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Double ionization of H_2 by fast bare-ion collisions

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A time-dependent close-coupling method is developed to treat the double ionization of H_2 by fast bare-ion collisions. At high incident energies, for which charge transfer to the projectile may be ignored, multipole expansions are made for the electron-electron and electron-projectile interactions in a fixed target nuclei coordinate system. The time-dependent Schrödinger equation for the six dimensional target electron wave function is reduced to a set of close-coupled equations on a four dimensional numerical lattice in $(r_1,\theta_1,r_2,\theta_2)$ center-of-mass spherical polar coordinates. Time-dependent close-coupling calculations are carried out for $p+H_2$ collisions at an incident energy of 1.0 MeV. The ratio of double to single ionization is found to be 0.3%, which is in reasonable agreement with experimental measurements.

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I. INTRODUCTION

The double ionization of atoms and molecules probes the long range interaction of two electrons in the field of a charged ion: the quantal three-body breakup problem. For atoms the two ejected electrons move in the spherical field of an atomic ion, while for molecules the two ejected electrons move in the nonspherical field of a molecular ion. Under photon-impact the two ejected electrons feel a dipolar interaction, while under fast bare-ion impact the two ejected electrons feel a multipolar interaction. From a theoretical perspective, the fast bare-ion-impact double ionization of a molecule is a quite challenging three-body problem.

In the last few years, several nonperturbative theoretical methods have been developed to treat photon-impact double ionization of atoms. Double ionization cross sections for He have been calculated using the extended R-matrix [1], converged close-coupling [2], R-matrix with pseudostates [3], hyperspherical close coupling [4], time-dependent close coupling [5,6], and exterior complex scaling [7] methods. Double ionization cross sections for the lightest alkaline earth metal atoms have also been calculated using the converged close-coupling [8,9], time-dependent close coupling [10], hyperspherical close coupling [11], and R-matrix with pseudostates [12] methods.

Recently, nonperturbative theoretical methods have been developed to treat both photon-impact double ionization of molecules and fast bare-ion-impact double ionization of atoms. Photon-impact double ionization cross sections for H_2 have been calculated using the time-dependent close-coupling [13,14], exterior complex scaling [15,16], and converged close-coupling [17,18] methods. Fast bare-ion-impact double ionization cross sections for He have been calculated using the time-dependent coupled channels [19,20] and time-dependent close-coupling [21,22] methods.

In this paper, we develop a nonperturbative time-dependent close-coupling method to calculate single and double ionization processes in fast bare-ion collisions with H_2. At high incident energies, charge transfer to the projectile may be ignored, so that multipole expansions are made for the electron-electron and electron-projectile interactions in a fixed target nuclei coordinate system. Due to the nonspherical field of the molecular target, the six-dimensional two-electron wave function is expanded in rotational functions. Reduction of the time-dependent Schrödinger equation yields a set of close-coupled equations on a four dimensional numerical lattice in $(r_1,\theta_1,r_2,\theta_2)$ center-of-mass spherical polar coordinates. The initial condition involves the solution of a set of close-coupled equations for the time-dependent Schrödinger equation in imaginary time including only the electron-electron interaction. The full set of close-coupled equations is propagated in real time for a number of projectile impact parameters. Single and double ionization cross sections are extracted by postcollision projection of the time evolved reduced wave functions onto bound single particle molecular orbitals. To compare with experimental measurements [23,24], time-dependent close-coupling calculations are carried out for $p+H_2$ collisions at an incident energy of 1.0 MeV.

The rest of the paper is organized as follows. In Sec. II we develop a time-dependent close-coupling method for ionization processes in fast bare-ion collisions with homonuclear diatomic molecules. In Sec. III, we apply the time-dependent close-coupling method to calculate single and double ionization cross sections for $p+H_2$ collisions. In Sec. IV, we conclude with a summary and an outlook for future work. Unless otherwise stated, all quantities are given in atomic units.

II. THEORY

The time-dependent Schrödinger equation for fast bare-ion scattering from a two-electron homonuclear diatomic molecule is given by

$$i\frac{\partial\Psi(\vec{r}_1,\vec{r}_2,t)}{\partial t}=[H_{tar}(\vec{r}_1,\vec{r}_2)+H_{proj}(\vec{r}_1,\vec{r}_2,t)]\Psi(\vec{r}_1,\vec{r}_2,t). \tag{1}$$

The target Hamiltonian is given by

$$H_{tar}(\vec{r}_1,\vec{r}_2) = \sum_{i=1}^{2}\left(-\frac{1}{2}\nabla_i^2 - \sum_{\pm}\frac{Z_t}{\sqrt{r_i^2 + \frac{1}{4}R_t^2 \pm r_iR_t\cos\theta_i}}\right) + \frac{1}{|\vec{r}_1 - \vec{r}_2|}, \tag{2}$$

where Z_t is the charge on each target nucleus and R_t is the internuclear distance. The projectile Hamiltonian is given by

$$H_{proj}(\vec{r}_1,\vec{r}_2,t) = \sum_{i=1}^{2}\left(-\frac{Z_p}{|\vec{r}_i - \vec{R}_p(t)|}\right), \tag{3}$$

where Z_p is the charge on the projectile. For straight-line motion, the magnitude of the time-dependent projectile position is given by

$$\vec{R}_p(t) = b\hat{i} + (d_0 + vt)\hat{k}, \tag{4}$$

where b is an impact parameter, d_0 is a starting distance ($d_0 < 0$), and v is the projectile speed.

The six-dimensional target electron wave function is expanded in rotational functions for each total angular momentum projection along the internuclear axis, M, and total spin angular momentum, S,

$$\Psi^{MS}(\vec{r}_1,\vec{r}_2,t) = \sum_{m_1,m_2}\frac{P^{MS}_{m_1m_2}(r_1,\theta_1,r_2,\theta_2,t)}{r_1r_2\sqrt{\sin\theta_1}\sqrt{\sin\theta_2}}\Phi_{m_1}(\phi_1)\Phi_{m_2}(\phi_2), \tag{5}$$

where

$$\Phi_m(\phi) = \frac{e^{im\phi}}{\sqrt{2\pi}}, \tag{6}$$

and $M = m_1 + m_2$.

Upon substitution of $\Psi^{MS}(\vec{r}_1,\vec{r}_2,t)$ of Eq. (5) into the time-dependent Schrödinger equation of Eq. (1), we obtain the following set of time-dependent close-coupled partial differential equations for each MS symmetry:

$$\begin{aligned} i\frac{\partial P^{MS}_{m_1m_2}(r_1,\theta_1,r_2,\theta_2,t)}{\partial t} &= T_{m_1m_2}(r_1,\theta_1,r_2,\theta_2)P^{MS}_{m_1m_2}(r_1,\theta_1,r_2,\theta_2,t) \\ &+ \sum_{m_1',m_2'} V^{M}_{m_1m_2,m_1'm_2'}(r_1,\theta_1,r_2,\theta_2)P^{MS}_{m_1'm_2'}(r_1,\theta_1,r_2,\theta_2,t) \\ &+ \sum_{m_1',m_2',M'} \dot{W}^{MM'}_{m_1m_2,m_1'm_2'}(r_1,\theta_1,R_p,\theta_p,t)P^{M'S}_{m_1',m_2'}(r_1,\theta_1,r_2,\theta_2,t) \\ &+ \sum_{m_1',m_2',M'} \ddot{W}^{MM'}_{m_1m_2,m_1'm_2'}(r_2,\theta_2,R_p,\theta_p,t)P^{M'S}_{m_1',m_2'}(r_1,\theta_1,r_2,\theta_2,t). \end{aligned} \tag{7}$$

The kinetic and nuclear interaction operator is given by

$$T_{m_1m_2}(r_1,\theta_1,r_2,\theta_2) = \sum_{i=1}^{2}\left(K(r_i) + \bar{K}(r_i,\theta_i) + A_{m_i}(r_i,\theta_i) + N(r_i,\theta_i)\right), \tag{8}$$

where $K(r)$ and $\bar{K}(r,\theta)$ depend on the lattice representation of derivative operators,

$$A_{m_i}(r_i,\theta_i) = \frac{m_i^2}{2r_i^2\sin^2\theta_i}, \tag{9}$$

and

$$N(r_i,\theta_i) = -\sum_{\pm}\frac{Z_t}{\sqrt{r_i^2 + \frac{1}{4}R_t^2 \pm r_iR_t\cos\theta_i}}. \tag{10}$$

The electron-electron interaction operator is given by

$$V^{M}_{m_1m_2,m_1'm_2'}(r_1,\theta_1,r_2,\theta_2) = 4\pi\sum_{\lambda=|q|}^{\lambda_{max}}\frac{(r_1,r_2)^{\lambda}_{<}}{(r_1,r_2)^{\lambda+1}_{>}}\frac{Y_{\lambda|q|}(\theta_1,0)Y_{\lambda|q|}(\theta_2,0)}{2\lambda+1}, \tag{11}$$

where $q = m_1 - m_1' = m_2' - m_2$ and $Y_{lm}(\theta,\phi)$ is a spherical harmonic. The electron-projectile interaction operators are given by

$$\begin{aligned} \dot{W}^{MM'}_{m_1m_2,m_1'm_2'}(r_1,\theta_1,R_p,\theta_p,t) &= -4\pi Z_p\delta_{m_2,m_2'}\sum_{\lambda=0}^{\lambda_{max}}\sum_{q=-\lambda}^{+\lambda}\delta_{q,m_1-m_1'} \\ &\times\frac{(r_1,R_p)^{\lambda}_{<}}{(r_1,R_p)^{\lambda+1}_{>}}\frac{Y_{\lambda|q|}(\theta_1,0)Y_{\lambda|q|}(\theta_p,0)}{2\lambda+1} \end{aligned} \tag{12}$$

and

$$\begin{aligned}\ddot{W}^{MM'}_{m_1m_2,m_1'm_2'}(r_2,\theta_2,R_p,\theta_p,t) &= -4\pi Z_p\delta_{m_1,m_1'}\sum_{\lambda=0}^{\lambda_{max}}\sum_{q=-\lambda}^{+\lambda}\delta_{q,m_2-m_2'}\\ &\quad\times\frac{(r_2,R_p)^{\lambda}_{<}}{(r_2,R_p)^{\lambda+1}_{>}}\frac{Y_{\lambda|q|}(\theta_2,0)Y_{\lambda|q|}(\theta_p,0)}{2\lambda+1}. \qquad (13)\end{aligned}$$

We choose the projectile to move in the xz plane, such that $\sin\,\theta_p=b/R_p(t)$, $\cos\,\theta_p=(d_0+vt)/R_p(t)$, and $\phi_p=0$. Thus, the projectile motion is aligned with the internuclear axis.

The initial condition for the solution of Eq. (1) is given by

$$\Psi(\vec{r}_1,\vec{r}_2,t=0)=\bar{\Psi}(\vec{r}_1,\vec{r}_2,\tau\to\infty), \qquad (14)$$

where $\bar{\Psi}(\vec{r}_1,\vec{r}_2,\tau\to\infty)$ is the ground state of the two-electron homonuclear diatomic molecule ($M=S=0$). The ground state may be obtained by relaxation of the Schrödinger equation in imaginary time ($t=i\tau$)

$$-\frac{\partial\bar{\Psi}(\vec{r}_1,\vec{r}_2,\tau)}{\partial\tau}=H_{tar}(\vec{r}_1,\vec{r}_2)\bar{\Psi}(\vec{r}_1,\vec{r}_2,\tau). \qquad (15)$$

The wave function $\bar{\Psi}^{MS}(\vec{r}_1,\vec{r}_2,\tau)$ is again expanded in products of rotational functions, substituted into Eq. (15), yielding a set of close-coupled partial differential equations for the ground MS symmetry

$$\begin{aligned}-\frac{\partial\bar{P}^{MS}_{m_1m_2}(r_1,\theta_1,r_2,\theta_2,\tau)}{\partial\tau} &= T_{m_1m_2}(r_1,\theta_1,r_2,\theta_2)\bar{P}^{MS}_{m_1m_2}(r_1,\theta_1,r_2,\theta_2,\tau)\\ &\quad+\sum_{m_1',m_2'}V^{M}_{m_1m_2,m_1'm_2'}(r_1,\theta_1,r_2,\theta_2)\bar{P}^{MS}_{m_1'm_2'}(r_1,\theta_1,r_2,\theta_2,\tau).\end{aligned} \qquad (16)$$

We solve the time-dependent close-coupling equations using lattice techniques to obtain a discrete representation of the reduced wave functions, $P(r_1,\theta_1,r_2,\theta_2,t)$ (or $\bar{P}(r_1,\theta_1,r_2,\theta_2,\tau)$), and all operators on a four dimensional radial and angular grid, $(r_i,\theta_j,r_{i'},\theta_{j'})$. For a low-order finite difference representation, the variational principle yields the kinetic energy operators

$$K_iP_{i,j,i',j'}(t)=-\frac{1}{2}\left[\frac{c_iP_{i+1,j,i',j'}(t)+c_{i-1}P_{i-1,j,i',j'}(t)-\bar{c}_iP_{i,j,i',j'}(t)}{\Delta r^2}\right], \qquad (17)$$

where $c_i=\frac{r^2_{i+1/2}}{r_ir_{i+1}}$ and $\bar{c}_i=\frac{r^2_{i+1/2}+r^2_{i-1/2}}{r_i^2}$, while

$$\bar{K}_{ij}P_{i,j,i',j'}(t)=-\frac{1}{2r_i^2}\left(\frac{d_jP_{i,j+1,i',j'}(t)+d_{j-1}P_{i,j-1,i',j'}(t)-\bar{d}_jP_{i,j,i',j'}(t)}{\Delta\theta^2}\right), \qquad (18)$$

where $d_j=\frac{\sin\,\theta_{j+1/2}}{\sqrt{\sin\,\theta_j\,\sin\,\theta_{j+1}}}$ and $\bar{d}_j=\frac{\sin\,\theta_{j+1/2}+\sin\,\theta_{j-1/2}}{\sin\,\theta_j}$. The coefficients reflect the adoption of half-spacing in all coordinate directions so that proper boundary conditions may easily be applied. The time-dependent close-coupling equations are propagated forward in time using an implicit algorithm,

$$\begin{aligned}P^{MS}_{m_1m_2}(t+\Delta t) &= \sum_{m_1',m_2',M'}e^{-i\Delta t/2(V^{M}_{m_1m_2,m_1'm_2'}(1,2)+W^{MM'}_{m_1m_2,m_1'm_2'}(1,2,t))}\left(1+\frac{i\Delta t}{2}U(1)\right)^{-1}\left(1+\frac{i\Delta t}{2}\bar{U}_{m_1'}(1)\right)^{-1}\\ &\quad\times\left(1+\frac{i\Delta t}{2}U(2)\right)^{-1}\left(1+\frac{i\Delta t}{2}\bar{U}_{m_2'}(2)\right)^{-1}\left(1-\frac{i\Delta t}{2}\bar{U}_{m_2'}(2)\right)\left(1-\frac{i\Delta t}{2}U(2)\right)\\ &\quad\times\left(1-\frac{i\Delta t}{2}\bar{U}_{m_1'}(1)\right)\left(1-\frac{i\Delta t}{2}U(1)\right)\sum_{m_1'',m_2'',M''}e^{-i\Delta t/2(V^{M}_{m_1'm_2',m_1''m_2''}(1,2)+W^{M'M''}_{m_1'm_2',m_1''m_2''}(1,2,t))}P^{M''S}_{m_1''m_2''}(t),\end{aligned} \qquad (19)$$

where $U(i)=K(r_i)+N(r_i,\theta_i)$ and $\bar{U}_{m_i}(i)=\bar{K}(r_i,\theta_i)+A_{m_i}(r_i,\theta_i)$.

For the extraction of ionization cross sections, we begin by defining asymptotic reduced wave functions. For the target channels (i.e., $M=S=0$),

$$\hat{P}^{MS}_{m_1m_2}(r_1,\theta_1,r_2,\theta_2)=P^{MS}_{m_1m_2}(r_1,\theta_1,r_2,\theta_2,t\to\infty)-\mathcal{L}\bar{P}^{MS}_{m_1m_2}(r_1,\theta_1,r_2,\theta_2,\tau\to\infty) \qquad (20)$$

and for all other channels

$$\hat{P}^{MS}_{m_1m_2}(r_1,\theta_1,r_2,\theta_2)=P^{MS}_{m_1m_2}(r_1,\theta_1,r_2,\theta_2,t\to\infty), \qquad (21)$$

where the overlap function

$$\mathcal{L} = \sum_{m_1,m_2} \int_0^\infty dr_1 \int_0^\pi d\theta_1 \int_0^\infty dr_2 \int_0^\pi d\theta_2 \bar{P}^{MS}_{m_1m_2}(r_1,\theta_1,r_2,\theta_2,\tau \to \infty) P^{MS}_{m_1m_2}(r_1,\theta_1,r_2,\theta_2,t \to \infty) \tag{22}$$

removes all ground-state character and thus prevents ground-state correlation from appearing as double ionization. The total single ionization probability, for a given velocity and impact parameter, is given by

$$\begin{aligned}\mathcal{P}_1(v,b) = 2\sum_M \sum_{m,m'} \sum_{n,l} \Bigg(& \int_0^\infty dr_2 \int_0^\pi d\theta_2 \left| \int_0^\infty dr_1 \int_0^\pi d\theta_1 P_{nlm}(r_1,\theta_1) \hat{P}^{MS}_{mm'}(r_1,\theta_1,r_2,\theta_2) \right|^2 \\ & - \sum_{n',l'} \left| \int_0^\infty dr_1 \int_0^\pi d\theta_1 \int_0^\infty dr_2 \int_0^\pi d\theta_2 P_{nlm}(r_1,\theta_1) P_{n'l'm'}(r_2,\theta_2) \hat{P}^{MS}_{mm'}(r_1,\theta_1,r_2,\theta_2) \right|^2 \Bigg).\end{aligned} \tag{23}$$

The total double ionization probability is given by

$$\begin{aligned}\mathcal{P}_2(v,b) = & \sum_M \sum_{mm'} \int_0^\infty dr_1 \int_0^\pi d\theta_1 \int_0^\infty dr_2 \int_0^\pi d\theta_2 |\hat{P}^{MS}_{mm'}(r_1,\theta_1,r_2,\theta_2)|^2 - \mathcal{P}_1(v,b) \\ & - \sum_M \sum_{m,m'} \sum_{n,l} \sum_{n',l'} \left| \int_0^\infty dr_1 \int_0^\pi d\theta_1 \int_0^\infty dr_2 \int_0^\pi d\theta_2 P_{nlm}(r_1,\theta_1) P_{n'l'm'}(r_2,\theta_2) \hat{P}^{MS}_{mm'}(r_1,\theta_1,r_2,\theta_2) \right|^2 .\end{aligned} \tag{24}$$

We note that the total single ionization probability of Eq. (23) is the sum of single ionization probabilities for all *nlm* states of the molecular ion. The bound single particle orbitals, $P_{nlm}(r,\theta)$, found in Eqs. (23) and (24) are obtained by direct diagonalization of the one-electron Hamiltonian,

$$H_m(r,\theta) = K(r) + \bar{K}(r,\theta) + A_m(r,\theta) + N(r,\theta). \tag{25}$$

Finally, the total cross section for both single and double ionization is given by

$$\sigma(v) = 2\pi \int_0^\infty \mathcal{P}(v,b) b db. \tag{26}$$

III. RESULTS

The time-dependent close-coupling method was used to calculate the ground state ($M=S=0$) of H_2 at $R_t=1.4$ using Eq. (16). We employed a $192\times16\times192\times16$ point lattice with a uniform mesh spacing of $\Delta r_1=\Delta r_2=0.20$ and $\Delta\theta_1=\Delta\theta_2=0.0625$. For the five coupled channels listed in Table I and $\lambda_{max}=4$ in Eq. (11), a fully converged ground state of H_2 on the lattice was obtained after 500 time steps with $\Delta\tau=0.02$ and a lattice energy of −52.7 eV. For $R_t=0.0$ we obtain a lattice energy of −81.1 eV, where the infinite lattice limit is −79.0 eV [25].

TABLE I. Ground state coupled channels for H_2.

Channel	m_1	m_2	M	S
1	0	0	0	0
2	+1	−1	0	0
3	−1	+1	0	0
4	+2	−2	0	0
5	−2	+2	0	0

The time-dependent close-coupling method was then used to calculate ionization cross sections for $p+H_2$ collisions at an incident energy of 1.0 MeV using Eq. (7). We again employed a $192\times16\times192\times16$ point lattice with a uniform mesh spacing of $\Delta r_1=\Delta r_2=0.20$ and $\Delta\theta_1=\Delta\theta_2=0.0625$. For the 19 coupled channels listed in Table II and $\lambda_{max}=2$ in Eqs. (12) and (13), the total wave function for H_2 was propagated

TABLE II. Scattering state coupled channels for H_2.

Channel	m_1	m_2	M	S
1	0	0	0	0
2	+1	−1	0	0
3	−1	+1	0	0
4	+2	−2	0	0
5	−2	+2	0	0
6	0	+1	+1	0
7	+1	0	+1	0
8	+2	−1	+1	0
9	−1	+2	+1	0
10	0	−1	−1	0
11	−1	0	−1	0
12	+1	−2	−1	0
13	−2	+1	−1	0
14	0	+2	+2	0
15	+2	0	+2	0
16	+1	+1	+2	0
17	−2	0	−2	0
18	0	−2	−2	0
19	−1	−1	−2	0

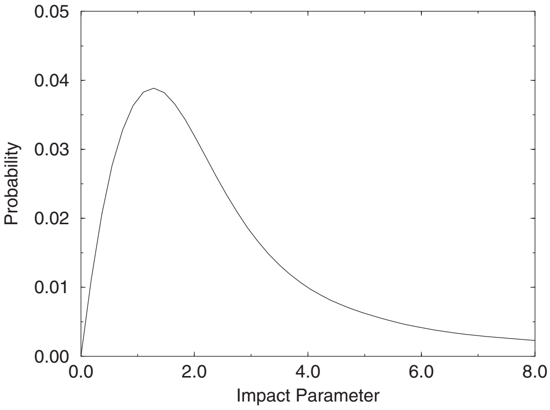

FIG. 1. Weighted probability $b\mathcal{P}_1(v,b)$ for single ionization in $p+H_2$ collisions at an incident energy of 1.0 MeV/amu. The impact parameter (b) is in atomic units.

for 3150 time steps with $\Delta t=0.005$. With a velocity of $v=6.35$, the proton moves from $z_i=-25.0$ to $z_f=+75.0$ at various impact parameters parallel to the internuclear axis ranging from $b=0.2$ to 9.0. The weighted single ionization probability, $b\mathcal{P}_1(v,b)$, from Eq. (23) is shown in Fig. 1 peaking at $b=1.2$. The weighted double ionization probability, $b\mathcal{P}_2(v,b)$, from Eq. (24) is shown in Fig. 2 peaking at $b=0.6$. Integrating the weighted probabilities using Eq. (26) yields a single ionization cross section of 21.5 Mb and a double ionization cross section of 62.0 kb.

As a test of the importance of electron correlation in the double ionization process, we carried out additional calculations in which electron-electron interaction operator of Eq. (11) was set to zero in the time-dependent close-coupling equations of Eq. (7). We found that the single ionization weighted probability at an impact parameter of 0.60 went from 2.92×10^{-2} to 3.11×10^{-2}, while the double ionization weighted probability went from 2.31×10^{-4} to 1.40×10^{-3}. The factor of six difference in the double ionization probabilities indicates the importance of including the full interaction between the two ejected electrons.

The ratio of double ionization to single ionization for $p+H_2$ collisions at 1.0 MeV is found to be 0.3%. The time-dependent close-coupling value is in reasonable agreement with time-of-flight beam-cell experiments which found 0.2% [23,24]. The present calculations assume the projectile moves in an xz plane parallel to the internuclear axis, while the experimental measurements average over all alignments of the projectile with the internuclear axis. An orientation average calculation is a much larger computational challenge.

For a projectile moving perpendicular to the internuclear axis, the electron-projectile interaction operators of Eqs. (12) and (13) need to be derived for projectile motion in the xy plane. As found before for $p+H_2^+$ collisions [26], the total cross section of Eq. (26) is modified to include impact parameters b and ϕ_b, calling for a full plane instead of just a line of projectile trajectories. In the studies of one-electron charge transfer in $p+H_2^+$ collisions at various projectile velocities and internuclear separations [26], the cross sections for perpendicular alignment were found to be 20% to 100% larger than the cross sections for parallel alignment. It will be interesting to see how much the single and double ionization cross sections for $p+H_2$ collisions change when the computationally more challenging calculations for the perpendicular alignment are carried out in the future.

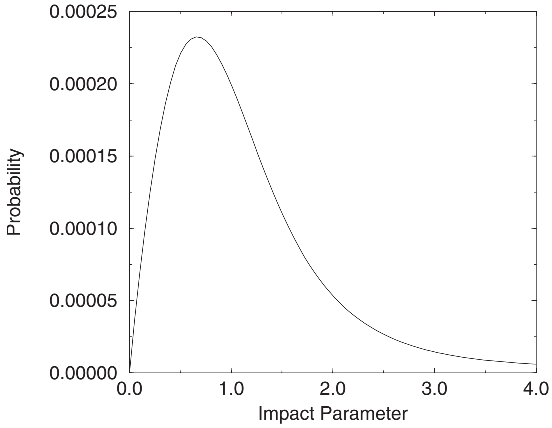

FIG. 2. Weighted probability $b\mathcal{P}_2(v,b)$ for double ionization in $p+H_2$ collisions at an incident energy of 1.0 MeV/amu. The impact parameter (b) is in atomic units.

IV. SUMMARY

A nonperturbative time-dependent close-coupling method has been developed to treat double ionization processes in fast bare-ion collisions with homonuclear diatomic molecules. This particular quantal three-body breakup problem is especially difficult due to the nonspherical field of the molecular ion and the strong multipolar interaction of the passing bare ion. A test calculation is then made for $p+H_2$ collisions at 1.0 MeV and reasonable agreement is found between theory and experiment for the ratio of double to single ionization.

In the future, we plan to apply the newly developed time-dependent close-coupling method to further $p+H_2$ collision studies. As found before for $\gamma+H_2$ collision studies [27], the time-dependent close-coupling method can be applied to study energy and angle differential cross sections for the ejected electrons as a function of internuclear orientation and separation. In support of experimental efforts, we also plan to study other ion-molecule collisions, including antiprotons on H_2 and alpha particles on Li_2.

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