Proton-impact excitation of laser-excited lithium atoms

M. S. Pindzola
Department of Physics, Auburn University, Auburn, Alabama, 36849
(Received 15 April 2002; published 23 September 2002)

A time-dependent solution of the Schrödinger equation on a three-dimensional lattice is used to calculate proton-impact excitation cross sections for both the ground ($2s$) and first excited ($2p$) states of the neutral lithium atom. Total cross sections for the $2s \rightarrow 3l$ and $2p \rightarrow 3l$ excitations are compared with atomic-orbital close-coupling calculations at incident energies of 15–50 keV. In support of future experiments involving crossed ion, atom, and laser beams, total aligned cross sections for the $2p\sigma \rightarrow 3l$ and $2p\pi \rightarrow 3l$ excitations are presented over the same energy range. The ratio of aligned cross sections for certain excitations and incident energies is found to be almost a factor of 2.

DOI: 10.1103/PhysRevA.66.032716 PACS number(s): 34.50.Fa

I. INTRODUCTION

Lithium beam spectroscopy has become a valuable diagnostic tool for many controlled fusion experiments [1]. The atomic database needed to model energetic lithium beams probing fusion edge plasmas includes proton-impact excitation of the neutral lithium atom. Crossed-beam experimental measurements [2] of the total cross section for the $2s \rightarrow 2p$ excitation are in reasonably good agreement with time-dependent atomic-orbital close-coupling [3], time-dependent Hartree-Fock [4], and time-dependent lattice [5] calculations for incident proton energies from 2–20 keV. Total cross sections for the $2s \rightarrow nl (2 < n < 6)$ excitations calculated in the time-dependent atomic-orbital close-coupling method, when combined with cascade branching ratios, are also found to be in reasonable agreement with crossed-beam emission measurements [6].

Future experiments involving crossed ion, atom, and laser beams hold the promise for measurements of total excitation cross sections from the excited states of the neutral lithium atom. A tunable dye laser can prepare the lithium atoms in specific excited states aligned parallel or perpendicular with the proton beam. In this paper we calculate proton-impact excitation cross sections for both the ground ($2s$) and first excited ($2p$) states of the neutral lithium atom. The total cross sections for the $2s \rightarrow 3l$ and $2p \rightarrow 3l$ excitations are calculated by direct solution of the time-dependent Schrödinger equation (TDSE) on a three-dimensional Cartesian lattice. This computationally intensive method has been recently applied to calculate proton-impact excitation cross sections for the neutral hydrogen atom over a wide energy range [7,8]. We compare the Li($2s$) and Li($2p$) excitation cross sections with time-dependent atomic-orbital close-coupling (AOCC) results [9] at incident-proton energies of 15–50 keV. We also present Li($2p\sigma$) and Li($2p\pi$) aligned excitation cross sections in support of future crossed ion, atom, and laser beams experiments. In Sec. II, we give an account of the theoretical and computational methods, proton-lithium excitation cross sections are presented in Sec. III, and a brief summary is given in Sec. IV. Atomic units are used throughout the paper, unless otherwise noted.

II. THEORY

The scattering geometry for an ion-atom collision is given in Fig. 1, where the ion beam is incident along the y axis. The time-dependent Schrodinger equation for a bare ion (Z) projectile colliding with the valence electron of an atom is given by

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

where for straight line trajectories,

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

b is the impact parameter, y_i is the starting position for the projectile, and v is the projectile velocity. 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 [5]. This prevents the

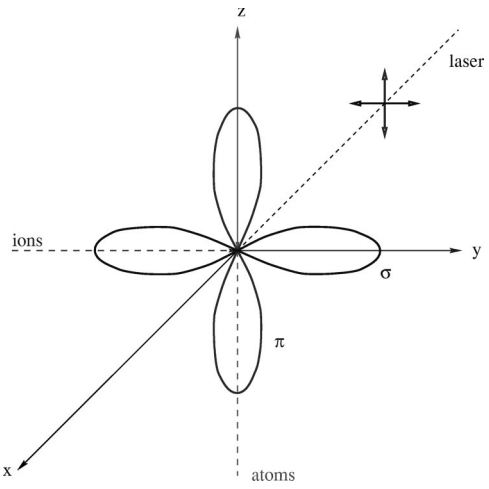

FIG. 1. Geometry for crossed ion, atom, and laser beams collision. σ orbitals are aligned parallel with the ion beam, while π orbitals are aligned perpendicular to the ion beam.

TABLE I. Summed excitation probabilities for the transition $2py \rightarrow nl$ at 15 keV and impact parameter $=5.0$ ($\wp_{2py\rightarrow nl} = \Sigma'_m \wp_{2py\rightarrow nlm}$).

Lattice	y_i	y_f	$2py \rightarrow 2s$	$2py \rightarrow 3s$	$2py \rightarrow 3p$	$2py \rightarrow 3d$
$30\times30\times30$ (0.2)	-15	$+30$	0.074	0.021	0.021	0.094
$30\times50\times30$ (0.2)	-25	$+50$	0.079	0.033	0.025	0.097
$45\times75\times45$ (0.3)	-38	$+75$	0.084	0.035	0.027	0.088
$45\times75\times45$ (0.3)	-38	$+118$	0.083	0.035	0.027	0.088
$45\times75\times45$ (0.3)	-38	$+274$	0.083	0.035	0.028	0.087
$48\times80\times48$ (0.4)	-40	$+116$	0.082	0.034	0.027	0.087
$48\times80\times48$ (0.4)	-40	$+271$	0.082	0.034	0.028	0.086

unphysical $2s \rightarrow 1s$ transition in the time evolution of the Schrodinger equation. Matrix diagonalization of the Hamiltonian

$$h(r) = -\frac{1}{2}\frac{\partial^2}{\partial r^2} + V_{core}(r), \tag{3}$$

on a radial mesh of $\Delta r = 0.1$, yields a set of radial orbitals $P_{nl}(r)$ whose eigenenergies are in reasonably good agreement with experimental removal energies [see Table I of previous work [5]]. The use of a pseudopotential is probably the largest single source of uncertainty in the calculational method. The full three-dimensional stationary states for the lithium atom are then found by relaxation of the time-dependent Schrödinger equation in imaginary time ($\tau = it$)

$$-\frac{\partial \psi_{nlm}(\vec{r},\tau)}{\partial \tau} = [-\tfrac{1}{2}\nabla^2 + V_{core}(r)]\psi_{nlm}(\vec{r},\tau), \tag{4}$$

where

$$\psi_{nlm}(\vec{r},\tau=0) = \frac{P_{nl}(r)}{r} Y_{lm}(\hat{r}). \tag{5}$$

We find that the energies of the fully relaxed stationary states $\psi_{nlm}(\vec{r})$ differ from the original eigenenergies by less than 1% for the range of grid spacings from $\Delta x = \Delta y = \Delta z = 0.1$ to $\Delta x = \Delta y = \Delta z = 0.4$.

The excitation probability for the transition $n_0 l_0 m_0 \rightarrow nlm$ at a specific velocity and impact parameter is given by

$$\wp_{n_0 l_0 m_0 \rightarrow nlm}(v,b) = \left| \int d\vec{r}\, \psi^*_{nlm}(\vec{r}) \Psi(\vec{r}, t=T) \right|^2, \tag{6}$$

where

$$\Psi(\vec{r}, t=0) = \psi_{n_0 l_0 m_0}(\vec{r}) \tag{7}$$

and $\Psi(\vec{r}, t=T)$ is the solution of Eq. (1) at a time $t=T$ following the collision. The time-dependent behavior of the excitation probability will be examined in the Sec. III when we quantify the value of T.

The total excitation cross section for the $2s$ ground state of lithium is given by

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

The total excitation cross section for the $2p$ excited state of lithium is given by

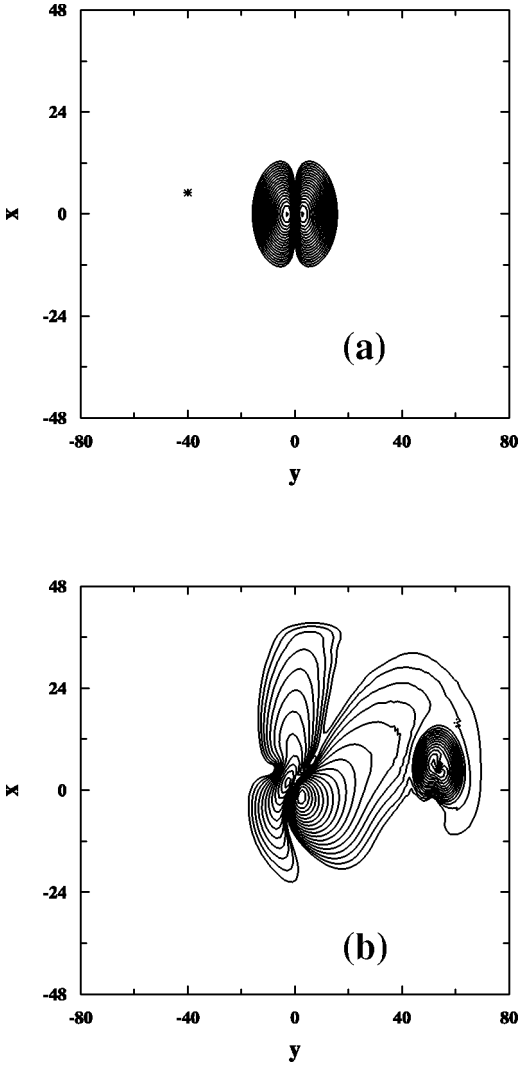

FIG. 2. Time evolution of the electron probability density in the $z=0$ scattering plane for a proton-Li($2py$) collision at 15 keV and an impact parameter of $b=5$. (a) $t=0$ and (b) $t=120$ (radial distances are in atomic units, 1.0 a.u.$=5.29\times10^{-9}$ cm).

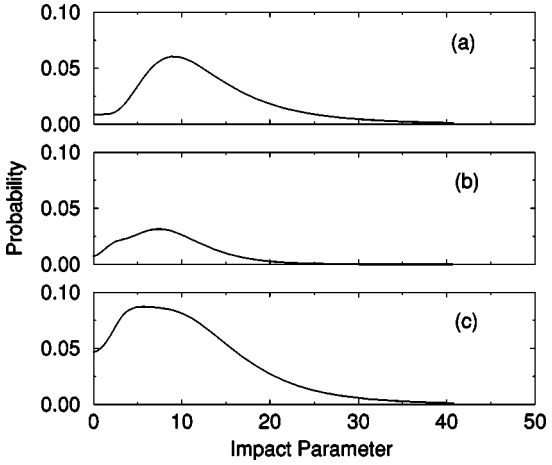

FIG. 3. Excitation probabilities versus impact parameter for a proton-Li($2py$) collision at 15 keV. (a) $2py \rightarrow 3s$ transition, (b) $2py \rightarrow 3p$ transition, and (c) $2py \rightarrow 3d$ transition (impact parameters are in atomic units, 1.0 a.u.$=5.29\times10^{-9}$ cm).

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

where the aligned parallel cross section is given by

$$\sigma_{2p\sigma\rightarrow nl}(v)=2\pi\sum_{m}{}' \int_0^\infty \wp_{2py\rightarrow nlm}(v,b)bdb \tag{10}$$

and the aligned perpendicular cross section is given by

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

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.

III. RESULTS

The proton-impact excitation cross sections for the neutral lithium atom are calculated by direct solution of the time-dependent Schrödinger equation of Eq. (1) on a three-dimensional Cartesian lattice. We tried several different lattices to gain an understanding of the sensitivity of excitation probabilities to lattice size, lattice spacing, and overall propagation time. An example of one of our tests is found in Table I for the transition $2py \rightarrow nl$ at an incident-proton energy of 15 keV and an impact parameter of 5.0. The $30\times30\times30$ (0.2) lattice is such that $-30\leqslant x\leqslant+30$, $-30\leqslant y\leqslant+30$, and $0\leqslant z\leqslant+30$, with a uniform grid spacing of $\Delta x=\Delta y=\Delta z=0.2$. Thus, the number of finite difference points in the lattice is $300\times300\times150$. The excitation probabilities were found to be most sensitive to the overall propagation time, given by $T=(y_f-y_i)/v$. For production runs using 35 impact parameters ranging from 0.0 to 40.8, we chose the $48\times80\times48$ (0.4) lattice in which the proton travels from $y_i=-40$ to $y_f=+116$, the latter being well beyond the lattice boundary at $+48$.

TABLE II. Proton-impact excitation cross sections for lithium (10^{-15} cm^2).

Transition	$E=15$ keV	$E=30$ keV	$E=50$ keV
$2s\rightarrow2p$	3.19	3.21	2.66
$2s\rightarrow3s$	0.03	0.05	0.05
$2s\rightarrow3p$	0.15	0.12	0.09
$2s\rightarrow3d$	0.35	0.28	0.18
$2p\rightarrow2s$	1.08	1.06	0.88
$2p\rightarrow3s$	1.45	1.12	0.81
$2p\rightarrow3p$	0.70	0.43	0.28
$2p\rightarrow3d$	3.10	3.11	2.56

We present probability density plots in the $z=0$ scattering plane in Fig. 2 for a proton collision at 15 keV and an impact parameter of $b=5$ with a lithium atom in a $2py$ excited state. In Fig. 2(a) the star is the initial position of the proton at the coordinates $(5,-40)$, while the probability density for the lithium atom, located at the coordinates (0,0), is aligned along the y axis. In Fig. 2(b) the proton has passed by the lithium atom and is located at the coordinates $(5,+55)$. Besides excitation of the target atom, one can also see substantial charge transfer to the projectile ion. We also present excitation probabilities as a function of impact parameter in Fig. 3 for a proton collision at 15 keV with a lithium atom in a $2py$ excited state. Since the integral in Eq. (10) is weighted towards large impact parameters (bdb), the TDSE lattice calculations must include quite large impact parameters.

Proton-impact excitation cross sections for a lithium atom in its ground and first excited state are presented in Table II, Figs. 4, and 5 for incident energies of 15, 30, and 50 keV. The total number of TDSE propagations needed to generate the cross sections is 420, given by the product of the number of initial states ($2s_0, 2px, 2py, 2pz$), the number of incident

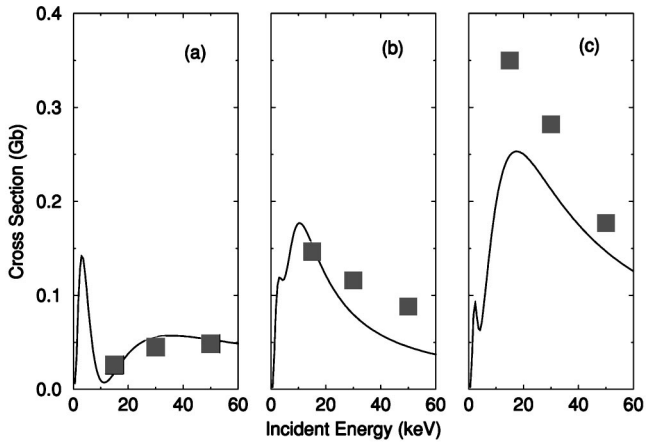

FIG. 4. Excitation cross sections for proton collisions with lithium in its ground state. (a) $2s\rightarrow3s$ transition, (b) $2s\rightarrow3p$ transition, and (c) $2s\rightarrow3d$ transition. Solid squares, TDSE calculations, solid line, AOCC calculations [9] (1.0 Gb$=1.0\times10^{-15}$ cm^2).

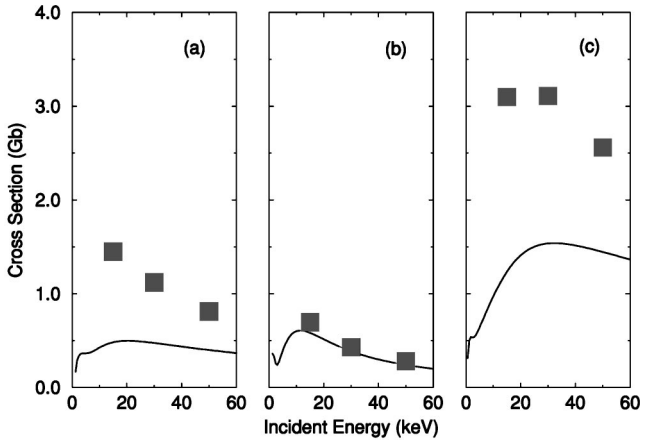

FIG. 5. Excitation cross sections for proton collisions with lithium in its first excited state. (a) $2p \rightarrow 3s$ transition, (b) $2p \rightarrow 3p$ transition, and (c) $2p \rightarrow 3d$ transition. Solid squares, TDSE calculations; solid line, AOCC calculations [9] (1.0 Gb $= 1.0 \times 10^{-15}$ cm^2).

energies (3), and the number of impact parameters (35). The ground-state cross sections at 15 keV are somewhat smaller than those reported before [5] for a $30 \times 30 \times 30$ (0.2) lattice with $y_f = +30$. The excitation probabilities on the current $48 \times 80 \times 48$ (0.4) lattice with $y_f = +116$ are simply better converged. A consistency check on the excited cross sections is that the $2p \rightarrow 2s$ cross section is $\frac{1}{3}$ the $2s \rightarrow 2p$ cross section to almost three significant figures. The TDSE results are compared with earlier AOCC results [9] in Figs. (4) and (5). The solid curves are obtained using the twelve parameter fitting formula from Eq. (3) of Schweinzer *et al.* [9]. The best agreement between the two methods is found for the $2s \rightarrow 3s$ and $2p \rightarrow 3p$ transitions, while the worst agreement is found for the $2p \rightarrow 3d$ transition.

As a challenge to the experiment, we present in Table III proton-impact excitation cross sections for a lithium atom in an excited-state aligned parallel or perpendicular to the ion-beam direction. The ratio of aligned cross sections, $R = \sigma_{2p\sigma \rightarrow nl} / \sigma_{2p\pi \rightarrow nl}$, varies from $R = 1.6$ for the $2p \rightarrow 3s$ cross sections at 15 keV to $R = 0.58$ for the $2p \rightarrow 3p$ cross sections at 50 keV. We note in particular that the alignment ratio for the $3s$ cross sections varies the most as a function of incident-proton energy.

TABLE III. Proton-impact excitation cross sections for lithium (10^{-15} cm^2).

Transition	$E = 15$ keV	$E = 30$ keV	$E = 50$ keV
$2p\sigma \rightarrow 3s$	1.92	1.05	0.56
$2p\sigma \rightarrow 3p$	0.56	0.30	0.19
$2p\sigma \rightarrow 3d$	2.87	3.06	2.57
$2p\pi \rightarrow 3s$	1.21	1.15	0.94
$2p\pi \rightarrow 3p$	0.77	0.50	0.33
$2p\pi \rightarrow 3d$	3.22	3.14	2.56

IV. SUMMARY

Proton-impact excitation cross sections of the lithium atom in its ground and excited states are calculated by numerical solution of the time-dependent Schrödinger equation on a three-dimensional Cartesian lattice. After the 11.52×10^6 points on the lattice are partitioned over the many processors on a distributed memory computer, the wave function for the valence electron of the lithium atom is time evolved subject to the motional field of an incident proton. Following the passage of the proton, the electron wave function is projected onto stationary states to obtain excitation probabilities. Hundreds of trajectories are used to calculate excitation cross sections from both the ground and first excited states of lithium. The agreement between the TDSE results and previous atomic-orbital close-coupling calculations is good for some excitations and relatively poor for others. We also present aligned excitation cross sections for the first excited state of lithium in support of future crossed ion, atom, and laser beam experiments.

ACKNOWLEDGMENTS

This work was supported in part by a grant for theoretical research in plasma and fusion science (Grant No. DE-FG02-96ER54348) and a grant for scientific discovery through advanced computing (Grant No. DE-FG02-01ER54644) to 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.

[1] K. McCormick, S. Fiedler, G. Kocsis, J. Schweinzer, and S. Zoletnik, Fusion Eng. Des. **34–35**, 125 (1997).
[2] F. Aumayr, M. Fehringer, and H. Winter, J. Phys. B **17**, 4185 (1984).
[3] R. Brandenburg, J. Schweinzer, F. Aumayr, and H.P. Winter, J. Phys. B **31**, 2585 (1998).
[4] K. Runge and D.A. Micha, Chem. Phys. Lett. **303**, 15 (1999).
[5] M.S. Pindzola, Phys. Rev. A **60**, 3764 (1999).
[6] J.W. Turkstra, D. Meyer, R. Hoekstra, R. Morgenstern, and J. Schweinzer, Phys. Rev. A **60**, 4627 (1999).
[7] A. Kolakowska, M.S. Pindzola, F. Robicheaux, D.R. Schultz, and J.C. Wells, Phys. Rev. A **58**, 2872 (1998).
[8] D.R. Schultz, M.R. Strayer, and J.C. Wells, Phys. Rev. Lett. **82**, 3976 (1999).
[9] J. Schweinzer, R. Brandenburg, I. Bray, R. Hoekstra, F. Aumayr, R.K. Janev, and H.P. Winter, At. Data Nucl. Data Tables **72**, 239 (1999).