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Polarization and localization in insulators: Generating function approach

Ivo Souza
Department of Physics and Astronomy, Rutgers University, New Jersey, USA

A theory is formulated, and practical expressions are derived, for the full quantum−mechanical distribution of the intrinsic macroscopic polarization of an insulator in terms of the ground state wave function [1]. The formalism applies to an insulating system of N correlated electrons obeying twisted boundary conditions over a finite volume. The central quantity is 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 **X**/N of the electrons ($\mathbf{X} = \sum^{N}_{i=1} \mathbf{x}_i$). The first moment is the average polarization, where we recover the well−known Berry phase expression [2]. The second cumulant gives the mean−square fluctuation of the polarization, which defines an electronic localization length squared $\xi_\propto^2$ along each direction $\propto$: $\xi_\propto^2 = (< X_\propto^2 > - < X_\propto >^2)/N$. It can be expressed in terms of a metric, which measures the infinitesimal distance between quantum states in a Hilbert space parametrized by the twisted boundary conditions [3,4]. The fluctuation−dissipation relation is used to show that in the thermodynamic limit $\xi_\propto^2$ diverges when the system becomes metallic and is a finite, measurable quantity in the insulating state [5], related to the optical gap by $\xi_\propto^2 \leq \hbar^2/(2\, m_e\, E_g)$. In one dimension this localization length coincides with the one recently introduced by Resta and Sorella [6]. In noninteracting systems it is related to the spread of the Wannier functions [4,6], and this picture is generalized to correlated insulators by defining the many−body analog of Wannier functions. In the limit of large N the maximally−localized ``many−body Wannier functions'' become localized in disconnected regions of the high−dimensional configuration space of the N electrons, establishing a direct connection with Kohn's theory of the insulating state [7]. By recasting the generating function in terms of these functions, it is shown that dielectric polarization results from the localized character of an insulating wave function in configuration space.

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