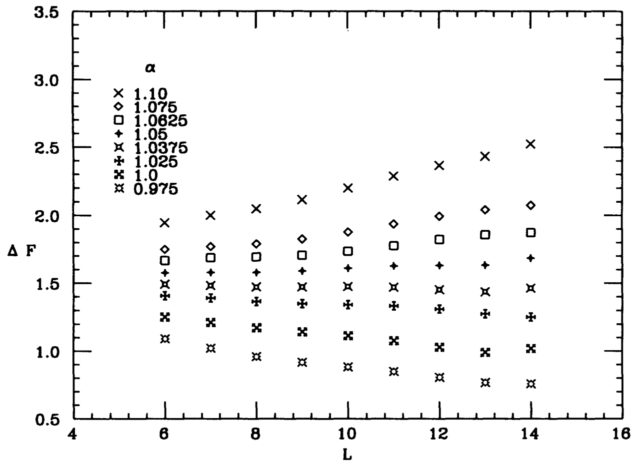


FIG. 2. Size dependence of $\Delta F = L^2 \Delta f(\alpha, L)$ for the kink energy gap.

Depending on the sign of $\delta$, it increases or decreases for increasing $L$, from a finite value $a$ at the transition, as in Fig. 2. From this change of behavior we can determine a critical value $\alpha_c = 1.042(6)$. The universal amplitude $a$ is related to the exponent $\eta$ as[22] $a = \pi\eta$, from which we estimate $\eta = 0.47(4)$ from the data in the figure. Sufficiently close to $\alpha_c$, where Eq. (5) is a good approximation, $1/\nu$ can be obtained from the slope of a log-log plot of $S = \partial \Delta F / \partial \alpha$ vs $L$ without requiring a precise determination of $\alpha_c$. On the other hand, $S$ can be obtained numerically from the slope of $\Delta F$ vs $\alpha$. Assuming that the data in Fig. 2, in the range $1.025 < \alpha < 1.075$, is in the linear regime of Eq. (5) we obtain the estimate of $S$ in Fig. 3. Data for $L < 8$ are clearly outside this regime. Using the results for larger systems we obtain, from the slope of the log-log plot, $\nu = 0.81(4)$.

One can also study the behavior of the helicity modulus. This measures the response of the system to an imposed phase twist. It vanishes in the disordered (incoherent) and is finite in the order (coherent) phase. We calculated this quantity by determining the free-energy differences, $\Delta F = L^2 \Delta f$, between strips with and without and additional phase mismatch of $\pi$ along the strip.[23] The helicity modulus is related to this quantity by $\gamma = 2\Delta F/\pi^2$ for large system sizes. The results are indicated in Fig. 4. The behavior is similar to the kink energy in Fig. 2 and quite different from what it would be expected if the transition was in the universality class of the 2D $XY$ model, where $\gamma$ is almost size independent in the ordered phase.[24] We have not attempted a finite-size-scaling analysis of these data as the scaling parameters are not as obvious as in Eq. (4). We note, however, that the helicity modulus, evaluated at the critical point determined from Fig. 2, appears to be smaller than the universal jump $2/\pi$ expected for a 2D $XY$ model transition.

Finally, from conformal invariance, the central charge $c$ can be related to the amplitude of the singular part of the free energy per site by[25] $f(\alpha_c, L) = f_0 + \pi c / 6L^2$. Using the data for values of $\alpha$ closest to the estimated critical value $\alpha_c$, we obtain $c = 1.67(4)$ from strips of $L > 8$.

The results for the critical exponents $\eta$ and $\nu$ differ significantly from pure 2D Ising exponents and the finite-size behavior of the helicity appears inconsistent with pure 2D $XY$ model behavior. Moreover, the central charge is large than $c = \frac{3}{2}$, which would be expected if the transition was single, but decoupled. All these results point to the single-transition scenario. In fact, they are consistent with a point along the line of single transitions[26] in the $XY$-Ising model[9] and support the conclusions of Ref. 16. Similar results have also been found for the 2D FC$XY$ model. From Monte Carlo simulations,[10] one finds $\nu = 0.85(3)$ and $\eta = 0.31(3)$, and an estimate of the central charge, from Monte Carlo transfer-matrix calculations,[8] gives $c = 1.66(4)$. The critical behavior of this model is also expected to be described by the same $XY$-Ising model and the results appear consistent with the line of single transitions. This, together with the present result, provides further support to the $XY$-Ising model as a correct description of the critical behavior in these systems. Also, in view of this overall agreement, one is led to suspect that the 1D FQ$XY$ may actually be directly relat-

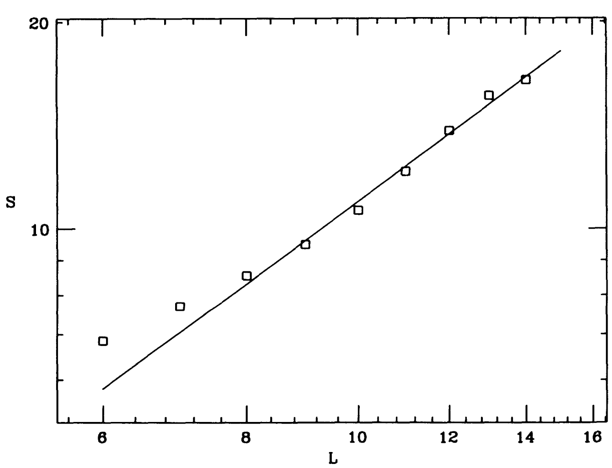


FIG. 3. $S = \partial \Delta F / \partial \alpha$ evaluated near $\alpha_c$ from Fig. 2. The exponent $1/\nu$ is obtained from the slope of $L > 8$.

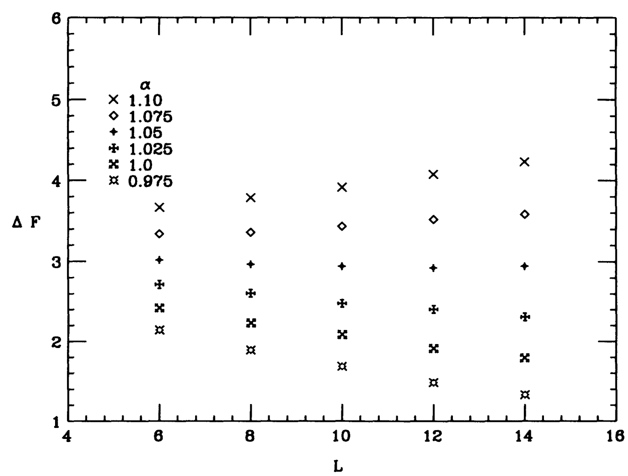


FIG. 4. Size dependence of $\Delta F = L^2 \Delta f(\alpha, L)$ for the helicity.

ed to the 2D FC$XY$ model. We note, however, that the quantum version is not just the Hamiltonian limit of the classical one.

In conclusion, we have studied a one-dimensional quantum version of the frustrated $XY$ model. The model can be physically realized as a ladder of Josephson junctions at half flux quantum per plaquette, which undergoes a zero-temperature superconductor-insulator transition as a function of charging energy. The critical behavior, expected to be in the universality class of the $XY$-Ising model, was studied using a Monte Carlo transfer matrix applied to the path-integral representation. The critical exponents and central charge appear to be consistent with the corresponding values for the $XY$-Ising model in the region of single transitions of the phase diagram. Similar result was recently obtained for the two-dimensional frustrated classical $XY$ model. The models are related by their universality classes, but the one-dimensional quantum version, apparently, is not the Hamiltonian limit of the two-dimensional one. The result of this paper together with the recent result for the two-dimensional classical version of the frustrated $XY$ model, provides further support to the relevance of the $XY$-Ising model for the critical behavior in these systems.

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