Evidence for a Berezinskii-Kosterlitz-Thouless phase in ferroelectric thin-films

YOUSRA NAHAS, SERGEI PROKHORENKO, University of Arkansas, IGOR KORNEV, CentraleSupelec, France, LAURENT BELLAICHE, University of Arkansas — The Berezinskii-Kosterlitz-Thouless (BKT) theory, discovered more than 40 years ago, has propelled the notion of topological phase transition, and has a venerable history and a seminal impact upon condensed matter physics and other areas in physics. So far, the question of whether low-dimensional ferroelectrics would manifest BKT physics has been eluded. Our work aims at bridging this gap as it focuses on the investigation of the critical properties of ferroelectric thin-films, namely BaTiO$_3$ under tensile strain. Using Monte Carlo simulations of a first-principles-based effective Hamiltonian scheme as well as scaling, symmetry, and topological arguments, we find that an intermediate critical BKT phase underlain by quasi-continuous symmetry emerges between the ferroelectric phase and the disordered paraelectric one. 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. Our results therefore highlight the subtle, fundamental richness of low-dimensional ferroelectrics and widen the realm of BKT transitions.

$^1$Y.N. and L.B. thank the support of ARO grant W911NF-16-1-0227 and S.P. acknowledges the DARPA grant HR0011-15-2-0038 (under the MATRIX program).