Homogeneous Electric and Magnetic Fields in Periodic Systems

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Because the application of external homogeneous electric or magnetic fields breaks the periodicity of a solid, the correct theoretical treatment of the response to such fields has been achieved remarkably recently. The modern theory of polarization showed how the polarization of an infinite solid could be obtained from consideration of the Bloch wavefunctions in a unit cell [1–3], and likewise recent work on the magnetization has yielded similar results [4, 5]. Both of these results can be understood in terms of geometric phase arguments.

In the present talk I will try to accomplish three objectives: to provide an overview of the geometric phase arguments that underpin these results; to discuss our recent extensions of the implementation of the polarization theory in a density-functional theory code to include the projector-augmented wave formalism [6] as well as spin-orbit coupling; and to outline our new theory of magnetic response in insulators and describe the current state of its implementation [7].

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