Bohmian-trajectories analysis of high harmonic generation from solids

Jinlei Liu^{*1}**, Lu Liu*****, Wenpu Dong*****, Yindong Huang*****, Jing Zhao*****, Jianmin Yuan***†**, Zengxiu Zhao**^{*2}

* Department of Physics, College of Science, National University of Defense Technology,
Changsha 410073, People's Republic of China
† IFSA Collaborative Innovation Center, Shanghai Jiao Tong University,
Shanghai 200240, People's Republic of China

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

$$i\frac{\partial\Psi(x,t)}{\partial t} = \{\frac{\hat{p}^2}{2} + \hat{V}(x) + xE(t)\}\Psi(x,t) \qquad (1)$$

, 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

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

, 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.

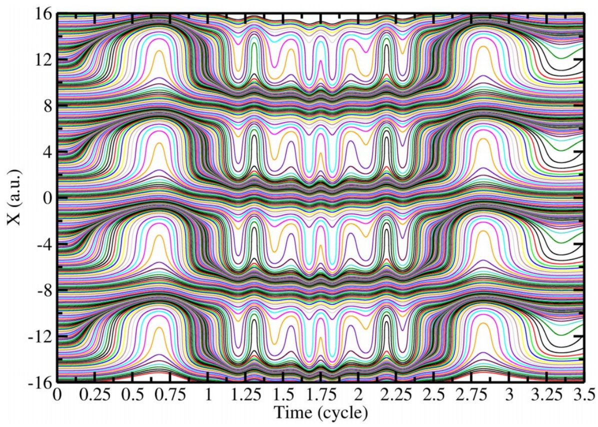

Figure 1. Bohmian trajectories at the laser intensities of $5\times 10^{12}W/cm^2$

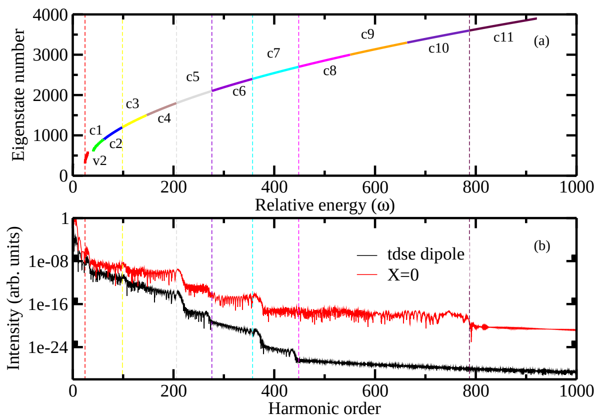

Figure 2. (b) Harmonic spectra of dipole and bohmian trajectory with $x(t=0) = 0$ and (a) corresponding band structure at the laser intensities of $5\times 10^{12}W/cm^2$

References

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[1]E-mail: liujinlei@nudt.edu.cn

[2]E-mail: zhao.zengxiu@gmail.com