Ionization of stabilized helium atoms by proton and antiproton impacts

S. Morita, N. Matsuda, N. Toshima, and K. Hino
Institute of Materials Science, University of Tsukuba, Tsukuba, Ibaraki 305-8573, Japan
(Received 24 June 2002; published 25 October 2002)

The classical trajectory Monte Carlo method is applied to the calculation of single- and double-ionization cross sections of helium atoms by proton and antiproton impacts. The classical helium atom is stabilized by the introduction of the Heisenberg core potentials that prevent autoionization of classical two-electron atoms under the constraint of the uncertainty principle. The ratio of the double- to single-ionization cross sections is larger for antiproton impact than for proton impact in agreement with measurements, though the difference is slightly smaller than the experimental findings. It is important to generate the initial distribution microcanonically taking all the possible configurations into account. Exclusive use of the circular orbits fails to account for the dependence on the projectile charge. The Bohr helium model without the stabilization is too fragile to be used for collision problems of charged particles even at high energies.

DOI: 10.1103/PhysRevA.66.042719 PACS number(s): 34.50.Fa

I. INTRODUCTION

Many years have passed since Andersen *et al.* [1] discovered that a large difference remains even at high energies above 1 MeV between the ratios of the double- to single-ionization cross sections of helium atoms for proton and antiproton projectiles. Shortly after the measurements, two types of theoretical calculations were reported; one is the classical trajectory Monte Carlo (CTMC) method by Olson [2] and the other one is the forced impulse method (FIM) by Reading and Ford [3]. Although both methods succeeded in producing the difference of the cross-sections ratios, the agreement with the measurement was not satisfactory in the energy dependence and in the absolute values. The FIM calculations were improved by adding *d* orbitals on the helium atom later [4] and good agreement was obtained with the measurement. No extended calculations have been done for the CTMC method.

Even if the coupling with the radiation field is disregarded, classical two-electron atoms are unstable through autoionization in which one electron falls into a deeper bound state ejecting the other to a continuum state through the correlation interaction. In order to circumvent this difficulty, Olson [2] adopted the Bohr helium-atom model where the two electrons stay in a common circular orbit with a phase difference of 180°. This model is stable only for an isolated helium atom, namely, when no other interaction is exerted onto the electrons. Even a small perturbation makes the electrons deviate from the circular orbit and the atom autoionizes quickly. They started to solve the scattering equations placing the projectile in the neighborhood of the target atom in order to finish the calculations before the atom autoionizes. It is a questionable procedure to avoid the autoionization by making the collision time artificially short.

In low collision-energy regions, the Bohr model becomes totally invalid since all the helium atoms autoionize completely before the projectile comes into the vicinity of the target atom. Beck *et al.* [5] incorporated a momentum-dependent potential named as Heisenberg core [6] to study antiproton capture on helium atoms,

$$V_H(r,p)=\frac{\xi^2}{4\alpha r^2}\exp\left\{\alpha\left[1-\left(\frac{rp}{\xi}\right)^4\right]\right\}, \tag{1}$$

where r and p are the radial parts of the position and momentum vectors of the electron and α and ξ are parameters. This potential becomes strongly repulsive for $rp\leqslant\xi$ to prevent the electron from falling into a deep bound state which is excluded by the Heisenberg uncertainty principle in the quantum mechanics.

In this paper we calculate single- and double-ionization cross sections by the CTMC method stabilizing the helium atom under the Heisenberg core potentials. Atomic units are used unless otherwise stated explicitly.

II. FORMULATION

The numerical procedure to solve the classical scattering equations is similar to that used by Beck *et al.* [5] except for the following two points.

We use the Jacobi coordinates without neglecting the terms of the order of the electron mass to the nuclear masses. The Hamiltonian of the unperturbed helium atom is then written as

$$H_{atom}=\frac{1}{2\nu_1}p_1^2+\frac{1}{2\nu_{2c}}p_{2c}^2-\frac{2}{r_1}-\frac{2}{r_2}+\frac{1}{r_{12}}+V_H(r_1,p_1)+V_H(r_2,p_2), \tag{2}$$

with

$$\nu_1=\frac{Mm}{M+m}, \tag{3}$$

$$\nu_{2c}=\frac{(M+m)m}{M+2m}, \tag{4}$$

where M and m are the masses of the helium nucleus and the electrons. $\mathbf{r}_1$ and $\mathbf{r}_2$ are the position vectors of the two electrons measured from the helium nucleus and r_{12} is the relative distance between the electrons. $\mathbf{r}_{2c}$ is the position vector

of the second electron measured from the center of mass of the system composed of the first electron and the helium nucleus. $\mathbf{p}_1$, $\mathbf{p}_2$, and $\mathbf{p}_{2c}$ are the conjugate momenta of the position vectors $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_{2c}$, respectively. Although the introduction of the core potential stabilizes the helium atom, a small difference in the equations of motion is sometimes amplified more than expected resulting in a large difference in the final distribution of the particles as a manifestation of the fact that the classical two-electron system is kinematically balanced very delicately. We exclude errors arising from the unnecessary approximation $M \gg m$ in the framework of the classical mechanics.

The other point is the choice of the parameters, α and ξ. Beck *et al.* adopted $\alpha=1.0$ and $\xi=2.767$. Their ξ is too large to make a proper classical model of helium atoms. The helium ground state with the energy $E=-2.9004$ takes, for example, the values $r=0.6035$, $p=1.703$, and $rp=1.028$ for the circular orbit of the Bohr model. Then the core potential (1) takes a large positive value 14.02, which is too high to bind even a single electron. Both electrons are ejected away with high energies from the nucleus. Since the total atomic energy is conserved, the ejected electrons have incorrectly high-energy distribution. *rp* can be smaller for other elliptic orbits and the repulsion by the core potential is more serious. Cohen [7] suggested $\alpha=2.0$ and $\xi=0.9343$, which give much more realistic helium model. In this case the core potential becomes 0.1184 for the Bohr model. We try to make the value ξ as small as possible in order to avoid unfavorable secondary effects of the core potential. We incorporate the core potential only for the purpose to prevent the collapse of electrons through autoionization. Numerical investigation shows that the autoionization never occurs for $\xi>0.78$ so that we adopt a marginal value $\xi=0.79$ for the present calculations. α is more insensitive to the kinematics of the orbits. We take $\alpha=2.0$ following Cohen. Then the core potential takes a negligibly small value 0.0051 for the Bohr model circular orbit. We do not use a core potential representing Pauli's exclusion principle for the correlation interaction between the two identical electrons [7] because it is not needed for the stabilization of the helium atom.

Hamilton's equations of motion are solved numerically adding to the atomic Hamiltonian (2) the kinetic-energy term of the relative motion of the projectile and the interaction potentials between the projectile and the target particles. We generate the microcanonical distribution of Kepler orbits under an effective charge $Z_{eff}=1.6875$ as a substitute of the initial distribution of the electrons of the helium atom since general analytic solution of the two-electron system is not known in the classical mechanics. The other parameters of the Kepler motion, namely, the eccentricity, the eccentric angle, and three Euler angles characterizing the orbital plane are generated randomly in the same manner as in the three-body CTMC calculations. [8,9] We adopt among the randomly generated Kepler orbits only the ones whose total atomic energy (2) stay in the energy interval $-80 \leqslant E \leqslant -78$ eV. We start to integrate the equations of motion at a distance of 20 a.u. from the target nucleus and stop the integration when the projectile is away by 100 a.u. from it. These distances are large enough to make the results independent of the choice.

TABLE I. Single- and double-ionization cross sections of helium atoms by antiproton and proton impacts (in units of cm^2). The numbers in brackets are the powers of 10 to be multiplied.

Projectile	Antiproton		Proton	
E (keV)	Single	Double	Single	Double
100	8.75[−17]	1.67[−18]	1.08[−16]	7.14[−19]
200	6.21[−17]	9.01[−19]	7.50[−17]	6.51[−19]
300	4.84[−17]	5.47[−19]	5.65[−17]	4.58[−19]
400	3.95[−17]	3.92[−19]	4.53[−17]	3.24[−19]
500	3.36[−17]	3.02[−19]	3.77[−17]	2.39[−19]
700	2.58[−17]	1.86[−19]	2.83[−17]	1.45[−19]
1000	1.91[−17]	1.20[−19]	2.04[−17]	8.66[−20]
1500	1.35[−17]	6.94[−20]	1.41[−17]	5.27[−20]
2000	1.04[−17]	4.96[−20]	1.08[−17]	3.43[−20]
3000	7.10[−18]	2.80[−20]	7.38[−18]	2.16[−20]
5000	4.17[−18]	1.36[−20]	4.30[−18]	1.02[−20]

III. RESULTS AND DISCUSSION

We generated 10^6 (at 100 keV) to 10^7 (at 5 MeV) trajectories for each collision energy increasing the number of the trajectories for higher energies. The statistical errors are kept within a few percents for the double-ionization cross sections and they are much smaller for the single-ionization cross sections.

The single- and double-ionization cross sections of the helium atom by proton and antiproton impacts are given in Table I and Figs. 1 and 2. The CTMC ionization cross sections are in good agreement with the measurement for both the projectiles over a wide energy range. The single-

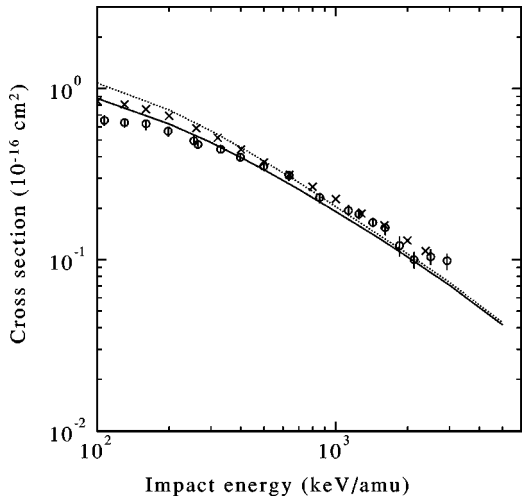

FIG. 1. Single-ionization cross sections of helium atoms. Present CTMC cross sections: solid line, antiproton impact; dashed line, proton impact. Experimental data: open circles, antiproton impact by Andersen *et al.* [1,11]; crosses, proton impact by Shah and Gilbody [12].

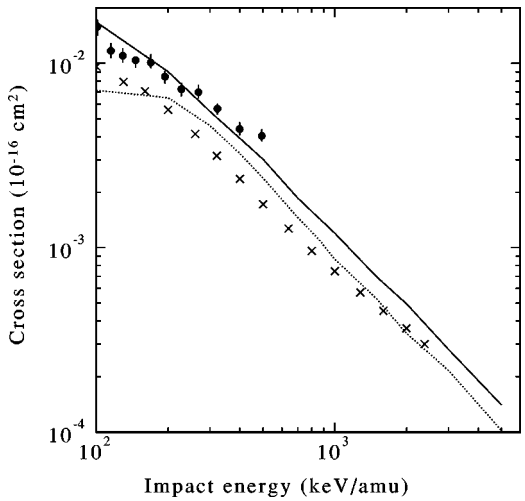

FIG. 2. Double-ionization cross sections of helium atoms. Present CTMC cross sections: solid line, antiproton impact; dashed line, proton impact. Experimental data: closed circles, antiproton impact by Hvelplund *et al.* [13]; crosses, proton impact by Shah and Gilbody [12].

ionization cross sections are slightly overestimated below 300 keV for both the projectiles. The double-ionization cross sections are also satisfactory though the proton cross sections tend to disagree with the measurements below 200 keV. The cross-section ratios are shown in Fig. 3. The ratios of the antiproton impact show the same energy dependence as the measurements, but the absolute values are a little smaller. The disagreement below 200 keV for the proton impact is

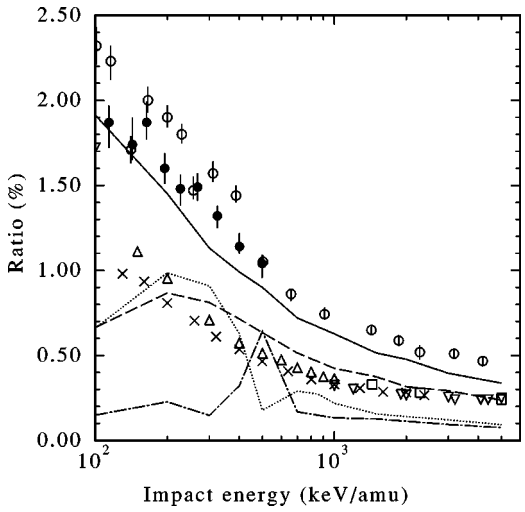

FIG. 3. The ratios of double- to single-ionization cross sections of helium atoms. CTMC calculations with microcanonical distribution: solid line, antiproton impact; dashed line, proton impact. CTMC calculations with the Bohr model: dotted line, antiproton impact; dotted-dashed line, proton impact. Experimental data: open circles, antiproton impact by Andersen *et al.* [1,11]; closed circles, antiproton impact by Hvelplund *et al.* [13]; crosses, proton impact by Shah and Gilbody [12]; squares, proton impact by Knudsen *et al.* [14]; inverted triangle, proton impact by Andersen *et al.* [11]; triangles, proton impact by Puckett and Martin [15].

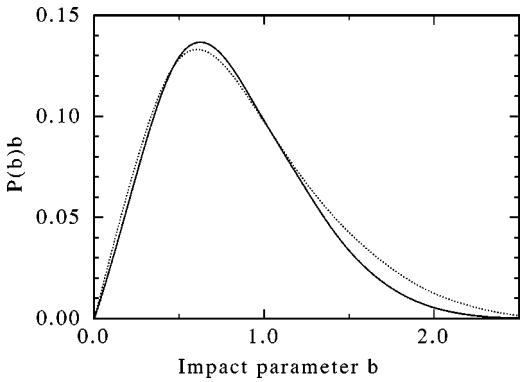

FIG. 4. The single-ionization probabilities as functions of the impact parameter *b* at the collision energy of 1 MeV. The solid line is for the antiproton impact and the dotted line is for the proton impact.

caused by the underestimate of the double-ionization cross section in this energy range. The difference of the ratios between the two projectiles is mainly caused by the double-ionization cross sections. The single-ionization cross sections do not differ much for these two projectiles at high energies as a result that the first-order Born approximation becomes valid for the single ionization. To compare with the results of Olson [2], we also carried out calculations for which only circular orbits (Bohr model) are used for the initial distribution. The results are also shown in Fig. 3. The cross-section ratios show wrong behavior below 700 keV and fail to reproduce the experimental findings.

The ionization probabilities as functions of the impact parameter *b* are shown in Figs. 4 and 5 at the collision energy of 1 MeV. The double-ionization probabilities are confined within a smaller impact-parameter region than the single-ionization probabilities, as one can easily expect from the fact that larger energy transfer is needed for the double ionization than for the single ionization. At this high energy, the integrated single-ionization cross section is about 7% larger for the proton impact than for the antiproton impact. This difference results mainly from the behavior of the transition probabilities at large impact parameters. The probabilities for the proton impact decay more slowly as the impact parameter becomes larger. This finding implies that the single ion-

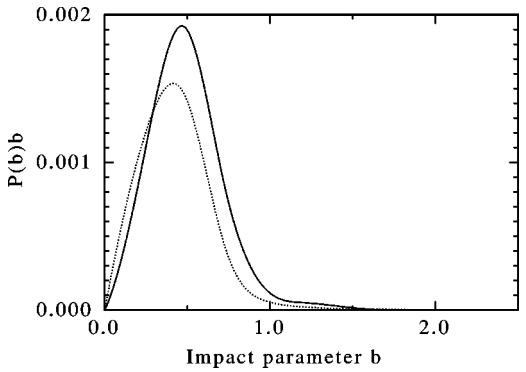

FIG. 5. The same as Fig. 4 but for the double-ionization probabilities.

ization by distant collisions is more effective for the attractive force than for the repulsive force. As we have seen before, the difference of the ratio of the double- to single-ionization cross sections is mainly due to that of the double-ionization cross sections. In contrast with the single-ionization probabilities, the double-ionization probabilities for the proton impact decay faster than for the antiproton impact at large impact parameters. When the antiproton ionizes the outer electron at first, the electron would be scattered inward owing to the repulsive interaction between the particles. On the other hand, the outer electron would be pulled outward from the target by the attractive interaction for the proton case. The probability of the ejected outer electron to kick off the inner electron is evidently larger for the antiproton impact in this picture.

Olson did not stabilize the helium atom in the course of the scattering calculations. We further tried to reproduce Olson's results removing the core potential from the classical equations of motion. The Bohr model is very fragile and most of the atoms autoionize before the projectile reaches the nearest encounter point if we start the calculations at a distance of 20 a.u. in the same way as we did for the stabilized model. Following McKenzie and Olson [10] we shortened the distance to 5 a.u. to avoid autoionization but we obtained too large ionization cross sections below 1 MeV as a result of the contamination of autoionization. The cross sections decrease rapidly as the energy increases and they become smaller than the measured values above 2 MeV. We decreased the starting point step by step down to 2 a.u. *to finish the calculations before the atom autoionizes* but we could not reproduce Olson's results. The cross-section ratios show completely incorrect energy dependence, that is, they increase for higher energies. The cross sections are strongly dependent where we start to solve the equations of motion and we could not achieve reliable results. In any case, such small distances are not acceptable as starting points for collision problems of charged particles.

The cross sections are insensitive to the choice of the effective charge Z_{eff} used for generating the initial Kepler orbits. We changed it from 1.5 to 1.8 and confirmed that the cross sections change within a few percent and the cross-section ratios remain almost the same. On the contrary, the cross sections are sensitive to the binding energy E of the initial state. It is important to choose the energy width of tolerance as small as possible centered on the correct eigenvalue, -78.919 eV.

We also carried out calculations of the antiproton capture at low energies to confirm the validity of our procedure. Since, as stated before, the value of $\xi=2.767$ is too large for the orbits of the ground-state helium atom, we used our present choice of the parameters, but the capture cross sections agree very well with those of Beck *et al.* [5]. Though we cannot clarify why so different choices of the core potential give similar capture cross sections, the satisfactory agreement ensures the correctness of our CTMC calculations.

In summary, we applied the four-body CTMC method to ionization processes of the helium atom by antiproton and proton impacts. The helium atom is stabilized incorporating the Heisenberg core potential. The single- and double-ionization cross sections, and hence their ratios agree well with the measurements. The Bohr helium model without the core potentials is so fragile that it cannot be used for collision problems of charged particles.

[1] L.H. Andersen, P. Hvelplund, H. Knudsen, S.P. Møller, K. Elsener, K.G. Rensfelf, and E. Uggerhøj, Phys. Rev. Lett. **57**, 2147 (1986).
[2] R.E. Olson, Phys. Rev. A **36**, 1519 (1987).
[3] J.F. Reading and A.L. Ford, Phys. Rev. Lett. **58**, 243 (1987).
[4] A.L. Ford and J.F. Reading, J. Phys. B **27**, 4215 (1994).
[5] W.A. Beck, L. Wilets, and M.A. Alberg, Phys. Rev. A **48**, 2779 (1993).
[6] C.L. Kirschbaum and L. Wilets, Phys. Rev. A **21**, 834 (1980).
[7] J.S. Cohen, Phys. Rev. A **62**, 022512 (2000).
[8] J.S. Cohen, Phys. Rev. A **26**, 3008 (1982).
[9] D.R. Schultz, Phys. Rev. A **40**, 2330 (1989).
[10] M.L. McKenzie and R.E. Olson, Phys. Rev. A **35**, 2863 (1987).
[11] L.H. Andersen, P. Hvelplund, H. Knudsen, S.P. Møller, A.H. Sørensen, K. Elsener, K.G. Resenfelt, and E. Uggerhøj, Phys. Rev. A **36**, 3612 (1987).
[12] M.B. Shah and H.B. Gilbody, J. Phys. B **18**, 899 (1985).
[13] P. Hvelplund, H. Knudsen, U. Mikkelsen, E. Morenzoni, S.P. Møller, E. Uggerhøj, and T. Worm, J. Phys. B **27**, 925 (1994).
[14] H. Knudsen, L.H. Andersen, P. Hvelplund, G. Astner, H. Cederquist, H. Danared, L. Liljeby, and K.G. Resnfelt, J. Phys. B **17**, 3545 (1984).
[15] L.J. Puckett and D.W. Martin, Phys. Rev. A **1**, 1432 (1970).