

## Argand diagram representation of orbiting resonance in proton-transfer collision

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Dynamic resonance in atom-diatom molecule collisions has been relatively well studied compared to orbiting resonance. We discuss orbiting resonance on reactive scattering involving proton (charge) transfer. Resonance structure is predicted to exist at forward-scattering angles in both the state-to-state angular distribution and the Argand diagram for the proton-transfer collision system of  $\text{He} + \text{H}_2^+ \rightarrow \text{HeH}^+ + \text{H}$ . The present study demonstrates the possibility of orbiting resonance particularly in proton (charge) -transfer reaction involving atom-diatom molecule systems.

### I. INTRODUCTION

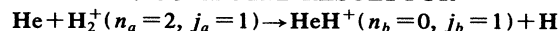
An extensive review of various types of resonance scattering was presented by Lane.<sup>1</sup> One of the areas of resonance scattering not covered in that review is the atom-diatom molecule collision, where resonance has recently been a subject of great interest. Numerous quantum-mechanical studies<sup>2-4</sup> of resonance have been presented in this area. However, a relatively small number of three-dimensional quantum-mechanical studies of resonant reactive scattering for atom-diatom molecule systems are presently available. Three-dimensional quantum reactive scattering calculations are most appropriate for treating nonzero angular momentum (impact-parameter) collision. The product rotational state distribution of the  $\text{F} + \text{H}_2$  system was observed by Polanyi and Woodall<sup>5</sup> to peak at a relatively high rotational angular momentum value of the product molecule. This means that transferred angular momenta in the reaction are definitely nonzero. Thus, one-dimensional (1D) quantum-mechanical approaches are not applicable to systems in which noncollinear collision dominates.

The exact three-dimensional (3D) quantum-mechanical study of Schatz and Kuppermann<sup>2(a)</sup> revealed evidence of dynamic resonance (internal excitation) for  $\text{H} + \text{H}_2$  reactive scattering. Walker, Stetchel, and Light<sup>3</sup> also presented a similar finding for the same system. Wyatt and co-workers<sup>4</sup> reported Feshbach dynamic resonance studies using a 3D  $j_z$ -conserving approximate method. Some review articles concerning the resonance scattering of the atom-diatom molecular systems have appeared.<sup>2(b),4(b)</sup> Experimental studies of note are various molecular-beam measurements.<sup>6-9</sup> In particular, Sparks *et al.*<sup>6</sup> and Hayden<sup>7</sup> suggest the presence of resonance scattering from their molecular-beam measurements of the  $\text{F} + \text{H}_2$  system.

Many of the one- to three-dimensional quantum-mechanical studies predict dynamic resonance in the transition-state region of the potential surface for the atom-diatom molecule system. Earlier we<sup>10</sup> presented a study of dynamic resonance involving electron-diatom

molecule systems, using an Argand diagram representation.<sup>11</sup> Our prime interest here is to explore yet another type of resonant reactive scattering without internal excitation; the possibility of orbiting resonance in atom-diatom molecule systems involving proton (charge) transfer. In this study, we emphasize the structures of the Argand diagrams and state-to-state reactive scattering angular distributions, in order to discuss the presence of orbiting resonance.

### II. COMPUTED RESULT FOR



We employ the potential-energy surface of Kuntz<sup>12</sup> and the potential parameters of Chapman and Hayes<sup>13</sup> for  $\text{HeH}^+$ . The DWBA (distorted-wave Born approximation) method that we employ for the present calculation is that of Suck Salk.<sup>14,15</sup> For other DWBA methods, we refer the readers to a recent study of Halvick *et al.*<sup>16</sup> We consider the DWBA that uses only the unperturbed diatomic molecular wave functions for both the entrance and exit channels. Accordingly the distorting potentials to be used are elastic. For this reason, we stress only the validity of relative cross sections.<sup>17</sup> The DWBA is expected to be accurate at low collision energies for weakly coupled systems. Relative translational energy in the  $\text{He} + \text{H}_2^+$  arrangement is higher than the value in the final  $\text{H} + \text{HeH}^+$  arrangement. Thus our calculated results are expected to be only qualitatively accurate. As is well known in nuclear physics,<sup>18</sup> DWBA treatments enable us to examine the possibility of orbiting resonance(s) in both the initial and final arrangement channels, or in one of the two arrangement channels. Indeed, such a DWBA application<sup>18</sup> has resulted in the correct prediction of orbiting resonances in nuclear heavy-ion reactions, in agreement with observation.

Figure 1 shows the DWBA predicted excitation function (cross section as a function of collision energy) for the low-lying rotational state transition of the charge (proton) -transfer system,  $\text{He} + \text{H}_2^+(n_a=2, j_a=1) \rightarrow \text{HeH}^+(n_b=0, j_b=1) + \text{H}$ . Here  $n_a$  and  $n_b$  are the vi-

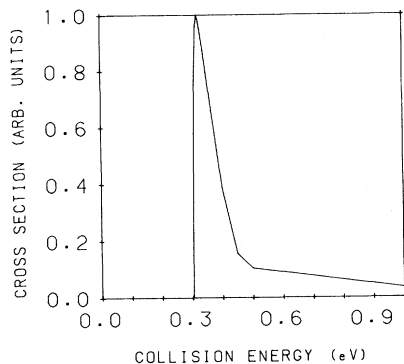


FIG. 1. Excitation function (total cross section as a function of collision energy) for  $\text{He} + \text{H}_2^+(n_a=2, j_a=1) \rightarrow \text{HeH}^+(n_b=0, j_b=1) + \text{H}$ . It is normalized at the resonance energy of 0.32 eV.

brational quantum number of the ionic molecules  $\text{H}_2^+$  and  $\text{HeH}^+$ , respectively, and  $j_a$  and  $j_b$  are the rotational quantum numbers corresponding to the ionic molecules. The predicted excitation function shows a peak at the incident collision (relative translational) energy of 0.32 eV.

In Fig. 2, we show the state-to-state reactive scattering angular distribution that enables us to examine the cause of this peak. Here we note that the oscillatory structure of the predicted angular distribution at the forward-scattering angles of  $\theta_{\text{c.m.}} = 5^\circ$  and  $\theta_{\text{c.m.}} = 25^\circ$  (with  $\theta_{\text{c.m.}}$  the center of mass angle) coincides well with that of  $|P_L(\theta)|^2$ , the Legendre polynomial of order  $L$ , at the orbital angular momentum value of  $L_b = 12$  for the final (product) channel. The state-to-state angular distributions at other collision energies did not reveal the same characteristics. This is consistent with the computed

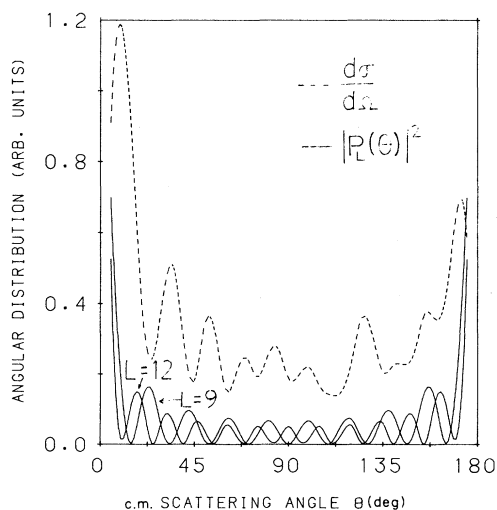


FIG. 2. State-to-state reactive scattering angular distribution at the incident collision energy of 0.32 eV and  $|P_{L_b}(\theta)|^2$  for  $L_b = 9$  and 12, respectively, in the final channel. They are in arbitrary units.

phase shift that showed a sudden increase by approximately  $\pi$  for the  $L_b = 12$  partial wave near the collision energy of 0.32 eV.

At the collision energy of 0.32 eV, this is consistent with the finding that the predicted  $L$  space (orbital angular momentum versus overlap integral) distribution for the system showed a peak at the product orbital angular momentum of  $L_b = 12$ . Due to the low-lying rotational reactive transitions from  $j_a = 1$  to  $j_b = 1$  in the state-to-state collision of interest, the maximum value of transferred angular momentum is  $j = 2$ . Thus, considering the angular momentum transfer  $j = L_a - L_b = j_b - j_a$  with  $L_b = 12$ , the partial waves of large-orbital angular momenta  $L_a$  in the initial (reactant) channel are expected to cause the forward-scattering peak. In general, large-orbital angular momenta contribute to forward scattering. Due to the small well depth and relatively large collision energy in the entrance channel, the computed distorted wave function did not show noticeably large enhancement in the region of the potential well. However, enhancement of the product channel distorted wave function was seen at  $L_b = 12$ . This is consistent with the peak value of  $L_b = 12$  in the  $L$ -space distribution.

The predicted state-to-state reactive scattering angular distribution is distinctively peaked at forward-scattering angles, showing the highest peak at the scattering angle of  $\theta_{\text{c.m.}} = 5^\circ$ , as shown in Fig. 2. The structure of the predicted angular distribution is relatively well characterized by  $|P_{L_b}(\theta)|^2$  with  $L_b = 12$ , particularly at forward-scattering angles. This indicates that there exists an orbiting resonance corresponding to the final (product) channel partial wave of relatively high-orbital angular momentum,  $L_b = 12$ , in addition to the contribution of direct scattering to the entire range of angular distribution. For a further check, in Fig. 3 we decompose the an-

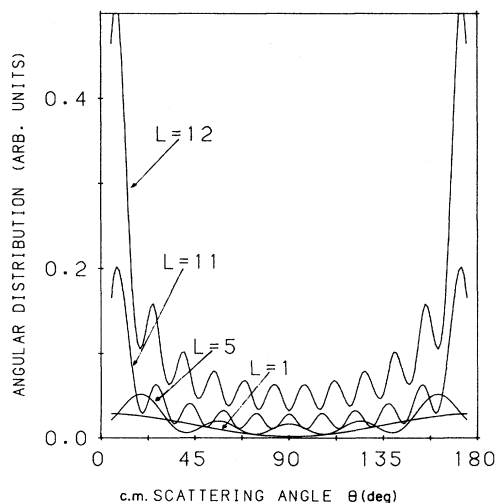


FIG. 3. State-to-state reactive scattering angular distributions corresponding to  $L_b = 1, 5, 11,$  and  $12$ , respectively, at the incident collision energies of 0.32 eV. They are in arbitrary units. The angular distribution here represents the contribution of only a single partial wave corresponding to each orbital angular momentum designated above in the final (product) channel.

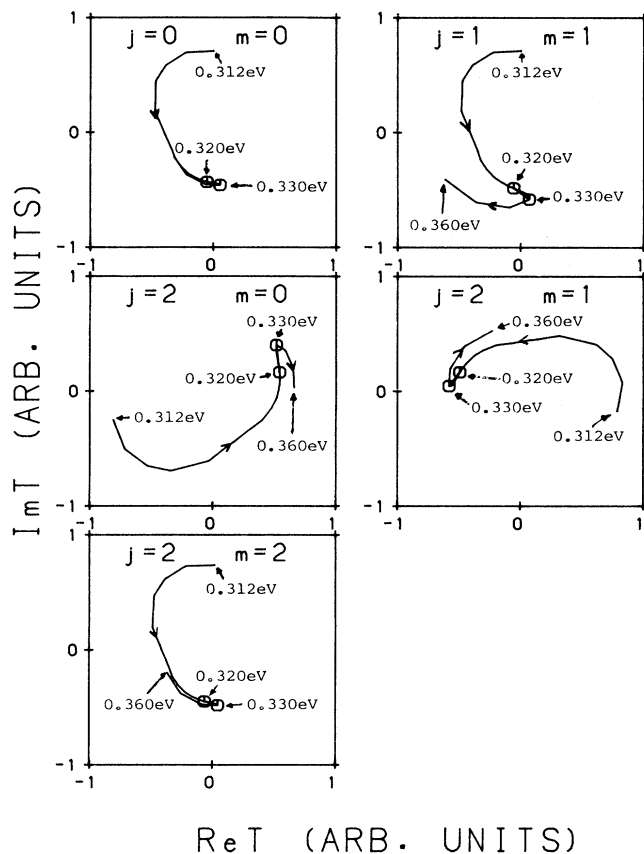


FIG. 4. Argand diagram representation of transition amplitude computed at  $\theta_{c.m.} = 5^\circ$  for the projection quantum numbers  $m$  corresponding to the transferred angular momenta of  $j=0$  and 2, respectively. Due to symmetry, Argand diagrams for the negative values of  $m$  are not shown here. Note that a turning point is seen at 0.33 eV.

gular distribution into contributions corresponding to each partial wave of  $L_b = 1, 5, 11,$  and  $12,$  respectively. As shown in the figure,  $L_b = 12$  yields the largest contribution to the magnitude of the angular distribution. Orbital angular momenta greater than  $L_b = 12$  (not shown) yielded a much smaller contribution.

To further confirm the presence of this resonance, we will examine the Argand diagram representation of the transition amplitude in order to show that the orbiting resonance at the product orbital angular momentum value of  $L_b = 12$  is indeed a consequence of orbiting motion associated with the quasibound triatomic system of  $\text{HeH}_2^+$ . We examine in Fig. 4 the Argand diagram representation of the  $T$  matrix computed at  $\theta_{c.m.} = 5^\circ$ . If

orbiting resonance occurs, the value of the transition amplitude in the complex plane is expected to move around a semicircle in a counterclockwise direction as the collision energy increases. For the reactive transition from the initial rovibrational state of  $n_a = 2$  and  $j_a = 1$  to the final rovibrational state of  $n_b = 0$  and  $j_b = 1$ , the transferred angular momentum  $j$  ranges between  $j = 0$  and 2. (The Argand diagrams for negative  $m$  are not shown here due to symmetry.) In all cases, counterclockwise semicircles between 0.31 and 0.33 eV at  $L_b = 12$  are predicted, indicating that there exists resonance in the state-to-state reactive transition involving proton (charge) transfer for  $\text{He} + \text{H}_2^+ \rightarrow \text{HeH}^+ + \text{H}$ . A turning point for clockwise rotation occurred at 0.33 eV in all cases, as shown in the figure.

### III. CONCLUSION

Earlier studies of reactive resonance scattering were mostly concerned with the dynamic resonance. In the present study, by examining both the angular distributions and Argand diagrams, we showed the possibility of orbiting resonance in charge (proton) -transfer collisions. By using the DWBA,<sup>18</sup> it is possible to find orbiting resonances in some atom-diatom molecule reactions. Note that orbiting resonances in nuclear reactions are well described by the DWBA, as mentioned earlier. In this paper we have demonstrated the possibility that the rotationally low-lying state-to-state reactive scattering of  $\text{He} + \text{H}_2^+(n_a = 2, j_a = 1) \rightarrow \text{HeH}(n_b = 0, j_b = 1) + \text{H}$  may occur through the presence of both the direct reaction process and orbiting resonance. The enhanced forward-scattering angular distribution is considered to be due to the single orbiting resonance associated with a large orbital angular momentum in the final (product) channel. At present, there seems to be experimental difficulty in measuring state-to-state angular distributions involving rotational transitions. To the best of our knowledge there are no experimental results available for comparison. It will be of great interest in the future to see if the orbiting resonance can be measured for state  $(n_a, j_a)$  to state  $(n_b, j_b)$  reactive scattering processes involving atom (proton) transfer.

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