Shift Vector Effects in High-Harmonic Generation by Massive Carriers in 2D Hexagonal Nanostructures

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The discovery of graphene [1] has catalyzed the search for novel nanomaterials with similarly exceptional electronic and structural properties [2]. Advances in nanotechnology over the past two decades have enabled the synthesis of graphene-like two-dimensional (2D) materials—such as silicene, germanene, and stanene [3]—that exhibit high carrier mobility and suppressed scattering. These materials consist of buckled honeycomb lattices with sublattices composed of A and B atomic sites. Unlike graphene, however, the Dirac quasiparticles in these systems acquire a finite mass due to strong spin–orbit coupling, reaching approximately 65 meV in stanene. Notably, this mass can be tuned via a perpendicular electric field, leading to nontrivial changes in the band topology [4]. Such tunability introduces a rich landscape of nonlinear optical phenomena not accessible in gapless graphene [5].

In this work, we investigate the nonlinear light–matter interaction in these 2D nanostructures using a four-band, second-nearest-neighbor tight-binding model that incorporates spin–orbit coupling and inversion symmetry breaking. Optical excitation in these systems induces a directional charge displacement described by the shift vector, a gauge-invariant quantity combining the derivative of the transition dipole phase and differences in intraband Berry connections. Alongside the Berry curvature [6], the shift vector plays a fundamental role in governing the optical and topological response of these materials.

Using time-domain numerical simulations of the quantum kinetic equation for the density matrix, we analyze the role of the shift vector in the high-harmonic generation (HHG) response. We demonstrate that time- and polarization-resolved HHG spectroscopy provides an all-optical, strong-field probe capable of revealing nontrivial band topology in these 2D hexagonal systems.

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