Intrinsic finite-size effects in the two-dimensional XY model with irrational frustration

Sung Yong Park¹,², M.Y. Choi², Beom Jun Kim³, Gun Sang Jeon⁴, and Jean S. Chung⁵

¹Lyman Laboratory of Physics, Harvard University, Cambridge, Massachusetts 02138
²Department of Physics, Seoul National University, Seoul 151-742, Korea
³Department of Theoretical Physics, Umeå University, 901 87 Umeå, Sweden
⁴Center for Strongly Correlated Materials Research, Seoul National University, Seoul 151-742, Korea
⁵Department of Physics, Chungbuk National University, Cheongju 361-763, Korea

This study investigates in detail the finite-size scaling of the two-dimensional irrationally frustrated XY model. By means of Monte Carlo simulations with entropic sampling, we examine the size dependence of the specific heat, and find remarkable deviation from the conventional finite-size scaling theory, which reveals novel intrinsic finite-size effects. Relaxation dynamics of the system is also considered, and correspondingly, finite-size scaling of the relaxation time is examined, again giving evidence for the intrinsic finite-size effects and suggesting a zero-temperature glass transition.

PACS numbers: 74.50.+r, 64.60.Cn, 74.60.Ge

The two-dimensional XY model with uniform frustration has attracted much interest in connection with quite a few physical realizations such as periodic arrays of coupled Josephson junctions in uniform magnetic fields. Of particular interest is the case of irrational frustration, where the possibility of a structural glass phase without intrinsic random disorder has been a long-standing question. In the model with irrational frustration, the periodicity of the ground state should be incommensurate with the underlying array periodicity and the ground states are infinitely degenerate, suggestive of the absence of a finite-temperature transition. It was thus argued that there is no phase transition at finite temperatures in the thermodynamic limit, which was also favored by numerical simulations of the current-voltage (IV) characteristics. The latter, performed with resistively shunted junction (RSJ) dynamics, demonstrated that the IV scaling is consistent with a zero-temperature vortex-glass transition proposed in Ref. 1. In other simulations, on the other hand, a metastable finite-temperature glass transition was proposed and the similarity of the relaxation dynamics to the primary relaxation in a supercooled liquid was pointed out. Subsequent Monte Carlo (MC) simulations of the original XY model and of the corresponding Coulomb gas then suggested the relevance of boundary conditions and dynamics in observing the reported glass effects, leaving the existence of a finite-temperature transition still inconclusive.

One way to resolve this is to attribute the observation of the finite transition temperature to intrinsic finite-size effects. In a finite system the effects of irrational frustration may not be distinguished from those of rational frustration, the value of which is given by a rational approximant sufficiently close to the irrational. Consequently, unlike the system in the thermodynamic limit, a finite system (with irrational frustration) tends to behave as if the value of the frustration were given by the rational approximant. Accordingly, the finite system may display such transition-like behavior as the specific heat peak (rounded off due to usual finite-size effects) at a finite temperature, even though the system in the thermodynamic limit undergoes a zero-temperature transition, as argued in Ref. 1. Here the approximant which properly describes a finite system depends on the system size, raising the interesting possibility of intrinsic finite-size effects in addition to the usual ones; this has not been probed in previous simulations, where, for simplicity, fixed rational approximants were mostly used instead of the actual irrational value of frustration.

In this Letter, we adopt the idea of the intrinsic finite-size effects to resolve the controversy on the phase transition in the two-dimensional irrationally frustrated XY (IFXY) model. For this purpose, we use the exact irrational number up to the machine precision, and perform extensive MC simulations with improved entropic sampling to compute the specific heat. The obtained data turn out to be inconsistent with the conventional scaling theory of either the first-order transition or the second-order one, revealing the presence of novel intrinsic finite-size effects. To confirm the existence of such intrinsic finite-size effects, we also study the relaxation dynamics of the system and construct the finite-size scaling theory of the relaxation time, on the basis of the zero-temperature glass transition together with the intrinsic finite-size effects. The size dependence of the relaxation time indeed agrees well with the scaling theory, providing strong evidence for the intrinsic finite size effects.

The Hamiltonian for the irrationally frustrated XY model on an $L \times L$ square lattice is given by

$$H = -J \sum_{(i,j)} \cos(\phi_i - \phi_j - A_{ij}),$$

where the angle $\phi_i$ corresponds to the phase of the superconducting order parameter at site $i$ and $J$ represents the Josephson coupling strength in the case of a Josephson junction array. The plaquette sum of the bond angle $A_{ij}$
is constant over the whole lattice, $\sum A_{ij} = 2\pi f$, where the frustration parameter $f$ is set equal to the golden mean: $f = \Omega \equiv (\sqrt{5} - 1)/2$.

To investigate the finite-size effects of this system, we consider systems of size $L = 5, 8, 13, 21$, and $34$, the entropies of which are computed by means of extensive MC simulations with entropic sampling. The entropy obtained for each system allows one to calculate the specific heat of the system. Both periodic boundary conditions (PBC) and free boundary conditions (FBC) are used and the results are compared with each other, from which two types of finite-size effects are identified. In principle both boundary conditions should yield correct limiting behavior as the system size $L$ is increased, although for finite $L$ the PBC induces mismatch at the boundary. The values of $L$ are thus chosen in such a way that the mismatch present in the PBC is kept minimum. In the case of the golden mean, it can be achieved by choosing the Fibonacci numbers.

Figure 4 presents the temperature dependence of the obtained specific heat in the PBC for various system sizes. For $L = 34$, in order to get reliable results, we have performed as many as $7.5 \times 10^{10}$ MC steps per site using a Cray T3E supercomputer system. As $L$ gets increased, the peak is shown to grow and the transition region to narrow whereas the peak position shifts toward lower temperatures. The position of the specific heat peak in the system of size $L$, denoted by $T_m(L)$, is expected to approach the critical temperature $T_c$ as $L$ is increased. The well-known finite-size scaling theory of the second-order transition \cite{12,13} gives the behavior

$$T_m(L) - T_c \propto L^{-1/\nu},$$

(2)

to which the least-square fit of our data leads to $T_c = 0$ and $1/\nu = 0.36$. On the other hand, the peak height in Fig. 4, expected to grow as $L^{\alpha/\nu}$, gives the value $\alpha/\nu \approx 0.17$, which, via the Josephson scaling relation $(2 - \alpha = d\nu$ with the system dimension $d = 2)$, leads to the value $\nu \approx 0.92$; this is consistent with the value $\nu \approx 0.9$ obtained in the numerical study of IV characteristics \cite{3}. Thus the result of the fit manifests inapplicability of the conventional finite-size scaling theory. Further, it is also inconsistent with the scaling theory of the first-order transition \cite{12,13}, according to which $1/\nu$ in Eq. (2) is replaced by the system dimension $d = 2$. It is thus concluded that the system does not display conventional finite-size effects associated with either a first-order transition or a second-order one. Still remains the possibility of a weakly first-order transition, in which case the system may appear to exhibit size dependence similar to that for a second-order transition \cite{12,13}. Such pseudo-divergent scaling behavior should disappear as the system size exceeds the correlation length of the system.

Deviation from these conventional (second-order, first-order, or weakly first-order) transitions can be observed most clearly in comparing the size dependences of the specific heat under PBC and under FBC. Periodic boundary conditions tend to suppress fluctuations, exhibiting the peak position at a temperature higher than the true critical temperature $T_c$. Under FBC, on the other hand, no such suppression exists and large fluctuations in general yield the peak at a lower temperature \cite{12}. Thus the ordinary finite-size effects are manifested by the shift of the peak position toward $T_c$ as the system size is increased, from higher temperatures in PBC and from lower temperatures in FBC, respectively. The results of test runs for the fully frustrated XY model with $f = 1/2$, shown in Fig. 5(a), indeed demonstrate such behavior of the ordinary finite-size effects: The data in both cases, PBC and FBC, follow Eq. (2) (up to the overall sign), and the least-square fit with the values of $T_c$ and $\nu$ in Ref. \cite{14} yields the lines displaying nice scaling behaviors \cite{3}. On the other hand, Fig. 5(b) reveals quite different features of the finite-size effects in the IFXY model. Here the peak position $T_m(L)$ in PBC is sensitive to the system size $L$, reducing rapidly with $L$, while it is not the case in FBC \cite{15}. In particular, unlike the case of rational frustration, the peak position in FBC does not shift toward higher temperatures, violating the conventional scaling given by Eq. (3).

Such peculiar behavior can be explained in terms of intrinsic finite-size effects present in addition to the ordinary ones \cite{10}: For the frustration given by the golden mean, the appropriate rational approximants are given by the ratios between adjacent pairs in the Fibonacci sequence, i.e., $f_k = q_{k-1}/q_k$, where $q_k$ denotes the $k$th Fibonacci number. Among these rational frustration values $f_k$’s, those satisfying the following condition determine nature of the transition in the (finite) system of size $L$:

$$q_k \ll L \ll |f - f_k|^{-1},$$

(3)

where $f = \Omega$. While the first inequality in Eq. (3) simply implies that the system size should be sufficiently larger than the size of a unit cell, the second one, related with the charge neutrality condition, gives the criterion that the defects due to the mismatch $f - f_k$ are negligible since the corresponding phase change across the system is $\propto L(f - f_k) \propto L^1$. Accordingly, as the system size $L$ is increased, the mismatch should get smaller and the bigger Fibonacci number $q_k$ is needed to describe the transition at the size. The transition temperature as well as nature of the transition depends on the frustration parameter or on $q_k$ \cite{12,13} and thus on the system size.

It is therefore plausible to replace $T_c$ in Eq. (2) by $T_c(L)$, the transition temperature of the system of size $L$, which yields

$$T_m(L) - T_c(L) = c_p L^{-1/\nu}$$

$$T_m(L) - T_c(L) = -c_f L^{-1/\nu}$$

(4)

with appropriate (positive) amplitudes $c_p$ and $c_f$ for PBC and for FBC, respectively. Here $T_c(L)$ is expected to decrease with the system size, approaching the true critical
value $T_c$ in the thermodynamic limit \[^{[1]}\]. Since the precise limiting behavior is unknown, we assume the simple behavior

$$T_c(L) - T_c = c_1 L^{-a}. \quad (5)$$

Note that in contrast to the ordinary finite-size effects, which depend crucially upon the boundary conditions, the intrinsic effects described by Eq. \[^{[2]}\] change the transition temperature itself, regardless of the boundary conditions.

Equations \[^{[1]}\] and \[^{[2]}\] thus yield the appropriate scaling form for the IFXY model: In PBC, both ordinary and intrinsic effects add up to give the finite-size scaling in the form

$$T_m(L) - T_c = c_1 L^{-a} + c_2 L^{-1/\nu}, \quad (6)$$

whereas in the case of FBC, the two effects give the convergence behavior in the opposite direction, leading to the form

$$T_m(L) - T_c = c_1 L^{-a} - c_3 L^{-1/\nu}. \quad (7)$$

Indeed using the value $\nu = 0.9$, we can fit the peak position data both in PBC and in FBC to Eqs. \[^{[1]}\] and \[^{[2]}\] with $T_c = 0$, respectively, to obtain the same value

$$a = 0.28 \pm 0.05. \quad (8)$$

The resulting scaling curves are displayed in Fig. 2(b), giving strong evidence for $T_c = 0$.

To confirm this, we also study the relaxation dynamics of an $L \times L$ RSJ array under PBC in both directions \[^{[9]}\]. To obtain dynamical behavior, we integrate directly the equations of motion with the time step $\Delta t = 0.05$, starting from random initial configurations and taking averages over 300 to 30000 independent runs. In the limit $t \to \infty$, the energy function is expected to approach the equilibrium value at given temperature $T$, allowing us to estimate the relaxation time $\tau$ of the energy function. The obtained behavior of $\tau$ is shown in Fig. 3 for various sizes $L = 5, 8, 13, 21$, and 34. Notice that for $T > 0.25$ the data do not depend appreciably on the system size, which explains why the size effects were not observed in Ref. \[^{[3]}\]. Still the scaling of IV characteristics, not relying much on the system size in the temperature region probed, can give an accurate value of the exponent $\nu$ \[^{[3]}\].

To examine the finite-size effects in the relaxation time data, we construct the suitable scaling form of the relaxation time. In the presumed zero-temperature glass transition, the relaxation has an activated form, and the relaxation time diverges exponentially as the temperature approaches zero, taking the form \[^{[28]}\]

$$\tau = A \exp(\Delta E/T). \quad (9)$$

Here $\Delta E$ is the typical barrier that a vortex should overcome to move across the correlation length $\xi$, and scales as $\Delta E \sim \xi^\psi$ with the barrier exponent $\psi$. In the presence of intrinsic finite-size effects, which lead to the size-dependent transition temperature $T_c(L)$, the correlation length should display the scaling behavior

$$\xi = L f(L^{1/\nu}[T - T_c(L)]) \quad (10)$$

with the appropriate scaling function $f(x)$ such that $f(x \to 0) \to \text{constant}$ and $f(x \to \infty) \to x^{-\nu}$. The corresponding finite-size scaling of the relaxation time thus takes the form

$$\log \tau = L^\psi \phi(L^{1/\nu}[T - T_c(L)]) \quad (11)$$

with the scaling function $\phi(x) \propto |f(x)|^\psi$.

Figure 3 presents the scaling plot of the relaxation time $\tau$ of the IFXY model, showing that the data indeed fit well to the finite-size-scaling form in Eq. \[^{[1]}\]. The critical temperature $T_c(L)$ at each size $L$ has been estimated from the specific heat data. From this scaling with $\psi = 0.54$, we obtain the exponent $\nu = 0.89 \pm 0.2$, which is in good agreement with the results of the specific heat data and of the IV characteristics in Ref. \[^{[3]}\].

In summary, we have studied the finite-size scaling of the specific heat and the relaxation time in the two-dimensional irrationally frustrated XY model. This has revealed intrinsic finite-size effects and a zero-temperature glass transition in the thermodynamic limit, thus resolving the controversy as to the existence of a finite-temperature transition. Since the analytic argument for the intrinsic effects is rather general \[^{[11]}\], we believe the conclusion to be valid for any irrational $\xi$; this is indeed supported by the preliminary results for the silver mean case, the detailed investigation of which is left for further study. Finally, we point out that for generic values of frustration, a quasiperiodic array displays behavior similar to that of a periodic array with irrational frustration \[^{[21]}\]. This suggests the presence of intrinsic finite-size effects also in the quasiperiodic array, as manifested by the apparent glass behavior reported in Ref. \[^{[3]}\].

MYC thanks D.J. Thouless for the hospitality during his stay at University of Washington, where part of this work was accomplished. SYP thanks D.R. Nelson, D.S. Fisher, and S. Teitel for useful discussions and acknowledges the fellowship from the Rotary Foundation. This work was supported in part by the NSF Grant DMR-9815932, by the Ministry of Education through the BK21 Program (MYC), and by the KRF Grant 99-005-D00034 (JSC).

\[^{[1]}\] For a list of references, see, e.g., (a) Proceedings of the 2nd CTP Workshop on Statistical Physics: KT Transition and Superconducting Arrays, edited by D. Kim, J.S. Chung, and M.Y. Choi (Min-Eum Sa, Seoul, 1993); (b)
Proceedings of the ICTP workshop on Josephson Junction Arrays, edited by H.A. Cerdeira and S.R. Shenoy, Physica B 222, 253 (1996).

[2] M.Y. Choi and D. Stroud, Phys. Rev. B 32, 7532 (1985).
[3] E. Granato, Phys. Rev. B 54, R9655 (1996).
[4] D.S. Fisher, M.P.A. Fisher, and D.A. Huse, Phys. Rev. B 43, 130 (1991).
[5] T.C. Halsey, Phys. Rev. Lett. 55, 1018 (1985).
[6] R.W. Reid, S.K. Bose, and B. Mitrović, Phys. Rev. B 54, R740 (1996); J. Phys.: Condens. Matter 9, 7141 (1997). Here quasiaperiodic arrays were also considered and no essential difference was observed, in agreement with Ref. [21].
[7] B. Kim and S.J. Lee, Phys. Rev. Lett. 78, 3709 (1997).
[8] C. Denniston and C. Tang, Phys. Rev. B 60, 3163 (1999).
[9] P. Gupta, S. Teitel, and M.J.P. Gingras, Phys. Rev. Lett. 80, 105 (1998).
[10] M.Y. Choi and D. Stroud, Phys. Rev. B 35, 7109 (1987).
[11] B.A. Berg and T. Celik, Phys. Rev. Lett. 69, 2292 (1992); J. Lee, ibid. 71, 211 (1993); S.Y. Park and M.Y. Choi, in preparation.
[12] J.L. Cardy, Scaling and Renormalization in Statistical Physics (Cambridge Univ. Press, Cambridge, 1996).
[13] V. Privman, Finite-Size Scaling Analysis and Numerical Simulation of Statistical Systems (World Scientific, Singapore, 1992).
[14] P. Peczak and D.P. Landau, Phys. Rev. B 39, 11932 (1989).
[15] M.Y. Choi and S. Doniach, Phys. Rev. B 31, 4516 (1985).
[16] P. Olsson, Phys. Rev. Lett. 75, 2758 (1995).
[17] There is controversy about the value of the exponent $\nu$ in the $f = 1/2$ case. See, e.g., G.S. Jeon, S.Y. Park, and M.Y. Choi, Phys. Rev. B, 55 14088 (1997). Here our purpose is not to distinguish which value is correct but merely to demonstrate the difference between PBC and FBC.
[18] Similar behavior was also reported in the approach using the approximate rational frustration given by the first few of the Fibonacci sequence. See Ref. [3].
[19] For the detailed method, see, e.g., B.J. Kim, M.Y. Choi, S. Ryu, and D. Stroud, Phys. Rev. B 56, 6007 (1997).
[20] R.A. Hyman, M. Wallin, M.P.A. Fisher, S.M. Girvin, and A.P. Young, Phys. Rev. B 51, 15304 (1995).
[21] J.S. Chung, M.Y. Choi, and D. Stroud, Phys. Rev. B 38, 11476 (1988).

FIG. 1. Specific heat versus temperature in the irrationally frustrated XY model under periodic boundary conditions, for size $L = 5, 8, 13, 21,$ and $34$. The peak position shifts toward lower temperatures as the system size is increased.

FIG. 2. Size dependence of the position of the specific heat peak. (a) In the rational case ($f = 1/2$), the data in both PBC and FBC follow Eq. (2), with the lines denoting the least square fits to Eq. (2). (b) In the irrational case ($f = \Omega$), the data fit to Eq. (6) (PBC) or (7) (FBC) rather than to Eq. (2). In (a) error bars are not larger than the symbols.
FIG. 3. Relaxation time $\tau$ versus the temperature $T$ in the semi-log scale for system size $L = 5, 8, 13, 21, \text{ and } 34$. Error bars have been estimated from the standard deviation and those data points without them have errors not larger than the size of the symbols. The dotted lines are merely guides to the eye.

FIG. 4. Fit of the relaxation time data to the finite-size-scaling formula given by Eq. (11), with $\psi = 0.54$ and $1/\nu = 1.12$. The critical temperature $T_c(L)$ has been obtained from the specific heat data.