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Contribution of Lattice Time-Dependent Schrödinger Equation Approach to the Controlled Fusion Atomic Data Center

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Abstract

We review the calculational method of the lattice time-dependent Schrödinger equation (LTDSE) approach. Parallel computing implementation of LTDSE is also discussed. We apply the LTDSE approach here to collisions of Be^{4+} ions on hydrogen atoms and demonstrate how it can contribute to the goals of the Controlled Fusion Atomic Data Center.

Keywords:

The Controlled Fusion Atomic Data Center, lattice time-dependent Schrödinger equation approach, parallel computing, message passing interface (MPI), Be^{4+}, electron capture

1. Introduction

The Controlled Fusion Atomic Data Center (CFADC) is supported through the U.S. Department of Energy, Office of Fusion Energy Sciences, and is part of the Oak Ridge National Laboratory's Physics Division. The CFADC's mission is to compile, evaluate, recommend, and disseminate atomic and molecular collision data relevant to fusion energy research and development. The CFADC also maintains a categorized bibliography of atomic and molecular collision references relevant to fusion energy research and development.

There are a variety of theoretical approaches to study ion-atom collisions which are relevant to fusion energy research. Widely known and used examples of such approaches include, various types of perturbation theory methods, the classical trajectory Monte-Carlo (CTMC) method, molecular orbital close coupling (MOCC) methods, atomic orbital coupled channel (AOCC) methods, and so forth. These approaches are, however, reliable only within certain limitations, which is a reflection of the validity conditions of the approximations each approach invokes.

In contrast to these approaches, the lattice time dependent Schrödinger equation (LTDSE) method is based on direct numerical integration of the time-dependent Schrödinger equation. Thus, the limitations are few regarding these approximations. On the other hand, since the LTDSE approach is computationally very intense, it is not always practical compared to other approaches. For these characteristics, LTDSE's suitable role, in present days, is to propose benchmarks for other approaches.

In this paper, we review the calculational method of the LTDSE approach and demonstrate its contributions to the CFADC. Similar to other theoretical approaches, LTDSE can provide a range of information concerning ion-atom collisions, such as excitation, ionization, charge transfer, and so forth [1-5]. In this paper, we focus on calculation of single electron capture from target atoms to projectile ions in ion-atom collisions. Atomic units are used throughout unless otherwise stated.

2. Calculational method

In the present treatment of ion-atom charge transfer, we employ the so-called semi-classical approximation in which the projectile ion travels along a straight line trajectory. The calculation is performed in the projectile frame for convenience to our numerical method. Therefore, the projectile ion is at rest at the center of the three-dimensional numerical grid and the target atom has a position vector given by $\vec{R}(t) = (0, b, -z_0 + v_P t)$, where b is the impact parameter, v_P is the collision velocity, and $-z_0$ is the initial internuclear coordinate along the z-axis.

In particular, we solve the time-dependent Schrödinger equation for one electron,

$$i\frac{\partial}{\partial t}\psi(\vec{r},t) = \{\mathcal{T} + V_T(\vec{r},t) + V_P(r)\}\,\psi(\vec{r},t) \qquad (1)$$

where $\psi(\vec{r},t)$ is the electronic wavefunction, $\vec{r}$ is the po-

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sition of the electron in the projectile frame, and $\mathcal{T}$ is the kinetic energy operator. $V_P(r)$ and $V_T(\vec{r},t)$ are potentials experienced by the electron due to the projectile (P) ion and the target (T) atom, respectively.

In the lattice approach, Eq. (1) is solved numerically by integrating it on a discretized three-dimensional space of finite volume. We adopt a cubic shape for this volume with sides of length $\mathcal{L}$. We set the origin of Cartesian coordinates at the center of the cube and the x-, y- and z-axis parallel to the sides, with N equally spaced points in each direction. The states of the projectile ion, which consist of the captured electron stay localized around this origin since we choose the projectile frame as mentioned above. The choice of the cubic volume with equally spaced lattice points is a consequence of the particular representation of the derivative operators and computer implementation that we have used.

The spatial points are denoted as (x_i, y_j, z_k) $(i, j, k = 1, 2, \cdots, N)$ and the wavefunction at a given time t is mapped to the vector $\psi(x_i, y_j, z_k, t)$ with dimension N^3. The potential operators are mapped to diagonal matrices, *e.g.*, $V_P(r) \to V_P(x_i, y_j, z_k)\delta_{i',i}\,\delta_{j',j}\,\delta_{k',k}$.

Regarding the configuration space kinetic energy operator, its discrete representation is in general not diagonal. Here, we exploit the fact that the kinetic energy operator is diagonal in momentum space. That is, after discretization this operator is

$$\tilde{\mathcal{T}}(\vec{p}) \to \frac{1}{2}\left\{(p_i^x)^2 + (p_j^y)^2 + (p_k^z)^2\right\}\delta_{i',i}\,\delta_{j',j}\,\delta_{k',k}, \quad (2)$$

where $\vec{p}$ is a coordinate vector in momentum space.

Using this property of $\mathcal{T}$, we can define its operation on the wavefunction $\psi(x_i, y_j, z_k, t)$, namely,

$$\mathcal{T}\psi(x_i, y_j, z_k, t) = \mathcal{F}^{-1}\left[\tilde{\mathcal{T}}\tilde{\psi}(p_i^x, p_j^y, p_k^z, t)\right], \quad (3)$$

where $\mathcal{F}[X]$ means the discrete Fourier transform of X and $\tilde{\psi}(p_i^x, p_j^y, p_k^z, t) = \mathcal{F}\left[\psi(x_i, y_j, z_k, t)\right]$.

Assuming one has defined the potentials in Eq. (1), which depend on collision systems being considered, we may calculate bound states of the target and projectile atoms. This is formally performed by diagonalizing the target Hamiltonian $\mathcal{H}_T = \mathcal{T} + V_T$ and the projectile Hamiltonian $\mathcal{H}_P = \mathcal{T} + V_P$

$$\mathcal{H}_T\phi_{nlm}^T = \phi_{nlm}^T E_{nlm}^T, \quad (4)$$

$$\mathcal{H}_P\phi_{nlm}^P = \phi_{nlm}^P E_{nlm}^P, \quad (5)$$

where ϕ_{nlm}^T and E_{nlm}^T are the eigenstates and the eigenenergies of the target and ϕ_{nlm}^P and E_{nlm}^P are the eigenstates and the eigenenergies of the projectile. The subscripts n, l, m denote the principal, azimuthal and magnetic quantum numbers, respectively. Since the complete diagonalization of the Hamiltonians is not practical for the very large dimensions of $\mathcal{H}_{\mathcal{T},\mathcal{P}}$ in the lattice representation, we use a partial eigensolution approach to calculate the ground state for the target (which is the initial state of the collision) and the low-lying states of the projectile (which are the final states that we consider here).

To initiate the calculation, the ground state of the target is used as the initial state of the system at $t = t_0$

$$\psi(\vec{r}, t_0) = \phi_{1s}^T(\vec{r} - \vec{R}(t_0))\exp(i\vec{v}_P \cdot \vec{r}) \quad (6)$$

where $\exp(i\vec{v}_P\cdot\vec{r})$ is the translation factor associated with the moving orbital. The time evolution of the wavefunction $\psi(x_i, y_j, z_k, t)$ is then carried out using the split operator method [6]. During the time evolution , the wavefunction is projected onto the projectile eigenstates,

$$\begin{aligned} a_{nlm} =& \langle\phi_{nlm}^P|\psi(t)\rangle \\ =& \left(\frac{\mathcal{L}}{N}\right)^3 \sum_{i,j,k} \phi_{nlm}^{P*}(x_i, y_j, z_k)\psi(x_i, y_j, z_k, t). \end{aligned} \quad (7)$$

Once the amplitude a_{nlm} reaches to its asymptotic limit, the time evolution is terminated. For a fixed kinetic energy of the projectile, since a_{nlm} depends on the impact parameter b, we rewrite the amplitudes as $a_{nlm}(b)$. The capture cross section to the state ϕ_{nlm}^P is, then,

$$\sigma_{nlm} = 2\pi \int_0^\infty \mathrm{d}b\, b\, |a_{nlm}(b)|^2 . \quad (8)$$

3. Numerical implementation for parallel computers

In some of our applications, the number of the lattice (N) points along one axis is as large as 320. Hence the dimension of the wavefunction vectors, $\psi(x_i, y_j, z_k, t)$ is 320^3 in such a case. If we use a 16-byte array with the dimension of 320^3 in computer calculations to store the wavefunction, we need about 500 Mega-bytes of memory for this array. This also applies to storages of the eigenstates, potential matrix (which is diagonal), and so forth. Therefore, a computer program for the numerical calculation requires a few Giga-bytes of storage memory, after all. Most common workstations in present days are not capable of handling programs with such large memory storages. For this reason, we utilize parallel computers (or a cluster of work stations) for the numerical calculations.

Our strategy to overcome the memory problem is to divide up the three-dimensional space in layers perpendicular to some coordinate axis (z-axis in our case). The wavefunctions and the Hamiltonian correspond to each

layer resides in memory devices that work with a single processor element. By this strategy, if we denote number of the processor elements invoked to solve Eq. (1) over the whole cube as N_{proc}, the required memory for each processor element reduces to $1/N_{proc}$ of the total required memory for the calculation. Each processor element performs time integration of the Schrödinger equation (1) on its own layer. However, operations such as Eq. (3) or Eq. (7) require information on the all layers. Communication between each processor element for this purpose is performed using the Message Passing Interface (MPI). MPI is a standard environment for parallel computing and is incorporated by a variety of architectures of parallel computers. We have chosen MPI to make our program code portable among various architectures.

Since the numerical integrations of the Schrödinger equation (1) with different impact parameters are independent each other, using parellel computers, we can perform them simultaneously. If we denote number of the impact parameters which we calculate simultaneously as N_b, the total number of the processor elements necessary for the calculation is $N_{tot} = N_{proc} \times N_b$.

4. Applications and results

We have applied the LTDSE method to the collisions of Be^{4+} on H(1s) and report our result briefly in this section. Further analysis of the result will be presented elsewhere. Beryllium is one of proposed plasma facing materials in future fusion reactors such as the International Thermonuclear Experimental Reactor, ITER. Evaporated beryllium ions may enter the plasma of the reactor as impurity and may affect conditions of controlling the plasma. Therefore this collision system is one of the most important elements of the controlled fusion atomic data.

For the present application, we have chosen the length of the sides of the cube being set at $\mathcal{L} = 40$ a.u. and the number of mesh points on the x-, y- and z-axis being $N = 245$. We also determined that a starting point of $z_0 = 10$ a.u. provided a sufficiently large internuclear distance to assure that we could neglect the interaction between the projectile and the target at $t = 0$.

Figure 1 shows cross sections for electron capture into each shell ($n = 1 - 3$) of the Be^{3+} ion. Result from the LTDSE method is compared with ones from the classical trajectory Monte-Carlo (CTMC) method [7], a perturbation method [8] and the molecular orbital close coupling (MOCC) method [9]. These references are listed in the bibliographic database of the CFADC. The most striking feature in the figure is that all calculations agree very well for the $n = 3$ shell. In contrast, bigger deviations exist between different methods for the $n = 1$ and the $n = 2$ shells. For the $n = 1$ shell, CTMC and LTDSE share the same trend but the magnitude differs greatly from each other. The difference between the two methods tends to increase for decreasing impact energy. On the other hand, the trend of the perturbation theory is very different from LTDSE. The cross section by LTDSE has a peak at around 200 keV/u, whereas the one by the perturbation theory monotonically decreases with increasing impact energy.

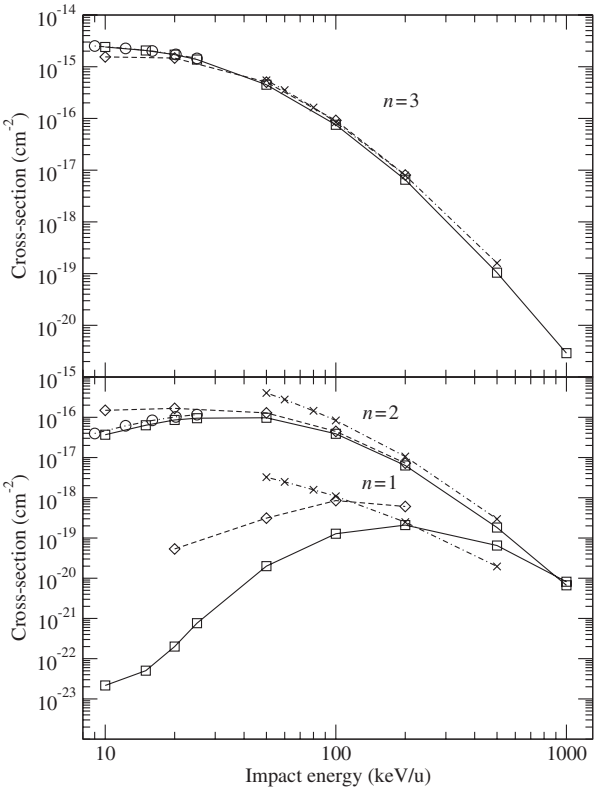

Fig. 1 Cross sections for the electron capture from the target hydrogen atom to each n shell of the projectile Be^{3+} ion. Square: present calculation. Diamond: CTMC from [7]. Cross: perturbation approach from [8]. Circle: MOCC from [9].

For the $n = 2$ shell, all the calculation methods seem to share the same trend. Especially, MOCC agrees very well with LTDSE. CTMC also agrees well with LTDSE over all but it tends to give bigger cross section than LTDSE and MOCC for 20 keV/u and less impact energy. The perturbation theory agrees with LTDSE much better compared to the case of the $n = 1$ shell, however it tends to give bigger cross section than LTDSE and CTMC.

In Figure 2, the electron-capture cross section into $n = 2$ shell is resolved in each azimuthal quantum number. For both states, CTMC and the perturbation method give bigger cross sections than LTDSE over all. The differences from LTDSE are the biggest at their

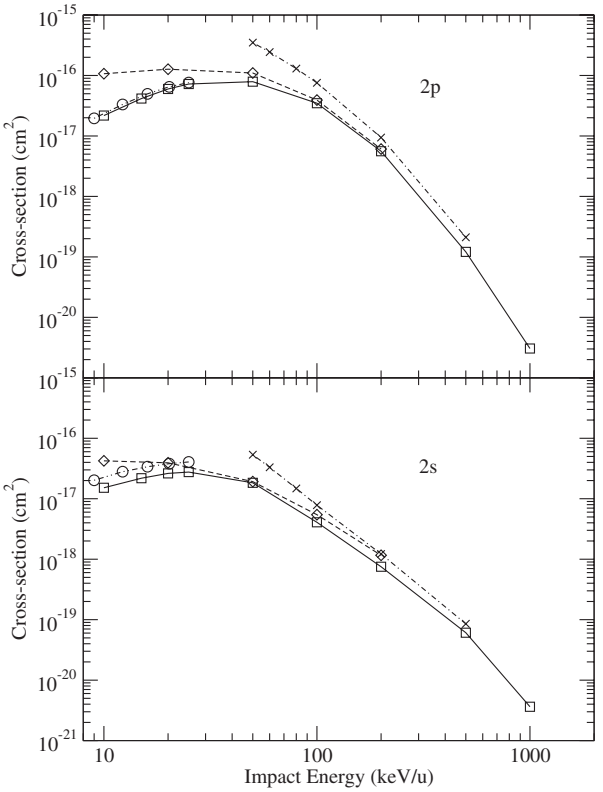

Fig. 2 Cross sections for electron capture from the target hydrogen atom to the 2s and 2p states of the projectile Be^{3+} ion. The same symbols in Fig. 1 are used.

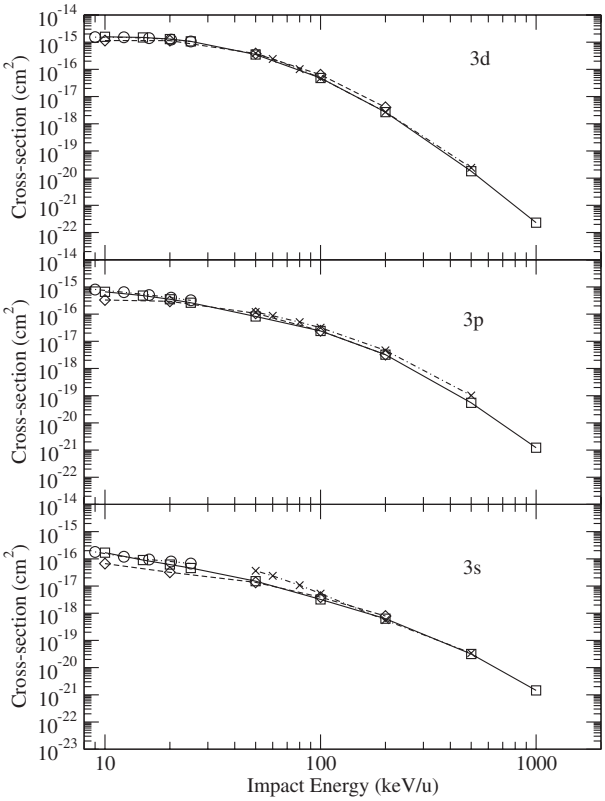

Fig. 3 Cross sections for electron capture from the target hydrogen atom to the 3s, 3p and 3d states of the projectile Be^{3+} ion. The same symbols in Fig. 1 are used.

lowest impact energy and tend to decrease with increasing impact energy. MOCC agrees with LTDSE for the both states very well. Especially for 2p state, the difference from LTDSE is very small. For the 2s state, MOCC gives a 10 % bigger cross section than LTDSE and each curve runs parallel to each other.

In Figure 3, the electron-capture cross section into $n = 3$ shell is resolved in each azimuthal quantum number. For the 3s state, CTMC gives 60 % smaller cross section than LTDSE at impact energy of 10 keV/u and the difference decreases with increasing impact energy. The perturbation method gives 60 % bigger cross section than LTDSE at the impact energy of 50 keV/u and the difference decreases with increasing impact energy. MOCC, again, agrees very well with LTDSE. For the 3p state, CTMC gives 50 % smaller cross section at the impact energy of 10 keV/u and the perturbation method gives 50 % bigger cross section at the impact energy of 500 keV/u. Otherwise, all the methods agree well for the 3p state. Lastly, for 3d state, all the calculations agree very well.

5. Summary

In this paper, we have discussed the calculational method of the lattice time-dependent Schrödinger equation approach and its numerical implementation for parallel computers. We have demonstrated how the LTDSE method can contribute to the goal of the Controlled Fusion Atomic Data Center. Finally, we have presented an application of the LTDSE method to collisions of Be^{4+} ions on hydrogen atoms and compared its result with other methods from the bibliographic database of the CFADC.

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