Polarization and Localization in Insulators: Generating Function Approach

Ivo Souza
Department of Physics and Materials Research Laboratory
University of Illinois at Urbana-Champaign

In the last decade there have been significant developments in the theory of insulators, coming mostly from the electronic structure community. First and foremost is the Berry phase theory of polarization [1], which extracts the average macroscopic polarization of an insulating crystal from the dependence of the bulk ground state wave function on the "twisted" boundary conditions. The Berry phase formula has become a standard tool in electronic structure calculations, having been applied to a wide range of problems.

Another basic property of insulators which is closely related to electronic polarization is electronic localization. In Refs. [2,3] the ideas from the Berry phase theory of polarization and the related theory of Wannier functions were extended in order to address this issue. The present work [4] is a contribution to this ongoing effort. In particular we show the connection between these recent ideas and the basic notion of localization in the insulating state, introduced by Kohn [5], as well as with the little known work of Kudinov [6].

Our starting point is the following question: Given the ground state wave function of a bulk insulating crystal with N electrons in a volume V obeying "twisted" boundary conditions, what is the quantum distribution of the macroscopic polarization ? We introduce a cumulant generating function which yields, upon successive differentiation, all the cumulants and moments of the probability distribution of an appropriately defined center of mass $\mathbf{X}/N$ of the electrons. This formulation is able to describe in appropriate limits both the Berry phase [1] and the "single-point" type of formulas [3,7]. For the first moment, the average electronic polarization $q_e\langle\mathbf{X}\rangle/V$, we recover the Berry phase expression. The second cumulant, the mean-square fluctuation of the polarization, can be used to define a localization length ξ_i for the electrons along each cartesian direction: $\xi_i^2 = (\langle X_i^2\rangle - \langle X_i\rangle^2)/N$. It follows from the fluctuation-dissipation theorem [6] that as $V \to \infty$, ξ_i diverges for a metal and is a finite, measurable quantity for an insulator. We show that it is related to the spread of the Wannier functions, and also to the optical gap $E_{\rm g}$, via the inequality $\xi_i^2 \leq \frac{\hbar^2}{2m_e E_{\rm g}}$. Similarly to the average polarization, which is given by a geometric phase, ξ_i^2 has a geometric interpretation as a "quantum distance".

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