Reply to “Incommensurate vortices and phase transitions in two-dimensional XY models with interaction having auxiliary minima” by S. E. Korshunov

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We present a rigorous proof and extensive numerical simulations showing the existence of a transition between the paramagnetic and nematic phases, in a class of generalized XY models. This confirms the topology of the phase diagram calculated by Poderoso et al. [PRL 106(2011)067202]. The results disprove the heuristic argument presented by Korshunov in [arXiv:1207.2349v1], against the existence of the generalized-nematic phase in a model with \( q = 3 \).

In a recent Letter [1], we have studied the phase diagram of a generalized XY model with Hamiltonian

\[
H = -\sum_{\langle ij \rangle} \left[ \Delta \cos(\theta_i - \theta_j) + (1 - \Delta) \cos(q\theta_i - q\theta_j) \right],
\]

where \( q > 1 \) is an integer and \( 0 \leq \Delta \leq 1 \). Using Monte Carlo (MC) simulations, we showed that for \( q = 3 \) and \( 0 < \Delta \lesssim 0.4 \), the model exhibits — depending on the temperature — three possible phases: paramagnetic (P), generalized-nematic (N), and ferromagnetic (UF). The phase transition between P and N was found to be in the Kosterlitz-Thouless (KT) universality class, while the transition between N and UF was found to belong to the 3-state Potts universality class. In his Comment on our work [2], Dr. Korshunov argued that the N phase cannot exist for \( q > 2 \), and that there should only be one “genuine phase transition” between the P and UF phases. We will now show that the argument of Ref. [2] is incorrect.

Let us first consider \( \Delta = 0 \). In this case the Hamiltonian becomes purely \( q \)-nematic. Changing variables in the partition function, \( q\theta_i \to \theta_i \), shows that the model is isomorphic to the usual XY model, but with the low temperature phase N, instead of UF. The phase transition from P to N will, therefore, occur at \( T_0 \approx 0.893 \), the same temperature as for the standard XY model and will belong to the KT universality class. This, clearly demonstrates that the N phase exists for \( \Delta = 0 \). Using Ginibre’s inequality [3] it is possible to show that the P to N transition will also extend to finite \( \Delta \) [4]. Furthermore, Ginibre’s inequality allows one to derive a rigorous lower bound [4] on the transition temperature between P and N phases, \( T_{\text{KT}}(\Delta) \geq (1 - \Delta)/T_0 \). Since at very low temperature the system must be in UF phase, this proves the existence of P, N and UF phases for small, but finite values of \( \Delta \), contradicting the heuristic argument of Ref. [2].

To precisely delimit the location of all three phases for the model with \( q = 3 \), we consider a specific example, \( \Delta = 1/4 \). For this \( \Delta \), and using finite size scaling (FSS), in Ref. [1] we have calculated the critical temperature for the N-UF transition to be \( T_{\text{Potts}} \approx 0.365 \), which was found to belong to the 3-state Potts universality class. The order parameter \( m_1 \) (magnetization) shows clearly this transition, see Fig. 1. On the other hand, at \( T_{\text{KT}} \), the nematic order parameter \( m_3 \) shows the transition between N and P phases. At the transition temperature, \( m_3 \) decreases with \( L \) as \( m_3(T_{\text{KT}}) \sim L^{-\beta/\nu} \), with \( \beta/\nu \approx 0.117 \). The exponent is very close to the theoretical value expected for the KT transition, \( 1/8 = 0.125 \). To further verify the “genuineness” of this transition, we calculated the helicity modulus \( \Upsilon \) [5], shown in the inset of Fig. 1 as a function of temperature, for several system sizes. The helicity modulus crosses the straight line \( 2T/\pi \) [6] at \( T_{\text{KT}}(L) \), when extrapolated to \( L \to \infty \), gives \( T_{\text{KT}} \approx 0.68 \).

In Fig. 2 we present the susceptibility \( \chi_3 \) as a function of \( T \) for different system sizes. The phase transition is very clear from the divergence of the susceptibility at \( T_{\text{KT}} \), as \( L \to \infty \). For a KT phase transition, the FSS predicts that \( \chi_3(T_{\text{KT}}) \sim L^{1.75} \), while our simulations find \( L^{-1.766} \). Finally, if we plot \( \chi_3L^{\eta - 2} \), with the KT \( \eta = 1/4 \), vs. the Binder cumulant, all the susceptibilities for different system sizes should collapse onto a universal curve [6]. This is precisely what is found in our MC simulations, see inset of Fig. 2.

Ref. [2] also questions the transition between the phases F1 and UF, in the model with \( q = 8 \), and the ab-

FIG. 1: Order parameters \( m_1 \) and \( m_3 \) (see Ref. [1]) for several system sizes \( L \) showing phase transitions at \( T_{\text{Potts}} \approx 0.365 \) and \( T_{\text{KT}} \approx 0.68 \). Inset: Helicity modulus \( \Upsilon \) versus \( T \). The crossing with the line \( 2T/\pi \) at \( T_{\text{KT}}(L) \), when extrapolated to \( L \to \infty \), gives \( T_{\text{KT}} \approx 0.68 \).
FIG. 2: The susceptibility $\chi_3$ associated with $m_3$ near the KT transition for various system sizes. Inset: rescaled susceptibility versus the Binder cumulant, $U_3 = \langle m_3^2 \rangle^2 / \langle m_3^4 \rangle$, showing a perfect collapse with the KT exponent $\eta = 1/4$. A similar collapse is also obtained for the magnetization [7].

In conclusion, we have presented a rigorous proof, as well as numerical evidence for the existence of a transition between the N and P phases belonging to the KT universality class, at odds with the heuristic argument of Ref. [2].

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