Bohmian-trajectories analysis of high harmonic generation from solids

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Synopsis High harmonic generation from solids driven by a strong midinfrared laser field are investigated in a Bohmian-mechanical perspective. Numerically solving the time-dependent Schrödinger equation (TDSE) in coordinate space, we find that the harmonic spectra obtained has the same structure as the harmonic spectra of a single Bohmian trajectory, indicating the non-local property of electron’s dynamics in solid.

Following the discovery of non-perturbative high-harmonic generation (HHG) in solids, several experimental and theoretical investigations have aimed to understand its detailed microscopic mechanism[1]. Bohmian trajectories method, as an alternative and complementary quantum approach, has a broad application in studying strong field processes. Bohmian trajectories method describes the probability-density flow associated with the quantum mechanical wave function in specific configuration-space regions, without losing phase information[2]. To the best of our knowledge, such a method has not been applied yet to investigate the high harmonic generation from solids.

We solve the one-dimensional time-dependent Schrödinger equation (TDSE) for solid’s interaction with the laser field in dipole approximation

\[
\frac{\partial \Psi(x,t)}{\partial t} = \left\{ \frac{\hat{p}^2}{2} + V(x) + xE(t) \right\} \Psi(x,t)
\]  (1)

, where \(E(t)\) is the electric field of laser pulse. The Mathieu-type potential \(V(x) = -V_0 [1 + \cos(2\pi x/a)]\) is used to describe a periodic potential of lattice, with \(V_0 = 0.37\) a.u. and lattice constant \(a_0 = 8\) a.u.. The Bohmian trajectories are obtained by integrating the equation of motion

\[
\dot{x} = \nabla S = Im \frac{\nabla \Psi(x,t)}{\Psi(x,t)}
\]  (2)

, where \(S\) is the real-valued phase of \(\Psi(x,t)\).

As shown in Fig.1, bohmian trajectories keep space-periodical at the laser intensities of \(5 \times 10^{12} W/cm^2\). Although most trajectories move in one lattice, several trajectories enter adjacent lattices several times. In Fig.2, harmonic spectra of TDSE dipole \(d(t) = \langle \Psi(t)|x|\Psi(t)\rangle\) and Bohmian trajectory with initial position \(x(t = 0) = 0\) are shown compared with the band structure of model potential. Two spectra obtained has the same structure indicating the non-local property of electron’s dynamics.

Figure 1. Bohmian trajectories at the laser intensities of \(5 \times 10^{12} W/cm^2\)

Figure 2. (b) Harmonic spectra of dipole and bohmian trajectory with \(x(t = 0) = 0\) and (a) corresponding band structure at the laser intensities of \(5 \times 10^{12} W/cm^2\)

References