Photon momentum transfer in one- photon ionization of H_2^+

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Background

In the one-photon ionization process, the electron and remaining ion would gain total momentum $\mathbf{q} = \hbar \mathbf{k}$ which equal to the momentum of one photon. The momentum participation between ion and electron varies from different atoms to molecules. For hydrogen-like atom, the average momentum of ionized electron is [1]

$$\langle \boldsymbol{q} \rangle = \frac{8(\omega + l_p)}{5c} \hat{\boldsymbol{k}} = \frac{8E_k}{5c} \hat{\boldsymbol{k}},$$
 (1)

proportion to final electron energy E_k . Things would be more complicate for molecules, here we investigate photon momentum transfer in single photon





ionization of H_2^+ .

The photon momentum transfer comes from 1st order non-dipole correlation of laser-matter interaction. In radiation gauge, the time-dependent Hamiltonian of electron interacting with laser field is

$$H = \frac{1}{2} [p + A(r, t)]^2 + \varphi_0, \qquad (2)$$

where **A** is the vector potential of laser field and φ_0 is the interaction potential between electron and nuclear. With plane wave approximation of laser field, we can expand the space-time distribution of vector potential as

$$A(r,t) = A(t - \hat{k} \cdot r/c) = A_0(t) + r \cdot \nabla A(r,t) + O\left(\frac{1}{c^2}\right)$$
$$= A_0(t) + \frac{\hat{k} \cdot r}{c} E_0(t) + O\left(\frac{1}{c^2}\right),$$
(3)

where A_0 , E_0 represents vector potential and electric field at r = 0 respectively. Take eq.(3) back to eq.(2), we get Hamiltonian to O(1/c):

$$\begin{aligned} \mathcal{H} = & \frac{p^2}{2} + \varphi_0 + \mathcal{A}_0(t) \cdot p + \frac{\mathcal{A}_0(t)^2}{2} \\ & + \frac{\hat{k} \cdot r}{c} \left[\mathcal{E}_0(t) \cdot p + \mathcal{E}_0(t) \cdot \mathcal{A}_0(t) \right] + \mathcal{O}\left(\frac{1}{c^2}\right), \end{aligned}$$

Eq.(4) is widely used when people consider the non-dipole effect.



Energy (a.u.)

Figure 1: (a-c) The 2D photoelectron momentum distributions in the polarization-propagation plane of a hydrogen molecule ion by a **20**-cycle linear polarized laser with $\omega = 2$ a.u. and $I = 5 \times 10^{12}$ W cm⁻² in *zx* (a), *xz* (b) and *yx* (c) configurations respectively. The electric field is polarized along vertical axis and wavevector is along horizontal axis. (d) The average momentum transfer of photo-electron ionized from H₂⁺ 1 s σ_g state along laser propagation direction as a function of electron energy. The direction of electric field and wavevector is abaaen to be *xz* (dot dashed blue line). *yx* (calid yellow line) and *zx* (dashed green line)

Method

In this work, we consider another gauge form which has been mentioned before [2]. Under gauge transformation

$$\Psi' = e^{i\Lambda}\Psi, \tag{5}$$

(4)

(6)

(8)

where $\Lambda = [A(\tau) + A_0(t)] \cdot r/2$. Hamiltonian transform as

$$H' = e^{i\Lambda} H e^{-i\Lambda} - \partial_t \Lambda$$

$$= \underbrace{\frac{p^2}{2} + \varphi_0}_{H_0} + \underbrace{r \cdot E_0(t)}_{\text{E-dipole}} - \underbrace{\frac{\hat{k} \cdot r}{2c}(r \cdot \partial_t E_0(t))}_{\text{E-quadrapole}}$$

$$+ \underbrace{\frac{1}{2c} L \cdot [\hat{k} \times E_0(t)]}_{\text{B-dipole}} + O\left(\frac{1}{c^2}\right).$$

Now it is clear that how the inhomogeneity of electric field and magnetic field affect the electron.

With above Hamiltonian, time-dependent Schrödinger equation is solved under fixed nuclear approximation in prolate spheroidal coordinates [3] (ξ , η , ϕ):

$$\xi = (r_1 + r_2)/R, \quad \eta = (r_1 - r_2)/R,$$
 (7)

where r_i is the distance between the electron and the *i*th nucleus, *R* is the internuclear distance, and ϕ is the azimuthal angle around the molecular axis. A Cartesian coordinate system in molecular frame with *z*-axis collinear with

chosen to be *xz* (dot-dashed blue line), *yx* (solid yellow line) and *zx* (dashed green line) respectively. Same quantity but for H atom (red dotted line) is plot for reference.



Figure 2: Average momentum transfer ratio of photo-electron from H_2^+ to those from H atom in (*E*, *R*) plane. Both two axises are in logarithmic scale. White lines with slope equal to -1/2 are plotted for reference.

molecular axis.

Result and Discussion [4]

Oscillation of electron average momentum is observed when change photon energy ω and internuclear distance **R**. We introduce the factor **F** to describe difference between molecule and atom

$$F = \frac{5c\langle q \rangle \cdot \hat{k}}{8 E_k}.$$

We plot ratio F as a function of internuclear distance and electron energy with double logarithm scale at zx configuration in Fig.2. Clear stripes with slope approximates to -1/2 can be observed, which corresponding to

$$\sqrt{2E_k}R = \text{const.}$$
 (9)

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Reference

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