Classical trajectory Monte Carlo model calculations for the antiproton-induced ionization of atomic hydrogen at low impact energy

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Abstract

The three-body dynamics of the ionization of the atomic hydrogen by 30 keV antiproton impact has been investigated by calculation of fully differential cross sections (FDCS) using the classical trajectory Monte Carlo (CTMC) method. The results of the calculations are compared with the predictions of quantum mechanical descriptions: The semi-classical time-dependent close-coupling theory, the fully quantal, time-independent close-coupling theory, and the continuum-distorted-wave-eikonal-initial-state model. In the analysis particular emphasis was put on the role of the nucleus-nucleus (NN) interaction played in the ionization process. For low-energy electron ejection CTMC predicts a large NN interaction effect on FDCS, in agreement with the quantum mechanical descriptions. By examining individual particle trajectories it was found that the relative motion between the electron and the nuclei is coupled very weakly with that between the nuclei, consequently the two motions can be treated independently. A simple procedure is presented by which the NN interaction effect can be included into the calculations carried out without it.

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I. INTRODUCTION

The ionization of the hydrogen atom by impact of antiprotons has attracted the attention of many theoreticians in the past decades. The great interest is explained by the fact that in the treatment of the process one is faced with a clean three-body break up problem: In contrast to proton impact there is no electron capture channel, and unlike the electron-induced ionization, the treatment is not complicated by electron exchange effects.

The enormous efforts devoted for the investigations of the collisions of antiprotons with atoms and molecules have been reviewed recently [1]. Besides the fundamental aspects of the topic, from the review the reader may learn about important, potential applications, for example, the radiation therapy for cancer treatment. Although the dominant process utilized in the therapy is the annihilation, there are several aspects of atomic physics relevance of this application, e.g., the slowing down process of the antiprotons in the biological issue, and the mechanism of creation of slow secondary electrons.

The subject of most of the research work carried out on the antiproton-induced ionization of the hydrogen atom was the energy-dependent total cross section. The few number of differential studies is explained partly by the present experimental limitations (first of all, the small intensity of the available antiproton beam), and theoretically the difficulties arising in the calculations of accurate partially or fully differential cross sections.

The deepest insight into the dynamics of the collision can be gained by kinematically complete experiments. A technique used widely for this purpose in the field of atomic collisions is COLTRIMS (cold target recoil ion momentum spectroscopy) [2]. COLTRIMS was applied in the only experimental study in which differential cross sections were measured for collisions involving antiprotons [3]. In the experiment carried out for helium target at 945 keV impact energy cross sections differential in the longitudinal electron and recoil-ion momenta were determined. The obtained data showed only a small (< 10%) difference from the corresponding cross sections measured by 1 MeV protons, as it is expected at such high impact energy.

The above experiment demonstrated the feasibility of differential measurements using antiprotons. This and future plans of facilities providing low-energy antiproton beams of high intensity (for a review see [4]) gave great momentum to the theoretical investigations of the differential properties of the antiproton-induced ionization. Another motivation towards
this direction was the clarification of the effect of nucleus-nucleus (NN) interaction on the fully differential cross sections (FDCS) in ion-atom collisions. The role of the NN interaction was one of the central questions of the attempts to solve the long-standing puzzle regarding discrepancies between theory and experiment in the FDCS for ionization in 100 MeV/amu C$^6^+$ + He collisions \[5\] (for a review see, e.g., \[6\]). The effect of the NN interaction on the ionization depends on the sign of the projectile charge, therefore it is expected to contribute to the particle-antiparticle differences in FDCS.

Exhaustive reviews of the available theoretical differential studies of the antiproton-induced ionization of hydrogen have been given in recent papers by Abdurakhmanov et al. \[7\] and Ciappina et al. \[8\]. In the followings we briefly summarize the models applied for calculation of FDCS. In most of the works the authors compare the results of their calculations with the predictions of the first Born approximations (FBA). Further, fully quantum mechanical first-order perturbation approaches that include the NN interaction are the continuum-distorted-wave-eikonal-initial-state (CDW-EIS) model of Voitkiv and Ullrich \[9\], that of Jones and Madison \[10\], and the 3C model of Berakdar et al. \[11\]. Voitkiv and Ullrich \[9\] have also made calculations in the second-order Born approximation.

Nonperturbative descriptions have also been applied in fully differential studies. McGovern et al. \[12, 14\] worked out a model within the framework of a time-dependent coupled pseudostate (CP) formalism. Although they used the straight-line approximation (SLA) for the projectile path, they could determine FDCS by establishing connection between the wave treatment of projectile motion and the SLA method. In this way their model gives account of the NN interaction. The fully quantal, time-independent convergent close-coupling (CCC) model of Abdurakhmanov et al. \[7\] has been developed along the lines of the CCC approach to electron-atom scattering. The model is also based on use of pseudostates, and as a fully quantal theory, it implicitly considers the NN interaction. Recently Ciappina et al. \[8\] investigated the differential properties of the antiproton-induced ionization within the framework of time-dependent close-coupling (TDCC) theory using SLA for the projectile path. They employed a Fourier transform method in order to extract FDCS for a specific value of projectile momentum transfer, and included the NN interaction into the model by a phase factor \[15, 16\] in the Fourier integral of the transition amplitude over the impact parameter. For the sake of completeness we mention that further investigations using semiclassical coupled-channel approaches \[17-20\] have also been reported in the literature, but in
these works only partially differential cross sections were calculated or some special aspects of the antiproton - hydrogen collision were analyzed.

In this paper we report the results of an analysis carried out by the classical trajectory Monte Carlo (CTMC) method. The motivation of the work was as follows. From the comparison of the FDCS predicted by the above models it turned out that there exist large discrepancies (more than factor of two) between the models, particularly at low impact energies ($\leq 200$ keV) [7, 8]. The reason of the discrepancies can be traced back to the approximations applied in the models. Most importantly, for the electronic wave function all the models use single-center expansion based on the target atom. The reasoning for this approximation is that the antiproton has no bound states of electrons, and therefore in lack of the electron capture channel there is no need to include projectile-centered states in the expansion of wave function. However, at low impact velocities a large distortion of the electron distribution – a strong reduction of the electron density near the antiproton – is expected which cannot be represented by the one-center expansion, as it was shown by Toshima [21]. Probably, as a consequence of the one-center approximation, in studies made with pseudostates the calculations were not repeated for protons, and therefore the analysis of one of the most interesting characteristics of the future antiproton experiments, the particle - antiparticle difference in FDCS is missing in these studies.

CTMC provides an exact description of the full dynamics of the three-body break up process, albeit classically. It is known to reproduce the main features of the excitation, ionization and charge transfer processes in ion-atom collisions. It can be successfully used for calculations of differential cross sections (as an example, see Ref. [22]). A further advantage of CTMC is that by analysis of the calculated trajectories one can gain a deeper insight into the dynamics of the collision processes. At the same time the model character of the method should be emphasized: Because of the neglect of quantum mechanical effects CTMC has a limited validity, in a number of applications it proved to be only a qualitative description. For example, for proton on hydrogen collision CTMC underestimates the total ionization cross section at 20 keV impact energy by more than a factor of two, and even at higher proton energies it fails to reproduce the observed angular distribution of the ejected electrons at backward angles [23].

We made the CTMC calculations at a relatively low impact energy of 30 keV where large particle - antiparticle differences in FDCS are expected. Another reason for the choice of
30 keV was that at this energy FDCS calculations were performed in most of the quantum mechanical models, providing a basis for the comparison of the various approaches. To the best knowledge of the author, until the present work the CTMC method has not been applied to study the full three-body dynamics of the antiproton-induced ionization of the hydrogen atom, and even the number of such studies for other collision systems involving positive ion projectiles is very scarce \[24, 25\]. At the same time, CTMC was applied in several works \[3, 26–28\] to calculate partially differential cross sections for the antiproton-induced ionization of the helium atom.

II. THEORETICAL METHOD

The CTMC method is based on the numerical solution of the classical equations of motion for a large number of trajectories of the interacting particles under randomly chosen initial conditions \[29, 30\]. The details of the used CTMC computer code are given in \[31\]. Briefly, it solves Newton’s non-relativistic equations of motion for the three particles (in atomic units):

\[
m_i \ddot{r}_i = \sum_{j(\neq i)=1}^{3} Z_i Z_j \frac{r_i - r_j}{|r_i - r_j|^3}, \quad (i = 1, 2, 3).
\]  

(1)

Here \(m_i, Z_i\) and \(r_i\) are the masses, charges and position vectors of the particles, respectively. The randomly selected initial conditions were the impact parameter and five further parameters defining the position and velocity vector of the target electron moving on Kepler orbits. The ranges of the latter parameters were constrained to give the binding energy of the hydrogen atom, 0.5 a.u.. For the generation of the initial values of the position and velocity coordinates of the electron from a set of uniformly distributed variables we applied the general procedure suggested by Reinhold and Falcón \[32\] for non-Coulombic systems which is equivalent to the original Abrines and Percival’s method \[29\] in the case of the Coulomb interaction.

The integration of the equations of motion was started at a large distance (138 a.u.) between the incoming projectile and the hydrogen atom. After the collision the calculations were made in two steps. In the first step the integration was continued until the internuclear distance \(R = 138\) a.u., where the main reaction channels (excitation, ionization, and charge transfer for proton impact) could be identified safely. In the second step only collision events
leading to ionization were regarded. For the accurate determination of the post-collisional effects on the electron emission \[33, 34\], in the second step the trajectories of the particles were calculated up to \( R = 10^8 \) a.u.

The fully differential cross section for ejection of the electron with energy between \( E_e \) and \( E_e + dE_e \) into solid angle \( d\Omega_e \), and for scattering of the projectile into solid angle \( d\Omega_p \) is expressed classically as

\[
\frac{d^3\sigma}{dE_e \, d\Omega_e \, d\Omega_p} = 2\pi \int_0^\infty b \frac{d^3P}{dE_e \, d\Omega_e \, d\Omega_p} (b) \, db ,
\]

(2)

where \( \frac{d^3P}{dE_e \, d\Omega_e \, d\Omega_p} \) is the fully differential ionization probability of the process, and \( b \) is the impact parameter. One can easily show that for large number \( N \) of collision events characterized by uniformly distributed \( b \) values in the range \((0, b_{\text{max}})\) the integral in (2) can be approximated by the following sum:

\[
\int_0^\infty b \frac{d^3P}{dE_e \, d\Omega_e \, d\Omega_p} (b) \, db \approx \frac{b_{\text{max}} \Sigma_j b_j^{(i)}}{N \Delta E_e \, \Delta\Omega_e \, \Delta\Omega_p} .
\]

(3)

Here \( b_j^{(i)} \) is the actual impact parameter at which the electron is emitted into energy and solid angle window \( \Delta E_e \) and \( \Delta\Omega_e \), and the projectile is scattered into solid angle window \( \Delta\Omega_p \). The solid angles \( \Delta\Omega_k \) \((k = e, p)\) are determined by the minimum and maximum values of the respective polar and azimuthal angles, \( \theta_k \) and \( \phi_k \):

\[
\Delta\Omega_k = \int_{\theta_k^{\text{min}}}^{\theta_k^{\text{max}}} \int_{\phi_k^{\text{min}}}^{\phi_k^{\text{max}}} \sin \theta_k \, d\theta_k \, d\phi_k = (\cos \theta_k^{\text{min}} - \cos \theta_k^{\text{max}})(\phi_k^{\text{max}} - \phi_k^{\text{min}}). \]

(4)

In our calculations we followed the history of \(8 \times 10^7\) \((1.6 \times 10^8)\) collision events with \( b_{\text{max}} = 3.5\) \((5)\) a.u. for antiproton (proton) impact. We carried out two series of calculations: We repeated the computer runs for the same collision events also without the NN interaction.

### III. RESULTS AND DISCUSSION

For the total cross section of the ionization of the hydrogen atom by impact of 30 keV antiprotons CTMC resulted in \(1.30 \times 10^{-16}\) cm\(^2\) that agrees with the measured value of \((1.14 \pm 0.25) \times 10^{-16}\) cm\(^2\) \[3, 35\] within the experimental error. At the same time, the corresponding value of \(0.76 \times 10^{-16}\) cm\(^2\) for proton impact is smaller by 35% than the
measured value of \((1.18 \pm 0.026) \times 10^{-16} \text{ cm}^2\) \[36\]. We note that in lack of experimental data exactly at 30 keV, we obtained the above cross section values by extrapolating and interpolating the published data for the antiproton and proton impact, respectively. As far as the NN interaction is concerned, it has a negligible (< 1%) effect on the calculated total cross sections for both projectiles.

From the results of the computer runs we derived FDCS values at electron energy \(E_e = (5 \pm 1) \text{ eV}\) and projectile scattering angle \(\theta_p = (0.35 \pm 0.05) \text{ mrad}\) in the laboratory reference system. The latter value corresponds to an average transverse momentum transfer \(q_\perp = 0.7\) a.u.. We considered coplanar collision geometry, i.e., electron emission events occurring in the collision plane were selected. The latter plane is defined by the initial and final momentum of the projectile, \(\mathbf{K}_i\) and \(\mathbf{K}_f\), respectively. The condition of the coplanar electron emission was fulfilled by the choice \(\phi_e - \phi_p = 0^\circ \pm 5^\circ\). The above choice of the collisional parameters means that for calculation of FDCS in Eq. \[3\] we used \(\Delta E_e = 2 \text{ eV}\), \(\Delta \theta_p = 0.1\) mrad and \(\Delta \phi_e = 10^\circ\). The azimuthally isotropic scattering of the projectile was expressed by taking \(\Delta \phi_p = 2\pi\). We mention here the main difficulty in calculation of FDCS by a Monte Carlo method, namely that the specification of the kinematical parameters of the collision by sufficiently narrow windows strongly reduces the number of the regarded ionization events, and to achieve a reasonable counting statistics one needs to follow the history of very large number of collisions.

The results of the calculations for antiproton and proton impact are presented in Fig. \[1\] and Fig. \[2\] respectively. In the figures we plotted also the prediction of FBA. The latter cross section can be expressed analytically (see, e.g., \[12\]). In the laboratory frame (in atomic units):

\[
\frac{\text{d}^3\sigma}{\text{d}E_e \text{d}\Omega_e \text{d}\Omega_p} = \frac{256 Z_p^2 m_p^2 v_f}{v_0 q^2 \pi [1 - \exp(-2\pi/\kappa)]} \times \\
\exp\left[-\frac{2}{\kappa} \arctan\left(\frac{2\kappa}{1+q^2-\kappa^2}\right)\right] \times \\
\frac{q^2 - 2\kappa q + \frac{(\kappa^2+1)(\kappa q)^2}{\kappa^2 q^2}}{(1 + q^2 + \kappa^2 - 2\kappa q)^4}. \tag{5}
\]

We note that the sign of the terms \(2\kappa q\) in Eq. \[5\] differs from that in Eq. (77) of Ref. \[12\], but agrees with that in Eq. (7.2.31) of Ref. \[37\].
In a naive view of the ionization the electron is expected to fly out from the atom in the direction of the transferred momentum due to the dominant electron-projectile interaction, i.e., the angular distribution of the electron is expected to be peaked at $\theta_e = \theta_q$ (at the present collisional parameters $\theta_q = 48^\circ$). This explains why FDCS is plotted against the relative electron emission angle $\theta_e - \theta_q$ in Figs. 1a and 2a. In panel (b) of the figures we plotted also the dependence of FDCS on $\theta_e$ in form of polar diagram. In the latter diagram the emphasis was put on the directional information, therefore the distributions were normalized at their maximum values.

As is seen from the figures, FBA predicts forward electron emission in the direction of the momentum transfer, in accordance with the aforementioned expectation. This can be understood considering that FBA accounts only for the projectile-electron interaction. Furthermore, FBA yields equal FDCS for antiproton and proton impact because of the $Z_p^2$ dependence on the projectile charge.

The FBA peak in Figs. 1 and 2 is a result of a direct momentum transfer in binary collision between the projectile and the electron, therefore it is called as ”binary peak”. At suitable collision conditions (higher collision velocity and lower projectile scattering angle) a second structure (called ”recoil peak”) also appears in the angular distribution. It has maximum in the direction of $-\mathbf{q}$, and it is interpreted as a double scattering process: First the electron is ejected via binary interaction with the projectile with momentum $\mathbf{q}$, then in its way out of the atom it backscatters elastically from the target nucleus (see, e.g., Ref. [5]).

For both projectiles the present CTMC calculations resulted in electron emission into completely different directions than that predicted by FBA. First we discuss the case of antiproton impact. Even without the NN interaction the obtained electron distribution is peaked at a backward angle, at $\theta_e \approx 120^\circ$ (see Fig. 1b). Interestingly, the shape of this latter distribution is similar to that of FBA: The two peaks have about the same width, but the distribution predicted by CTMC shows some asymmetry. This is in a qualitative agreement with the TDCC results of Ciappina et al. [8] obtained without inclusion of the NN interaction. Concerning the peak intensities, the CTMC result is smaller by a factor of 3 than that of FBA. The inclusion of the NN interaction led to a dramatic effect: The FDCS is further reduced by a factor of 5, and the angular distribution completely changed. In this case the electrons are emitted at even larger backward angles. The distribution has
FIG. 1: (Color online) FDCS for ionization of the hydrogen atom by impact of 30 keV antiprotons in the scattering plane. The energy of the ejected electron is 5 eV, the scattering angle of the projectile is 0.35 mrad. Open circles, CTMC including the NN interaction; solid circles, CTMC neglecting the NN interaction; thick solid line (blue), CDW neglecting the NN interaction; dotted line (red), FBA. (a) The angular distribution of the electron as a function of the difference between the electron ejection angle $\theta_e$ and the direction of the momentum transfer vector $\theta_q$. (b) Polar diagram of the electron electron emission as a function of the electron ejection angle $\theta_e$. The distributions in the polar diagram are normalized at their maximum values. The arrow labeled by q shows the direction of the momentum transfer. The z axis defines the direction of the incoming projectile beam. The thin solid and dashed lines through the CTMC results are only to guide the eye.
maximum at $\theta_e \approx 220^\circ$, but a smaller peak is also visible at $\theta_e \approx 110^\circ$. Similar double-peak structure has been observed in quantum mechanical calculations [7–9]. In the latter works the smaller and the larger peak were identified as the binary and the recoil peak. In the followings we will refer the two peaks using these notations.

A very different result was obtained for proton impact. Our both calculations without and with inclusion of the NN interaction show an opposite shift of the binary peak as compared to antiproton impact: The electrons are emitted at small angles in forward direction. The widths of the distributions are much narrower than that predicted by FBA. This indicates the presence of a strong two-center effect. The intensities of the peaks are smaller than that predicted by FBA, but the difference is smaller for protons than for antiprotons.

In Figs. 1 and 2 we plotted also FDCS data obtained from CDW-EIS calculations [15].

FIG. 2: (Color online) The same as Fig. 1 but for proton impact.
without considering the NN interaction. CDW-EIS is also a perturbation theory as FBA, but unlike FBA it accounts for the distortion of the electronic states in the presence of the projectile. Therefore, CDW-EIS is expected to provide FDCS data that are closer to the CTMC results. Indeed, for antiproton impact of the binary peak predicted by CDW-EIS is very similar to that obtained from CTMC, regarding both its the intensity and shape. At the same time, CDW-EIS predicts a smaller shift of the peak from the direction of $q$ than CTMC. The widths the peaks also differ slightly, the CDW-EIS peak is broader. For proton impact CDW-EIS predicts much smaller two-center effect than CTMC, the CDW-EIS peak does not show the strong narrowing effect observed for CTMC.

In Figs. 3 and 4 we compare the present FDCS and DDCS results with those of quantum mechanical calculations. In Fig. 3 the quantum mechanical models used in the comparison are the TDCC theory of Ciappina et al. \cite{8}, the CCC approach of Abdurakhmanov et al. \cite{7}, and the CDW-EIS model of Voitkiv and Ullrich \cite{9}. The FDCS data of the latter model were taken from Ref. \cite{7}, as well as we made independent CDW-EIS calculations also in the present work.

We note that the present CTMC data were evaluated in the laboratory reference system. At the same time, the published FDCS results of the above models were expressed in the relative coordinate system. To convert the latter data to the laboratory system we multiplied them with the factor $(m_p/\mu)^2$ (see, e.g., \cite{14}), where $\mu_p$ is the reduced mass of the projectile:

$$\mu_p = \frac{m_p m_H}{m_p + m_H}.$$  

Here $m_p$ and $m_H$ are the mass of the projectile and that of the hydrogen atom, respectively. For proton (antiproton) on hydrogen scattering to a good approximation $(m_p/\mu)^2 \approx 4$. Unlike FDCS, the DDCS values are the same in the two reference systems (due to the integration over $\theta_p$), therefore we did not need to correct the DDCS data.

From Fig. 3 we can establish only qualitative agreement between CTMC and the quantum mechanical models. The disagreement is particularly large for the binary peak concerning both its intensity and position. While all the three quantum mechanical models predict a peak position of about $45^\circ$, according to CTMC the peak appears at about $65^\circ$. CTMC predicts a greatly suppressed binary peak. For the recoil peak a better agreement is observed. In the latter case a striking feature of the CTMC results is the narrower peak width compared to other theories.
Concerning the greatly suppressed binary peak predicted by CTMC, we note that the description of this peak seems to be very sensitive to the applied theoretical approach: Even for the quantum mechanical models the peak maximum varies by a factor of more than two. Furthermore, we note that the coupled pseudostate (CP) calculations of McGovern et al. [14] carried out under identical collision conditions with the present work resulted in also a greatly suppressed binary peak relative to the recoil peak (see the 3D plot of FDCS in Fig. 1 of Ref. [14]).

There may be several reasons of the discrepancies between CTMC and the quantum mechanical models. As is seen from Fig. 1, the inclusion of the NN interaction has a profound effect on FDCS, therefore its approximate treatment may introduce uncertainties into the calculations.

As it is discussed in the Introduction, the coupled-states descriptions (TDCC, CCC) are based on one-center expansion of the electronic wave function. This approximation is questionable at low impact energy [21], thus the neglect of the two-center effects may be a further reason of the discrepancies. We note that in CDW-EIS the distortion factors applied at the initial- and final-state wave function give account of the two-center effect. However, CDW-EIS is a perturbation theory, its use is justified at high impact energy.
FIG. 4: DDCS for ejection of electrons of energy 5 eV as a function of the emission angle. The dotted line denotes FBA. The present CTMC results are shown by open and solid circles for antiproton and proton impact, respectively. Quantum mechanical models for antiproton impact: solid line, CCC [7]; dashed line, CP [12].

As far as CTMC is concerned, it remains a question how far FDCS is affected by the neglect of the quantum mechanical effects. Anyhow, CTMC seems to be suitable for the differential characterization of the antiproton-induced ionization of the hydrogen atom, and may contribute in this way to a deeper understanding of the process.

In Fig. 4 the present DDCS results are compared with those of the CCC approach of Abdurakhmanov et al. [7] and the CP model of McGovern et al. [12] as a function of the electron emission angle. The energy of the electron is 5 eV. The CTMC data are plotted for both antiproton and proton impact, and demonstrate well the expected large particle-antiparticle difference. CTMC predicts dominant electron emission at backward directions for antiproton impact, in qualitative agreement with the quantum mechanical models.

To investigate the role of the NN interaction in the antiproton-induced ionization, we analyzed particle trajectories at various collision conditions. As a great surprise, practically no difference was observed in the electron trajectories when the NN interaction was turned on and off. This is in contrast to the previous explanation of the NN interaction effect given by Abdurakhmanov et al. [7], who assumed an interference effect that takes place between the interactions of the target electron and proton with the outgoing antiproton. According to the authors, the outgoing scattered antiproton is decelerated in the attractive field of the target nucleus, resulting in a stronger final-state interaction between the antiproton and
The electron. This leads to the polarization of the target electron cloud and a shift of the electron density away from the projectile path.

The insensitivity of the electron trajectories on the NN interaction observed in the present work indicates that the effect assumed by Abdurakhmanov et al. is probably very small at the collision energies regarded also by the authors (≥ 30 keV). Then the question is: How can one explain the drastic change of FCDS seen in Fig. 1 when the NN interaction is turned on?

The answer was found by analyzing the trajectory of the target nucleus. We found that it changed in a large extent when the NN interaction was turned on. The change is caused by the momentum transferred by the projectile to the target nucleus in the NN scattering. As a result, the total momentum transferred to the whole atom is also changed which leads to the rearrangement of the collision events and to a modified angular distribution.

The finding that the nucleon-nucleon scattering has practically no effect on the motion of the electron is understandable considering the very small scattering angle and the negligible change in collision velocity, as well as the length scale difference of three orders of magnitude between the motion of the electron and that of the target nucleus. The rigidity of the angular distribution of the electron on the NN interaction is well reflected by the ratio of DDCS values for ejection of electrons of 5 eV calculated with and without the NN interaction. The ratio is plotted in Fig. 5 for electron ejection angles $\theta_e > 50^\circ$ at which DDCS takes appreciable values. Although systematical deviations from unity can be observed at smaller and larger electron ejection angles.
angles, the effect is small ($< 2\%$) and within the error of the calculations.

Our finding that the relative motion between the electron and the nuclei is coupled very weakly with that between the nuclei indicates that two motions can be treated independently. This led us to show that the NN interaction can be be included in the calculations in the form of the following simple correction procedure. Let us denote the additional momentum transfer vector due to the NN scattering by $q_{\text{NN}}$. For small scattering angles the longitudinal component of $q_{\text{NN}}$ can be neglected, and the transversal component is given as

$$q_{\perp}^{\text{NN}} \approx k_i \theta_p^{\text{NN}}.$$  

(6)

$\theta_p^{\text{NN}}$ is the NN two-body scattering angle that can be obtained from the relationship

$$\theta_p^{\text{NN}} = 2 \arctan \left( \frac{b}{a} \right),$$

(7)

where $a = Z_p Z_t / 2 E_p$ is the half distance of closest approach ($E_p$: the energy of the projectile).

The correction procedure is simply the replacement of the momentum transfer vector $q$ by the vector $q + q_{\text{NN}}$ for all the collision events that were calculated without the NN interaction. The FDCS data derived from the modified collision events are compared with those obtained with the "exact" treatment of the NN effect in Fig. 6. We may conclude from the figure that the correction procedure is excellent, thus proving the weak coupling between the electron-nuclei and the nucleon-nucleon relative motion. We note that the success of the presented approximate treatment of the NN effect gives a strong support to the procedure applied by Schulz et al. [38] in the analysis of their experimental FDCS results obtained for ionization in 100 MeV/amu $\text{C}^{6+}$ + He collisions. The latter authors used the Monte Carlo event generator (MCEG) method in FBA to account for the additional momentum transfer due to the elastics scattering of the projectile ion on the target nucleus. The application of MCEG was necessary, because such a correction can be made only event-by-event, in a way as it was done in our present CTMC investigation.

IV. CONCLUSIONS

We investigated the three-body dynamics of the ionization of the atomic hydrogen induced by antiprotons. To this end, we calculated fully differential cross sections by applying the CTMC method. The calculations were made at relatively low impact energy of 30 keV
FIG. 6: Comparison of FDCS values obtained by approximate treatment of the NN interaction effect (solid circles) with the exact results (open circles).

where large deviations from the predictions of the first Born approximation are expected. The kinematical parameters (electron energy, projectile scattering angle) were chosen to be those of quantum mechanical investigations of the process available in the literature. The calculations made also for proton impact under the same collision conditions revealed large particle-antiparticle differences in FDCS. Comparing the CTMC results with the predictions of quantum mechanical models (CCC, TDCC, CDW-EIS) we concluded that the classical mechanical description can reproduce the main features of the antiproton-induced ionization of the hydrogen atom, and thereby it helps the deeper understanding of the process. We analyzed the possible reasons of the observed discrepancies between CTMC and the quantum mechanical models: The approximate treatment of the NN interaction and the use of the one-center expansion of the electronic wave function in the quantum mechanical descriptions on one side, and the neglect of quantum effects in CTMC on the other side.

To clarify the role of the NN interaction in the ionization, we examined individual particle trajectories. We established that the relative motion between the electron and the nuclei is coupled very weakly with that between the nuclei, consequently the two motions can be treated independently. This was convincingly proved by a calculation in which the additional momentum transfer due to the elastics scattering of the projectile on the target nucleus was taken into account by a simple correction procedure for collision events obtained without inclusion of the NN interaction.
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