Supplementary Material: Generation of Ultrafast Attosecond Magnetic Field from Ne Dimer in Circularly Polarized Laser Pulses

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Part 1. Ne atom electron current density distribution under two schemes of coherent resonance and direct ionization.

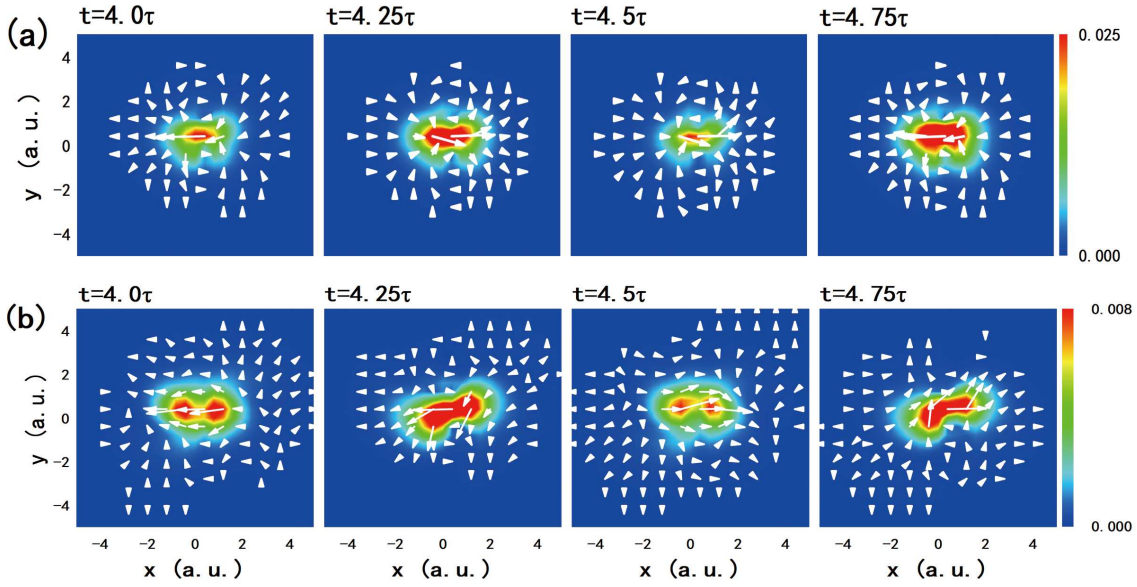

Fig. S1. (Color online) Electron dynamics in CM process of Ne atom under two conditions of coherent resonance excitation and direct ionization with $2p$ state as the initial state. Electron density distribution and electron current density distribution at four moments under (a) coherent resonance excitation ($\lambda = 76$ nm, $\omega = 0.6$ a.u.) and (b) direct ionized ($\lambda = 38$ nm, $\omega = 1.2$ a.u.). The white arrow indicates the direction of the electron current.

We consider CP laser pulses acting on Ne atom, using $2p$ state as the initial state, the coherent electron density $A(\boldsymbol{r},t)$ and electron current density of Ne atom at different wavelength at different time are calculated. It can be found in Fig. S1. that the electron density $A(\boldsymbol{r},t)$ inside Ne atom changes to the left or right under resonance excitation ($\lambda = 76$ nm, $\omega = 0.6$ a.u.), which indicates that the internal charge of the atom moves to the right or left and that can be explain through Eq (10), under resonance excitation, there is strong coherence between electron wave packets, so the CM efficiency is strong. In addition, in the case of direct ionization

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($\lambda = 38$ nm, $\omega = 1.2$ a.u.), the internal electron density of the atom rotates counterclockwise, that indicate the weak coherence of electron wave packets by direct ionization.

Part 2. Time-dependent electron current $j(t)$ and induced magnetic field $B(0,t)$ of Ne atom under schemes (i) and (ii)

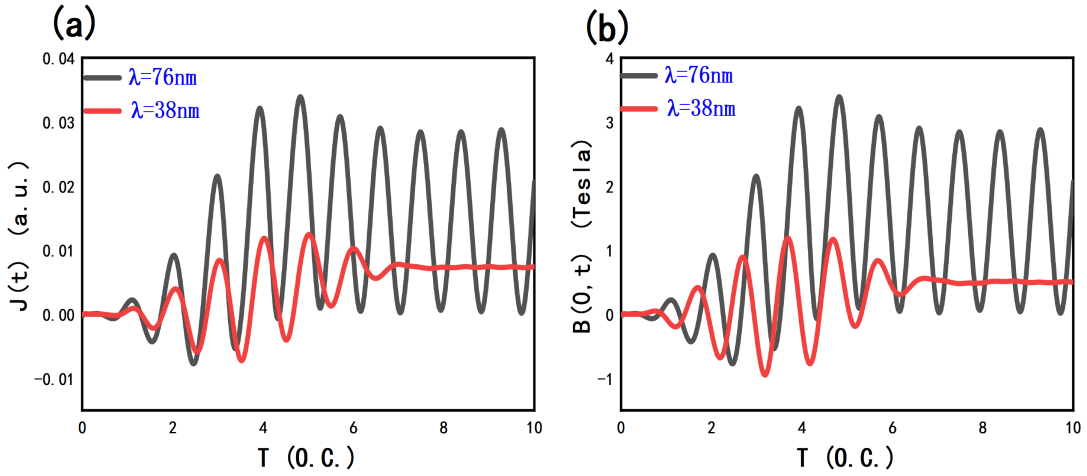

Fig. S2. (Color online) In the case of coherent resonance excitation and direct ionization, the electron current $j(t)$ and magnetic field intensity $B(0,t)$ at the center of Ne atom as functions of time. (a) Electron current as functions of time at $r = 0$; (b) Induced ultrafast magnetic field at $r = 0$.

Based on the calculation results of Ne dimer and Ne atom, it is reasonable to guess that the time-dependent induced current and ultrafast magnetic field intensity of Ne atom under resonance excitation are stronger than those under direct ionization. As shown in Fig. S2.(a) that when the laser pulse interacts with Ne atom ($t < 7\tau$), the electron current at $\lambda = 76$ nm is significantly stronger than that at $\lambda = 38$ nm, and when lase pulse was turn off ($t > 7\tau$), in the case of resonance excitation, periodic oscillating electron current is generated, and the current intensity does not fluctuate under direct ionization, the induced magnetic field intensity is consistent with the electronic current and at $\lambda = 76$ nm the maximum magnetic field is 3.4 T. Besides, we found that the ultrafast magnetic field and electron current generated by CP laser pulse with Ne atom shift along the y axis, and in the case of direct ionization, when the laser pulse is turned off, the electron current and magnetic field do not return to 0 as that of Ne dimer, this is because when the laser interacting with the Ne atom, the Ne will drift, while the Ne dimer has a large weight, and will not drift. In addition, when the same CP laser pulse is applied to Ne dimer and Ne atom, the electron current and magnetic field intensity generated by Ne atom are one order of magnitude stronger than that of Ne dimer.

Part 3. The PMD and PAD of Ne atom under scheme (i) and scheme (ii)

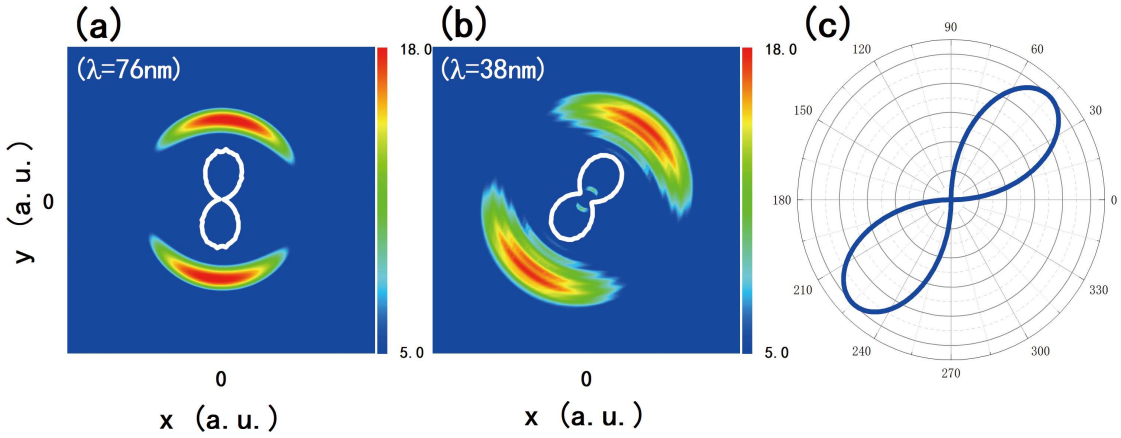

Fig. S1. (Color online) (a) PMD and PAD of Ne atom by resonant excitation; (b)PMD and PAD of Ne atom by direct ionization; (c) PAD prediction of Ne dimer using two-center interference model in Eq (3).

Finally, we investigate the PMD of the final time of Ne atom under resonant excitation (i) and direct ionization (ii) and the theoretical results predicted by the ultrafast ionization model. As shown in Fig. S3., for both cases, the PMD shows a two-lobe structure, and under direct ionization ($\lambda = 38$ nm), both Ne dimer and Ne atom of PMD appear interference fringes. Then, we use the ultrafast ionization model to interpret the PMD results, for Ne atom, the transition amplitude of single-photon ionization can be expressed as:

$$\begin{aligned} A^{(x)} &= \langle \psi_c | \boldsymbol{r} \cdot \boldsymbol{E}_x | \psi_0 \rangle = \sigma^{(x)} E_x \cos(\theta) \\ A^{(y)} &= \langle \psi_c | \boldsymbol{r} \cdot \boldsymbol{E}_y | \psi_0 \rangle = \sigma^{(y)} E_y \sin(\theta), \end{aligned} \tag{1}$$

where, $\sigma^{(x)} = \langle \psi_c | x \cdot E_x | \psi_0 \rangle$ and $\sigma^{(y)} = \langle \psi_c | y \cdot E_y | \psi_0 \rangle$ represent transition matrix elements in the x and y directions, respectively, θ is the angle between the momentum of the photoelectron and the x axis, $|\psi_0\rangle$ and $|\psi_c\rangle$ are initial state and continuous state wave functions, E_x and E_y are the Fourier transform of the electric field in the x and y directions, respectively. The total distribution is the modulus square of the transition amplitudes in the x and y directions plus the interference terms in both directions:

$$|A|^2 = |A^{(x)}|^2 + |A^{(y)}|^2 + |A^{(x,y)}|, \tag{2}$$

and

$$\begin{aligned} A^{(x,y)} &= A^{(x)^*} A^{(y)} + A^{(y)^*} A^{(x)} \\ &= \sigma^{(x)} \sigma^{(y)} E_x E_y \sin(2\theta). \end{aligned} \tag{3}$$

According to Eq (3), we find the PMD and PAD in case of direct ionization (Fig. S3.(b)) $\lambda = 38$ nm is keep with ultrafast ionization model and they all have a two-lobe structure, the intensity distribution of the actual calculation results agrees well with the theoretical prediction result. Meanwhile, PMD is mainly distributed along the y axis and under direct ionization, there is a deflection angle between the PMD and the y axis, which is derived from the interaction between the laser pulse and the Coulomb potential, and the deflection direction is consistent with the laser pulse deflection direction. In addition, the PMD intensity under direct ionization ($\lambda = 38$ nm) stronger than that under resonance excitation ($\lambda = 76$ nm), for Ne atom, the reason for the difference in PMD intensity in the two ionization cases is consistent with Ne dimer. From the PMD results of Ne dimer and Ne atom in two ionization cases, it can be found that resonance excitation cannot be explained by the traditional ultrafast ionization model, which contains a more complex physical mechanism.