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MeV Cations and Coulomb Explosion Threshold of 1D Atomic Hydrogen Cluster: Simplified Numerical Simulation

Zhang Zhe[1] Zhang Guizhong[1] Xiang Wanghua[1] W. T. Hill Ⅲ[2]

[1] *College of Precision Instrument and Optoelectronics Engineering, Tianjin University Key Laboratory of Optoelectronic Information and Technical Science, Ministry of Education, Tianjin University, Tianjin, 300072, China*

[2] *Institute for Physical Science and Technology, University of Maryland, College Park, MD20742, USA*

Abstract A simplified version together with a double-array 1D atomic hydrogen cluster model is presented for simulating cluster dynamics when exposed to intense light. The computed maximum kinetic energy and cation number distributions were in fair agreement with numerical results and experimental observations. An expression for determining the abundance variation of ionized cations with exciting laser intensity was proposed from which the threshold laser intensity of cluster Coulomb explosion could be extracted.

Key words atomic hydrogen cluster; Coulomb explosion; 1D model

一维氢原子团簇模型下的兆电子伏离子与库仑爆炸：简化的数值模拟

张 喆[1] 张贵忠[1] 向望华[1] W. T. Hill Ⅲ[2]

[1] 天津大学精密仪器与光电子工程学院，教育部光电信息技术科学实验室，天津 300072

[2] Institute for Physical Science and Technology, University of Maryland, College Park, MD20742, USA

摘要 本文使用一维双列氢原子团簇模型对强激光场中的团簇动力学过程进行了数值模拟。计算所得的质子最大动能和能谱均与他人的计算或实验结果符合较好，但计算大为简化。表明本文所述模型适用于氢原子团簇模拟。本文亦根据逸出质子数量随入射激光强度变化的规律总结出一个描述团簇库仑爆炸的光强阈值公式。

关键词 氢原子团簇；库仑爆炸；一维模型

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In the past decade, interaction of intense lasers with clusters has become another research focus in the field of atomic, molecular and optical physics[1~7]. In theory, full quantum treatment is beyond the current computability, so that the well developed classical particle-in-cell (PIC) benchmark calculation scheme for plasma[8] and a simplified Coulomb explosion model[2] are the way out. In experiment, cluster dynamics is characterized by three prominent aspects for ionized cations[2,9] as follows: (1) maximum kinetic energy saturation with light intensity; (2) distribution of number abundance versus kinetic energy with a sharp cut-off in the high-energy end; and (3) proportionality of maximum kinetic energy to initial cluster radius.

In this paper we present a simplified simulation method for a novel one-dimensional (1D) cluster model on which the interaction of strong laser pulses with atomic hydrogen cluster is calculated using Newton's law of motion with scattering taken into account. Rather than calculating electric field strength by solving Poisson equation, this simplified method takes Coulomb actions only from five neighbor particles in a cluster, because farther charge particles (either protons or electrons) essentially diminish forces on the charged particle under consideration. This means profoundly reduces computation cost while maintaining the essential physics and numerical precision for conceptual understanding. With this proposed model, we study the

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maximum kinetic energy of dislodged protons and their energy distribution. The numerical experimental results show that a laser-intensity threshold for cluster's Coulomb explosion could be extracted from a suggested expression. The fairly reproduced cluster dynamics corroborated the validity of the proposed method. We think that it is suitable for three-dimensional (3D) simulations of cluster interaction with intense light.

The 1D model of atomic hydrogen cluster is illustrated in Fig. 1. This prototypical cluster contains 1000 hydrogen nuclei (protons) aligned along the x-axis with equal nearest-neighbor spacing of 4.5 a.u.. The spatial extension in simulation is 5400 a.u., where a central section of 4500 a.u. is the grids for the 1000 protons, two end sections of 450 a.u. each are buffer grids. Any proton escaped upon ionization into the buffer region is tracked for both its identity number and energy. More importantly, protons' orderly dislodging in accordance with their identity numbers is guaranteed due to the 1D nature in the model. Like the cations, electrons are deposited also along the x-direction, but with a transverse displacement of $a = 1$a.u., the softening parameter in the smoothed Coulomb force is relative to the cation array. The electron array has identical spatial ranges of simulation to those of the cations.

Prior to laser excitation, protons are deposited on the grid points (upper line in Fig. 1) in the proton array and electrons are deposited on the grid points (lower line in Fig. 1) in the electron array. The double-array 1D model ensures that the same species of particles move along their own lined track and no collisions between cations and electrons occur. Initially, the protons are assigned to be motionless while the electrons' velocities are small values determined thermally by $\sqrt{2K_{\mathrm{B}}T/m_{\mathrm{e}}}$ with $T = 300$ K.

The incident laser pulses are of wavelength of 800 nm, with electric field $E(t)$ polarized along the x-axis:

$$E(t) = E_0 \cdot \sin(\omega_0 t + \phi) \cdot \exp\left[-\left(\frac{t-\tau/2}{\tau/5}\right)^2\right], \quad (1)$$

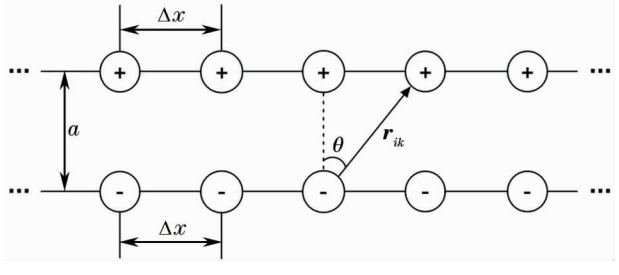

Fig. 1 Spatial grid configuration of 1D atomic hydrogen cluster. Positively and negatively signed circles stand for protons and electrons, respectively

where E_0 is the peak field strength, τ is a 5-cycle duration of the pulse. ϕ is the carrier-envelope phase difference(CEPD). E_0 value is varied in the calculation between 4～9 a.u.

Coulomb's law is used directly for calculating electric force between charged particles. The double-array 1D model has the Coulomb force on the ith particle as

$$\boldsymbol{F}_i = -\sum_{j(\neq i)} \frac{\boldsymbol{r}_{ij0}}{|\boldsymbol{r}_{ij}|^2} + \sum_k \frac{\boldsymbol{r}_{ik0}\sin\theta_{ik}}{|\boldsymbol{r}_{ik}|^2}, \quad (2)$$

where $\boldsymbol{r}_{ij}$ is the vector from the ith particle to the jth of the same species, $\boldsymbol{r}_{ik}$ is the vector from the ith particle to the kth of the other species. θ_k is the angle between $\boldsymbol{r}_{ik}$ and the y-axis which is perpendicular to the double-array, as illustrated in Fig. 1.

At every time step, the velocity of the ith particle by Newton's second law of motion was written as

$$v_{i,\mathrm{new}} = v_{i,\mathrm{old}} + a_i \cdot \Delta t, \quad a_i = \frac{F_i}{m_i}, \quad (3)$$

while the new position of this particle is

$$x_{i,\mathrm{new}} = x_{i,\mathrm{old}} + v_{i,\mathrm{new}} \cdot \Delta t, \quad (4)$$

As mentioned above, the 1D double-array model had already avoided collisions between the protons and electrons. In view of electrons' small size, we did not consider collisions between electrons either. Collisions among protons were the only scattering in our model. At every time step, collisions took place between two adjoining protons only if (1) their spacing was less than some critical internuclear distance while the relative speed of the rear proton with respect to the front one in the pair was negative; or (2) the two protons were reversed in position. The collisions were considered to be elastic for retrieving protons' new velocities after a collision, in terms of classical motion laws.

For protons, quantity and kinetic energy were tracked on escaping from the cluster bulk after laser excitation. Thus, quantity and maximum kinetic energy of the emitted cations were obtained. The computation was repeated for different laser strengths.

Figure 2 presents the maximum kinetic energies and a fitting with either a second-order or third-order polynomial. This downward-curved fitting is a signature of the onset of cation energy saturation although the complete saturation effect was not computationally observed. This saturation effect is typical of cluster behavior when exposed to intense light, as evidenced by Ref. [2].

Figure 3 is the normalized distribution of kinetic energy for four laser field strengths with $E_0 \leqslant 7.5$a.u. (laser intensity is $I \leqslant 3.95 \times 10^{18}$ W/cm^2). All these distribution functions manifest that (1) a peak feature appears in high energy regime; (2) this relatively broad

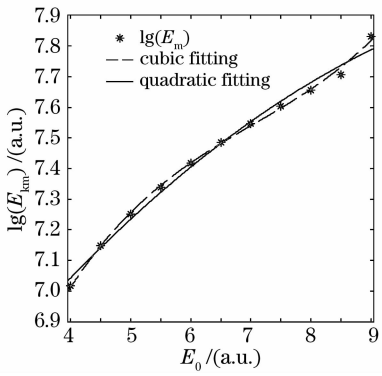

Fig. 2 Logarithmic plot of maximum kinetic energy versus laser field strength

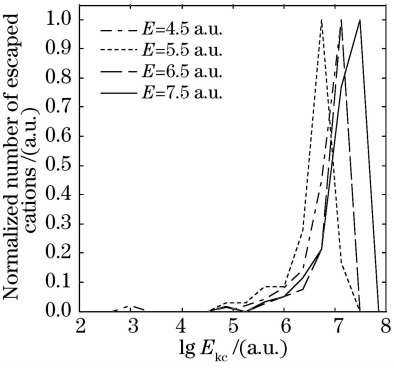

Fig. 3 Variations of normalized cation number versus cation kinetic energy for different excitation laser intensities

peak blue-shifts and broadens with increasing laser intensity. It is implied that both the protons' maximum and average kinetic energies increase with increasing light intensity. When $E_0 \geqslant 8$ a.u., however, another peak emerges and shows a similar blue-shift and widening behavior, as given in Fig. 4. Shao *et al*. has measured a two-peak feature but for electrons in the experiment[10]. To some extent, this sort of relatively broad peak structure has also been observed in other

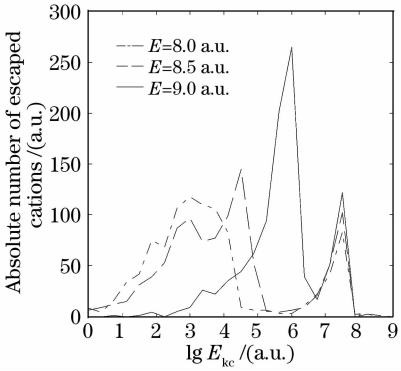

Fig. 4 When $E_0 \geqslant 8$ a.u., a second broad peak feature appears compared with Fig. 3. The secondary peak narrows up and blue-shifts with increasing light strength

numerical experiment[11].

We also computed cation number N if they were dislodged into the buffer region, as shown in Fig. 5. After some trial and error, we achieved

$$N(E_0) \approx \frac{\tanh[6(E_0 - E_{th})] + 1.2}{2.2}, \qquad (5)$$

there E_{th} is the threshold peak electric field at which half of the protons had left the cluster. Fitting of the curve (solid line) with Eq. (5) was fairly acceptable. From it, $E_{th} \approx 7.7$ a.u. was extracted. This electric field strength corresponds to a laser intensity of 4.2×10^{18} W/cm^2, which could be defined as some threshold light intensity for Coulomb explosion in the cluster[2,9]. The threshold scenario was qualitatively: below the threshold, only a fraction of the protons were kicked out of the cluster which just expanded without breaking apart; above this threshold, Coulomb explosion happened due to the repulsive force when the electrons were all removed. As to the physical significance of Eq. (5), we do not have any deeper understanding except for a nice fit.

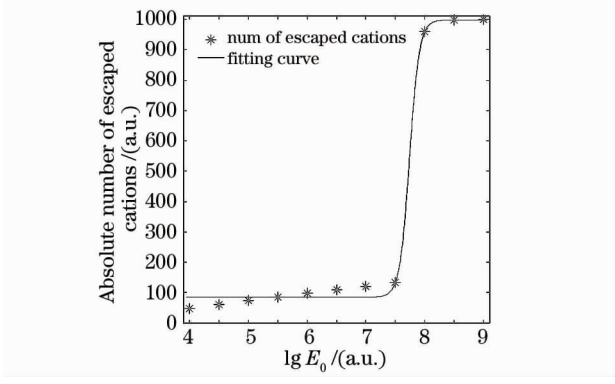

Fig. 5 Dependence of absolute number of escaping cations after ionization on peak electric field E_0 of the exciting laser pulses

In summary, we presented a relatively simplified method for calculating cluster dynamics taking into account of proton-proton collision, and tested this method on a 1D double-array atomic hydrogen cluster model. The essential points of the proposed method are of twofold: simplify computation by taking actions from only five near-neighbor particles, and smooth Coulombic singularity by arranging protons and electrons along two parallel grids. On the basis of having maintained numerical precision, the simulated cluster phenomena, such as maximum kinetic energy saturation and kinetic energy distribution, were in fair agreement with others' numerical experiments, which corroborated the feasibility of the method.

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