Berry curvature effects in high-order wave mixing in biased bilayer graphene

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In recent decades, there has been a growing interest in extending atomic high-order harmonic generation (HHG) and high-order wave mixing (HWM) into novel nanostructures [1]. The progress of recent decades in the field of nanotechnology enabled the synthesis of a new class of optical materials, namely two-dimensional nanostructures with extreme high carrier mobility and extraordinary properties [2]. Among these materials, gapped graphene-like systems with non-trivial topology of energy bands are of particular interest. Examples include atomically thin monolayer transition metal dichalcogenides (TMDCs), monolayer hexagonal boron nitride (hBN), and biased bilayer graphene with Bernal stacking. These materials exhibit nontrivial Berry curvatures in their energy bands. In this aspect, biased bilayer graphene has a practical importance, where the band gap can be tuned up to approximately 0.3 eV. Moreover, the Berry curvature near the band edge in biased bilayer graphene is about two orders of magnitude larger than that in monolayer TMDCs or hBN. This unique feature provides an unprecedented opportunity to investigate the influence of Berry curvatures on the HHG process. In a previous study [3], we investigated HWM in TMDCs and found that the impact of Berry curvature on the generation process was minimal. Instead, we observed that many-body electron-electron Coulomb interaction played a significant role in altering both HWM and HHG processes in TMDC nanostructures.

In this study, we present a microscopic quantum theory elucidating the nonlinear and nonperturbative optical response of biased bilayer graphene to a two-color strong laser field, employing a four-band Hamiltonian. This Hamiltonian is derived through ab-initio calculations utilizing the HSE06 functional and a 12×12 Monkhorst-Pack grid with the Quantum Espresso code [4]. Subsequently, we project onto the pz orbitals and employ the wannierization procedure to obtain the Hamiltonian using the Wannier90 software [5]. For the laser-stimulated dynamics, we employ a 300×300 Monkhorst-Pack grid to accurately describe the evolution of the single-particle density matrix across the entire Brillouin zone.

The resonant generation of electron-hole pairs by the high-frequency component of the field, coupled with the induction of HWM and HHG by the low-frequency strong field component, leads to a significant alteration of the HWM/HHG spectra due to the Berry curvature effect. This effect modifies the relative contributions of the interband and intraband channels, fundamentally reshaping the radiation spectra.

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References

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