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Model-potential approach to electron—hydrogen-molecule scattering at low energies

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An investigation of electron—hydrogen-molecule scattering has been performed using the method of model potentials. A modified form of the Hara free-electron-gas exchange potential has been employed to take account of exchange. Two different adiabatic polarization potentials have been used to make the comparative study. Our model exchange potential is found to be suitable in predicting the cross sections. The results for the differential and total cross sections have been given in the energy range 0.3 to 10 eV. Comparisons are made with the available experimental and theoretical findings.

I. INTRODUCTION

The problem of electron-molecule scattering is highly complicated. Recently, Lane[1] and Burke[2] have reviewed the various aspects of this problem. Repeated attempts have been made to understand the physics of this problem. The complexity of the problem demands rigorous calculations. One has to indulge approximate methods in solving the problem. The fixed nuclei approximation is most commonly used. In addition, the treatment of exchange is simplified by developing approximate models. Two different model exchange potentials, the semiclassical exchange (SCE) and free-electron-gas exchange (FEGE) potential, are used. The semiclassical exchange potential is proposed by Furness and McCarthy[3] for electron-atom scattering. The other potential is based on free-electron-gas approximation due to Slater[4] and is applied to this problem by Hara[5] (HFEGE). There are different variants of these two model exchange potentials (see Riley and Truhlar,[6] Baille and Darewych,[7] and Gibson and Morrison[8]).

Baille and Darewych[7] have concluded that the effect of exchange is most accurately represented by the SCE potential. On the other hand, Morrison and other[8-10] have found that the exchange effect is well represented by using FEGE potential. The SCE model is mostly used at intermediate energies.

There are important variants of the FEG model potential. Hara[5] himself had pointed out that the assumption on which his HFEGE potential is based is incorrect for large separation. Riley and Truhlar[6] have modified this by putting the correct asymptotic energy of the electron (AAFEGE) that tends to $\frac{1}{2}k_0^2$. The exchange potential suggested by them is more attractive than the desired one for small separation. There is another semiempirical version of the HFEGE potential due to Morrison and Collins,[9] where the value of the ionization potential is varied to obtain the cross sections which are in tune with the exact static exchange (ESE) results and it is termed as tuned free-electron-gas exchange potential (TFEGE). By investigating the utility of several model exchange potentials for e^--H_2 collisions Gibson and Morrison[8] obtained the best agreement with the ESE and ESEP e-H_2 cross sections by using the TFEGE potential of Morrison and Collins.[9] In a very recent attempt, Morrison and Collins[10] have observed that the combined use of orthogonality constraints of continuum and bound orbitals (Lippman and Schey[11]) and FEGE potential accounts for the effect of exchange reliably.

Recent measurements of cross sections for e^--molecule scattering give impetus to theoretical workers to investigate the problem. A large number of theoretical works were performed during the last few years (see Refs. 1 and 2). Here we have calculated the total cross section for elastic scattering of electrons by hydrogen molecules following the work of Hara.[5] We have used two sets of polarization potentials, one given by Hara,[5] and the other by Henry and Lane.[12] This has been done to find the suitable form for the effective polarization potential. By considering the exchange potential for the e^--H_2 collision it has been found[8-10] that each of the two FEG potentials, i.e., HFEGE and AAFEGE requires modification. This has led us to construct a model FEGE potential which tends to that of Hara[5] for small separation, and to that of Riley and Truhlar,[6] for large separation. In other words, our potential gives the correct value for energy at all separations. This modification is physically sound and it does not increase the complexity of calculations over and above that present in Hara's[5] potential.

II. THEORY

We have taken the polar axis of our system along the direction of the incidental particle. We have strictly followed Hara[4] in carrying out our calculations and so we are not giving the details of the procedure.

The scattered wave $F(\vec{r})$ satisfies the following partial differential equation:

$$[-\tfrac{1}{2}\nabla^2+V_0(r)+V_2(r)P_2(\cos\theta)-\tfrac{1}{2}k_0^2]F(\vec{r})=0\,, \tag{1}$$

where

$$V_0(r)=V_s^0(r)+V_p^0(r)+V_{\mathrm{ex}}(r) \tag{2}$$

and

$$V_2(r)=V_s^2(r)+V_p^2(r)+V_q^2(r)\,, \tag{3}$$

where $V_0(r)$ and $V_2(r)$ are the spherical and nonspherical parts of the effective potential. Here θ is the angle between $\hat{r}$ and $\hat{s}$, $\hat{s}$ being the unit vector along the molecular axis. Thus we have

$$P_2(\cos\theta)=\tfrac{4}{5}\pi\sum_{m=-2}^{2}Y_{2m}^{*}(\hat{s})Y_{2m}(\hat{r})\,. \tag{4}$$

The partial-wave expansion of the scattered wave is given by

$$F(\vec{r})=\sum\frac{u_{lm}(r)}{r}Y_{lm}(\hat{r})\,. \tag{5}$$

Now we substitute (5) and (4) in (1) and assume $m=0$ for the incident wave and neglect the orbital angular momentum coupling. Then, one gets the following differential equation (notations are same as that used by Hara):

$$\left[\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}-2\langle l\mid V\mid l\rangle+k_0^2\right]u_l(r)=0\,, \tag{6}$$

where

$$\langle l\mid V\mid l\rangle=V_0(r)+\frac{l(l+1)V_2(r)}{(2l-1)(2l+3)}P_2(\cos\theta)\,. \tag{7}$$

A. Effective potential

The interaction potential for the *e*-molecule system may be represented as

$$V(\vec{r},\vec{s})=\sum_{\lambda}v_\lambda(r,s)P_\lambda(\hat{r}\cdot\hat{s})\,. \tag{8}$$

We have retained only the first two terms in the expansion, i.e., $\lambda=0$ and 2. The static, polarization, and exchange interactions constitute the effective potential which governs the behavior of cross sections for low-energy e^--H_2 collisions.

1. Static potential

The static potential is obtained by using the simple H_2 wave function of Wang[13] in two-center formalism and is given by

$$V_s(r)=V_s^0(r)+\left[-\frac{Q}{r^3}+V_s^2(r)\right]P_2(\cos\theta)\,, \tag{9}$$

where the explicit forms of $V_s^0(r)$ and $V_s^2(r)$ are given by Bhattacharya[14] *et al.* It has been found that Hara's[5] values of static potentials are slightly erroneous. The value of the quadrupole moment Q has been taken to be 0.49 (Kolos and Wolniewicz[15]).

2. Polarization potential

We have used two models for the polarization potential and the quadrupole tail of the static potential, one due to Hara[5] and the other due to Henry and Lane.[12]

Model A (Hara[5])

$$V_q^2(r)=-Qr^3(r^2+R_0^2)^{-3}\,,$$

$$V_p^0(r)=-\tfrac{1}{2}\alpha_0(r^2+R_0^2)^{-2}\,,$$

$$V_p^2(r)=-\tfrac{1}{2}\alpha_2r^2(r^2+R_0^2)^{-3}\,,$$

where α_0 and α_2 are the linear combinations of the static parallel and perpendicular polarizabilities ($\alpha_{||}$, $\alpha_\perp$) are given by

$$\alpha_0=\tfrac{1}{3}(\alpha_{||}+2\alpha_\perp)\,,$$

$$\alpha_2=\tfrac{2}{3}(\alpha_{||}-\alpha_\perp)\,.$$

Model B (Henry and Lane[12])

$$V_q^2(r)=-Qr^{-3}(1-e^{-(r/r_0)^6})\,,$$

$$V_p^0(r)=-\tfrac{1}{2}\alpha_0(r^2+R_1^2)^{-2}(1-e^{-(r/R_a)^3})\,,$$

$$V_p^2(r)=\begin{cases} 0, & r<0.5a_0 \\ -\frac{1}{2}\alpha_2(r^2-R_2^2)^{-2}(1-e^{-(r/R_b)^4}), & r\geq 0.5a_0 \end{cases}$$

where in model A the cutoff parameter R_0 is taken to be equal to $1.6a_0$ and in model B, $R_1=1.22a_0$, $R_2=0.1a_0$, $R_a=1.7a_0$, $R_b=2.0a_0$, and $r_0=1.8a_0$. In both the models, Q, α_0, α_2 are taken to the $0.49e^2a_0^2$, $5.1786e^2a_0^2$, and $1.2019a_0^3e^2$, respectively.

B. Exchange potential

To calculate the exchange potential Hara[5] followed Slater[4] and obtained

$$V_{\text{ex}}(r)=\frac{-1}{\pi K_0}\left[\frac{1}{2}(K_0^2-k_{\max}^2)\ln\left[\frac{K_0-k_{\max}}{K_0+k_{\max}}\right]+K_0k_{\max}\right], \tag{10}$$

where $k_{\max}$, the maximum momentum of the molecular electrons, is related to the charge density $\rho(r)$ of the bound electrons by

$$k_{\max}=[3\pi^2\rho(r)]^{1/3}. \tag{11}$$

Hara[5] assumed that the incident and the molecular electrons are in the same potential field. To be consistent with this assumption, he used the following equation to determine $K_0^2/2$, the energy of the electron:

$$\frac{K_0^2}{2}=\frac{k_0^2}{2}+\frac{k_{\max}^2}{2}+I, \tag{12}$$

where I is the ionization potential. This assumption is incorrect for large r. Since $\rho(r)$ and hence $k_{\max}(r)$ goes to zero as r tends to infinity, asymptotically the electron energy tends to $\frac{1}{2}k_0^2+I$ instead of $\frac{1}{2}k_0^2$. Riley and Truhlar[6] have suggested the following modified form of Eq. (12):

$$\frac{K_0^2}{2}=\frac{k_0^2}{2}+\frac{k_{\max}^2}{2}. \tag{12a}$$

This potential is more attractive at all separations than that of Hara.[5] We have chosen a modified form of the HFEGE potential, by taking

$$\frac{K_0^2}{2}=\frac{k_0^2}{2}+\frac{k_{\max}}{2}+I/(1+k_0^2/2). \tag{12b}$$

TABLE I. e^--He s-wave phase shifts in radians.

Energy (eV)	k_0 (a_0^{-1})	Riley and Truhlar	Present	Hara
1.22	0.3	2.731	2.6384	2.607
3.4	0.5	2.442	2.34798	2.304
13.6	1.0	1.867	1.8161	1.769
21.26	1.25	1.662	1.6295	1.589
41.67	1.75	1.371	1.3576	1.331
217.68	4.00	0.832	0.83079	0.829

One can see that our model exchange tends to that of Hara[5] for small separation and to that of Riley and Truhlar[6] asymptotically.

Validity of the proposed exchange potential

In order to examine the validity of our exchange potential we have considered the problem of e^--He scattering. We have solved the following differential equation for e^--He scattering:

$$\left[\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+V(r)+k_0^2\right]u_l(r)=0\,,$$

where $V(r)=V_s(r)+V_{\text{ex}}(r)$, $V_s(r)$ being the static potential. The s-, p-, and d-wave phase shifts for three different model exchange potentials are displayed in Tables I, II, and III, respectively. It is evident from these tables that our phase shifts nearly coincide with that of Hara[5] at low energies and with that of Riley and Truhlar[6] at comparatively higher energies.

In support of our model for exchange, we have also compared the differential cross sections for

TABLE II. e^--He p-wave phase shifts in radians.

Energy (eV)	k_0 (a_0^{-1})	Riley and Truhlar	Present	Hara
1.22	0.3	0.268	0.0071098	0.00565
3.4	0.5	0.0680	0.02951	0.0233
13.6	1.0	0.178	0.13975	0.116
21.26	1.25	0.221	0.1945	0.167
41.67	1.75	0.279	0.268686	0.247
217.68	4.00	0.337	0.336799	0.334

TABLE III. e^--He d-wave phase shifts in radians.

Energy (eV)	k_0 (a_0^{-1})	Riley and Truhlar	Present	Hara
1.22	0.3	0.000431	0.0000768	0.0000603
3.4	0.5	0.00243	0.0008577	0.000648
13.6	1.0	0.0179	0.013099	0.0104
21.26	1.25	0.0301	0.025488	0.0211
41.67	1.75	0.0581	0.05525	0.0494
217.68	4.00	0.150	0.150059	0.148

e^--H_2 collisions (model B) at the incident energy 0.04 Ry (Fig. 1), with the exact static exchange (ESE) results (as quoted by Gibson and Morrison[8]) and that of TFEGE due to Morrison and Collins. The effective potential used these three calculations are more or less similar. The discrepancy between our results and that of ESE may be due to the fact that we have neglected the orbital angular momentum coupling. It may be noted that as compared to the results of Morrison and Collins our results are in better agreement with the ESE results.

III. RESULTS AND DISCUSSIONS

In Fig. 2 we have presented our results for differential cross sections at four incident energies. Theoretical results wherever available have also been displayed. We have compared our results with the unnormalized results of Linder and Schmidt.[16] This allows us to avoid the error that comes from the normalization procedure. Experimental results of Trajmar[17] *et al.* which correspond to an incident energy of 10 eV have been given for comparison in the figure. All the theoretical results have been normalized with respect to the experimental one. The present results agree well with the measured values of Linder and Schmidt.[16] at each of the energies chosen, It is evident from Fig. 2 that the present method overestimates the cross sections at 10 eV in comparison with the experimental as well as the other theoretical results. In the present calculations we have neglected the orbital angular momentum coupling and the value of the magnetic quantum number has been taken to be zero throughout. Moreover, we have averaged the cross sections over different molecular orientations in an approximate way. With the increase of energy, the contribution to the cross sections from the nonspherical part of the potential, increases. Thus the way of averaging becomes less suitable at higher energies. These may be the possible reasons behind the observed discrepancy between our results and the others quoted at 10 eV. However, the qualitative agreement of the present results with the measurements is reasonably good.

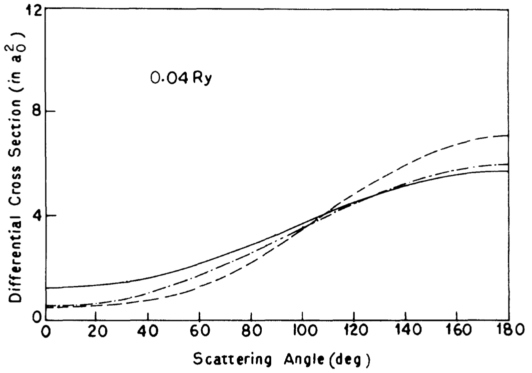

FIG. 1. Differential static exchange polarization cross sections for the following treatments of exchange: ——, present (B); —·—·—·, exact; — — —, tuned FEG.

Our total cross sections have been given in Table IV along with the theoretical results of Hara[5] and Henry and Lane.[12] The measured values of different workers have been given as well as the most recent measurements of Dalba[18] *et al.* Our results lie below that of Dalba[18] *et al.* in the energy range 3–4.5 eV. Our results with model B are in better agreement with the experimental values than those with model A. Both results are more or less in agreement with those of Dalba[18] from 6 eV onwards. Experimental results (Golden[19] *et al.* and

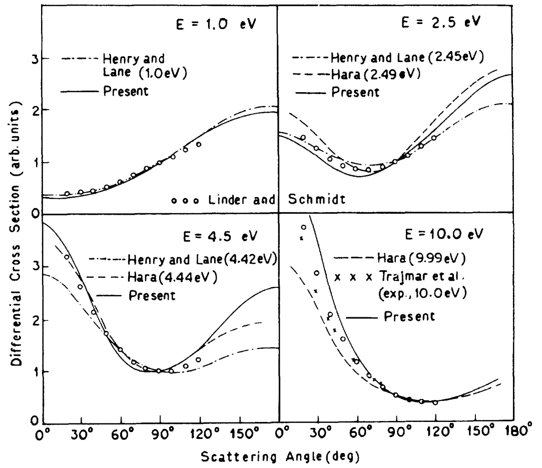

FIG. 2. Differential cross sections for elastic e-H_2 scattering.

TABLE IV. e^--H_2 total scattering cross section (in units of a_0^2).

Energy (eV)	Present A	Present B	Dalba *et al.*	Golden *et al.*	Henry and Lane	Hara
0.3	25.57	39.69	33.1	34.8		
0.6	29.14	42.63	42.3	41.4	38.5	
1.0	32.63	44.87	50.0	46.5	46.8	44.1
1.5	35.96	47.25	54.9	50.3	55.2	49.2
2.0	38.92	48.60	57.7	53.4	61.0	52.8
2.5	41.63	50.41	59.5	55.2	66.7	56.1
3.5	45.85	51.25	59.1		68.8	
4.5	48.14	52.14	56.4			
6.0	50.86	49.93	50.8	46.0	57.7	46.6
8.0	44.66	44.85	44.1	38.7	47.9	42.8
10.0	39.43	39.9	38.5	33.2	41.0	37.4

Dalba[18] *et al.*) differ appreciably among themselves. The best theoretical predictions are due to Henry and Lane.[12] The results of Hara[5] do not agree with those of Henry and Lane.[12] Our finding also differ from their results. In the low-energy region (below 6 eV) all the results (theoretical and experimental) differ amongst themselves appreciably. The present situation is very much unsatisfactory. This warrants further experimental and theoretical studies.

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