Real-time dynamics of spin, orbit, charge via time-dependent density functional theory: Ab initio access to geometric or topological natures of solid states

Noejung Park,
Ulsan National Institute of Science and Technology (UNIST), Department of Physics,
UNIST-gil 50, Ulsan, 44919 Korea

We have performed the real-time time-dependent density-functional theory calculations, mostly within the adiabatic local density approximation(ALDA), to access to various Berry-curvature characteristics of solid states. We demonstrate that the quantum anomalous Hall conductivity and the quantum spin Hall conductivity of real-material bulk topological insulators can be directly obtained through the real-time profile of the electrons velocity. We extend our methods to nonlinear optical responses associated with spin-orbit dynamics, particularly focusing on the situation when a built-in geometrical chirality is linked to an electric field and/or magnetic field with even a non-zero topological term $\mathbf{E}\cdot\mathbf{B}$. We show that the spin structure emerging over the charge-orbit dynamical state has a quite different characters from the models commonly cited in the interpretations of experimental results. The analogy of these real-time dynamics with the Thouless pump model in the extreme adiabatic limit and the possible realization of axial anomaly as a lattice gauge theory are also discussed. This talk also includes the limitation and utility of ALDA of the exchange-correlation magnetic field in for the aforementioned spin-orbit dynamics.