Emergent Berezinskii-Kosterlitz-Thouless phase in low-dimensional ferroelectrics

Y. Nahas[1], S. Prokhorenko[1], I. Kornev[2], L. Bellaiche[1]

[1]University of Arkansas

[2]CentraleSupelec

In two-dimensional systems with continuous symmetry and short-range interactions, strong fluctuations prevent the formation of long range order, and rather than a spontaneous symmetry breaking, a topological phase transition driven by the unbinding of vortex-antivortex pairs can occur, the so-called Berezinskii-Kosterlitz-Thouless or BKT transition. It is an infinite-order phase transition and is paradigmatically captured by the two-dimensional XY-model that has attracted much interest for it astutely describes, amongst others, the physics of superfluid helium films, superconducting films, the Coulomb gas model, Josephson junction arrays, and nematic liquid crystals. Ferroelectrics on the other hand, which constitute an important class of materials, are prima facie not expected to exhibit BKT transition, owing to their discrete symmetry stemming from the cubic anisotropy of both the lattice and the ferroelectric interactions, which include the long-range dipolar ones. Whether the BKT behavior would be robust against the introduction of symmetry-breaking ferroelectric anisotropy remains unsettled. Here we show, using Monte Carlo simulations of a first-principles-based effective Hamiltonian scheme as well as scaling, symmetry, and topological arguments, that an intermediate critical BKT phase underlain by quasi-continuous symmetry emerges between the ferroelectric phase and the disordered paraelectric one in tensily strained thin-film of BaTiO3, a prototypical ferroelectric. We find that this overlooked intermediate phase supports quasi-long-range order reflected in the algebraic decay of the correlation function and sustained by the existence of neutral bound pairs of vortices and antivortices, in accordance with defining characteristics of a BKT phase. Its lower and upper critical temperatures, T_c and T_{BKT}, are associated with the condensation and unbinding of vortex-antivortex pairs, respectively. Moreover, we also find that upon reaching T_{BKT}, the correlation function's critical exponent acquires a value close to the theoretical predictions 0.25 of the XY-model, further indicating that the upper transition is likely to be of the BKT type. Our results therefore highlight the subtle, fundamental richness of low-dimensional ferroelectrics and widen the realm of BKT transitions.

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