Laser-modified charge-transfer processes in proton collisions with lithium atoms

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(Received 9 April 2003; published 11 July 2003)

A time-dependent semiclassical lattice solution of the Schrödinger equation is used to calculate charge-transfer processes in proton collisions with lithium atoms. State-selective cross sections are obtained at 5–15 keV incident energy for laser excited $2p\sigma$ states aligned parallel and $2p\pi$ states aligned perpendicular to the ion beam. State-selective cross sections are also obtained at 5 keV for $1s^2 2s$ ground states in which the polarization of a moderately intense pulsed laser is aligned parallel and perpendicular to the ion beam. The addition of a pulsed laser is found to have a strong effect on the charge-transfer cross sections to the $n=3$ excited states of hydrogen.

DOI: 10.1103/PhysRevA.68.013404 PACS number(s): 34.50.Rk

I. INTRODUCTION

The addition of a laser beam to an experiment involving crossed ion and atom beams holds the promise of finding means to control the strength of excitation and charge-transfer processes. Already lasers have been used in proton and α- particle collisions with sodium atoms to resonantly populate excited states [1]. The resulting charge-transfer processes are now from excited states that are aligned parallel or perpendicular to the ion beam. Recent theoretical work [2,3] has suggested that if laser and ion beams can simultaneously interact with a target atom, then it may be possible to obtain a wide range of strengths for selected excitation and charge-transfer processes.

In this paper we solve the time-dependent Schrödinger equation on a three-dimensional Cartesian lattice to calculate charge-transfer processes in proton-lithium collisions, in which a laser resonantly populates the $1s^2 2p$ excited state and in which a laser simultaneously excites the $1s^2 2s$ ground state. Previously, the time-dependent semiclassical lattice method has been used to examine various inelastic-scattering processes in antiproton-hydrogen collisions [4–6], antiproton-helium collisions [7], proton-hydrogen collisions [8–13], and α-particle collisions with hydrogen [14]. Recently we have applied the same computational method to examine excitation and charge transfer from the $1s^2 2s$ ground state of lithium [15] and to examine excitation from the $1s^2 2p$ excited state of lithium [16]. This paper's charge-transfer cross-section results from the resonantly populated $1s^2 2p$ excited state are in support of planned experiments. We hope the charge-transfer cross-section results for the simultaneous laser interaction with the $1s^2 2s$ ground state will stimulate future experimental design. In Sec. II we give an outline of the theoretical methods, charge-transfer cross-section results are presented in Sec. III, and a brief summary is given in Sec. IV. Atomic units are used throughout the paper, unless otherwise stated.

II. THEORY

For charge-transfer processes in a laser field, we solve the time-dependent Schrödinger equation in the frame of reference of a bare ion Z projectile:

$$i\frac{\partial \Psi(\vec{r},t)}{\partial t} = \left(-\frac{1}{2}\nabla^2 - \frac{Z}{r} + V_{core}(R(t)) + V_{laser}(\vec{r},t) \right) \Psi(\vec{r},t), \quad (1)$$

where for straight-line trajectories (in the y direction)

$$R(t) = \sqrt{(x-b)^2 + [y-(y_i+vt)]^2 + z^2}, \quad (2)$$

b is the impact parameter, y_i is the starting position for the target, and v is the relative velocity. The laser field potential $V_{laser}(\vec{r},t)$ is given by

$$V_{laser}(\vec{r},t) = E(t) f(\vec{r}) \cos(\omega t), \quad (3)$$

where $E(t)=E_0[\sin(\pi t/2)]^2$ for $0<t<t_i$ and $t_f<t<t_{pulse}$, $E(t)=E_0$ for all other times, E_0 is the electric-field amplitude, and ω is the radiation field frequency. Thus, t_i is the initial ramp-on time, t_f is the final ramp-off time, and t_{pulse} is the total pulse time of the electromagnetic field. For light polarization perpendicular to the ion beam, $f(\vec{r})=x$; while for light polarization parallel to the ion beam, $f(\vec{r})=y$. We note that the collision Hamiltonian has reflection symmetry with respect to the $z=0$ plane.

The $1s^2$ core potential $V_{core}(r)$ for lithium was constructed previously as a pseudopotential in order to eliminate the inner node of the $2s$ valence orbital [15]. This prevents the unphysical $2s\rightarrow 1s$ transition in the time evolution of the Schrödinger equation. The full three-dimensional stationary states for the lithium atom are found by relaxation of the time-dependent Schrödinger equation in imaginary time ($\tau = it$):

$$-\frac{\partial \psi^A_{nlm}(\vec{r},\tau)}{\partial \tau} = \left(-\frac{1}{2}\nabla^2 + V_{core}(r) \right) \psi^A_{nlm}(\vec{r},\tau), \quad (4)$$

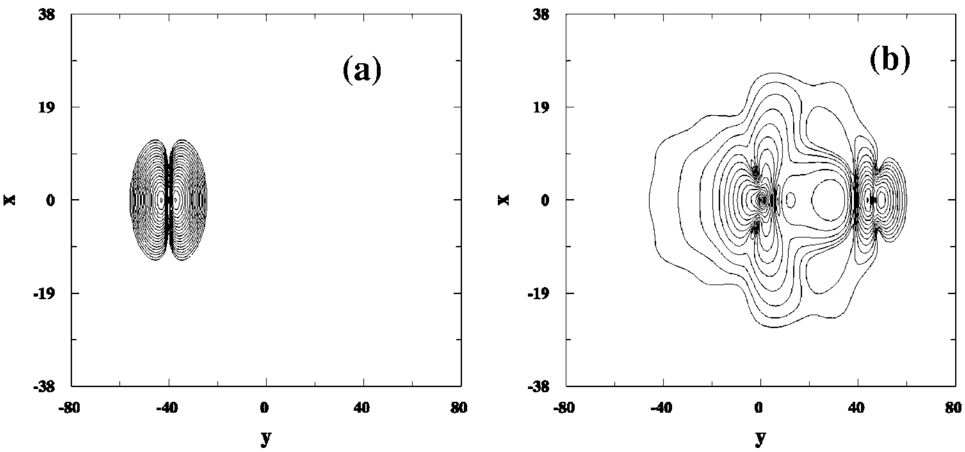

FIG. 1. Time evolution of the electron probability density in the $z=0$ scattering plane for a proton-Li($2py$) collision at an incident energy of $E=5$ keV and an impact parameter of $b=0$. (a) $t=0$, (b) $t=192$ (radial distances are in atomic units; 1.0 a.u. $=5.29\times10^{-9}$ cm).

while the three-dimensional stationary states for the hydrogenic ion are found by relaxation of

$$-\frac{\partial\psi^{I}_{nlm}(\vec{r},\tau)}{\partial\tau}=\left(-\frac{1}{2}\nabla^2-\frac{Z}{r}\right)\psi^{I}_{nlm}(\vec{r},\tau). \qquad (5)$$

The relaxed spectrum for the atom and ion incorporates effects due to finite grid spacing and size of the lattice.

The charge-transfer probability for the transition $A(n_0l_0m_0)\rightarrow I(nlm)$ at a specific velocity and impact parameter is given by

$$\wp_{n_0l_0m_0\rightarrow nlm}(v,b)=\left|\int d\vec{r}\,\psi^{I*}_{nlm}(\vec{r})\Psi(\vec{r},t=T)\right|^2, \qquad (6)$$

where

$$\Psi(\vec{r},t=0)=\psi^{A}_{n_0l_0m_0}(x-b,y-y_i,z)e^{ivy} \qquad (7)$$

and $\Psi(\vec{r},t=T)$ is the solution of Eq. (1) at time $t=T$ following the collision. The total charge-transfer cross section for the $1s^22s$ ground state of lithium is given by

$$\sigma_{2s\rightarrow nl}(v)=2\pi{\sum_m}'\int_0^\infty\wp_{2s0\rightarrow nlm}(v,b)b\,db. \qquad (8)$$

The total charge-transfer cross section for the $1s^22p$ excited state of lithium is given by

$$\sigma_{2p\rightarrow nl}(v)=\tfrac{1}{3}\sigma_{2p\sigma\rightarrow nl}(v)+\tfrac{2}{3}\sigma_{2p\pi\rightarrow nl}(v), \qquad (9)$$

where the aligned parallel cross section is given by

$$\sigma_{2p\sigma\rightarrow nl}(v)=2\pi{\sum_m}'\int_0^\infty\wp_{2py\rightarrow nlm}(v,b)b\,db, \qquad (10)$$

and the aligned perpendicular cross section is given by

$$\sigma_{2p\pi\rightarrow nl}(v)=\pi{\sum_{m_1}}'\int_0^\infty\wp_{2px\rightarrow nlm_1}(v,b)b\,db+\pi{\sum_{m_2}}'\int_0^\infty\wp_{2pz\rightarrow nlm_2}(v,b)b\,db. \qquad (11)$$

In all cases, the sums over m are restricted to those final states with the same $(-1)^{l+m}$ reflection number as the initial state, for example, -1 for the $2pz$ state. We note that a straight-line trajectory for the incident proton has been found to be an excellent approximation for calculating collision cross sections with hydrogen down to incident energies of 1.0 keV [9], due, in part, to the small projectile-target interaction times and the weighting of the collision probabilities in Eqs. (8)–(11) by the impact parameter.

III. RESULTS

Charge-transfer cross sections for collisions of protons with the $1s^22p$ excited states of Li are first calculated by direct solution of Eq. (1) on a three-dimensional Cartesian lattice with the laser potential of Eq. (3) set to zero. We employ a $192\times400\times96$ point lattice with a uniform grid spacing of $\Delta x=\Delta y=\Delta z=0.4$. We present probability density plots in the $z=0$ scattering plane in Fig. 1 for a proton collision at 5 keV with the $1s^22py$ excited state of Li. In Fig. 1(a) the $2py$ probability density for Li is found centered at $\vec{r}_A=(0.0,-40.0,0.0)$ as it begins a zero impact parameter collision. During the time propagation of the Schrödinger equation, the center of the electronic wave function moves to larger values of y. In Fig. 1(b) the atom has passed by the proton and is now located on the lattice at $\vec{r}_A=(0.0,+46.2,0.0)$. The probabilities for charge transfer to the excited states of hydrogen, centered at $\vec{r}_I=(0.0,0.0,0.0)$, are calculated at increments of a change in y of 10.0. The probabilities begin to approach their asymptotic limits only when the atom has moved to distances roughly twice the lattice maximum of $y=+80.0$. Spurious wave reflection at the lattice boundary is eliminated through the use of exponential masking. The charge-transfer probabilities for the $2py$ excited state are obtained using Eq. (6) and impact parameters ranging from 0.0 to 20.0.

Charge-transfer cross sections for the transitions Li($2p\sigma$)→H(n) and Li($2p\pi$)→H(n) with $n=2$ and $n=3$ are presented in Fig. 2. In general, we find good agreement between the time-dependent semiclassical (TDSE) lattice calculations and the time-dependent atomic-orbital close-coupling (TD-AOCC) calculations of Hansen *et al.* [17]. In this energy range the more recent TD-AOCC calculations of

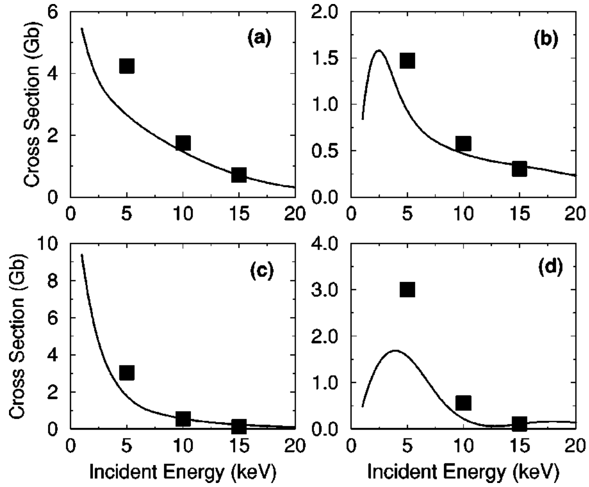

FIG. 2. Charge-transfer cross sections for proton collisions with lithium in the $1s^22p$ excited state. (a) $\mathrm{Li}(2p\sigma)\rightarrow\mathrm{H}(n=2)$, (b) $\mathrm{Li}(2p\sigma)\rightarrow\mathrm{H}(n=3)$, (c) $\mathrm{Li}(2p\pi)\rightarrow\mathrm{H}(n=2)$, (d) $\mathrm{Li}(2p\pi)\rightarrow\mathrm{H}(n=3)$. Solid squares, TDSE calculations; solid line, spline fit to TD-AOCC calculations [17]; ($1.0\ \mathrm{Gb}=1.0\times10^{-15}\ \mathrm{cm}^2$).

Lundsgaard *et al.* [18] are also in good agreement with the time-dependent lattice calculations and the original TD-AOCC calculations of Hansen *et al.* [17]. On the other hand, although we find our $\mathrm{Li}(2pm)\rightarrow\mathrm{H}(2)$ results are in reasonable agreement with the time-dependent molecular-orbital close-coupling (TD-MOCC) calculations of Salas [19], we also find that our $\mathrm{Li}(2pm)\rightarrow\mathrm{H}(3)$ results are substantially below the TD-MOCC calculations of Salas [19].

TABLE I. Proton-impact charge-transfer cross sections for the $1s^22p$ excited state of Li for incident energies of $E=5-15$ keV (units of $10^{-15}\ \mathrm{cm}^2$).

Transition	$E=5$ keV	$E=10$ keV	$E=15$ keV
$\mathrm{Li}(2p\sigma)\rightarrow\mathrm{H}(2s)$	0.34	0.22	0.17
$\mathrm{Li}(2p\sigma)\rightarrow\mathrm{H}(2p)$	3.90	1.53	0.55
$\mathrm{Li}(2p\sigma)\rightarrow\mathrm{H}(3s)$	0.26	0.14	0.10
$\mathrm{Li}(2p\sigma)\rightarrow\mathrm{H}(3p)$	0.68	0.34	0.17
$\mathrm{Li}(2p\sigma)\rightarrow\mathrm{H}(3d)$	0.53	0.11	0.03
$\mathrm{Li}(2p\pi)\rightarrow\mathrm{H}(2s)$	0.25	0.05	0.02
$\mathrm{Li}(2p\pi)\rightarrow\mathrm{H}(2p)$	2.91	0.53	0.11
$\mathrm{Li}(2p\pi)\rightarrow\mathrm{H}(3s)$	0.60	0.08	0.03
$\mathrm{Li}(2p\pi)\rightarrow\mathrm{H}(3p)$	1.65	0.38	0.08
$\mathrm{Li}(2p\pi)\rightarrow\mathrm{H}(3d)$	1.05	0.14	0.02

Charge-transfer cross sections for the transitions $\mathrm{Li}(2p\sigma)\rightarrow\mathrm{H}(nl)$ and $\mathrm{Li}(2p\pi)\rightarrow\mathrm{H}(nl)$ with $nl=2s,2p,3s,3p,3d$ are presented in Table I for incident energies of 5, 10, and 15 keV. Moderate differences are found in the cross sections for $\mathrm{Li}(2pm)$ states aligned parallel or perpendicular to the ion beam.

Charge-transfer cross sections for collisions of protons with the $1s^22s$ ground state of Li are then calculated by

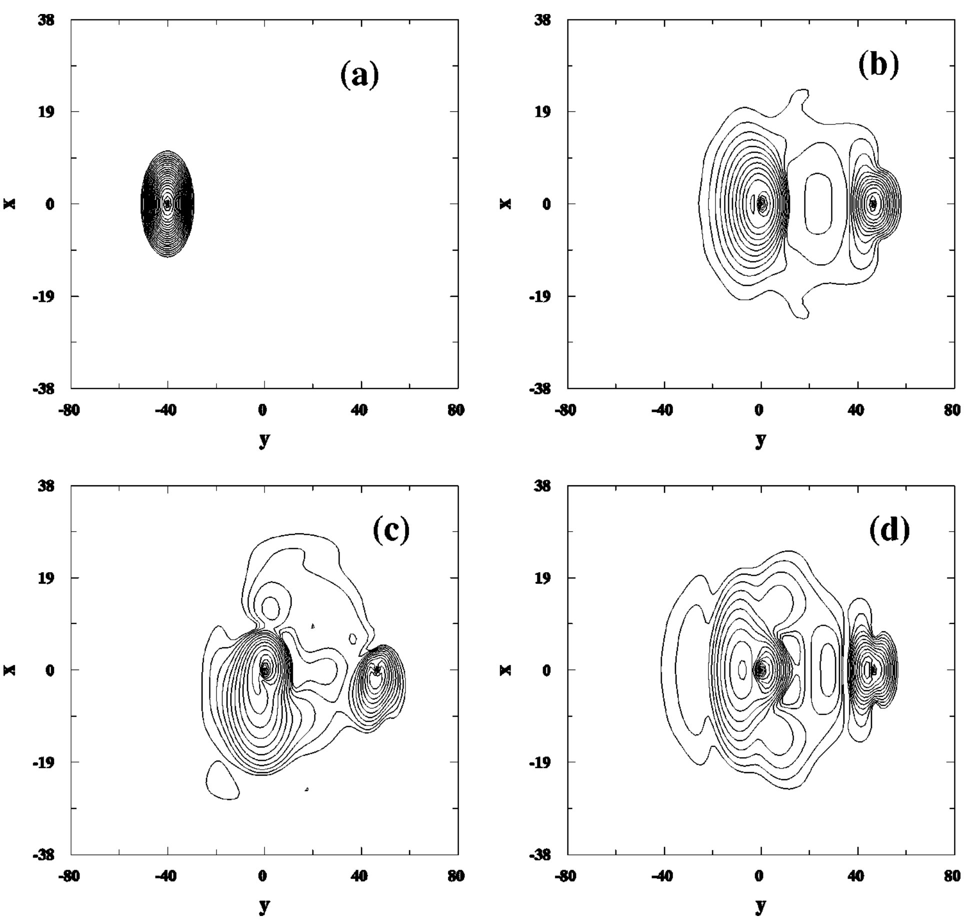

FIG. 3. Time evolution of the electron probability density in the $z=0$ scattering plane for a proton-$\mathrm{Li}(2s)$ collision at an incident energy of $E=5$ keV and an impact parameter of $b=0$. (a) $t=0$, (b) $t=192$ for no laser field, (c) $t=192$ for a laser field with light polarization perpendicular to the ion beam, (d) $t=192$ for a laser field with light polarization parallel to the ion beam (radial distances are in atomic units; $1.0\ \mathrm{a.u.}=5.29\times10^{-9}$ cm).

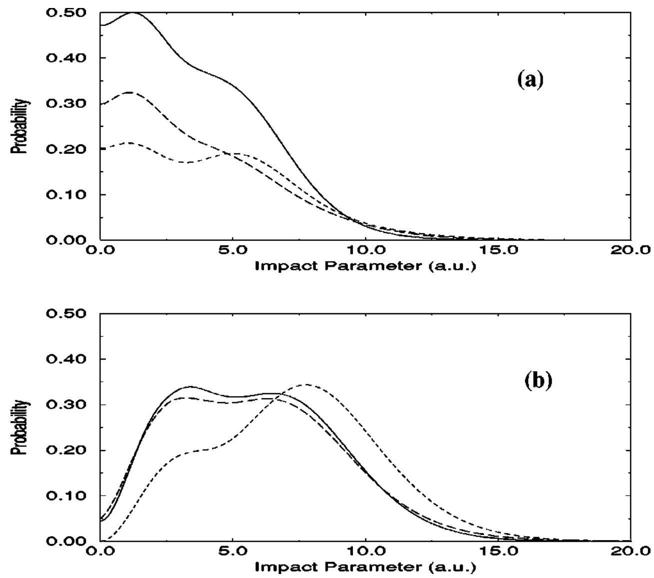

FIG. 4. Charge-transfer probabilities versus impact parameter for a proton-Li($2s$) collision at an incident energy of $E=5$ keV. (a) Li($2s$)→H($2s$), (b) Li($2s$)→H($2p$). Solid line, no laser; long-dashed line, laser with perpendicular polarization; short-dashed line, laser with parallel polarization (impact parameters are in atomic units; 1 a.u. $=5.29\times10^{-9}$ cm).

direct solution of Eq. (1) on a three-dimensional Cartesian lattice with the laser potential of Eq. (3) set to a nonzero value. The laser photon energy is chosen to be $\omega=2.27$ eV, corresponding to the energy difference between

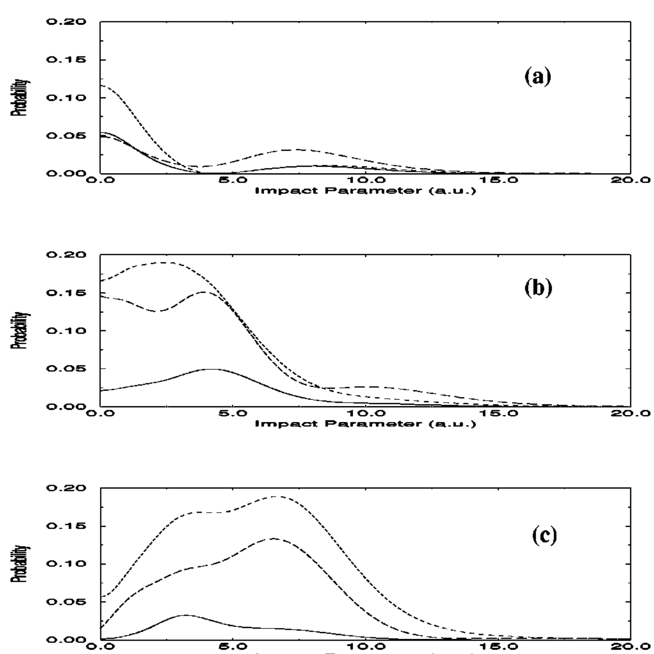

FIG. 5. Charge-transfer probabilities versus impact parameter for a proton-Li($2s$) collision at an incident energy of $E=5$ keV. (a) Li($2s$)→H($3s$), (b) Li($2s$)→H($3p$), (c) Li($2s$)→H($3d$). Solid line, no laser; long-dashed line, laser with perpendicular polarization; short-dashed line, laser with parallel polarization (impact parameters are in atomic units; 1 a.u. $=5.29\times10^{-9}$ cm).

TABLE II. Proton-impact charge-transfer cross sections for the $1s^2 2s$ ground state of Li in a laser field for an incident energy of $E=5$ keV (units of 10^{-15} cm^2).

Transition	$I=0$ W/cm^2	$I=10^{12}$ W/cm^2 $f(\vec{r})=x$	$I=10^{12}$ W/cm^2 $f(\vec{r})=y$
Li($2s$)→H($2s$)	1.96	1.27	1.28
Li($2s$)→H($2p$)	3.03	3.00	3.54
Li($2s$)→H($3s$)	0.09	0.28	0.14
Li($2s$)→H($3p$)	0.23	0.82	0.76
Li($2s$)→H($3d$)	0.13	0.96	1.68

the $1s^2 2s$ and $1s^2 2p$ states of Li on the lattice. By tuning to the $2s\rightarrow 2p$ resonance, we minimize phase difference effects between the laser pulse and the ion beam [2]. The pulse time $t_{pulse}=3T$ where $T=2\pi/\omega$, while the turn-on time $t_i=T$ and the turn-off time $t_f=2T$. Thus, the laser-pulse time of 5.5 fsec is approximately equal to the 5.4 fsec transit time associated with the Li atom, at a relative energy of 5 keV, moving from $y=-40.0$ to $y=+60.0$ on the lattice. Finally, the peak intensity of the laser field is chosen to be 10^{12} W/cm^2, yielding an electric-field amplitude $E_0=0.0053$. If the peak intensity is much higher, laser ionization of the target Li atom reduces the probability of capture to the projectile.

We present probability density plots in the $z=0$ scattering plane in Fig. 3 for a proton collision at 5 keV with the $1s^2 2s$ ground state of Li. In Fig. 3(a) the $2s$ probability density for Li is found centered at $\vec{r}_A=(0.0,-40.0,0.0)$ as it begins a zero impact parameter collision. In the remaining frames of Fig. 3 the atom has passed by the proton and is now located on the lattice at $\vec{r}_A=(0.0,+46.2,0.0)$. The probability density left behind at the center of the lattice is due to charge transfer into bound excited states of hydrogen. In Fig. 3(b) the laser potential is zero; in Fig. 3(c) the laser potential is nonzero with $\omega=2.27$ eV, $I=10^{12}$ W/cm^2, and light polarization perpendicular to the ion beam; and in Fig. 3(d) the laser potential is nonzero with the same laser frequency and intensity, but with the light polarization parallel to the ion beam. In comparison with Fig. 3(b), we find electron density in Fig. 3(c) driven in the x direction perpendicular to the ion beam, while in Fig. 3(d) we find electron density driven in the y direction parallel to the ion beam.

We present charge-transfer probabilities as a function of the impact parameter in Figs. 4 and 5 and total charge-transfer cross sections in Table II for proton-Li($2s$) collisions with and without a pulsed laser field at an incident energy of $E=5$ keV. The laser field is found to slightly reduce the Li($2s$)→H($2s$) cross section by reducing the collision probability at small impact parameters, increase slightly the Li($2s$)→H($2p$) cross section by shifting the collision probability to larger impact parameters, and strongly increase the Li($2s$)→H($3l$) cross sections by substantially increasing the collision probabilities at all impact parameters. In particular, the charge-transfer cross section for the Li($2s$)→H($3d$) transition is an order of magnitude larger than the zero-field result for laser light polarized parallel to the ion beam. In general, the overall strength of the Li($2s$) $\rightarrow$H($3l$) cross sections of 2.06 Gb for laser light polarized perpendicular to the ion beam and of 2.58 Gb for laser light polarized parallel to the ion beam lies between the field-free cross sections of 1.47 Gb for the Li($2p\sigma$)$\rightarrow$H($3l$) transitions and 3.30 Gb for the Li($2p\pi$)$\rightarrow$H($3l$) transitions, and much higher than the field-free Li($2s$)$\rightarrow$H($3l$) cross sections of 0.45 Gb. Thus, the two-step process of laser excitation of the target followed by charge transfer to the proton is more than likely to be a dominant quantum-mechanical pathway.

IV. SUMMARY

Proton-impact charge-transfer cross sections from the ground and excited states of the Li atom to the low-lying excited states of the H atom are calculated by a numerical lattice solution of the time-dependent Schrödinger equation. Charge-transfer cross sections for Li($2p$)$\rightarrow$H(nl) transitions are found to be in good agreement with previous time-dependent atomic-orbital close-coupling calculations [17]. Moderate differences are found for state-selective charge-transfer cross sections for laser excited $2p\sigma$ states aligned parallel and $2p\pi$ states aligned perpendicular to the ion beam. Further, charge-transfer cross sections for Li($2s$) $\rightarrow$H(nl) transitions in the simultaneous presence of a pulsed laser field of moderate intensity are also obtained by direct solution of the time-dependent Schrödinger equation. The presence of the radiation field is found to have a strong effect on charge-transfer cross sections for Li($2s$)$\rightarrow$H($3l$) transitions. In conclusion, we hope this work will stimulate further experimental investigation of laser control of charge-transfer processes in ion-atom collisions.

ACKNOWLEDGMENTS

This work was supported in part by a grant for theoretical research in plasma and fusion science (Grant No. DE-FG02-96ER54348) to Auburn University and a grant for scientific discovery through advanced computing (Grant No. DE-FG02-01ER54644) to a US/UK consortium through Auburn University by the U.S. Department of Energy. Computational work was carried out at the National Energy Research Scientific Computing Center in Oakland, CA, and the Center for Computational Sciences in Oak Ridge, TN.

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