Lattice Schrödinger-equation approach for excitation and ionization of He^+ by antiproton impact

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Cross sections for excitation to low-lying states and ionization of He^+ by antiproton impact are calculated in the energy range 1–500 keV by solving the time-dependent Schrödinger equation on a numerical lattice. The results are compared with those of other theoretical approaches. Such comparisons allow a strenuous test of the lattice Schrödinger-equation approach for this fundamental collision system. [S1050-2947(97)04311-4]

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I. INTRODUCTION

The advent of powerful computer workstations has led to the fulfillment of the goal of performing full three-dimensional lattice solutions of the time-dependent Schrödinger equation (TDSE) regarding fundamental atomic collisions systems for which unresolved questions have existed (see, e.g., Refs. [1,2]). Earlier pioneering applications were restricted to fewer dimensions and suffered as well from relatively small, sparse grids and in some cases significant physical approximations (see, e.g., Refs. [3–7]). Even present computational resources and approaches encounter significant challenges in attempting to treat fully two-center, multielectron collisions without severe approximations. Further, a difficult aspect of the approach is the development of methodology to treat both the close collision and the evolution of the dynamic two-center continuum wave function to asymptotically large distance scales.

A problem well suited for application of the lattice approach to solving the TDSE is that of antiproton impact of hydrogenic atomic systems. In this case, one need only treat a one-electron Hamiltonian unless the collision energy is so small (e.g., $\lesssim 100$ eV) that the nuclear motion would have to be treated quantum mechanically as well. Further, since the antiproton ($\bar{p}$) is negatively charged, electron transfer to the projectile is not possible, greatly simplifying the approach since in this event only elastic scattering, excitation, and ionization are possible. For this collision system and covering a wide range of collision energies, one can represent on a lattice the dominant reaction channels with a modest grid size. In addition, recent experiments and theoretical treatments have highlighted the physical interest in considering antiproton impact as a way of probing atomic collision dynamics by changing the projectile charge sign in comparison to proton impact (see Refs. [1,8,9] and references therein).

In previous work [1] we have applied the lattice TDSE (LTDSE) approach to study ionization in collisions of antiprotons with atomic hydrogen and He^+, finding good agreement with the best available theoretical treatments in the various regimes of their validity. We refer the interested reader to this work for the basic formulation and application of the method. Here we provide an even more strenuous test by comparing the LTDSE results with various theoretical approaches regarding excitation of low-lying levels of He^+. Advantages of the LTDSE approach include the fact that it provides a nonperturbative method with very little bias in basis-set selection and interaction potentials. Additionally, it spans a large molecular (two-center) basis of moving continuum states without the need to develop *ad hoc* translation factors. By solving the Schrödinger equation as directly as possible numerically, it provides a compellingly simple conceptual approach that is applicable from low energies where close-coupling treatments require large bases of molecular states and careful treatment of electron translation factors, up to high energies, providing a linkage to results of perturbation theories.

II. RESULTS AND DISCUSSION

In Fig. 1 we display the results of our LTDSE approach for excitation to the $2s$, $2p$, $3s$, $3p$, and $3d$ states of He^+ by antiproton impact, as well as the cross sections summed over subshells. The lattice used to support the electronic wave function was analogous to that previously described for $\bar{p}+H$ [1] and consisted of 135^3 points extending from -13 a.u. to $+13$ a.u. in all three Cartesian directions. Eigenenergies of the first 14 bound states of He^+ were determined by partial lattice eigensolution with deviations from the exact values of between 0.01% and 0.5%. Similarly, expectation values of angular momentum, radius, and parity were well reproduced. The antiproton projectile was placed at the edge of the numerical grid and followed a straight-line trajectory throughout the collision with the initial $He^+(1s)$ state for a range of impact parameters. Throughout the collision, the overlap of the wave function with each of the 14 bound eigenstates was periodically monitored and time evolution was carried out until the probabilities had converged. From these impact-parameter and energy-dependent prob-

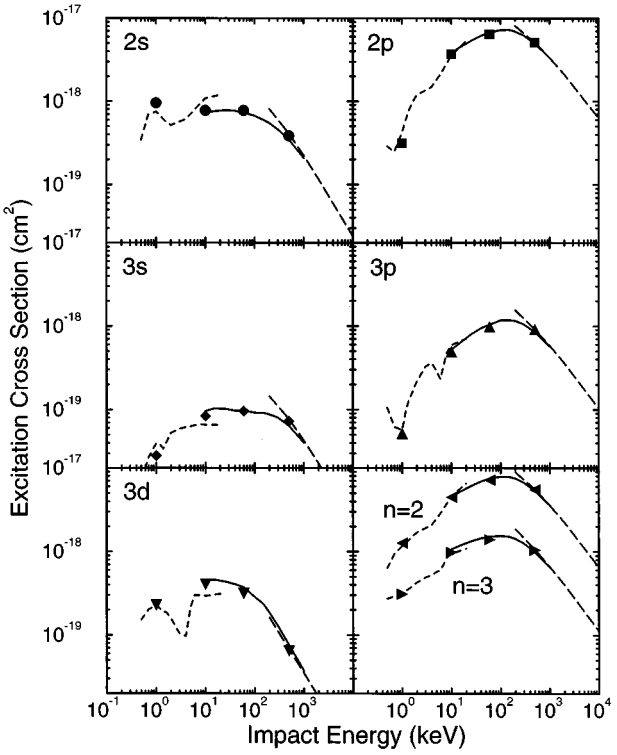

FIG. 1. Excitation cross section over a wide range of impact energy for antiproton impact of He^+. Shown are the results for excitation to the $2s$, $2p$, $3s$, $3p$, and $3d$ states, and for $n=2$ and $n=3$, using the present LTDSE approach (solid symbols), the present MOCC method (short-dashed curves), the AOCC method of Ford *et al.* (solid curves) [10], and the present 16-state AOCC method (long-dashed curve).

abilities, total cross sections were computed. For simplicity, we display here results summed over the magnetic quantum number.

Also shown in the figure are the results of three theoretical approaches that should provide benchmarks in each of the three impact energy ranges for which they are applicable. For example, at high energies, we compare with our 16-state atomic-orbital close-coupling (AOCC) calculations involving only the first few bound states of He^+. For energies above ~ 1 MeV, these results tend to the first Born approximation. The 500-keV LTDSE points agree well with these results, as do the impact-parameter-dependent probabilities. At intermediate energies we compare with the large-scale single-centered Hilbert basis-set close-coupling calculations (labeled AOCC) of Ford *et al.* [10]. Their basis included 13 complex radial functions for each angular momentum ℓ and m value, up through $\ell=6$, for a maximum of 299 coupled channels. The LTDSE results agree extremely well with the AOCC results. For example, averaging over the deviations between the LTDSE and AOCC results for the $2s$, $2p$, $3s$, $3p$, and $3d$ states, we find that they differ by 8.4% at 500 keV, 7.5% at 60 keV, and 8.4% at 10 keV. Ford *et al.* estimate that their AOCC results are accurate to within 5% or better for the lowest energies (e.g., 10–15 keV) and 2% for the higher energies. Thus the LTDSE results for the present grid size and density may be estimated to be accurate to within about 10%. Summing the cross sections over subshells, we find that the differences are 3.3%, 4.3%, and 2.0% for $n=2$ at 10, 60, and 500 keV, respectively, and 5.9%, 8.7%, and 9.3% for $n=3$.

In order to provide a state-of-the-art calculation for low energies (i.e., 0.5–10 keV), we have developed a molecular-orbital close-coupling (MOCC) treatment. Specifically, the radial and rotational matrix elements of nonadiabatic couplings are calculated using the standard truncated adiabatic basis in prolate elliptical coordinates. These are calculated on a fine radial grid extending from 0.02 to 140 a.u. and fitted to an analytical form to speed the solution of the close-coupling equations. The basis contained all adiabatic molecular states up to $n=4$ (in the united-atom spherical quantum numbers) and additional states from the $n=5-7$ manifolds. The convergence of the $2s$-$3d$ components of the cross section was monitored separately with respect to basis size. In particular, convergence at 10 keV was reached with 18 basis states for the $n=2$ components, but required 34 basis states for the $n=3$ components. No translation factors are involved in the calculation. Their effect is greatly reduced since all states are localized on the target He^+ ion, which was chosen as the origin of electronic coordinates.

Agreement between the LTDSE and MOCC results is good, especially considering the difficulty of these low-energy calculations. A remarkable feature of the low-energy results is the exhibition of Stark oscillations in the cross section (see, e.g., Ref. [11]). This effect arises from the beating of the population of spherical states within a given manifold in the receding portion of the collision due to the Stark splitting induced by the time-dependent electric field of the projectile. This effect is certainly present in collisions involving positively charged projectiles (e.g., proton impact), but is often entangled with oscillations due to strong charge transfer.

In the course of investigating these low-energy oscillations, we also applied the classical trajectory Monte Carlo (CTMC) method to compute the excitation cross sections to explore the possible role played by classical collision dynamics. Figure 2 displays our results for excitation to the $n=3$ subshells using both the CTMC and MOCC methods. Clearly, a classical analog of the oscillations is also present in the CTMC method, but is observed to be shifted to lower energies. It is reasonable to expect the Stark oscillations to be present in the CTMC results since Born [12] originally predicted this phenomenon on the basis of purely classical dynamics. The reason why more oscillations are present in the MOCC result is that the quantum atom can beat with multiples of the classical Stark frequency.

Also, to further test the agreement between the LTDSE and MOCC results, we computed the excitation probability as a function of impact energy (0.5–10 keV) for a fixed impact parameter ($b=0.25$ a.u.). We note that to obtain convergence of these probabilities, or indeed the cross sections reported here, the time evolution had to be computed out to long times (e.g., 500 a.u. or more of time past the closest approach of the nuclei). Figure 3 shows a comparison of the LTDSE and MOCC results for this fixed impact parameter, the oscillatory behavior of the probability again being due to Stark splitting of the energy levels in the outgoing phase of the collision. Results of the two methods agree best regarding the probability summed over subshells, as observed re-

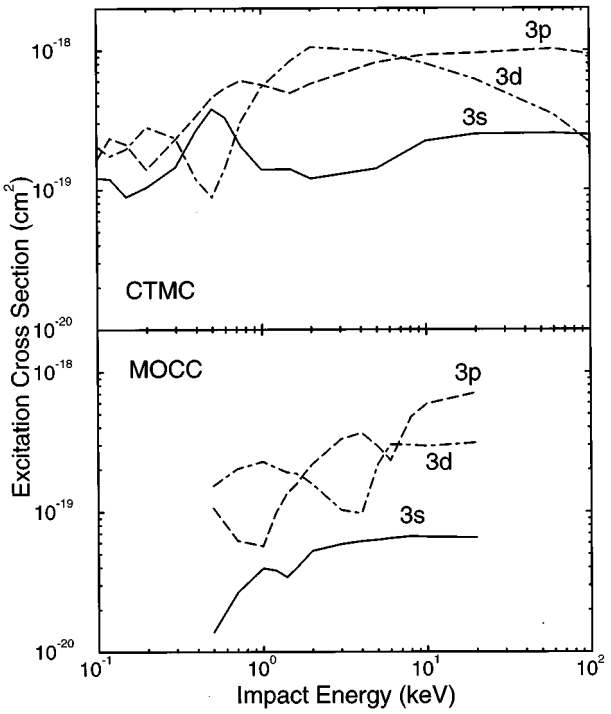

FIG. 2. Excitation cross section in antiproton impact of He^+ computed using the CTMC and MOCC approaches for the $n=3$ manifold.

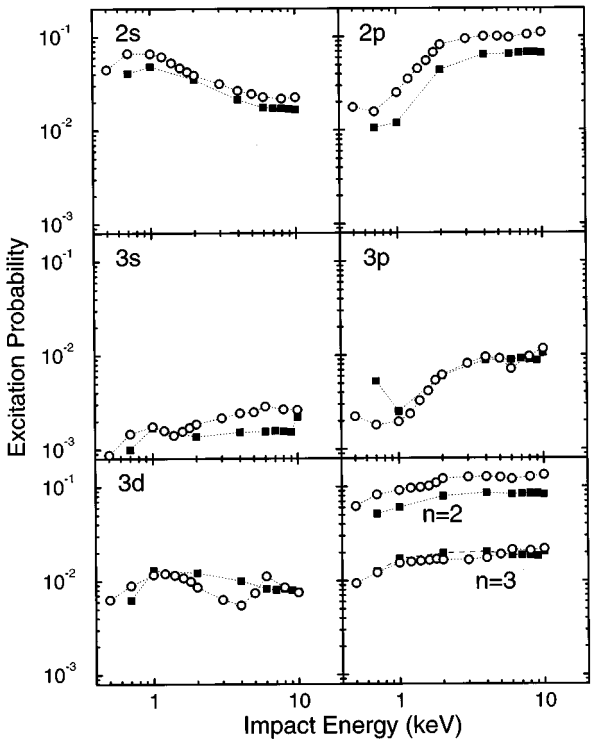

FIG. 3. Excitation probability for a fixed impact parameter ($b=0.25$ a.u.) illustrating the low-energy Stark oscillations in $\overline{p}+He^+$ collisions. The solid symbols indicate the present LTDSE results and the open symbols indicate the present MOCC results. Thin dashed lines connect the points to guide the eye.

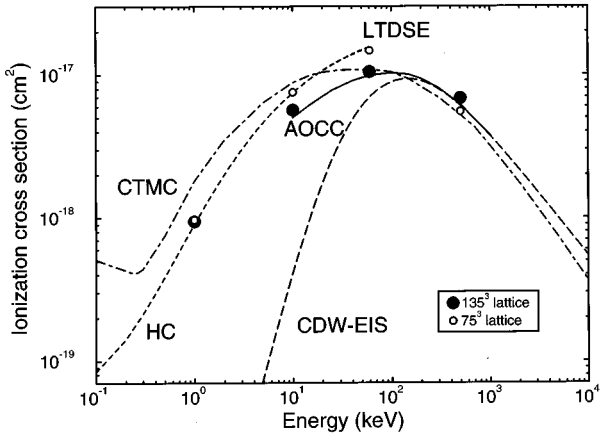

FIG. 4. Ionization cross section as a function of collision energy for $\overline{p}+He^+$. Shown are the results of the CTMC method (dash-dotted curve [1]), the LTDSE method (open circles, 75^3 grid [1]), the LTDSE method (filled circles, present 135^3 grid), the continuum-distorted-wave–eikonal-initial-state method (CDW-EIS, dashed curve [1]), the hidden-crossing method (HC, short-dashed curve [1,13]), and the AOCC results of Ford *et al.* [10]).

garding the total cross sections. This occurs since the beating changes as a function of time the subshell probabilities, but not the n-level probability. Agreement between the two approaches is also better for the $2s$ and $2p$ levels than for the $3s$, $3p$, and $3d$ levels since the time required for their convergence is much shorter. Running the LTDSE solutions out to extremely long times is not an efficient method to propagate the beating between just a few atomic states. We plan to combine our AOCC and LTDSE methods to compute the electronic evolution for large internuclear seperations in the future.

Finally, we have computed the ionization cross section for $\overline{p}+He^+$ collisions and compared with other theoretical results using the present 135^3 lattice point grid. Specifically, ionization is computed using the unitarity of probabilities as $1-\Sigma P_{bound}$, where P_{bound} are the probabilities of remaining in any of the bound states of the target supported on the lattice. In our previous work that focused on resolving a controversy regarding ionization in $\overline{p}+H$ collisions [1], we also performed a calculation for $\overline{p}+He^+$, but too optimistically used a smaller grid composed of 75^3 points. Results of our present calculations on the larger lattice are depicted in Fig. 4. The overestimation of the ionization cross section using the 75^3 grid results from supporting fewer bound states. The larger lattice supports more excited states and therefore reduces the ionization cross section, particularly for the results computed at impact energies of 10 and 60 keV, where excitation to higher-n levels is large. Shown for comparison in the figure are the results of the continuum-distorted-wave–eikonal-initial-state and hidden-crossing methods as presented in our previous work [1].

Also shown in the figure are the AOCC results of Ford *et al.* [10], which agree with the LTDSE results to within about 10%. The fact that the LTDSE results are still larger than the AOCC results indicates that it is likely that excitation to He^+ ($n\geq 4$), which is incorrectly treated as ionization on the present LTDSE grid, might account for the remaining difference. A rough estimate of the degree to which using a

grid large enough to support more states would actually make up this difference can be obtained by summing the excitation cross sections for $n \geq 4$ using the AOCC $n=3$ result and a $1/n^3$ scaling. Unfortunately, this procedure overestimates the difference by about a factor of 2. Thus we can conclude that treatment of excitation to $n \geq 4$ would be important, but that other factors such as grid spacing would also have to be carefully examined in order to confidently improve the ionization results beyond an accuracy of 10%.

III. CONCLUSION

Using a lattice approach to solve the time-dependent Schrödinger equation for collisions of antiprotons with He^+ for impact energies between 1 and 500 keV, we have computed the cross sections for excitation to He^+ ($2s$, $2p$, $3s$, $3p$, and $3d$) and the ionization cross section through the condition of unitarity of transition probabilities. We have compared these results with those of other theoretical methods that provide benchmarks in the low-, intermediate-, and high-impact-energy regimes, finding very good agreement. Even for low energies where the excitation process displays strong Stark oscillations, the results are in good agreement with the best available theoretical approach. Thus the LTDSE approach has been shown to provide an accurate method for treating simple ion-atom collisions across a broad range of impact energies. The lattice approach is therefore a viable addition to other means at our disposal to explore strongly interacting atomic systems.

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