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Orientation dependence in electron capture to arbitrary projectile *n* states from molecular hydrogen

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The dependence on the orientation of the intermolecular axis of cross sections for electron capture from molecular hydrogen by bare ions is calculated in a two-center approximation, which ignores multiple scattering between atomic centers and is compared to experiment. Electron-capture cross sections are calculated as functions of both projectile principal quantum number *n* and molecular orientation angles. Orientation-averaged cross sections are compared with recent measurements of $O^{8+}+H_2$ at $E=8$, 10, 12.5, 16, and 20 MeV. Comparisons are also made between our calculations for electron capture into projectile *n* states by H^+ from H_2 and the available calculation for *ns* states from $E=50$ keV to 5 MeV. The orientation-dependence differential in the molecular-orientation angle is studied in dissociative ionization and excitation of the molecular ion following single-electron capture from H_2 using a two-step independent-electron model. The calculated orientation dependence is in qualitative agreement with preliminary experimental observations as a function of the orientation angle done with O^{8+} ions at $E=10$ MeV, where capture to $n>1$ state is significant.

I. INTRODUCTION

Single-electron capture from molecular hydrogen by heavy-ion projectiles at high collision velocities has received increasing experimental and theoretical attention in recent years [1–6]. The capture cross section as a function of orientation of the molecular axis connecting the two nuclei is of particular interest, since it provides direct information on how the two atomic centers in the molecule respond to the external interactions and produce various two-center interference patterns according to the relative geometry and collision velocities. Although such a two-center interference effect was first defined some time ago by Tuan and Gerjuoy [7], it was not until recently that calculations for molecular-orientation effects in electron capture from molecular hydrogen began [3, 4, 6]. In a previous paper [6] (here-after referred to as I), an impact-parameter treatment is formulated to study scattering from a diatomic molecule and applied to H^+ and He^{2+} incident on H_2. Electron capture from H_2 to the 1*s* projectile state was then calculated in the Oppenheimer-Brinkman-Kramers [8] (OBK) approximation at high collision velocities v, for a fixed molecular orientation. One advantage of using the impact-parameter representation is that one may consider multiple-electron processes such as transfer excitation by using the independent-electron approximation where single transition probabilities are simply multiplied to form a multiple transition probability.

For projectiles with nuclear charge Z, when $Z/v>1$, capture to excited states becomes dominant. At intermediate velocities, Shingal and Lin [4] have applied atomic orbital expansion for capture from H_2 by He^{2+}, where capture into $n=2$ prevails. However, to our knowledge, there is no calculation explicitly giving orientation dependence for arbitrary *n* (here we sum over substate quantum numbers *l* and *m*) states at high collision velocities. Ray and Saha did the first OBK calculation [9] for electron capture to projectile *ns* states in $p+H_2$ collisions at high velocities. But their calculation averaged out the orientation dependence. Here we present a calculation based on a simple extension of our previous general study to obtain orientation dependence for electron capture to arbitrary *n* states. In high velocity ion-atom collisions, electron capture mainly populates the *ns* projectile states. For example, in $p+H(1s)$ collisions [10], capture to *ns* is predicted to be more than 90% of the total *n* at 1 MeV, and more than 98% at 2 MeV in atoms. We shall consider this question in H_2 molecules. The OBK calculation for total *n* is simpler than the corresponding calculation for *ns*. Thus it is convenient to do a calculation for capture into arbitrary *n* states and compare to experiments where sums over all final projectile states are taken.

In this paper we calculate orientation-dependent single capture cross sections for O^{8+} on H_2 at MeV energies where significant contributions occur for capture into $n>1$ states. An ongoing measurement [11] of orientation dependence in total dissociative excitations and dissociative ionizations following single-electron capture from H_2 by O^{8+} at 10 MeV is providing the first experimental observation of molecular-orientation dependence in electron capture by heavy ions from molecular hydrogen. In Sec. III we compare to preliminary data from this experiment.

II. SINGLE CAPTURE TO ARBITRARY *n* STATES

In I we discussed [6] a general procedure to treat electron capture from a homonuclear diatomic molecule at high velocities in the impact-parameter formulation. By neglecting nuclear motion of a diatomic molecule and rescattering between each center, the scattering amplitude

$a_M(\mathbf{B})$ is a superposition of individual scattering amplitudes from each atomic center of the molecule and the probability is given by

$$P_M=|a_M|^2=|a_1|^2+|a_2|^2+2\,\mathrm{Re}(a_1^* a_2 e^{i\delta}) \,. \tag{1}$$

The individual amplitudes a_1 and a_2 carry a phase difference $\delta=\alpha_z\rho_z$, where α_z (ρ_z) is the projection of momentum transfer (orientation axis) along the incident beam. For electron capture [12], $\alpha_z \cong v/2-\Delta E/v$, where $\Delta E=E_f-E_i$. We use the two-center Weinbaum [13] wave function for H_2,

$$\Phi_M(1,2)=N_M\{\phi^a(1)\phi^b(2)+\phi^a(2)\phi^b(1)$$
$$+c[\phi^a(1)\phi^a(2)+\phi^b(1)\phi^b(2)]\} \tag{2}$$

where the two hydrogen nuclei are formally labeled as a and b, having two electrons (1 and 2) attached to them. In Eq. (2), ϕ is a 1s hydrogenic orbital with effective charge Z_M and c is a constant. Supposing electron 1 is captured to the projectile and electron 2 ends up in the ground ${H_2}^+$ state (nondissociative), the ionic wave function is then taken as a linear combination of 1s hydrogenic orbitals centered on a and b with a different effective charge Z_I,

$$\Phi_I(2)=N_I[u^a(2)+u^b(2)] \,. \tag{3}$$

In the simple OBK approximation, we obtained the probability for capturing one electron to $n=1$ projectile state from H_2 and leaving the other electron in the ground state of ${H_2}^+$, namely [6],

$$P^c_{n=1}(Z,\mathbf{B})=|N|^2\left[\frac{2}{v}\right]^2\frac{(ZZ_M)^5}{(Z_M^2+\alpha_z^2)^4}$$
$$\times[x_-^4K_2^2(x_-)+x_+^4K_2^2(x_+)$$
$$+2x_-^2x_+^2K_2(x_-)K_2(x_+)\cos(\alpha_z\rho_z)] \tag{4}$$

where $x_\pm=(Z_M^2+\alpha_z^2)^{1/2}|(\mathbf{B}\pm\boldsymbol{\rho}_\perp/2)|$ is a scaled distance corresponding to impact trajectory passing through each center. The z axis, passing through the midpoint of the molecular axis, is taken as $B=0$ trajectory. Here $\boldsymbol{\rho}_\perp$ is the projection of molecular-orientation axis perpendicular to the incident beam direction. The first two terms in the square brackets are due to contributions from each atomic center and the last term is due to interference.

In Eq. (4), $|N|^2$ may be interpreted as a shake probability for the uncaptured electron making a transition to a final state of ${H_2}^+$, here the ground ionic state. If we write the wave function for the uncaptured electron as either $\Phi_M^a(2)$ or $\Phi_M^b(2)$ [compare Eq. (2)],

$$\Phi_M^{a,b}(2)=N_M(1+c)\phi^{a,b}(2) \,, \tag{2$'$}$$

then N is given by

$$N=\langle\Phi_I(2)|\Phi_M^a(2)\rangle$$
$$=\langle\Phi_I(2)|\Phi_M^b(2)\rangle=N_MN_I(\Delta_{IM}+\chi_{IM})(1+c) \tag{5}$$

where

$$\begin{aligned}
N_M&=1/\{2[(1+c^2)(1+\Delta_M^2)+4c\Delta_M]\}^{1/2}\,,\\
\Delta_M&=\int\phi^{a*}(\mathbf{r})\phi^b(\mathbf{r})d\mathbf{r}\\
&=(1+Z_M\rho+\tfrac{1}{3}Z_M^2\rho^2)\exp(-Z_M\rho)\,,\\
N_I&=1/[2(1+\Delta_I^2)]^{1/2}\,,\\
\Delta_I&=\int u^{a*}(\mathbf{r})u^b(\mathbf{r})d\mathbf{r}\\
&=(1+Z_I\rho+\tfrac{1}{3}Z_I^2\rho^2)\exp(-Z_I\rho)\,,\\
\Delta_{IM}&=\int u^{a*}(\mathbf{r})\phi^a(\mathbf{r})d\mathbf{r}\\
&=\int u^{b*}(\mathbf{r})\phi^b(\mathbf{r})d\mathbf{r}\\
&=8(Z_IZ_M)^{3/2}/(Z_I+Z_M)^3\,,\\
\chi_{IM}&=\int u^{a*}(\mathbf{r})\phi^b(\mathbf{r})d\mathbf{r}\\
&=\int u^{b*}(\mathbf{r})\phi^a(\mathbf{r})d\mathbf{r}\\
&=\frac{8(Z_IZ_M)^{3/2}}{\rho\nu^3}[Z_I(\rho\nu-4Z_M)e^{-Z_M\rho}\\
&\qquad+Z_M(\rho\nu+4Z_I)e^{-Z_I\rho}]\,,\\
\nu&=Z_I^2-Z_M^2\,.
\end{aligned} \tag{6}$$

In our calculations we choose $Z_M=1.193$, $Z_I=1.4$, $c=0.256$, and $\rho=1.4$ a.u. The simple shake probability N^2 in this case is about 30%. This is consistent with a recent measurement (Table III of Ref. 1). One can similarly estimate shake probability for transition to other ${H_2}^+$ states after electron capture from H_2.

After integrating over impact parameter $\mathbf{B}$ in Eq. (4), the total capture cross section as a function of molecular-orientation angle θ_ρ is given by

$$\frac{d\sigma_{n=1}(Z)}{d(\cos\theta_\rho)}=|N|^2(2\sigma^A_{n=1}+\sigma_{12}) \tag{7}$$

where $\sigma^A_{n=1}$ is the OBK cross section for electron capture into the projectile ground state from a hydrogenic atom (with effective nuclear charge Z_M), namely,

$$\sigma^A_{n=1}=\frac{2^8(ZZ_M)^5}{5v^2(Z_M^2+\alpha_z^2)^5} \,. \tag{8}$$

By using the identity

$$\frac{x^2K_2(x)}{(Z_M^2+\alpha_z^2)^2}=\int d\boldsymbol{\alpha}_\perp\frac{2^4\pi e^{i\boldsymbol{\alpha}_\perp\cdot\mathbf{B}}}{(Z_M^2+\boldsymbol{\alpha}^2)^3} \tag{9}$$

the interference term σ_{12} may also be evaluated in close form

$$\sigma_{12}=\sigma^A_{n=1}[\tfrac{1}{192}y^5K_5(y)]\cos(\alpha_z\rho_z) \tag{10}$$

where $y=(Z_M^2+\alpha_z^2)^{1/2}\rho_\perp$.

As the projectile charge Z increases, capture from atoms into higher n becomes more important. In ion-atom collisions, it is known that, due to Fock's sum rules

[14, 15] for hydrogenic wave functions, there exists an analytical expression for OBK cross-section summing over all projectile substate quantum numbers (l,m). For capture from molecular hydrogen, Fock's sum rules can also be applied since the molecular T matrix T^M is connected to the atomic T matrix t^A through a phase factor, i.e., $T^M = t^A \cos[\boldsymbol{\alpha}\cdot(\boldsymbol{\rho}/2)]$. The phase factor, though depending on projectile principal quantum number n, may be approximately taken as independent of projectile substate quantum numbers (l and m). With this in mind, capture to an arbitrary projectile n state, summing over all substate quantum numbers l and m, can be written as

$$\frac{d\sigma_n(Z)}{d(\cos\theta_\rho)} = n^2 \frac{d\sigma_{n=1}(Z/n)}{d(\cos\theta_\rho)} . \tag{11}$$

Orientation-dependent cross sections can therefore be calculated for an arbitrary n state. From Eq. (11), for large n or high v, we expect the well-known n^{-3} law for OBK cross section in ion-atom collision will also follow in ion-molecule collisions.

III. DISSOCIATIVE EXCITATION AND IONIZATION

Molecular dissociation caused by an external force has been a long-standing subject, especially for dissociation induced by electron-impact collisions [16]. Such processes are generally complicated due to the coupling among internal molecular motions and the external interactions. However, the situation is a little simpler when considering dissociation induced by fast heavy ions, such as we study here.

In a fast collision between a bare heavy ion and a molecular hydrogen, if one of the electrons is captured or stripped off, the other may end up in either the stable ground state or the excited repulsive states of the hydrogen molecular ion. When molecular excitation occurs (i.e., transfer excitation or transfer ionization), the molecular ion will dissociate and produce two fragments (two protons or one proton plus one hydrogen atom) leaving each other in a direction closely related to the orientation of molecular axis. Since the collision time is much shorter than characteristic times for nuclear motions in the molecular hydrogen, the departing fragments will travel away from each other in the direction aligned with the initial orientation of the molecular hydrogen to a good approximation. This makes it possible to compare the orientation dependence obtained in the preceding section, where the hydrogen molecular ion is in the nondissociative stable ground state, with the direct observations of dissociation fragments.

For this transfer excitation and transfer ionization we introduce an independent electron model treating capture and dissociation as two independent processes. First direct single capture of one of the electrons from H_2 into a projectile leaves the other in the ground (nondissociative) state; subsequently the molecular hydrogen ion is excited to dissociative states by the same projectile. In the impact-parameter picture, we can write the total probability as a product of probabilities for each of the two processes, namely,

$$P(B) = P^c(B) P_f^{\mathrm{ex}}(B) \tag{12}$$

where P^c stands for the single capture probability and P_f^{ex} is the probability for excitation of $H_2{}^+$ to a particular state f (excluding elastic scattering). Orientation dependence can be caused by both single capture from H_2 and also by the subsequent excitation of $H_2{}^+$. In principle, ion-H excitation [17] could be computed in detail and applied to ion-$H_2{}^+$ excitation. Here we will deal with a simpler situation. In the observations [11] with which we compare there is a sum over all excited final $H_2{}^+$ states including continuum (i.e., transfer ionization). Using closure we can sum over final states and rewrite Eq. (12) as

$$P(B,v) = P^c(B,v)[1 - P_0(B,v)] \tag{13}$$

where $P_0(B,v)$ is the probability for elastic scattering between the projectile and the ground-state $H_2{}^+$ ion which is nondissociative.

Let us consider the scattering regions for single capture and elastic processes appearing in Eq. (13). At high collision velocities, elastic scattering usually takes place at impact parameters larger than the size of the target while electron capture occurs at much smaller distances. Our previous calculations [6] for probabilities of electron capture by protons (where capture to projectile ground state dominates) show $P^c(B)$ peaks at B values that correspond to the positions of the nuclei, i.e., $\mathbf{B} = \pm\boldsymbol{\rho}/2$ in Eq. (4). For beams passing the molecular axis, the probability $P(B)$ peaks at $B=0$; for beams perpendicular to the axis, it peaks parallel to $B = \rho/2 \approx 0.7$ a.u. On the other hand, for elastic scattering at relatively high velocities, we take $P_0(B=0.7) \approx P_0(B=0)$, roughly approximating $P_0(B,v) \approx P_0(v)$, an energy-dependent constant. Consequently, orientation dependence in dissociation following electron capture dominantly comes from the electron-capture channel. According to an estimate from experimental data [1], $P_0 \approx 30\%$ for the system we consider (i.e., consistent with the shake picture in Sec. II). Hence here we do not differentiate orientation dependence in single capture and orientation dependence in total molecular dissociation at high velocities.

In concluding this section, we remark that orientation dependence for processes other than electron capture can also be studied. In fact, calculation of angular distribution in direct excitation of $H_2{}^+$ by electrons and protons was done quite some time ago [18]. Observations of orientation dependence in dissociation of $H_2{}^+$ following ionization of H_2 by protons have also been carried out recently [19]. We also note that pure ionization of H_2 by proton impact at high velocities (where first Born approximation is valid) provides relatively little orientation dependence [20] (typically 20%) as compared to the much larger dependence in electron capture reported in I. For these systems, in Eq. (1) $\delta = \alpha_z \rho_z \approx (\Delta E/2v)\rho_z \ll 1$ for ionization so that there is relatively little variation of the ionization cross sections with molecular orientation.

IV. RESULTS AND DISCUSSION

In the following we concentrate on presenting calculations for electron capture by O^{8+} ions with H_2. For this

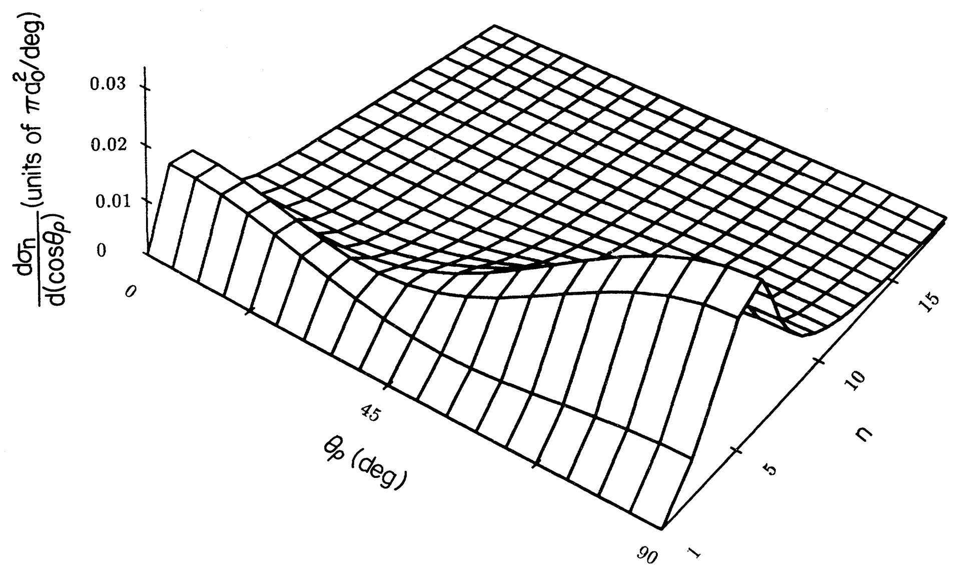

FIG. 1. Cross sections for single-electron capture from H_2 by O^{8+} as functions of molecular-orientation angle θ_p and projectile principal quantum number n at $E = 10$ MeV. The discrete n have been connected to guide the eye. Here $n = 4$ has the largest population.

system there have not been many experiments or theoretical calculations at higher energies. It is also the only system in which an experiment has been done observing the orientation dependence discussed in the preceding section. We also briefly compare our results for $p + H_2$ collisions with those of Ray and Saha [9].

Let us first consider calculations of the orientation dependence at 10 and 16 MeV for single capture to projectile $n = 1$ to 19. Figures 1 and 2 show both the orientation dependence and population of each n state. At 10 MeV, capture into $n = 4$ has the largest cross section. At 16 MeV, $n = 3$ is dominant. In both figures the n^{-3} law holds for $n > 10$, typical of OBK approximation in ion-atom collisions. The orientation dependence varies strongly with n since the interference is mainly determined by the phase factor $\cos(\alpha_z \rho_z)$ which is a function of n. It is well known OBK cross sections are generally a factor of 3–20 bigger than the true cross sections. Nevertheless, in ion-atom collisions, OBK cross sections usually have the same energy dependence as the measured

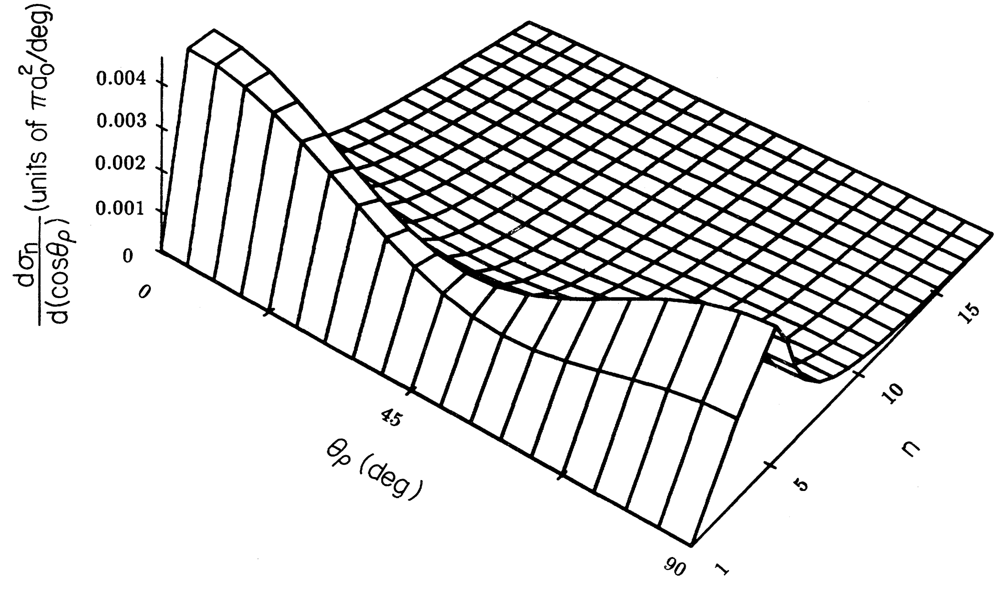

FIG. 2. Same as Fig. 1 except at $E = 16$ MeV. The largest populated state is now shifted to $n = 3$.

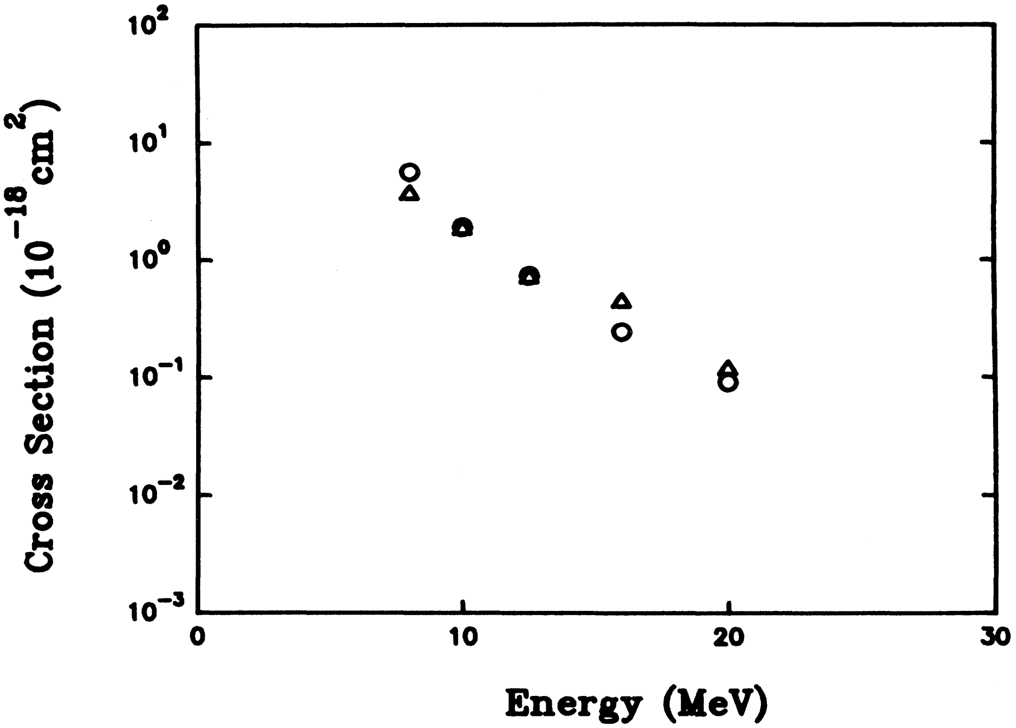

FIG. 3. Total single-capture cross sections (summed over n and orientation angles) at $E=8$, 10, 12.5, 16, and 20 MeV. △: experimental results from Ref. 1; ○: calculated OBK cross sections (multiplied by 0.1).

cross sections. In Fig. 3, we compare orientation-averaged cross sections with recent experimental measurement [1] at 8, 10, 12.5, 16, and 20 MeV. The calculated OBK cross sections shown in the figure have been simply reduced by an overall factor of 10.

In order to compare scattering of H_2 with 2H, we have evaluated the cross-section ratio $R_n=\sigma_n(H_2)/[2\sigma_n(H)]$ as a function of both n and impact energy. For a fixed velocity (or impact energy), this ratio varies strongly with n. This is obvious since both v and n affect the phase term in Eq. (10). In $p+H_2$ collisions, comparing our numerical results of $\sigma_n(H_2)$ at energies between 50 keV and 5 MeV with the corresponding $\sigma_{ns}(H_2)$ cross sections [i.e., capture to H(ns) states] of Ray and Saha [9], we found that cross-section ratio R_n follows the same energy dependence as $R_{ns}=\sigma_{ns}(H_2)/2\sigma_{ns}(H)$. Also, $\sigma_{ns}(H_2)$ is about 90% of $\sigma_n(H_2)$ at 1 MeV and more than 98% at 2 MeV, very similar to $p+H$ collisions. It is also useful to consider total cross-section ratio $R=\sum_n\sigma_n(H_2)/[2\sum_n\sigma_n(H)]$, for high-$Z$ projectiles where capture into larger n prevails. Contrary to R_n, R is only dependent on impact velocity and gives the influence of interference at each energy. We find for O^8+H_2 R is close to 1 (within 10%) at energies between 8 and 16 MeV, although R_n can vary from as big as 1.4 (for $n=1,2$) down to smaller than 1 (for larger n) in this energy range. We also find $R\approx 1.2$ at $E=20$ MeV.

We now turn to the dissociation of a molecular hydrogen ion subsequent to capture. In Fig. 4 we compare the calculated orientation dependence (obtained by adding up

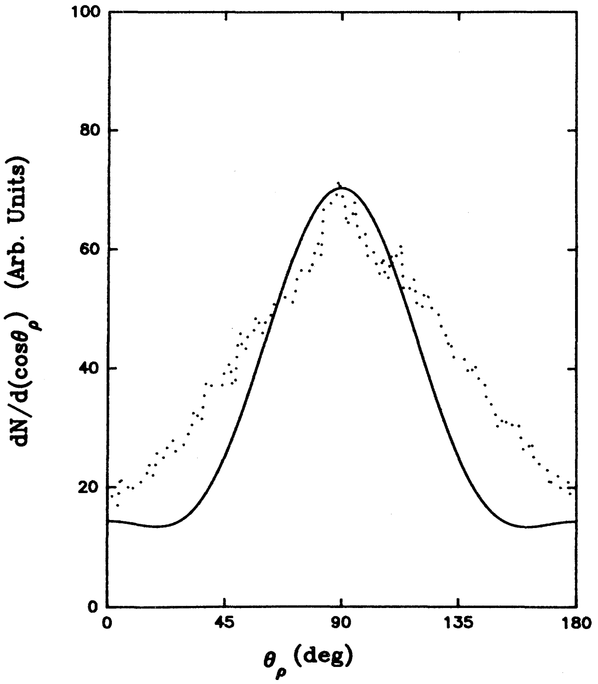

FIG. 4. Orientation dependence in dissociation of $H_2{}^+$ following single-electron capture from H_2 by O^{8+} ions at $E=10$ MeV. Dots: preliminary experimental data (yield, N, of all dissociation products as function of orientation angle θ_p) from Ref. 11; solid line: calculated OBK cross section normalized to experiment.

all cross sections in Fig. 1 and normalizing to experiment) with the preliminary result of a recent experiment of Cheng *et al.* [11]. In the experiment, the total dissociative ionization and excitation events are collected for a fixed molecular orientation. Both the position and the height to the base of the peak are in agreement with our simple OBK calculation, although the calculated shoulders are a little sharper than those observed. This comparison between theory and experiment provides the first direct test of a molecular-orientation effect in electron capture by heavy ions in collision with molecular hydrogen. The discrepancy with respect to experimental data may be partially attributed to the crude approximation of setting $P_0(\mathbf{B},v)\approx P_0(v)$, i.e., neglecting orientation dependence from the excitation part.

Comparisons with experiment in both total cross sections and orientation-dependent cross sections seem to support our two-step model. Yet a number of limitations may stimulate further investigation. First, the validity of first-order perturbation theory is questionable for $Z/v\approx 1$, although for the dominant excited states $(Z/n)/v$ is less than one in our studies. It would be more convincing to compare to experiments with lower-Z projectiles or high-Z projectiles at higher energies (above 1 MeV/u). Second, for electron capture to higher n excited states, it has been argued [21] that any first-order theory, such as the OBK theory, should not be applied even in ion-atom collisions. While we favor our use of final-state excitation by independent scattering from the projectile described in Sec. III, it may be possible to describe this excitation at least in part by final-state rearrangement of the molecule after capture as described in Sec. II. It is also possible that higher-order theories introduce additional phase terms in the capture amplitude that we have not included. There is evidence [22] that, even at not too high velocities, rescattering between molecular nuclei is not negligible. Further studies are needed in this respect.

In summary, we have calculated electron capture into arbitrary n states of a bare projectile from H_2 as a function of molecular orientations in the OBK approximation. Using a simple two-step independent-electron model, calculated orientation dependence is found to be in qualitative agreement with the observations in dissociation of $H_2{}^+$ following single-electron capture from H_2 by O^{8+} ions at 10 MeV.

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[1] S. Cheng, C. L. Cocke, E. Y. Kamber, C. C. Hsu, and S. L. Varghese, Phys. Rev. A **42**, 214 (1990).
[2] W. Schwab, G. B. Baptista, E. Justiniao, R. Schuch, H. Vogt, and E. W. Weber, J. Phys. B **20**, 2825 (1987).
[3] N. C. Deb, A. Jain, and J. H. McGuire, Phys. Rev. A **38**, 3769 (1988).
[4] R. Shingal and C. D. Lin, Phys. Rev. A **40**, 1302 (1989).
[5] L. Meng, C. O. Reinhold, and R. E. Olson, Phys. Rev. A **40**, 3637 (1989).
[6] Y. D. Wang, J. H. McGuire, and R. D. Rivarola, Phys. Rev. A **40**, 3673 (1989).
[7] T. F. Tuan and E. Gerjuoy, Phys. Rev. **117**, 756 (1960).
[8] J. R. Oppenheimer, Phys. Rev. **31**, 349 (1928); H. C. Brinkman and H. A. Kramers, Proc. Acad. Sci. Amsterdam **33**, 973 (1930).
[9] P. P. Ray and B. C. Saha, Phys. Lett. **71A**, 415 (1979); P. P. Ray and B. C. Saha, Phys. Rev. A **23**, 1807 (1981).
[10] N. C. Sil, B. C. Saha, H. P. Saha, and P. Mandal, Phys. Rev. A **19**, 655 (1979).
[11] S. Cheng, C. L. Cocke, V. Frohne, E. Y. Kamber, and S. L. Varghese, Nucl. Instrum. Methods (to be published).
[12] M. R. C. McDowell and J. P. Coleman, *Introduction to the Theory of Ion-Atom Collisions* (North-Holland, Amsterdam, 1970), Chap. 8.
[13] S. Weinbaum, J. Chem. Phys. **1**, 593 (1933).
[14] V. Fock, Z. Phys. **98**, 145 (1935).
[15] J. Eichler and F. T. Chan, Phys. Rev. A **20**, 104 (1979).
[16] J. W. McConkey, S. Trajmar, and G. C. M. King, Comments At. Mol. Phys. **22**, 17 (1988).
[17] M. R. C. McDowell and J. P. Coleman, Ref. 12, Chap. 4.
[18] R. N. Zare, J. Chem. Phys. **47**, 204 (1967).
[19] A. K. Edwards (private communication).
[20] Y. D. Wang and J. H. McGuire (unpublished).
[21] L. Dube and J. Briggs, J. Phys. B **14**, 4593 (1981).
[22] P. Hvelplund and A. Andersen, Phys. Scr. **26**, 375 (1982).