Hydrogen atom ionization in femtosecond laser field: Numerical solution of the TDSE using CWFDVR method

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We present an discrete variable representation for solving the time-dependent Schrodinger equation for an atomic system interacting with an intense laser pulse. Instead of the usual finite difference (FD) method, the radial coordinate is discretized using the discrete variable representation (DVR) constructed from Coulomb wave functions. Our results are in excellent agreement with other accurate theoretical calculations using different methods.

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INTRODUCTION

The study multiphoton ionization of atom by femtosecond laser pulse is a subject of interest for both experiments and theory. One way to describe such process is numerical solution of the time dependent Schrodinger equation (TDSE). "Exact" solution of TDSE with minimal computational effort still remain challenge for researchers. Different numerical methods for solution of TDSE are tested and give promising results. Among them should be emphasized the generalized pseudospectral method (GPSM) of Shih I Chu and coworkers [1-3], and matrix- iterative method of Grum Grzhimailo et al [4]. The former method based on Crank-Nicholson approximation of TDSE, gives most accurate results for ejected electron spectrum. The GPSM attractive in that, it uses the "exact" integration of TDSE by split operator method, discretizing differential operators on the pseudospectral Legendre basis, not only avoiding the Coulomb singularity, but also uses several times less, non-uniform radial grid nodes, which make this method computationally more effective. Limitation of this method is the Legendre basis doesn't possess correct asymptotic behavior. Peng and Starace [5] developed Coulomb wave function discrete variable representation method (CWFDVR) for solution of TDSE for an atom in intense laser field. In comparison with the GPSM, the basis has correct Coulomb wave asymptotic form. In this paper, we propose Coulomb wave function discrete variable representation method to solve the TDSE.

THEORY

We solved the time-dependent Schrodinger equation (TDSE) for atomic hydrogen in an intense laser field to calculate electron energy spectra with the hydrogen atom initially in the ground state. The Schrodinger equation for atomic hydrogen in the presence of linearly polarized fields E $\vec{}$(t) can be written as (in atomic units)

$$i\frac{\partial\Psi(\vec{r},t)}{\partial t} = \hat{H}\Psi(\vec{r},t) = \left[\hat{H}_0 + \hat{V}(\vec{r},t)\right]\Psi(\vec{r},t). \quad (1)$$

Here $\hat{H}_0$ is the unperturbed H atom Hamiltonian and $\hat{V}$ is the atom-field interaction:

$$\hat{H}_0 = -\frac{1}{2}\frac{d^2}{dr^2} + \frac{\hat{L}^2}{2r^2} - \frac{1}{r}$$

$$\text{and } V(\vec{r},t) = \vec{p}\cdot\vec{A}(t). \quad (2)$$

A linearly polarized laser field is used in the calculation. One can choose pulse shape either for $\vec{A}(t)$ or for $\vec{E}(t)$. Grum Grzhimailo et al pointed out that the photoelectron spectrum depends on, which one of the two vectors have a sin^2 pulse envelope. If one choose for example

$$\vec{E}(t) = E_0 sin(\omega t + \varphi_0) sin^2\left(\frac{\pi\, t}{\tau}\right), \quad (3)$$

$0 \le t \le \tau$ the in this case the $A(t)$ determined by simple integration:

$$A(t) = -\int_0^t E(t)dt = \frac{1}{4}E_0\left(-\frac{2\cos[\phi 0]\cos[\omega t]}{\omega} + \frac{\tau\cos\left[\frac{2\pi t}{\tau}-\phi 0-\omega t\right]}{-2\pi+\tau\omega} + \frac{\tau\cos\left[\frac{2\pi t}{\tau}+\phi 0+\omega t\right]}{2\pi+\tau\omega} + \frac{2\sin[\phi 0]\sin[\omega t]}{\omega}\right) \quad (4)$$

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On the other hand, we choose the vector potential in the similar form of (3):

$$A(t) = A_0 cos(\omega t + \varphi_0) sin^2\left(\frac{\pi t}{\tau}\right) \qquad (5)$$

The electric field can be determined by differentation:

$$\vec{E}(t) = -\frac{1}{c}\frac{dA(t)}{dt} \qquad (6)$$

We shall use the second-order split-operator technique in spherical coordinates for the time propagation of the Schrodinger equation:

$$\Psi(\vec{r}, t + \Delta t) \cong \exp\left(-i\hat{V}(\vec{r}, t + \Delta t)\frac{\Delta t}{2}\right) \times exp\left(i\hat{H}_0 \Delta t\right) \times exp\left(-i\hat{V}(\vec{r}, t)\frac{\Delta t}{2}\right)\Psi(\vec{r}, t) + O(t^3) \quad (7)$$

To pursue the time propagation, we expand the total wavefunction $\Psi(\vec{r}, t)$ in Legendre polynominals:

$$\Psi(r_i, \theta_j, t) = \sum_{l=0}^{l_{max}} g_l(r_i, t)\, P_l(cos\theta_j) \quad (8)$$

where the P_l is the normalized Legendre polynomails. $g_l(r_i, t)$ can determined accurately by the Gauss-Legendre quadrature

$$g_l(r_i) = \sum_{k=1}^{l_{max}} w_k\, P_l(cos\theta_k)\Psi(r_i, \theta_k, t) \quad (9)$$

Where $(cos\theta_k)$ are the L+1 zeros of the Legendre polynomial $P_{L+1}(cos\theta_k)$ and w_k are the corresponding quadrature weights.

The present method discretizes the radial coordinate using the discrete variable representation CWFDVR constructed from the positive energy Coulomb wave function. The CWFDVR greatly simplifies the evaluation of Hamiltonian matrix elements. Let us consider the following equation

$$\frac{d^2}{d\tilde{r}^2}\phi(\tilde{r}) + \left[1 + \frac{2Z}{\tilde{r}\sqrt{2E}} - \frac{L(L+1)}{\tilde{r}^2}\right]\phi(\tilde{r}) = 0 \quad (10)$$

with the solution given by regular Coulomb function

$$\phi(r) = F_0\left(-\frac{Z}{\sqrt{2E}}, r\sqrt{2E}\right) \qquad (11)$$

where E-energy, Z- nuclear charge.

We define the Lagrange interpolation cardinal function $C(r)$ as

$$C_i(r) = \frac{1}{\phi'(r_i)}\frac{\phi(r)}{r - r_i} \qquad (12)$$

where r_i is the ith zero of $\phi(r)$and $\phi'(r_i)$ is its first derivative at r_i.

$C_i(r)$ satisfies the cardinality condition

$$C_i(r_j) = \delta_{ij} \qquad (13)$$

The Coulomb wave function DVR basis function defined in the following way

$$f_i(r) = \frac{1}{\sqrt{\omega_i}}C_i(r) = \frac{1}{\sqrt{\omega_i}}\frac{1}{\phi'(r_i)}\frac{\phi(r)}{r - r_i} \qquad (14)$$

The potential matrix elements to draw in merely the evaluation of the interaction potential at the CWFDVR grid points. The kinetic energy matrix elements can also be calculated [5].

RESULTS

TDSE for hydrogen atom in a femtosecond laser field solved with the CWFDVR method in the following cases.

A. 2-cycle laser pulse with the peak intensity I = $10^{15} W/cm^2$ and central frequency of $\omega = 0.2$, (Fig.1)

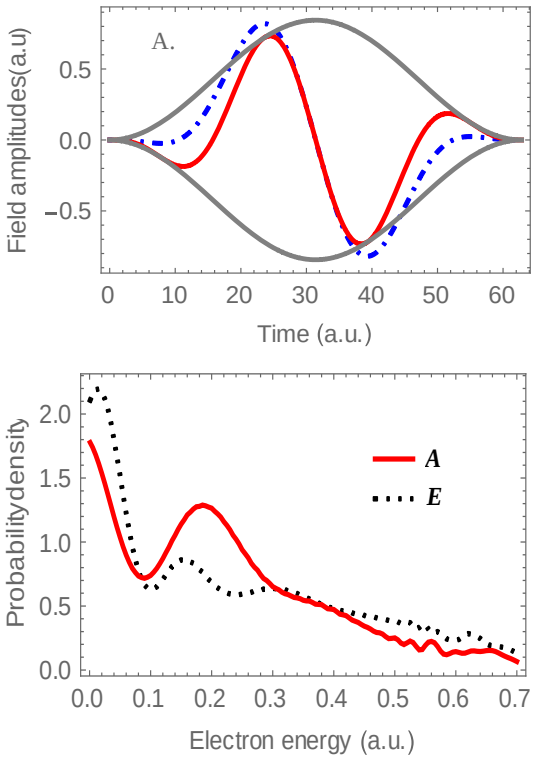

Figure 1. Laser pulse with a sin² envelope. Ionization of atomic hydrogen in ***A****. 2 cycle, a peak intensity of* $10^{15} W/cm^2$*, and central frequency of 0.2 a.u, corresponding to a wavelength of 227.75 nm.*

In this case first we compare the laser pulse vector potentials and found different shape as seen from Figure 1A, and the corresponding probability density of ejected electron spectrum also strongly different from each other (Figure 1B).

B. 4-cycle laser pulse with the peak intensity *I*= $10^{15} W/cm^2$ and central frequency of $\omega = 0.3$ (Fig.2).

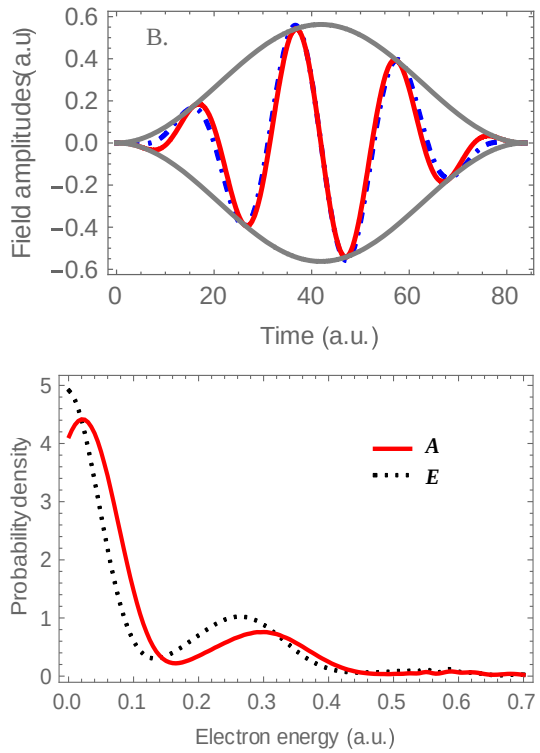

*Figure 2. Laser pulse with a sin² envelope. Ionization of atomic hydrogen in **B**. 4 cycle laser pulse with a sin² envelope, a peak intensity of $10^{15}W/cm^2$, and central frequency of 0.3 a.u, corresponding to a wavelength of 151.84 nm.*

C. 20-cycle laser pulse with the peak intensity $I= 10^{14}W/cm^2$ and central frequency of $\omega =$ 0.114 3 (Fig.3).

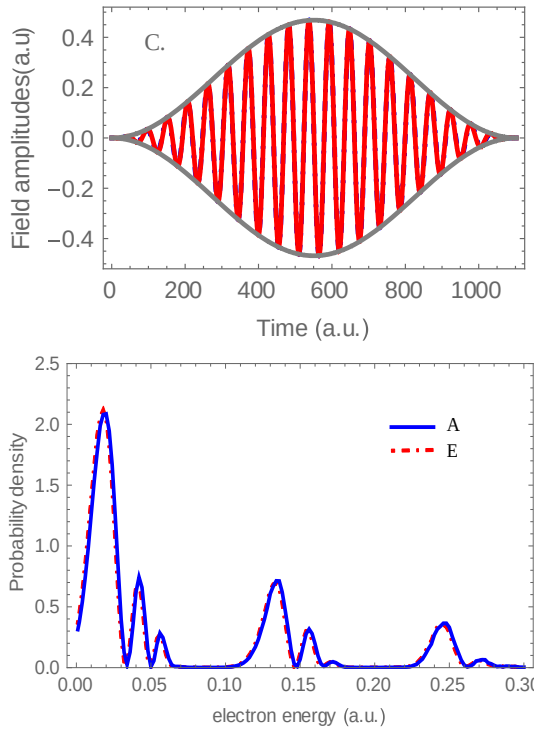

Figure 3. Laser pulse with a sin² envelope. Ionization of atomic hydrogen in C. 20 cycle laser pulse with a sin² envelope for the electric field, a peak intensity of $10^{14}W/cm^2$, and central frequency of 0.114a.u, corresponding to a wavelength of 399.57nm.

As seen from the Fig.1, in the first case (A), didn't fit both the envelope and carrier shapes and corresponding electron spectrums are different from each other. Analogically to present case, we compare pulse shape and electron spectrum for four cycle laser pulse (case B). In this case the pulses have slightly different shape and the corresponding spectrum also differs from each other. Third we consider 20 cycle laser pulse. Figure 3 shows that both the vector potential pulse shape and the electron spectrum nearly coincides for this longer pulse. Notice that our spectrum B and C in agreement with the corresponding spectrum given in reference [2].

CONCLUSIONS

We apply the CWFDVR method to the numerical solution of TDSE for ionization of atomic hydrogen in intense laser field. The choice of sin² envelope either for *E(t)* or for *A(t)* give nearly the same electron spectrum for longer (20cycle) pulse, but for four and specially for two cycle case, electron spectrum differs from each other. In the case of central frequency of 0.3 and 0.114, our calculated electron spectrums are in excellent agreement with other accurate theoretical calculations using different methods.

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