MAR17-2016-020108

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

The theory of polarization: From its origins to the modern day

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Textbooks define macroscopic polarization **P** as the dipole of a bounded sample, divided by its volume, in the large sample limit. When instead we address unbounded samples within periodic boundary conditions (PBCs) the above definition cannot be adopted. The breakthrough came 25 years ago, when the focus was shifted from **P** itself to adiabatic changes in **P**, and it was soon realized that such changes take the form of a Berry phase of the electronic wavefunction. Even **P** itself can be defined, but it is *not* a vector: it is a lattice. Such exotic feature has outstanding physical consequences. For instance for an insulating centrosymmetric polymer P is a Z_2 invariant: either P=e/2 mod e, or P=0 mod e: the Z_2 class depends on the bulk, while the "mod" value depends on actual termination of the bounded sample. Besides **P**, other quantum-mechanical observables are based on the "bare" position **r**, which is not a legitimate operator within PBCs: foremost among them is orbital magnetization **M**. Here I express such observables in terms of a "projected" position operator $\tilde{\mathbf{r}}$, which is legitimate for both bounded and unbounded samples, and yields very compact expressions for the relevant PBCs formulae. Besides **P** and **M**, I will also express in terms of $\tilde{\mathbf{r}}$ the anomalous Hall conductivity (for insulators and metals), and the Marzari-Vanderbilt gauge-invariant quadratic spread.