

Vortex lines at the intersection of domain walls in ferroelectrics

Sergei Prokhorenko,* Yousra Nahas, and L. Bellaïche
*Physics Department and Institute for Nanoscience and Engineering,
University of Arkansas, Fayetteville, Arkansas 72701, USA*

In this study we qualitatively investigate the geometric properties of intersecting ferroelectric domain walls. Such intersections, being the locus of two vanishing polarization components, represent topological defects of reduced dimensionality [1] as compared to the domain walls themselves, and therefore can possess advanced functionalities for the design and implementation of novel electronic devices [2, 3]. However, despite the considerable interest in nontrivial ferroelectric domain patterns [2–5], the full topological classification of inhomogeneous polarization structures in the vicinity of the domain walls intersection lines has not been fully developed. For instance, the description of the intersection of two domain walls has been thoroughly investigated in the sole case of ferroelectric systems described by two-component order parameter [7]. Herein, we attempt to advance the methodology described in Ref. [7] to the three dimensional case.

Our discussion is limited to intersecting domain walls that do not carry any bound electric charge density [9]. Without any loss of generality, we choose the line at the intersection of the domain walls as being along the z -axis, and the domain walls coinciding with the xz and yz coordinate planes. Since $\nabla \cdot P = 0$, only P_x (P_y) and P_z components of polarization can change upon crossing the xz (yz) plane. Two simple illustrative cases under study are presented in Fig.1. In the first case (Fig.1(a.1)), only P_x and P_y components change across the xz and yz planes, respectively. The presented configuration corresponds to a flux-closure pattern of polarization for the P_x and P_y components, while additionally featuring a nonzero constant P_z component. Notably, similar polarization structures have been predicted from first-principles calculations in (Ba,Sr)TiO₃ nanocomposites [5]. One instructive topological characteristic of this configuration can be obtained by mapping the flux of polarization through a contour in real space to the flux in the order parameter space. The topological flux in real space can be defined as $\Phi = \int_S n \cdot (\partial_x n \times \partial_y n)$ [8], where n represents the normalized polarization vector field, and S denotes a specific simply connected region in real space. In the case under study, topological flux represents a characteristic of particular importance. Indeed, the translational invariance of the considered polarization distributions along the domains intersection line makes the system effectively two-dimensional, allowing to keep Φ well defined. Practically, the first step of the calculation of topological flux generated by the intersection line (its topological charge), is achieved by defining a closed contour in the xy plane enclosing the intersection line (blue circle in Fig.1(a.3)). Secondly, one maps the orientation of the dipoles along this path onto the unit sphere. In our case this yields a square whose nodes (red dots in Fig.1(a.2) and (a.3)) intercept the sphere at the latitude defined by P_z . The topological flux is equal to the area of the spherical cap with cut edges (Fig.1(a.2)) obtained by projection of the obtained square on the sphere surface. As one can immediately see, the obtained topological charge monotonically increases upon decreasing $|P_z|$, however showing a discontinuity at $P_z = 0$. Indeed, in contrast to magnetic systems, for which the magnitude of individual spins can be assumed constant, Φ is equal to zero at $P_z = 0$, while having a limit of $\pi/2$ at $P_z \rightarrow 0$. The existence of such limiting point configuration would correspond to a ferroelectric analogue of the so-called Bloch-line in magnetic materials. Finally, it is worthwhile noticing that in this domains configuration, the variation of P_x and P_y along the path are encompassed in the cross product term $\partial_x n \times \partial_y n$ appearing in the chiral charge definition. Hence, considering these two components only, yields a vortex singularity in the xy plane, thereby enabling the identification of the intersection line with a vortex line.

The second case is concerned with the domain walls intersection for which only P_z and P_x components change across the yz and xz planes, respectively (Fig.1(b.1)). This configuration is assumed to have a constant P_y component. The mapping of the flux in real space to the order

*Electronic address: prokhorenko.s@gmail.com

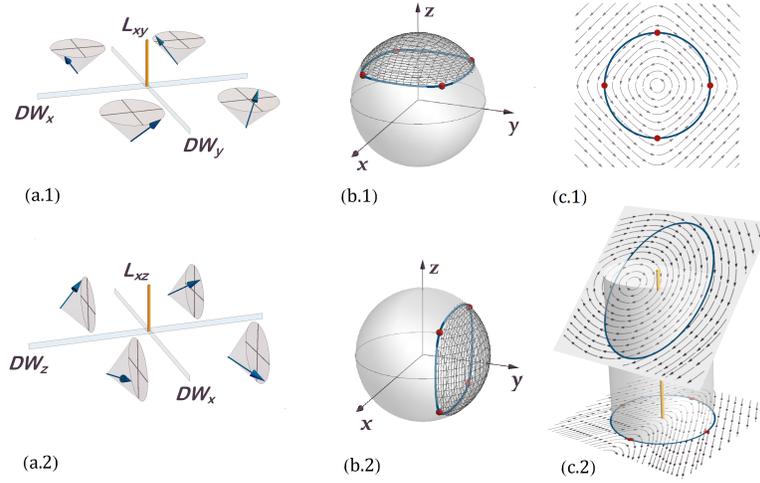


FIG. 1: (a) Dipolar structure in the vicinity of intersecting domain walls. In (a.1) is displayed the case of intersecting P_x and P_y domain walls (denoted by DW_x and DW_y), while (a.2) corresponds to the case of intersecting P_x and P_z domain walls (DW_x and DW_z). In both cases, the intersection line is along the z -axis (L_{xy} in (a.1) and L_{xz} in (a.2)). (b) Mapping of the polarization orientation onto the unit sphere when circulating along a closed path in xy -plane enclosing L_{xy} (b.1) and L_{xz} (b.2). (c) Projection of polarization field depicted in (a.1) on xy plane (c.1). Projection of polarization distribution (b.1) on two differently oriented planes. In the inclined plane, the projection of the vector field reveals its vortex singularity.

parameter space yields the same result as in the former case, however having the truncated spherical cap revolving around the y -axis, in accordance with the constant P_y component. Notably, one does not observe the vortex singularity in the xz plane, but rather an Ising domain profile, which in our case corresponds to the stacking of the vortices in xz plane along the intersection line contained within this plane. Later can be verified by projecting the polarization vector field on xy plane rotated around x axis by the angle ϕ gradually approaching $\pi/2$. The projection corresponding to $\phi = \pi/4$ is depicted in Fig.1(b.3), for which the vortex nature of the intersection line is retrieved. At $\phi \rightarrow \pi/2$ the distance between the core of the projected vortex observed in Fig.1(b.3) and the domain walls intersection line tends to zero along with the elongation of the vortex projection along the rotated y axis. Moreover, the vortex nature of the intersection line can be confirmed by the existence of a global transformation of the vector field corresponding to a passive coordinate rotation around x axis by an angle of $\pi/2$ which conserves the topological flux.

Finally, we show, that realistic patterns of polarization field yielding an integer topological flux can be allowed in ferroelectric systems thereby allowing to predict dipolar configurations analogous to magnetic skyrmionic structures.

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- [1] T. C. Proctor, D. A. Garanin, and E. M. Chudnovsky, *Phys. Rev. Lett.*, 112, 097201 (2014)
 - [2] N. Balke, B. Winchester, W. Ren, Y.H. Chu, A.N. Morozovska, E.A. Eliseev, M. Huijben, R.K. Vasudevan, P. Maksymovych, J. Britson, S. Jesse, I.A. Kornev, R. Ramesh, L. Bellaiche, L.Q. Chen, and S.V. Kalinin, *Nature Physics*, 8, 8188 (2012)
 - [3] T. Choi, Y. Horibe, H. T. Yi, Y. J. Choi, Weida Wu, and S.-W. Cheong, *Nature Mat.*, 9, 253 (2010)
 - [4] Jia, C. L. , K. W. Urban , M. Alexe , D. Hesse , and I. Vrejoiu *Science*, 331, 1420 (2011)
 - [5] L. Louis, I. Kornev, G. Geneste, B. Dkhil, and L. Bellaiche, *J. Phys.: Condens. Matter*, 24, 402201 (2012)
 - [6] S. Prosandeev, A. Malashevich, Z. Gui, L. Louis, R. Walter, I. Souza, and L. Bellaiche, *Phys. Rev. B*, 87, 195111 (2013)
 - [7] E. B. Sonin, and A. K. Tagantsev, *Sov. Phys. JETP*, 67, 396 (1988)
 - [8] N.D. Mermin, *Rev. Mod. Phys.*, 51, 591 (1979)
 - [9] P. Marton, I. Rychetsky, and J. Hlinka, *Phys. Rev. B*, 81, 144125 2010