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Exploration of the electron multiple recollision dynamics in intense laser fields with Bohmian trajectories

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41 cut-off expansion and multiple plateau generation requires accurate quantum mechanical
42 treatment [7]. Detailed analysis of energy features of the strong field ionization has been also the
43 focus of many studies [8-11]. Yan et al., [11] presented a semi-classical approach based on
44 quantum orbits to provide a physically intuitive interpretation analysis of the low-energy
45 structures (LES). Liu et al. [10] has shown that the LES arises due to an interplay between
46 multiple forward scattering of an ionized electron and the electron momentum disturbance by the
47 Coulomb field immediately after the ionization. Hickstein et. al [12] used a simple model to
48 associate the shape of these structures with the number of times the ionized electron is driven
49 past its parent ion in the laser field before strongly scattering away. Consequently, multiple
50 rescattering has been essentially reported to be responsible for the appearance of some of the
51 primary features of the above-threshold ionization (ATI) spectra [10-14]. At the same time,
52 many reports have been dedicated to directly probe and visualize the electron recollision process
53 [12,15-18].

54
55 Since introduced by Bohm [19], Bohmian mechanics has been applied, as an alternative and
56 complementary quantum approach, to the study of a broad range of problems. One approach to
57 Bohmian mechanics is the hydrodynamics formulation of quantum mechanics, in which the
58 probability amplitude and the phase of the wave function are transported along the quantum
59 trajectories and observables may be computed directly in terms of this information. In the de
60 Broglie-Bohm framework, on the other hand, the individual tracer particles are evolved along
61 quantum trajectories with the velocities generated by the time-dependent wave function field.
62 The patterns developed by these quantum trajectories as they emerge from an ensemble of initial
63 points exactly define the history of the system as it evolves from the initial to final state. This
64 allows one to employ de Broglie–Bohm’s framework of Bohmian mechanics (BM) to provide an
65 accurate trajectory-based scheme to interpret the electron wave packet dynamics [20]. The BM
66 approach has been successfully applied to the model study of problems such as photo-
67 dissociation [21], tunneling [22], atom diffraction by surface [23], etc., in the past. More
68 recently, it has been also used in the model study of strong field processes such as HHG [24],
69 laser-driven electron dynamics [25-32], etc. Although many of the BM studies of strong field
70 processes so far have adopted either 1D or soft-potential models, there are also some promising
71 reports that used the de Broglie-Bohm formalism by means of *ab initio* three-dimensional
72 numerical approach [33].

73
74 Although the well-known semiclassical model takes into account the electron-core interaction,
75 due to the lack of phase information, it was proven that this approach may not be suitable to
76 investigate the coherent dynamic processes such as the momentum distribution of the low-energy
77 ATI [15]. An ensemble of individual Bohmian trajectories, within the De Broglie–Bohm’s
78 framework, on the other hand, contains all the information embedded in the time-dependent
79 wave function. This accurate numerical scheme, therefore, allows tracing the few percentage of
80 the ionized wave packet involved in the rescattering process to reveal the quantum electron

81 dynamical origin of the major features appearing in ATI spectra. This method would be a
82 promising candidate to serve as the electron-dynamical analysis tool, in order to provide an
83 intuitive perspective to explain the experimental and numerical observations.

84

85 We have recently employed Bohmian mechanics to demonstrate the effect of laser pulse shape
86 on the characteristic properties of high-order harmonic generation [7] and the sub-cycle
87 ionization dynamics [34]. In Ref. [34] we showed that, within each optical cycle of the external
88 laser field, some portion of the ionized wave packets, represented by various groups of Bohmian
89 trajectories, return to the parent ion when the laser field changes sign. Since the returning
90 trajectories travel different distances before they change direction and return to the core, each of
91 them would have different return energies. This causes transitions to excited bound and
92 continuum states over time. Therefore, when the next ionization is about to happen (during the
93 subsequent optical cycle), these oscillations of the electron density give rise to multiple wave
94 packets, instead of just one. This effect becomes more and more influential for longer pulse
95 durations (laser field with more number of optical cycles). Similar reasoning can be utilized to
96 interpret the HHG and ATI results by evaluating the harmonic emission and energy content of
97 various group of Bohmian trajectories, which in turn represent the dynamics of different wave
98 packets detached from the parent ion and traveling under the external laser field.

99

100 It has been reported [3,12] that the shape and spacing of the photoelectron interference structures
101 in ATI spectra correspond to the specific number of times the electron reencounters its parent ion
102 before scattering away. Our Bohmian calculations indicate that, driven by a 1600nm laser field, a
103 hydrogenic returning electron wave packet passes the parent ion only if the peak intensity of the
104 laser is as high as $2 \times 10^{14} W / cm^2$. Furthermore, we found that the electrons cannot pass the
105 parent ion if the higher frequency lasers (e.g. 800nm) are used, even with the intensity of
106 $2 \times 10^{14} W / cm^2$. Consequently, the presence of the low energy photoelectron interference
107 structures for the wavelengths above 800nm does not necessarily require the multiple electron
108 recollision with its parent ion to happen. This, at the same time, implies that observation of such
109 common structures in ATI spectra is not sufficiently enough to be taken as an evidence for the
110 existence of multiple electron revisits.

111

112 II. THEORY AND NUMERICAL PROCEDURES

113

114 In this paper, we present our results from a fully *ab initio* three-dimensional and accurate
115 treatment of the Bohmian trajectories to explain the role of multiple recollision of photoelectron
116 in HHG and ATI processes. The time-dependent generalized pseudo-spectral (TDGPS) method
117 [35] is used to solve the TDSE in spherical coordinates accurately and efficiently and to obtain
118 the time-dependent wave functions for Bohmian mechanics calculations. This method takes
119 advantage of the generalized pseudo-spectral (GPS) technique for non-uniform optimal spatial
120 discretization of the coordinates and the Hamiltonian using only a modest number of grid points.

121 Atomic units (a.u.) are used throughout the paper unless specified otherwise. The time
 122 propagation of the wave function under this method is performed by the split operator method in
 123 the energy representation [35]:

$$\begin{aligned}
 & \psi(r, t + \Delta t) \\
 & \cong \exp\left(-i\hat{H}_0 \frac{\Delta t}{2}\right) \times \exp\left[-iV\left(r, \theta, t + \frac{\Delta t}{2}\right) \Delta t\right] \\
 & \times \exp\left(-i\hat{H}_0 \frac{\Delta t}{2}\right) + O(\Delta t^3). \tag{1}
 \end{aligned}$$

128 For atoms in linearly polarized laser fields, the angular momentum projection onto the
 129 polarization direction of the field (the z-axis) is conserved. That means the dependence of the
 130 wave function on the angle φ (rotation angle about the z-axis) is reduced to the factor
 131 $\exp(im\varphi)$, where m is the angular momentum projection. For $m=0$ the wave function does not
 132 depend on φ at all, thus the gradient of the wave function ψ can be calculated with respect to
 133 the coordinates r (radial coordinate) and θ (angle between the radius-vector and z-axis):

$$\nabla \psi = \mathbf{e}_r \frac{\partial \psi}{\partial r} + \mathbf{e}_\theta \frac{1}{r} \frac{\partial \psi}{\partial \theta} = \mathbf{e}_r \frac{\partial \psi}{\partial r} - \mathbf{e}_\theta \frac{\sin\theta}{r} \frac{\partial \psi}{\partial \cos\theta}. \tag{2}$$

136 \mathbf{e}_r and \mathbf{e}_θ are the unit vectors of spherical coordinate system. The equation for the Bohmian
 137 trajectories reads as

$$\frac{d\mathbf{r}}{dt} = \text{Im} \frac{\nabla \psi}{\psi}, \tag{3}$$

141 Since the velocity $\frac{d\mathbf{r}}{dt}$ has the following expansion in the spherical coordinate system,

$$\frac{d\mathbf{r}}{dt} = \mathbf{e}_r \frac{dr}{dt} + \mathbf{e}_\theta r \frac{d\theta}{dt} + \mathbf{e}_\varphi r \sin\theta \frac{d\varphi}{dt}, \tag{4}$$

143 the vector equation (3) is equivalent to a set of three 1D equations:

$$\frac{dr}{dt} = \text{Im} \left(\frac{1}{\psi} \frac{\partial \psi}{\partial r} \right), \tag{5}$$

$$\frac{d\theta}{dt} = -\frac{\sin\theta}{r^2} \text{Im} \left(\frac{1}{\psi} \frac{\partial \psi}{\partial \cos\theta} \right), \tag{6}$$

$$\frac{d\varphi}{dt} = 0. \tag{7}$$

150

151 Obviously, the angle φ does not change, and the trajectory lies in the plane defined by the
 152 initial (at $t = t_0$) radius-vector and the z -axis. One has to solve the Cauchy problem for the set of
 153 two equations (5) and (6). In the generalized pseudo-spectral (GPS) discretization, we use the
 154 Gauss-Lobatto scheme for the variable r (with the appropriate mapping transformation) and the
 155 Gauss scheme for the variable $\cos\theta$. The expressions for the first derivatives with respect to r
 156 and θ appear in detail in our previous works [7,34]. This set of coupled ordinary differential
 157 equations is solved numerically with the help of the 4th order Runge-Kutta (RK4) method,
 158 yielding the electron quantum trajectories.

159

160 To obtain the ATI spectra, within the Kramers-Henneberger (KH) frame, we start from the
 161 expression for the differential ionization probability corresponding to ejection of the electron
 162 with the energy E_f within the unit energy interval and unit solid angle under the specified
 163 direction:

$$164 \quad \frac{\partial^2 P}{\partial E_f \partial \Omega} = \sqrt{2E_f} |T_{fi}|^2. \quad (8)$$

165 where Ω denotes the solid angle. For the transition matrix element T_{fi} we use the expression
 166 suggested in Ref. [9].

167

$$168 \quad T_{fi} = -i \int_0^{t_f} dt \exp\left(iE_f t + \frac{i}{2} \int_0^t \dot{\mathbf{b}}^2 d\tau\right) \int d^3 r \psi_f^*(\mathbf{r} - \mathbf{b}) \\ \times [U(\mathbf{r}) - U(\mathbf{r} - \mathbf{b})] \exp[-i(\dot{\mathbf{b}} \cdot \mathbf{r})] \psi(\mathbf{r}, t). \quad (9)$$

169 Here, the time-dependent quantity \mathbf{b} has the meaning of the displacement of the ‘‘classical’’
 170 electron under the influence of the laser field only; a dot above \mathbf{b} denotes the first derivative with
 171 respect to time. The potential $U(\mathbf{r})$ represents the interaction with the atomic core; the term $U(\mathbf{r})$
 172 $- U(\mathbf{r} - \mathbf{b})$ decreases at least as $1/r^2$ at large r ; therefore, the spatial integration in Eq. (9)
 173 emphasizes the core region of the wave packet. The wave function $\psi(\mathbf{r}, t)$ satisfies the time-
 174 dependent Schrödinger equation:

$$175 \quad i \frac{\partial}{\partial t} \psi(\mathbf{r}, t) = \left[-\frac{1}{2} \nabla^2 - (\ddot{\mathbf{b}} \cdot \mathbf{r}) + U(\mathbf{r}) \right] \psi(\mathbf{r}, t). \quad (10)$$

176 It takes into account the interactions with both the atomic core and laser field (the latter
 177 interaction is described in the length gauge; $\ddot{\mathbf{b}}$ is the classical acceleration). Before the laser
 178 pulse, this function coincides with the initial bound state of the electron.

179

180 The final state of the electron $\psi_f(\mathbf{r})$ describes motion in the atomic field only. As discussed in
 181 the scattering theory [36], the correct final states for calculation of the angular distributions are
 182 the functions $\bar{\psi}_k(\mathbf{r})$ which have plane waves and incoming spherical waves asymptotically at
 183 large distances. They satisfy the following orthogonality and normalization condition:

$$184 \langle \bar{\psi}_{k'}(\mathbf{r}) | \bar{\psi}_k(\mathbf{r}) \rangle = \delta^{(3)}(\mathbf{k} - \mathbf{k}').$$

185
 186 (11)

187
 188 The final continuum states $\bar{\psi}_k(\mathbf{r})$ in the Coulomb field are known in a closed form:

$$189 \bar{\psi}_k(\mathbf{r}) = \frac{1}{2\pi} \sqrt{\frac{\nu}{\exp(2\pi\nu) - 1}} \exp[i(\mathbf{k} \cdot \mathbf{r})] \quad (12)$$

$$\times M(iv, 1, -i[kr + (\mathbf{k} \cdot \mathbf{r})]).$$

190 where $M(a, c, x)$ is the confluent hypergeometric function. ν is the Coulomb parameter,
 191 $\nu = -Z_c/k$.

192
 193 All the calculations for the current study are performed for hydrogen atom subject to linearly
 194 polarized mid-infrared laser fields. The laser pulse has a sine-squared envelope,
 195 $F(t) = F_0 \sin^2(\frac{\pi t}{T}) \sin(\omega t)$, where F_0 is the peak field amplitude, ω is the carrier frequency, and
 196 T is the pulse duration. First, we study the mechanism of multiple recollision when $\lambda = 1600 \text{ nm}$
 197 (Corresponding to $\omega = 0.0285 \text{ a.u.}$) with two peak intensities, 5×10^{13} and $2 \times 10^{14} \text{ W/cm}^2$. In our
 198 investigations, we have considered several wavelengths, finding that for $\lambda = 1600 \text{ nm}$ the multiple
 199 recollision effect is more pronounced and the results are more striking, which are the ones here
 200 reported. To be able to better identify and understand the role of multiple recollision in HHG and
 201 ATI processes, we limit our results for the case of 4 optical cycle laser fields.

202
 203 The expectation value of the dipole acceleration, is obtained from the time-dependent wave
 204 function:

$$205 d_A(t) = \langle \psi(\mathbf{r}, t) | -\frac{z}{r^3} + F(t) | \psi(\mathbf{r}, t) \rangle. \quad (13)$$

206
 207 The corresponding HHG power spectrum from hydrogen atom exposed to the laser field is
 208 obtained, on the single-atom level, by the Fourier transformation of time-dependent dipole
 209 acceleration as follows [37]:
 210

211

$$P_A(\omega) = \left| \frac{1}{t_f - t_i} \frac{1}{\omega^2} \int_{t_i}^{t_f} d_A(t) e^{-i\omega t} \right|^2. \quad (14)$$

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III. RESULTS AND DISCUSSION

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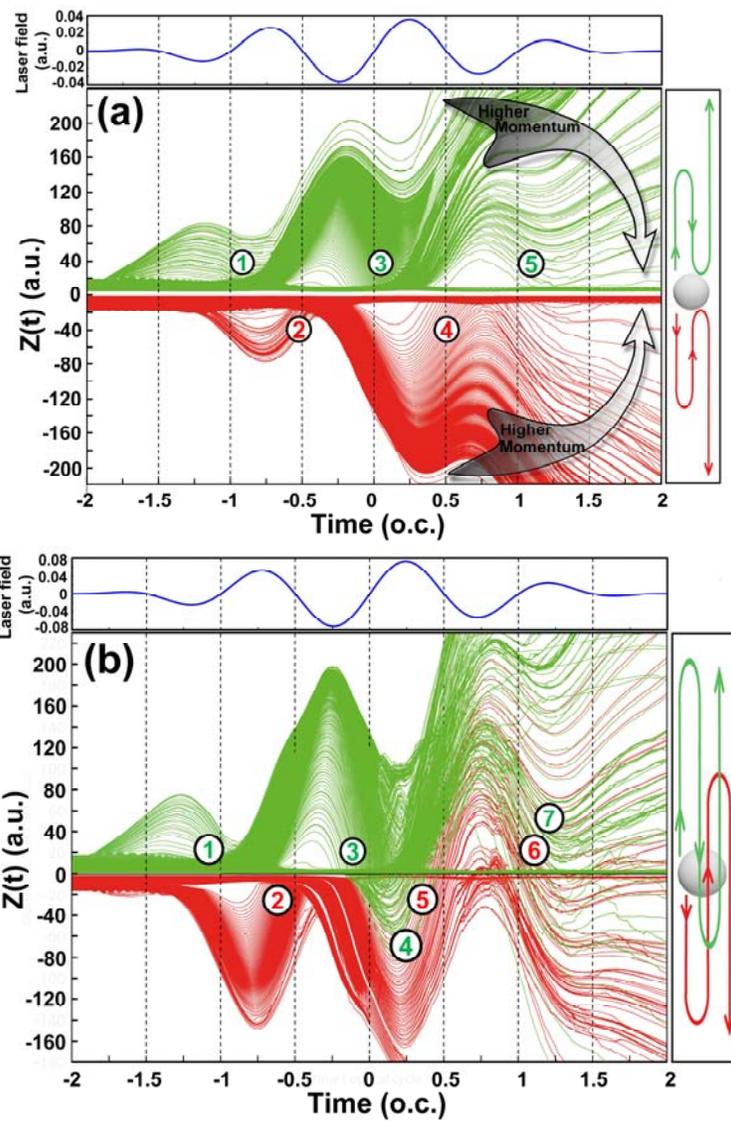
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In Fig.1, we use Bohmian trajectories to provide a complete illustrative picture of the hydrogenic photoelectron dynamics under four optical cycle 1600nm sine-squared laser pulses with two different intensities of 5×10^{13} and $2 \times 10^{14} W / cm^2$ (presented in the top boxes in Fig.1). The red and green trajectories presented in Fig.1 are obtained from two separate sets of Bohmian calculations. For the green trajectories we set the initial condition in the z -direction to be $+1 \leq z_0 \leq +20$, and for the red trajectories we use $-1 \leq z_0 \leq -20$. For both cases, $x_0 = 1$ (all in atomic units). Although the proposed method is robust and is not sensitive to the selected initial conditions, we found that this set best represents the dynamics of electron under the given laser fields. The right panels, in Fig.1, schematically display the characteristic trajectories for each case. The first immediate observation is presence of multiple revisits under the stronger laser pulse, Fig.1(b); this feature is obviously absent in the case of a weaker laser field, Fig.1(a). Under the $5 \times 10^{13} W / cm^2$ laser pulse, Fig.1(a), the emitted electron traveling toward positive or negative z -direction stays on one side of the parent ion. In this case the electron is pulled back when the laser field changes sign, and eventually scatters away from the same side of the atom (after some oscillations under the influence of the laser field). At the higher intensity, $2 \times 10^{14} W / cm^2$, [Fig.1(b)] however, the returning trajectories are strongly pulled over the parent ion and therefore penetrate into the opposite z -direction. As can be seen in Fig.1(b), this effect is influential only around and after the laser peak, when the driving external field is strong enough. In both cases, all the sequential returning groups of Bohmian electron trajectories are numerically labeled for further analysis. In particular, it is worth mentioning that in Fig.1(b) the trajectories exhibiting two rescattering events are marked by “4” and “6”. The second return of the green trajectories is labeled by “4”, and the one corresponding to the red trajectories is labeled by “6”. These groups of Bohmian trajectories represent the electron wave packets that return to the core from the opposite direction of their initial detachment. In the remaining part of this article we will investigate the contribution of each of these ensemble trajectories to harmonic generation. The big circular arrows in Fig.1(a) schematically display how the ejected electrons are distributed in momentum content.

The tail of these arrows correspond to the higher momentum traveling electrons. These are electrons that are expected to have higher velocities, due to the fact that they are represented by trajectories with higher slopes, dZ/dt , in the presented plots in Fig.1. Being valid for the other laser field cases, this roughly represented feature will help us to better interpret some of the structural aspects of the ATI spectra. Time evolution of individual trajectories will be closely

247 analyzed to address some of the main features of the photoelectron angular distributions for
 248 atoms subject to intense mid-infrared laser fields.
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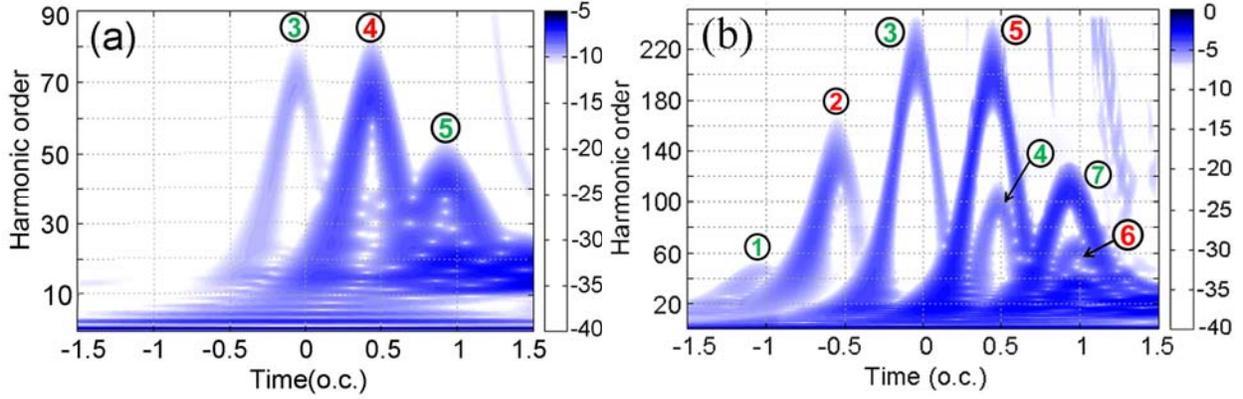


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 255 FIG.1. (Color online) Bohmian trajectories illustrating the dynamics of hydrogenic electron wave
 256 packets initially traveling toward negative (red) and positive (green) z -direction; **time is**
 257 **measured in optical cycles (o.c.)**. These results are obtained by solving the coupled system of
 258 Eqs. (5) and (6). The driving laser field is a four optical cycle 1600nm sine-squared laser pulse
 259 with (a) $5 \times 10^{13} W / cm^2$ and (b) $2 \times 10^{14} W / cm^2$ peak intensity. In each case, the sequential
 260 returning groups of Bohmian electron trajectories are numerically labeled for further analysis.
 261 The top panels present the driving laser fields and the right panels schematically display the

262 characteristic trajectories for each case. Double revisits is the characteristic feature under study,
263 which is only present when the electron is traveling under high intensity mid-infrared laser field,
264 (b). The big circular arrows in (a) schematically display how the ejected electrons are distributed
265 in momentum content. This roughly represented feature is valid for other laser field cases in this
266 study.

267 The results presented in Fig.2 are the HHG time-frequency profiles obtained by the wavelet
268 transformation of the dipole acceleration [Eq. (13)] of the hydrogen atom driven by the two
269 given laser fields. The HHG wavelet time-frequency profile is considered as unambiguous
270 evidence of the existence of the Bremsstrahlung radiation which is emitted by the re-collision of
271 the electron wave packet with the parent ionic core. In each presented profile, the deeper blue
272 color indicates that relatively larger number of electron trajectories contribute to generation of
273 those particular harmonics. The presented wavelet profiles, together with the information
274 obtained from the Bohmian mechanics, Fig.1, provide a comprehensive and intuitive picture of
275 the HHG process and the role of multiple rescattering events. For each case in Fig.2(a,b), the
276 dominant groups of the trajectories in generation of the emission peaks in the wavelet profiles
277 are indicated by the same numbers as in Fig.1. This correlation is made by close comparison
278 between the harmonic peaks' emission times in Fig.2 and the return time period of each group of
279 the Bohmian trajectories in Fig.1. The first noticeable difference between the two wavelet
280 profiles is the existence of three main peaks in Fig.2(a) contrary to five peaks in Fig.2(b). This
281 difference can be simply explained by observing the strongly driven/returning trajectories
282 labeled "1" and "2" in Fig.1(b), on the contrary of similarly labeled groups of slightly driven
283 trajectories under weaker laser field in Fig.1(a). In other words, the initially detached traveling
284 trajectories under $5 \times 10^{13} W / cm^2$, labeled "1" and "2" in Fig.1(a), do not gain enough energy
285 under the external field to be able to have noticeable contribution in the harmonics generation
286 upon the return. In addition, one of the most prominent features in Fig.2(b) is the appearance of
287 two sub-peaks (indicated by arrows and labeled by "4" and "6") at the second half of the time
288 propagation of the electron under the driving high intensity laser field. These harmonic emissions
289 are considered to be caused by the recombination of the second revisiting electron wave packets
290 with the parent ions. The trajectories representing these electrons have labels "4" and "6" in
291 Fig.1(b).

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301 FIG.2. (Color online) HHG time-frequency profile obtained by the wavelet transformation of the
 302 dipole acceleration [Eq. (13)] of the hydrogen atom driven by a four optical cycle 1600nm sine-
 303 squared laser pulse with the peak intensities of (a) $5 \times 10^{13} W / cm^2$ and (b) $2 \times 10^{14} W / cm^2$. Time is
 304 measured in optical cycles (o.c.), and the color scale is logarithmic. The numerical labels are the
 305 same as appeared in Fig.1. These numbers indicate which groups of the Bohmian trajectories
 306 have dominant contributions to each main harmonic emission peak. The sub-peaks indicated by
 307 the arrows in (b) are due to the recombination of the second-revisiting electrons marked by “4”
 308 and “6” in Fig.1(b).

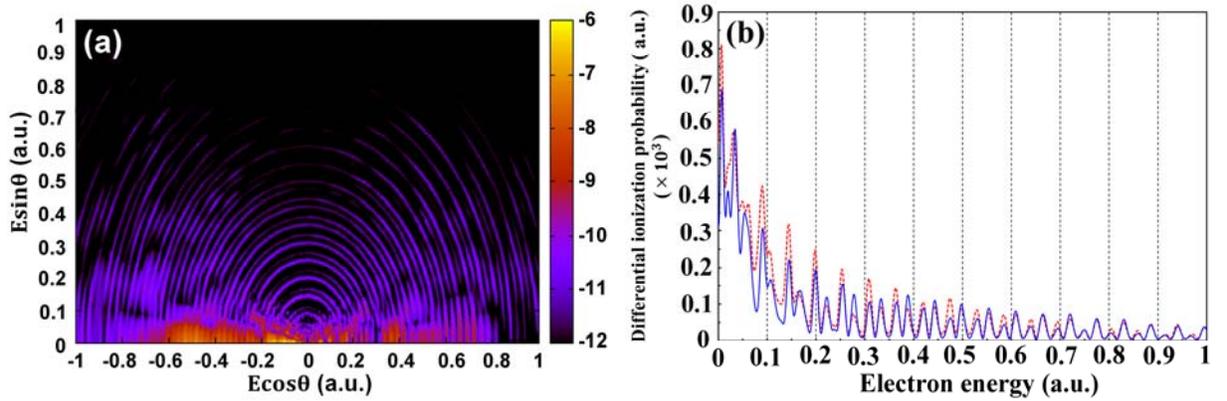
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310 The differential ionization probabilities, obtained from Eq. (8), at the end of each of these laser
 311 pulses are presented in Fig. 3. The polar surface plots of the differential ionization probabilities
 312 are shown in Fig.3(a,c). The radial distance on these plots represents the energy and the angle
 313 points to the direction where the electron is ejected (with respect to the polarization of the laser
 314 field). The density (color) shows the differential ionization probability (in logarithmic scale).
 315 There are two immediate observations: (i) Regarding the angular distributions, one can see that
 316 in Fig.3(a) the electrons (under the $5 \times 10^{13} W / cm^2$ laser field) are mostly ejected in the field
 317 direction; however, noticeable side lobes are present in Fig.3(c) (the $2 \times 10^{14} W / cm^2$ laser field),
 318 which indicates the prominent distribution of the electron wave packets toward x -direction. (ii) In
 319 Fig.3(c), close comparison of the positive and negative momentum distributions shows fine
 320 structure of each ATI peak in the right half-space. This also can be seen on panels (b) and (d),
 321 which compare the corresponding energy spectrum for the electrons emitted in the polarization
 322 direction of these laser fields, respectively. In each case, the dashed red line shows the spectrum
 323 for the electrons ionizing toward negative z -direction, and the solid blue line is presenting the
 324 electrons traveling toward positive z -direction. In Fig.3(b), one can see a similar pattern (position
 325 and the intensity of the peaks) for the both presented plots. Both of these energy spectra exhibit
 326 the well-known ATI structure with the peaks separated by a photon energy ω . The similarity
 327 between these two plots demonstrates the relatively equal contribution of the electron wave
 328 packets traveling toward negative and positive z -direction. The energy spectra under the
 329 $2 \times 10^{14} W / cm^2$ laser field, however, illustrate clearly different patterns for the opposite direction

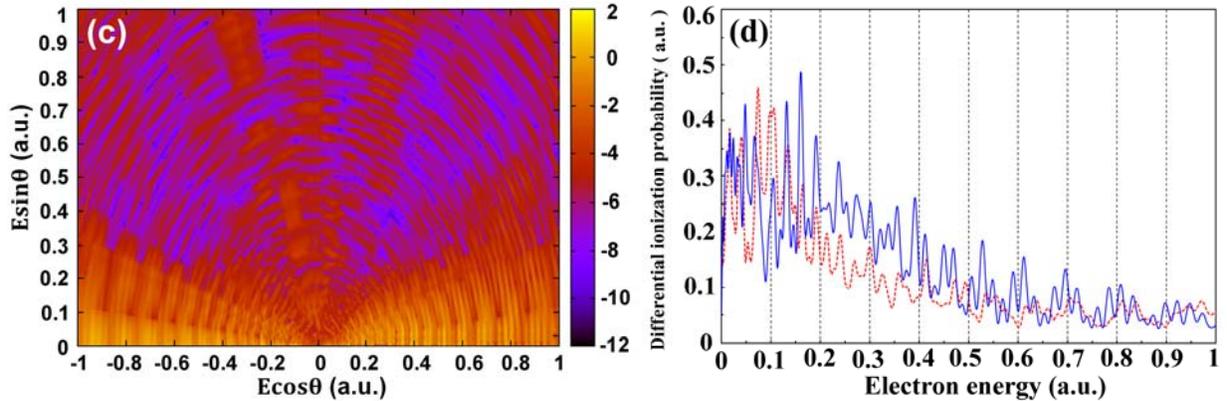
330 traveling electron wave packets. Along with the comprehensive picture provided by the Bohmian
 331 trajectories, this can serve as an evidence for the existence of multiple (in this case, two) revisits
 332 of the electron. Fig.1(b) shows that under the incident laser field, big portions of the electron
 333 wave packets that initially detached toward negative z -direction (represented by the red-
 334 trajectories in Fig.1(b)) end up scattering away from the positive z -direction. Close contribution
 335 (in energy) of these electron trajectories (in red) with the ones that are initiated and scattered
 336 away from the positive z -direction (in green) should be held responsible for the appearance of the
 337 fine structure in the right half-space of Fig.3(c), which is reflected in the corresponding energy
 338 spectrum in Fig.3(d) (blue solid line) as well.

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342 FIG.3. (Color online) (a,c) Energy-angle polar surface plots of differential ionization probability.
 343 The color scale represents logarithm of the quantity defined by Eq. (8). θ is the ejection angle
 344 with respect to the polarization of the laser field. The carrier wavelength of the laser pulse is
 345 1600 nm and duration is four optical cycles. The peak intensity is $5 \times 10^{13} W / cm^2$ for (a), and
 346 $2 \times 10^{14} W / cm^2$ for (c). For each case, the energy spectrum for the electrons emitted in the
 347 polarization direction of the laser field is given on panels (b) and (d), respectively. The dashed
 348 red line shows the spectrum for the electrons traveling toward negative z -direction, and the solid
 349 blue line is presenting the electrons traveling toward positive z -direction.

350

351 In Fig.4, we study the time evolution of some selected individual Bohmian trajectories, for the
352 case of the laser fields with the peak intensities of $5 \times 10^{13} W / cm^2$ (Figs.4(a-c)) and $2 \times 10^{14} W / cm^2$
353 (Figs.4(d-f)). In resemblance to Fig. (1), in each case, the displacement of the electron particle
354 tracer in z -direction is given in panels (a) and (d). The number of revisits of the electron under
355 the stronger ($2 \times 10^{14} W / cm^2$) laser field is also given in Figs.4(d,f). Comparison of the
356 trajectories in xz plane from the panels (b) and (e) provides the explanation for the first
357 observation, (i), we made around Fig.3. As one can see in Fig.4(b), under the weaker laser field,
358 the detached electron wave packets are mainly distributed in the direction of the laser field and
359 have only small spreading in the x -direction (maximum traveling distance in this direction is less
360 than 16 a.u.). As illustrated in Fig.4(e), however, the detached electron may travel up to about 90
361 a.u. perpendicular to the field direction with the peak intensity of $2 \times 10^{14} W / cm^2$. This
362 observation explains the presence of noticeable side lobes in ATI spectrum in Fig.3(c). This can
363 also serve as an additional evidence for multiple transit of the electron over its parent ion subject
364 to a strong mid-infrared laser field. Panels (c) and (f) show how the momentum is changing with
365 respect to the distance in the direction of the driving laser field for the selected individual
366 Bohmian trajectories. The prominent observation here is that the trajectories traveling close to
367 each other in space would be carrying close energy content at their final state. This observation,
368 therefore, supports our previous statement regarding the presence of the fine structure in the ATI
369 spectrum in Fig.3(c), and the corresponding energy spectrum in Fig.3(d) (blue solid line).

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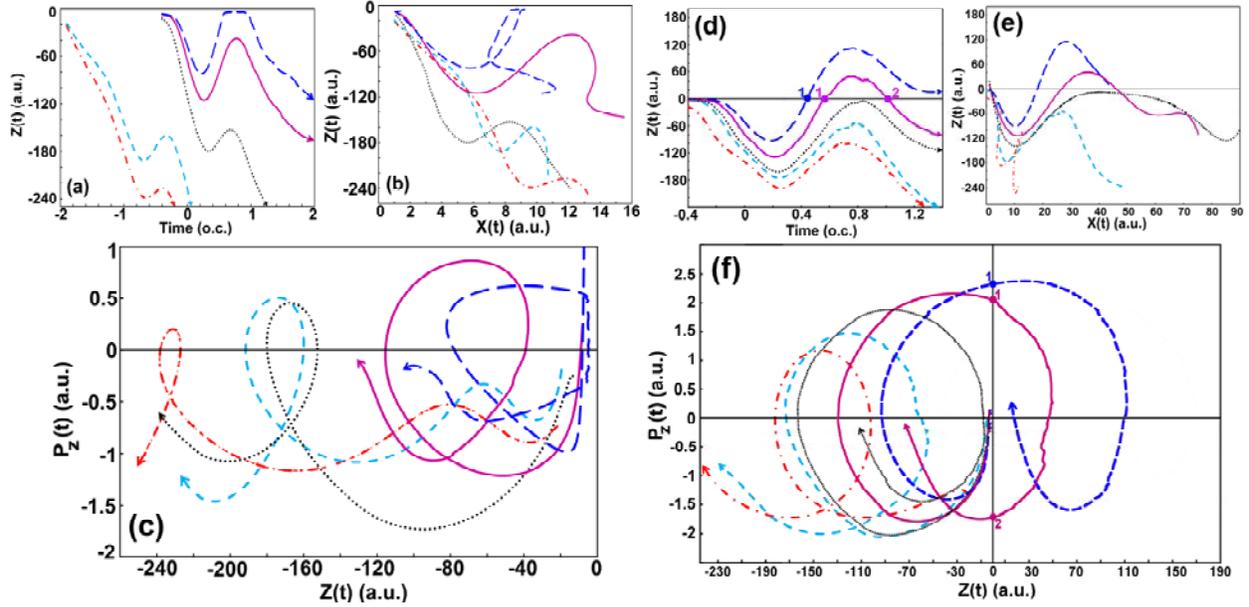
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377 FIG.4. (Color online) Selected Bohmian trajectories, representing various groups of trajectories
 378 from Fig.1. (a-c) illustrate the dynamics of the electron wave packets which are initiated, travel
 379 and scatter away from the negative z -direction, under the influence of a 1600nm four optical
 380 cycle \sin^2 laser pulse with the peak intensity of $5 \times 10^{13} W / cm^2$; time is measured in optical
 381 cycles (o.c.). (a) The time evolution of the electron position in z -direction. (b) The same
 382 trajectories in xz plane. (c) The phase diagram showing how the momentum changes with the
 383 distance in the field direction. (d-f) present the similar results when the laser peak intensity is
 384 $2 \times 10^{14} W / cm^2$. The revisits of the electron are labeled by '1' and '2' in panels (d) and (f). These
 385 results are obtained by solving the coupled system of Eqs. (5) and (6).

386

387 IV. SUMMARY

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389 In summary, we used a fully *ab initio* three-dimensional and accurate Bohmian mechanics results
 390 to illustrate the role of electron multiple re-collisions in some of the main features observed in
 391 HHG and ATI spectra. Contrary to semi-classical calculations, Bohmian trajectories contain all
 392 the information embedded in the time-dependent wave function. This makes the method suitable
 393 to investigate the coherent dynamic processes for which the phase information is crucial. In this
 394 study, the appearance of the sub-peaks in the high harmonic generation time-frequency profiles
 395 and the asymmetric fine structures in the above-threshold ionization spectrum were analyzed by
 396 the comprehensive and intuitive picture provided by Bohmian mechanics. The commonly
 397 accepted evidence for multiple revisits of an electron in the ATI spectra was re-evaluated and a
 398 clear distinct pattern in the HHG spectra which demonstrates the occurrence of multiple revisits
 399 in wavelet time-frequency profiles is explained by comprehensive picture provided by Bohmian
 400 mechanics.

401

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412 **REFERENCES**

413

- 414 [1] P. B. Corkum, *Phys. Rev. Lett.* **71**, 1994 (1993).
415 [2] M. Lewenstein *et al.*, *Phys. Rev. A* **49**, 2117 (1994).
416 [3] U. Mohideen *et al.*, *Phys. Rev. Lett.* **71**, 509 (1993).
417 [4] X. M. Tong, P. Ranitovic, D. D. Hickstein, M. M. Murnane, H. C. Kapteyn, and N. Toshima, *Phys.*
418 *Rev. A* **88**, 013410 (2013).
419 [5] T. Tate, T. Auguste, H. G. Muller, P. Salieres, P. Agostini, and L. F. DiMauro, *Phys. Rev. Lett.* **98**,
420 013901 (2007).
421 [6] Y. Mairesse *et al.*, *Phys. Rev. Lett.* **93**, 163901 (2004).
422 [7] H. Z. Jooya, D. A. Telnov, P. C. Li, and S. I. Chu, *J. Phys. B: At. Mol. Opt. Phys.* **48**, 195401 (2015).
423 [8] D. A. Telnov, and S. I. Chu, *Phys. Rev. A* **83**, 063406 (2011).
424 [9] D. A. Telnov, and S. I. Chu, *Phys. Rev. A* **79**, 043421 (2009).
425 [10] C. Liu, and K. Z. Hatsagortsyan, *Phys. Rev. Lett.* **105**, 113003 (2010).
426 [11] T. M. Yan, S. V. Popruzhenko, M. J. J. Vrakking, and D. Bauer, *Phys. Rev. Lett.* **105**, 253002
427 (2010).
428 [12] D. D. Hickstein, *et. al.* *Phys. Rev. Lett.* **109**, 073004 (2012).
429 [13] A. Gazibegovic-Busuladzic, D. B. Milosevic, W. Becker, B. Bergues, H. Hultgren, and I. Yu. Kiyan,
430 *Phys. Rev. Lett.* **104**, 103004 (2010).
431 [14] M. Li, X. Sun, X. Xie, Y. Shao, Y. Deng, C. Wu, Q. Gong, and Y. Liu, *Scientific Reports* **5**, 8519
432 (2015).
433 [15] X. M. Tong, S. Watahiki, K. Hino, and N. Toshima, *Phys. Rev. Lett.* **99**, 093001 (2007).
434 [16] O. Smirnova, S. Patchkovskii, and M. Spanner, *Phys. Rev. Lett.* **98**, 123001 (2007).
435 [17] M. H. Xu, L. Y. Peng, Z. Zhang, Q. Gong, X. M. Tong, E. A. Pronin, and A. F. Starace, *Phys. Rev.*
436 *Lett.* **107**, 183001 (2011).
437 [18] A. Kastner, U. Saalman, and J. M. Rost, *Phys. Rev. Lett.* **108**, 033201 (2012).
438 [19] D. Bohm, *Phys. Rev.* **85**, 166 (1952).
439 [20] R.E. Wyatt, *Quantum dynamics with trajectories, Interdisciplinary applied mathematics, Vol. 28*
440 (Springer, 2000).
441 [21] F. S. Mayor, A. Askar, and H. Rabitz, *J. Chem. Phys.* **111**, 2423 (1999).
442 [22] C. L. Lopreore and R. E. Wyatt, *Phys. Rev. Lett.* **82**, 5190 (1999).
443 [23] R. Guantes, A. Sanz, J. Margalef-Roig, and S. Miret-Artes, *Surf. Sci. Rep.* **53**, 199 (2004).
444 [24] J. Wu, B. B. Augstein, and C. F. d. M. Faria, *Phys. Rev. A* **88**, 023415 (2013).

- 445 [25] P. Botheron and B. Pons, Phys. Rev. A **82**, 021404 (R) (2010).
446 [26] R. Sawada, T. Sato, and K. L. Ishikawa, Phys. Rev. A **90**, 023404 (2014).
447 [27] J. Wu, B. B. Augstein, and C. F. de Morisson Faria, Phys. Rev. A **88**, 063416 (2013).
448 [28] S. S. Wei, S. Y. Li, F. M. Guo, Y. J. Yang, and B. Wang, Phys. Rev. A **87**, 063418 (2013).
449 [29] J. Stenson, and A. Stetz, Eur. J. Phys. **34**, 1199 (2013).
450 [30] N. Takemoto, and A. Becker, J. Chem. Phys. **134**, 074309 (2011).
451 [31] S. Dey, and A. Fring, Phys. Rev. A **88**, 022116 (2013).
452 [32] Y. Song, F. M. Guo, S. Y. Li, J. G. Chen, S. L. Zeng, and Y. J. Yang, Phys. Rev. A **86**,
453 033424 (2012).
454 [33] A. Picon, A. Benseny, J. Mompert, J.R. Vazquez de Aldana, L. Plaja, G.F. Calvo, and L. Roso, New.
455 J. Phys. **12**, 083053 (2010).
456 [34] H. Z. Jooya, D. A. Telnov, P. C. Li, and S. I. Chu, Phys. Rev. A **91**, 063412 (2015).
457 [35] X. M. Tong, and S. I. Chu, Chem. Phys. **217**, 119 (1997).
458 [36] R. G. Newton, Scattering Theory of Waves and Particles (McGraw-Hill, New York, 1966).
459 [37] H. Z. Jooya, P. C. Li, S. L. Liao, and S. I. Chu, Phys. Lett. A **380**, 316 (2016).