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Are Polarization and Magnetization really Bulk Properties?[1]
RAFFAELLO BIANCO, RAFFAELE RESTA, Physics Dept., U. Trieste — Microscopic understanding of P and of (orbital) M was achieved only recently; the modern theories express both as BZ integrals. Since k-space is an artificial construct, all bulk properties must be embedded in the ground state density matrix $\rho(\mathbf{r},\mathbf{r}')$, "nearsighted" in insulators, independently of the boundary conditions, either periodic (PBCs) or open (OBCs). A basic tenet of the modern theory is that the bulk electron distribution determines P only modulo a "quantum": therefore P is not independent of the boundaries. Instead M is not affected by any quantum indeterminacy and an expression in terms of the bulk ρ is not ruled out: we explicitly find such expression. In a finite homogeneous sample, within OBCs, the macroscopic magnetization is cast as a function of the bulk $\rho(\mathbf{r},\mathbf{r}')$. Remarkably, our approach applies even to topological (Chern) insulators, where M explicitly depends on the chemical potential. The boundary currents contribute to M, but even their contribution is "bulk" in the above sense; the value of M is robust and cannot be altered by acting on the boundaries only. Instead, P can be varied (by a quantum) by acting on the boundaries only. Simulations performed on a 2d model Hamiltonian within OBCs demonstrate our approach.

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