Fluctuations and topological defects in ferroelectrics

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Topologically nontrivial patterns like vortices, hedgehogs (monopoles), skyrmions are not commonly expected to play an important role in statistical mechanics of lattice models whose Hamiltonians possess only a finite set of symmetries. Indeed, in the absence of quenched disorder, the ground state of such models is defect-free, while the classical "topological protection" mechanisms cannot be realized due to a nearly trivial topology of the order parameter space that reduces the set of possible topological defects to domain walls (kinks). Proper ferroelectric materials correspond to one of the real-world prototypes for such models. Specifically, bulk ferroelectric crystals exhibit neither depolarizing nor random local fields that can render topological defects energetically favorable, while strong crystalline anisotropies characteristic for these materials reduce underlying Hamiltonian symmetries to point groups comprising finite number of elements. It is therefore not surprising, that until the recent experimental observation of ferroelectric vortices, domain walls very thought to be the only topological defects exhibited by ferroelectric materials.

In this study, we combine homotopy theory and first-principles-based effective Hamiltonian approach to explore stability of topological defects in bulk BaTiO3 and resolve the aforementioned controversy between theoretical expectations and recent experimental results. Specifically, our results show that this proper ferroelectric material can exhibit stable topological point defects in its tetragonal polar phase and stable topological line defects in its orthorhombic polar phase. The stability of such defects originates from a novel mechanism of topological protection related to finite-temperature fluctuations of local dipoles. Large-scale effective Hamiltonian Monte Carlo simulations are then conducted to confirm these theoretical predictions. The results of our work, hence, reveal a novel mechanism of topological protection that can be realized in proper ferroelectrics and provide a theoretical framework for investigations of topological defects in systems with finite underlying symmetries.

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