Study interaction between intensive circularly polarized laser and hydrogen atom using a matrix method *

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Abstract. Recently the study of intensive laser and atom interaction is one of the most interesting topics in laser and atom interdisciplinary physics. Study of interaction of hydrogen atom and intense laser using a matrix method is reported in this paper. This method includes Givens reduction for real symmetric tridiagonal matrix form of Hamiltonian matrix, Thomas algorithm for eigenvectors, and bisection algorithm with Sturm theorem for eigenvalues. Some preliminary results and progress for this study are presented.

Keywords: intensive laser, hydrogen atom, matrix method.

1. Introduction

In recent decades, with development of high intensity laser, the intensive laser and matter interaction have become a hot topic in both experimental and theoretical physics [1-2]. Because the hydrogen is the simplest system for studying the interaction of an atom system with a laser field, without interference from multi-electron effects, the study of interaction between hydrogen atom and a laser provides a clean test case for theoretical calculation. Therefore, we develop an approach to solve the time dependent Schrödinger equation (TDSE) of hydrogen atom in the presence of circularly polarized laser field [3].

The remaining of this paper is organized as follows: Section 2 describes our theoretical approach. In Section 3 the corresponding eigenvalues and eigenvectors are calculated and checked. Section 4 concludes the paper and discusses possible future research directions.

2. Theoretical approach

Considering the hydrogen atom in the presence of a relative long pulse and circularly polarized laser field,
the TDSE of the electron can be changed into a non time dependent Schrödinger equation (NTDSE) by some rotation and unitary transformation \[4\]

\[H'_e |i\rangle = E |i\rangle \]  

(1)

where \( E \) is Eigen energy of eigenvector \(|i\rangle\) and

\[H'_e = \frac{p^2}{2\mu} + V(r) - \frac{k}{\mu} p_x l_x + \frac{k^2}{2\mu} l_x^2 + \frac{\hat{A} e^2}{2\mu} + \frac{eA}{2\mu} p_x + kcl_z. \]  

(2)

Here, \( V(r) \) is coulomb potential, \( c \) is light velocity, \( \mu \) is the mass of electron, \( k \) is wave number, \( p \) is momentum, \( p_x \) and \( p_y \) are \( x \) and \( y \) direction components of \( p \) respectively, \( l_z = ml \) is the z-component of the angular momentum, and \( m \) is the magnetic quantum number.

At first, we only consider the part of bound stationary state of hydrogen atom \( \psi_{k(nlm)} \) (or \( \Psi^k_{nlm} \)) to be basis to combine the eigenvector \(|i\rangle\) of \( H'_e \), and in the coordination it can be written as

\[|i\rangle = \sum_{k(nlm)} C^i_{k(nlm)} |k(nlm)\rangle \]  

(3)

Where \( C^i_{k(nlm)} \) is the coefficient of the orthogonal basis vector \( |k(nlm)\rangle \).

Then using the matrix form of \( H'_e \) (NTDSE), secular Eq. 1 can be written as

\[
\begin{bmatrix}
H'_{e11} & H'_{e12} & \cdots & H'_{e1f} \\
H'_{e21} & H'_{e22} & \cdots & H'_{e2f} \\
\vdots & \vdots & \ddots & \vdots \\
H'_{ef1} & H'_{ef2} & \cdots & H'_{eff}
\end{bmatrix}
\begin{bmatrix}
c^i_1 \\
c^i_2 \\
\vdots \\
c^i_f
\end{bmatrix}
= \epsilon^i
\begin{bmatrix}
c^i_1 \\
c^i_2 \\
\vdots \\
c^i_f
\end{bmatrix}
\]  

(4)

in which,

\[H'_{ekk} = \langle k' | H'_e | k(nlm) \rangle, \]  

(5)

\( C^i_k \) is abbreviation of \( C^i_{k(nlm)} \), \( \epsilon^i \) is the eigenvalue of effective Hamiltonian \( H'_e \) for eigenvector \(|i\rangle\), and \( H'_e \) can be specifically rewritten as

\[H'_{ekk} = \left( \frac{p^2}{2\mu} + V(r) + k^2\frac{\hbar^2}{2\mu} + \frac{\hat{A} e^2}{2\mu} + kcmh \right) c^i_k + \frac{\hat{A} e^2}{2\mu} \langle \psi^k_\mu | p_x | \psi^i_\mu \rangle - \frac{kmh}{\mu} \langle \psi^k_\mu | p_z | \psi^i_\mu \rangle. \]  

(6)

Fig. 2.1 shows the process of our matrix method. After we calculate the element of effective Hamiltonian \( H'_e \), the real symmetric tridiagonal matrix form of Hamiltonian matrix is obtained by Givens reduction \[5\]. The related eigenvalues are then calculated by bisection algorithm with Sturm theorem \[6\], and eigenvectors are computed by Thomas algorithm \[7\] with well-separated eigenvalue. Finally, we can obtain some physics quantities, such as ionization cross section and laser intensity dependence \[8\]. In this paper, we will only present some results of eigenvalue and eigenvector of \( H'_e \).
3. Some results

Before giving some results of eigenvalue and eigenvector of $H_e'$, we would like to check the reliability and accuracy for Givens reduction and Bisection algorithm used in our approach. We compare the eigenvalues and eigenvectors from our approach to a known result. The matrix used for comparison is a five order square matrix $M_0$ [5] (shown in Table 3.1).

![Fig. 2.1. Flowchart of our approach.](image)

Table 3.1. A five order square matrix $M_0$.

<table>
<thead>
<tr>
<th>Table 3.1</th>
<th>A five order square matrix $M_0$.</th>
</tr>
</thead>
</table>
| $M_0$     | \[
\begin{bmatrix}
0.71235 & 0.33973 & 0.28615 & 0.30388 & 0.29401 \\
0.33973 & 1.18585 & -0.21846 & -0.06685 & -0.37360 \\
0.28615 & -0.21846 & 0.18159 & 0.27955 & 0.38898 \\
0.30388 & -0.06685 & 0.27955 & 0.23195 & 0.20496 \\
0.29401 & -0.37360 & 0.38898 & 0.20496 & 0.46004
\end{bmatrix}
\]

### Table 3.2. Eigenvalue.

<table>
<thead>
<tr>
<th>Method</th>
<th>No.1</th>
<th>No.2</th>
<th>No.3</th>
<th>No.4</th>
<th>No.5</th>
</tr>
</thead>
<tbody>
<tr>
<td>Matrix calculator</td>
<td>-0.141269eV</td>
<td>0.050511eV</td>
<td>0.092036eV</td>
<td>0.092036eV</td>
<td>0.092036eV</td>
</tr>
<tr>
<td>Givens+Besction*</td>
<td>-0.141269eV</td>
<td>0.050511eV</td>
<td>0.092036eV</td>
<td>0.092036eV</td>
<td>0.092036eV</td>
</tr>
</tbody>
</table>

### Table 3.3. No.1. Eigenvector.

<table>
<thead>
<tr>
<th>Method</th>
<th>Givens+ Thomas</th>
<th>Matrix calculator</th>
</tr>
</thead>
<tbody>
<tr>
<td>index</td>
<td>No.1</td>
<td>No.1</td>
</tr>
<tr>
<td>1</td>
<td>-0.0000000</td>
<td>-3.316883E-07</td>
</tr>
<tr>
<td>2</td>
<td>0.004647</td>
<td>0.004647</td>
</tr>
<tr>
<td>3</td>
<td>0.826421</td>
<td>0.826421</td>
</tr>
<tr>
<td>4</td>
<td>-0.401293</td>
<td>-0.401293</td>
</tr>
<tr>
<td>5</td>
<td>-0.394932</td>
<td>-0.394932</td>
</tr>
</tbody>
</table>

### Table 3.4. No.3. Eigenvector.

<table>
<thead>
<tr>
<th>Method</th>
<th>Givens+ Thomas</th>
<th>Matrix Calculator</th>
</tr>
</thead>
<tbody>
<tr>
<td>index</td>
<td>No.3</td>
<td>No.3</td>
</tr>
<tr>
<td>1</td>
<td>-0.000001</td>
<td>-8.184097E-07</td>
</tr>
<tr>
<td>2</td>
<td>0.161946</td>
<td>0.161946</td>
</tr>
<tr>
<td>3</td>
<td>-0.057399</td>
<td>-0.057399</td>
</tr>
<tr>
<td>4</td>
<td>-0.747648</td>
<td>-0.747648</td>
</tr>
<tr>
<td>5</td>
<td>0.641484</td>
<td>0.641484</td>
</tr>
</tbody>
</table>

Except No.1 and No.3 eigenvectors, other eigenvectors are completely same. Only No.1 and No3 eigenvectors with some slight differences are shown in Table 3.3 and Table 3.4, respectively. Therefore, we can easily conclude that the result of our model has a 5-digit precision for eigenvector and has more than 5-digit precision for eigenvalue.

As we set laser parameters $A=1.8 \times 10^{-3} V \cdot s / m$, and $k = 1.03 \times 10^7 / m$ (wave lengthy $\lambda = 1.64 \times 10^{-6} m$), the eigenvalue $E$ of Hamiltonian $H_e'$, and corresponding eigenvector $|i\rangle$ in the presence of this laser field are calculated based on our approach. Table 3.5 shows the first ten items of eigenvector $\psi_{E=4.65eV}$ of
Hamiltonian $H_e$ (which has a largest component of ground state of atomic hydrogen) based on the basis of bound states of hydrogen atom, and its corresponding eigen energy $E= 4.65\text{eV}$.

Table 3.5. Data for the first ten items of eigenvector $\psi_{E=4.65\text{eV}}$.

<table>
<thead>
<tr>
<th>Index of $c_i$</th>
<th>Value of $c_i$</th>
<th>Index of $c_i$</th>
<th>Value of $c_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.7570579446137287</td>
<td>6</td>
<td>0.00208548190289008</td>
</tr>
<tr>
<td>2</td>
<td>0.09483098226226934</td>
<td>7</td>
<td>-0.17854082543374933</td>
</tr>
<tr>
<td>3</td>
<td>-0.3767373556802446</td>
<td>8</td>
<td>-4.97999186909243E-7</td>
</tr>
<tr>
<td>4</td>
<td>-0.0000012743403275</td>
<td>9</td>
<td>0.1615973380163324</td>
</tr>
<tr>
<td>5</td>
<td>0.33683326841968736</td>
<td>10</td>
<td>0.11358396205104035</td>
</tr>
</tbody>
</table>

Using data in Table 3.5, one can plot $\psi_{E=4.65\text{eV}}$, an eigenvector of effective Hamiltonian $H_e$, with mathematic software.

![Graphs showing probability distributions for $\psi_{E=4.65\text{eV}}$ and ground state of atomic hydrogen.](image)

Fig. 3.6. Probability for $\psi_{E=4.65\text{eV}}$, an eigenvector of effective Hamiltonian $H_e$ (left picture), and the probability for ground state of atomic hydrogen with laser off (right picture). White color represents a large probability and blue represents a low probability in both pictures.

Because $\psi_{E=4.65\text{eV}}$ has a largest component of ground state of atomic hydrogen without laser among all eigenvectors of $H_e$, the ground state $\psi_{E=-13.6\text{eV}}$ of atomic hydrogen will most likely transit to eigenvector $\psi_{E=4.65\text{eV}}$ of effective Hamiltonian $H_e$ as a laser field ($A=1.8\times10^{-3}V\cdot s/m$, and $k=1.03\times10^7/m$) is employed. The transition probability is calculated as 0.57 by our approach. However, from both plots in Fig. 3.6, one can clearly see that the spherical symmetry of the ground state of atomic hydrogen is broken as the circularly polarized laser field is employed.
4. Conclusion and outlook

In this paper, we have briefly described the process of how to establish the approach, and checked its reliability and accuracy with an example when the eigenvalues are well-separated. One of the eigenvector of $H_e$ with a largest component of ground state of hydrogen atom has been studied. In the future, we will study the eigenvectors when the corresponding eigenvalues are not well-separated, ionization cross section , transition rate between two discrete states, and especially the effect of continuum part of hydrogen atom wave function on our approach in the presence of the circularly polarized laser field.

5. References


