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Algebraic eikonal approach to electron-molecule scattering. II. Rotational-vibrational excitations

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The algebraic eikonal approach to electron-molecule scattering is applied to electron scattering off HF and HCl, for which rotational-vibrational excitation cross sections were recently measured. Calculations are done with realistic interactions that include improved dipole, quadrupole, and polarization interactions. Good agreement with the data is obtained in the vibrational elastic channels.

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I. INTRODUCTION

Electron scattering from a polar molecule is a complex process that involves many channels. Various approximations and techniques were developed [1] to solve the coupled-channel equations [2]. *Ab initio* coupled-channel calculations were performed for diatomic and some triatomic [3] molecules. For polyatomic molecules the approach becomes difficult to apply due to the large number of coupled channels, although some *ab initio* calculations were recently done [4] for molecules such as formaldehyde using an optical potential model. An alternative method was recently developed [5,6] in which the algebraic treatment of the rotational-vibrational molecular states (vibron model [7]) is combined with the eikonal (Glauber) approximation. The advantage of the algebraic eikonal approach is that the S matrix is given in a closed form to all orders in the interaction as a representation matrix of the corresponding dynamical group of the molecule.

In a previous paper [8] (which we refer to as paper I), we have generalized the algebraic approach to include more realistic interactions that are not necessarily linear in the generators of the dynamical algebra. In particular we have used a more realistic form for the dipole operator of the molecule, which resulted in the enhancement of the vibrational inelastic cross section.

Recent measurements [9] of differential cross sections of individual rotational-vibrational states make a more detailed comparison between theory and experiment possible. When the vibrational cross sections are resolved into their rotational content, it is essential to include additional long- and medium-range interactions [1,2,10] beside the dominant dipole interaction. The purpose of this paper is to apply the methods of paper I to such situations. In particular we include a quadrupole interaction and a polarization potential [11], which results from the molecular dipole moment induced by the electron field. The agreement with the data is significantly improved, in particular in the vibrational elastic channels. In the vibrational inelastic channels, though we obtain a significant enhancement as compared with previous algebraic calculations [5], we still underestimate the data, especially at backward angles. This is mostly since we have not yet incorporated the exchange interaction [12,13] in the algebraic formulation. This interaction is known to play an important role in the inelastic vibrational channels [10] and at higher energies.

The outline of the paper is as follows. In Sec. II we briefly review the multichannel generalized algebraic eikonal approach to electron-molecule scattering and in Sec. III we discuss several realistic electron-molecule interactions: the dipole, quadrupole, and polarization interactions. The dipole operator of the molecule in the vibron model has already been discussed in paper I, so here we discuss in detail only the quadrupole operator. The methods developed in paper I are then applied in Sec. IV to electron scattering off molecules using the above interactions. Results for electron scattering from LiF, HF, and HCl are presented in Sec. V and compared with experimental data [9,14]. A comparison with other calculations is made.

II. ALGEBRAIC EIKONAL APPROACH

The Hamiltonian of an electron colliding with a molecule is given by

$$H=\frac{\mathbf{p}^2}{2m}+H_0(\xi)+V(r,\xi) \ , \tag{2.1}$$

where $\mathbf{r}$ and $\mathbf{p}$ are the relative coordinate and momentum of the electron, and ξ are the molecule internal coordinates. H_0 is the molecule's Hamiltonian and V is the electron-molecule interaction. In paper I it was shown that in the eikonal approximation, the scattering amplitude from an initial molecular state i to a final state f can be expressed as an integral over an impact parameter b

$$\mathscr{f}_{fi}(\mathbf{q})=ki^{|m_i-m_f|-1}\int_0^\infty b\,db J_{|m_i-m_f|}(qb) \times\langle f|U_I(b)-1|i\rangle \ . \tag{2.2}$$

Here it is assumed that the initial and final states have good angular momentum projection m_i and m_f, respectively, along the collision z axis. $\mathbf{q}$ is the momentum

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transfer $\mathbf{q}=\mathbf{k}_f-\mathbf{k}_i$ and $J_{|m|}$ is the Bessel function of order $|m|$. $U_I(b)$ is the propagator (S operator) in the interaction picture for a straight-line trajector at an impact parameter $\mathbf{b}$ that is parallel to $\mathbf{q}$.

In the Glauber approximation one assumes in addition to the eikonal, the sudden limit, for which the incoming electron is moving fast compared with a time scale characterizing the vibrational and rotational motion in the molecule. In this limit, the rotational-vibrational excitation energies in the molecule are small compared with the collision energy and $[H_0,V]\approx 0$. The potential V_I in the interaction picture can be approximated by V, and $U_I(b)$ in Eq. (2.2) is replaced by the sudden propagator

$$U(b)=\mathcal{T}_z\exp\left[-i\frac{m}{\hbar^2 k}\int_{-\infty}^{\infty}dz\,V(b,z)\right], \qquad (2.3)$$

where $\mathcal{T}_z$ denotes z ordering.

In the algebraic approach, the molecular Hamiltonian H_0 is expanded in the generators G_n of a dynamical algebra $\mathcal{G}$. We assume that the interaction V can be written in the form

$$V=V_0+V_1\ , \qquad (2.4)$$

where $V_0=\sum_n v_n G_n$ is a linear combination of the generators of the algebra and V_1 is weak relative to V_0. V_1 is in general a nonlinear function of G_n. In some realistic situations V_1 may be quadratic in G_n. If $V_1=0$, then the sudden propagator $U_0(b)$, given by (2.3) with V_0 replacing V, is an element of the group G

$$U_0(b)=\exp\left[-i\sum_n\theta_n G_n\right], \qquad (2.5)$$

where θ_n are some parameters that depend on the impact parameter b and the coefficients v_n. The matrix elements $\langle f|U_0(b)|i\rangle$ describe a representation matrix of the group and can therefore be evaluated in a closed form. For $V_1\neq 0$ and nonlinear in G_n, $U(b)$ is not a group element. In paper I it was shown that an algebraic evaluation of $U(b)$ is still feasible if V_1 is weak compared with V_0. For example, if V_1 is quadratic in G_n, then

$$\langle f|U(b)|i\rangle=\sum_{i'}\langle f|U_0(b)|i'\rangle \times\left[\delta_{ii'}+\sum_{m,n}\gamma_{m,n}(b)\langle i'|G_mG_n|i\rangle\right], \qquad (2.6)$$

where $|i'\rangle$ is a finite number of intermediate states, which are connected to the initial state $|i\rangle$ by G_mG_n. The coefficients $\gamma_{m,n}$ are determined from v_n, as is explained in paper I. In Eq. (2.6) the matrix elements of both $U_0(b)$ and G_mG_n can be evaluated algebraically.

III. ALGEBRAIC DESCRIPTION

A. Electron-molecule interaction

In the present algebraic eikonal approach to electron scattering off molecules, the molecule is described in the Born-Oppenheimer approximation, and no electronic excitations are taken into account. We can then average the electron-molecule interactions over the electronic ground-state molecular wave function to obtain an effective interaction $V(\mathbf{r},\xi)$, which depends only on the nuclear coordinates ξ (as well as the scattered electron coordinate $\mathbf{r}$), but not on the coordinates of the molecule's electrons. If the incoming electron is not too close to the molecule, we can expand its Coulomb interaction with the molecule in multipoles to obtain

$$V(r,\xi)=-\sum_{\lambda,\mu}(-1)^{\mu}\frac{4\pi e}{2\lambda+1}\frac{\mathcal{Y}_{\lambda-\mu}(\hat{\mathbf{r}})}{r^{\lambda+1}}Q_{\lambda\mu}\ , \qquad (3.1)$$

where $\hat{\mathbf{r}}$ denotes a unit vector specifying the direction of the electron, and Q_λ is the electric 2^λ pole moment of the molecule and is a function of the nuclear coordinates ξ. Because the molecule is electrically neutral, there is no monopole term in (3.1) and the leading term is the dipole interaction. In this paper we shall investigate also the quadrupole interaction.

For $\lambda=1$, the dipole contribution to (3.1) can be rewritten as

$$V_d=\alpha_1(r)\hat{\mathbf{r}}\cdot\mathbf{T}\ , \qquad (3.2)$$

where $\mathbf{T}$ is the dipole operator of the molecule

$$\mathbf{T}=\left[\frac{4\pi}{3}\right]^{1/2}Q_{\lambda=1}\ , \qquad (3.3)$$

and $\alpha_1(r)$ is

$$\alpha_1(r)=-\frac{e}{r^2+R_0^2}\ . \qquad (3.4)$$

In Eq. (3.4) we have added a cutoff radius R_0 to avoid the nonphysical singularity of the dipole interaction at short range.

For $\lambda=2$, the quadrupole contribution to (3.1) is

$$V_q=\alpha_2(r)\sum_\mu\mathcal{Y}^*_{2\mu}(\hat{\mathbf{r}})Q_{2\mu}\ . \qquad (3.5a)$$

Here

$$\alpha_2(r)=-\frac{4\pi}{5}\frac{e}{(r^2+R_0^2)^{3/2}}\ , \qquad (3.5b)$$

where we have introduced a cutoff radius R_0 similar to the one in (3.4).

The multipole expansion (3.1) assumes that the molecule is not affected by the incoming electron. An important correction to (3.1) is obtained by considering the interaction between the electron and the induced dipole moment caused by the electric field of the electron. This interaction is known as the polarization potential V_p. Denoting by $\mathbf{E}$ the electric field of the electron at the molecule and by $\mathbf{T}_{\text{ind}}$ the induced dipole moment, we have

$$V_p=-\tfrac{1}{2}\mathbf{E}\cdot\mathbf{T}_{\text{ind}}=-\frac{e}{2}\frac{\hat{\mathbf{r}}}{r^2}\cdot\mathbf{T}_{\text{ind}}\ . \qquad (3.6)$$

The polarizability tensor is diagonal in the intrinsic molecular frame and we denote by $\alpha_\parallel$ and $\alpha_\perp$ its components along the molecular axis (of the diatomic molecule) and perpendicular to it, respectively. Then

$$\mathbf{T}_{\text{ind}}=\alpha_\parallel \mathbf{E}_\parallel+\alpha_\perp \mathbf{E}_\perp \ . \tag{3.7}$$

Denoting by Θ the angle between $\hat{\mathbf{r}}$ and the molecule axis we obtain

$$V_p=-\frac{e^2}{2r^4}(\alpha_\parallel \cos^2\Theta+\alpha_\perp \sin^2\Theta) \ . \tag{3.8}$$

Defining an average polarizability α and an anisotropic polarizability α' by

$$\alpha=\frac{2\alpha_\perp+\alpha_\parallel}{3} \ , \quad \alpha'=\alpha_\parallel-\alpha \ , \tag{3.9}$$

we can rewrite (3.8)

$$V_p=-\frac{e^2}{2r^4}[\alpha+\alpha' P_2(\cos\Theta)] \ . \tag{3.10}$$

Thus, V_p has both a monopole and a quadrupole contribution. To rewrite the quadrupole part in a more general way, we assume an axially symmetric rigid molecule that has an intrinsic quadrupole moment Θ_v,

$$Q_{2\mu}=\sum_{\mu'} D^{(2)*}_{\mu\mu'}(\Omega) Q^{\text{int}}_{2\mu'}=\mathcal{Y}_{2\mu}(\Omega)\Theta_v \ , \tag{3.11}$$

where Ω denotes the orientation of the molecule's axis in the laboratory frame. Using the addition theorem for the spherical harmonics we can rewrite P_2 in (3.11) in terms of the molecule's quadrupole moment:

$$P_2(\cos\Theta)=\frac{4\pi}{5}\Theta_v^{-1}\sum_\mu \mathcal{Y}^*_{2\mu}(\hat{\mathbf{r}})Q_{2\mu} \ . \tag{3.12}$$

The polarization potential is then more generally written as a sum of monopole and quadrupole contributions

$$\begin{aligned} V_p &= V_p^0+V_p^2 \\ &=\alpha\alpha_0(r)+\frac{4\pi}{5}\frac{\alpha'}{\Theta_v}\alpha_0(r)\sum_\mu \mathcal{Y}^*_{2\mu}(\hat{\mathbf{r}})Q_{2\mu} \ , \end{aligned} \tag{3.13}$$

where $\alpha_0(r)$ is given by

$$\alpha_0(r)=-\frac{e^2}{2r^4} \ . \tag{3.14}$$

Here too, we have to introduce a cutoff to suppress (3.14) at short distances. Various cutoffs have been considered in the literature. We shall use

$$\alpha_0(r)=-\frac{e^2}{2(r^2+R_{0p}^2)^2} \ . \tag{3.15}$$

The total electron-molecule interaction potential considered in this paper is then

$$\begin{aligned} V(\mathbf{r}) &= V_d+V_q+V_p^{(0)}+V_p^{(2)} \\ &=\alpha_1(r)\hat{\mathbf{r}}\cdot\mathbf{T}+\alpha_2(r)\sum_\mu \mathcal{Y}^*_{2\mu}(\hat{\mathbf{r}})Q_{2\mu} \\ &\quad +\alpha_0(r)\alpha+\frac{4\pi}{5}\alpha_0(r)\sum_\mu \mathcal{Y}^*_{2\mu}(\hat{\mathbf{r}})\left[\frac{\alpha'}{\Theta_v}Q_{2\mu}\right] \ . \end{aligned} \tag{3.16}$$

Another important contribution to the electron-molecule interaction is the exchange interaction [13], but we have not yet included it in our algebraic formulation.

B. Vibron model

The rotational-vibrational structure of molecules can be described algebraically in the vibron model [7], using the algebra u(4). The model is described in terms of four bosons, one scalar with a creation operator $s^\dagger$ and three spherical components of a vector $p^\dagger_\mu$ ($\mu=-1,0,1$). Most diatomic molecules are described well by a Hamiltonian that is a linear combination of Casimir invariants in the chain u(4)$\supset$o(4)$\supset$o(3). The molecule's eigenstates are $|\sigma,j,m\rangle$ with $\sigma(\sigma+2)$ the eigenvalue of an o(4) Casimir invariant, j is the angular momentum of the molecule, and m is its projection. The vibrational quantum number v is related to σ by $v=(N-\sigma)/2$. As in paper I we shall exploit the isomorphism of o(4) to su(2)$\times$su(2). The calculations are then done in a basis $|\kappa m_1,\kappa m_2\rangle$, where $\kappa=\sigma/2$ is the SU(2) quasispin.

The dipole and quadrupole moments of the molecule play an important role in the long- and medium-range electron-molecule interaction. The dipole operator $\mathbf{T}$ of the molecule was already discussed in paper I. It is a nonlinear function of the u(4) generators

$$\mathbf{T}=d_0\mathbf{D}+\tfrac{1}{2}d_1(\hat{n}_p\mathbf{D}+\mathbf{D}\hat{n}_p) \ . \tag{3.17}$$

Here $D_\mu=(s^\dagger\tilde{p}+p^\dagger s)^{(1)}_\mu$ is an o(4) dipole operator, $\hat{n}_p=p^\dagger\cdot\tilde{p}$ and d_0,d_1 are parameters.

C. Quadrupole moment

The leading contribution to the quadrupole moment of the molecule is the quadrupole operator of u(4),

$$Q_{2\mu}=q_0(p^\dagger\times\tilde{p})^{(2)} \ . \tag{3.18}$$

The constant q_0 is determined from the measured quadrupole moment of the molecule. For that purpose we recall that

$$Q_{2\mu}=\sum_{\mu'} D^{(2)*}_{\mu\mu'}(\Omega)Q^{\text{int}}_{2\mu'} \ , \tag{3.19}$$

where $Q^{\text{int}}_{2\mu'}$ are the quadrupole components in the intrinsic frame. For a diatomic molecule, the charge distribution is axially symmetric and $Q^{\text{int}}_{2\mu'}=0$ for $\mu'\neq 0$. We find

$$Q_{2\mu}=\left[\frac{4\pi}{5}\right]^{1/2}\mathcal{Y}_{2\mu}(\hat{\mathbf{R}})Q^{\text{int}}_{20}(R) \ , \tag{3.20}$$

where $\mathbf{R}$ is the vector connecting the two nuclei. The reduced matrix elements of (3.20) in a vibrational state v are given by

$$\begin{aligned} (v,j'\|Q_2\|v,j) &= (-1)^{j'}\sqrt{(2j'+1)(2j+1)} \\ &\quad \times \begin{pmatrix} j' & 2 & j \\ 0 & 0 & 0 \end{pmatrix}\langle v,j'|Q^{\text{int}}_{20}|v,j\rangle \ . \end{aligned} \tag{3.21}$$

For a rigid molecule $\langle v,j'|Q^{\text{int}}_{20}|v,j\rangle$ is independent of j and j' and it defines the intrinsic quadrupole moment of the molecule Θ_v:

$$\Theta_v = \left[\frac{4\pi}{5}\right]^{1/2} \langle v | Q_{20}^{\rm int} | v \rangle \; . \tag{3.22}$$

The factor $\sqrt{4\pi/5}$ is due to the fact that Θ_v is related to the Cartesian component $Q_{zz}^{\rm int}$, while $Q_{20}^{\rm int}$ is the spherical component [for a charge distribution ρ, we have $\Theta_v = (e/2)\int \rho(3Z^2 - R^2) d^3R$]. We conclude

$$(v,j' \| Q_2 \| v,j) = \left[\frac{5}{4\pi}\right]^{1/2} \Theta_v (-1)^{j'} \sqrt{(2j'+1)(2j+1)} \times \begin{bmatrix} j' & 2 & j \\ 0 & 0 & 0 \end{bmatrix} \; . \tag{3.23}$$

We adopt (3.23) as the definition of Θ_v. For special values of j and j' we obtain

$$\Theta_v = \left[\frac{4\pi}{5}\right]^{1/2} (v,j'=2 \| Q_2 \| v,j=0) \; , \tag{3.24a}$$

$$\Theta_v = -\left[\frac{2\pi}{3}\right]^{1/2} (v,j'=1 \| Q_2 \| v,j=1) \; , \tag{3.24b}$$

$$\Theta_v = -\left[\frac{14\pi}{25}\right]^{1/2} (v,j'=2 \| Q_2 \| v,j=2) \; . \tag{3.24c}$$

In the vibron model Q_2 is given by (3.18). To calculate its matrix elements, we note that the u(4) generators can be expressed [15] as irreducible tensors $T_{(s,m_s)(t,m_t)}$ of su(2)×su(2) with $s,t=0,1$. The su(2)×su(2) reduced matrix elements of $T_{(s,t)}$ are defined through a Wigner-Eckart theorem and are tabulated in Ref. [16],

$$\langle \kappa_1', m_1'; \kappa_2', m_2' | T_{(s,m_s)(t,m_t)} | \kappa_1, m_1; \kappa_2, m_2 \rangle = \frac{1}{\sqrt{(2\kappa_1'+1)(2\kappa_2'+1)}} (\kappa_1 m_1 s m_s | \kappa_1' m_1') \times (\kappa_2 m_2 t m_t | \kappa_2' m_2') (\kappa_1', \kappa_2' \| T_{(s,t)} \| \kappa_1, \kappa_2) \; . \tag{3.25}$$

o(3) rotational tensors can be constructed by a recoupling of the su(2)×su(2) tensors. Their o(3) reduced matrix elements are then related to the su(2)×su(2) ones. In particular $(p^\dagger \times \tilde{p})^{(2)}$ is given by

$$(p^\dagger \times \tilde{p})^{(2)}_\mu = \sum_{m,m'} (1m1m'|2\mu) T_{(1,m)(1,m')} \; , \tag{3.26}$$

and its reduced o(3) matrix elements are

$$(\sigma',j' \| (p^\dagger \times \tilde{p})^{(2)} \| \sigma,j) = \sqrt{5(2j+1)(2j'+1)} \times \begin{Bmatrix} \sigma'/2 & \sigma'/2 & j' \\ \sigma/2 & \sigma/2 & j \\ 1 & 1 & 2 \end{Bmatrix} \times (\kappa'=\sigma'/2, \kappa'=\sigma'/2 \| T_{(1,1)} \| \kappa=\sigma/2, \kappa=\sigma/2) \; . \tag{3.27}$$

TABLE I. Theoretical values of the quadrupole parameter q_0 derived from Eqs. (3.24) and (3.29) for the molecules LiF, HF, and HCl. The experimental values [17] of θ_v are listed in the last column.

	q_0 (e Å^2)			
Molecule	$j=0,\ j'=2$	$j=j'=1$	$j=j'=2$	Θ_v (e Å^2)
LiF	0.016 219	0.016 214	0.016 209	1.207
HF	0.016 504	0.016 476	0.016 443	0.491
HCl	0.021 316	0.021 292	0.021 265	0.786

In particular, the reduced matrix elements in a vibrational state v (for which $\sigma = \sigma' = N - 2v$) are

$$(\sigma/2, \sigma/2 \| T_{(1,1)} \| \sigma/2, \sigma/2) = -(N+2)(\sigma+1)/2 \; . \tag{3.28}$$

Therefore, in the vibron model

$$(v,j' \| Q_2 \| v,j) = -\frac{q_0}{2}(N+2)(N-2v+1) \times \sqrt{5(2j+1)(2j'+1)} \times \begin{Bmatrix} N/2-v & N/2-v & j' \\ N/2-v & N/2-v & j \\ 1 & 1 & 2 \end{Bmatrix} \; . \tag{3.29}$$

Comparing Eqs. (3.29) and (3.23), we can calculate q_0 from the measured value Θ_v. Since the vibron model does not describe necessarily a rigid molecule [for which Θ_v in (3.23) is independent of j,j'], we expect to find a slight dependence of q_0 on the values of j and j' used to determine Θ_v in (3.23). For example, if $v=0$ and $j=0, j'=2$, we find

$$q_0 = \frac{1}{N+2} \left[\frac{15N(N+2)}{2\pi(N-1)(N+3)}\right]^{1/2} \Theta_{v=0} \; . \tag{3.30}$$

Table I lists several such values for q_0 for the three molecules discussed in this paper: LiF, HF, and HCl. They are derived from Eqs. (3.24) and (3.29) using the experimental values of Θ_v. q_0 is seen to be very weakly dependent on j and j'.

D. Born approximation

If the electron-molecule interaction is weak enough, we can use the Born approximation to calculate the cross section $v,j \to v',j'$. Using the multipole expansion (3.1) for the electron-molecule interaction, we obtain

$$f_{fi} \approx \frac{m}{2\pi\hbar^2} \sum_{\lambda,\mu} (-1)^\mu \frac{4\pi e}{2\lambda+1} \left[\int d^3\mathbf{r}\, e^{i\mathbf{q}\cdot\mathbf{r}} \frac{\mathcal{Y}_{\lambda-\mu}(\hat{\mathbf{r}})}{r^{\lambda+1}}\right] \times \langle f | Q_{\lambda\mu} | i \rangle \; . \tag{3.31}$$

The contribution of the 2^λ pole to the unpolarized cross section (sum over final m' and average over initial m) is then

$$\left[\frac{d\sigma}{d\Omega}\right]_{v,l\to v,l'} \approx 2\left[\frac{4\pi m e}{(2\lambda+1)\hbar^2}\right]^2 \times \frac{|(v',j'\|Q_\lambda\|v,j)|^2}{(2j+1)(2\lambda+1)} F_\lambda(q) , \qquad (3.32)$$

with

$$F_\lambda(q) = \sum_{\mu=-\lambda}^{\lambda} \left| \int_0^\infty db\, bJ_{|\mu|}(qb) \int_{-\infty}^{\infty} dz \frac{\mathcal{Y}_{\lambda\mu}(\hat{\mathbf{r}})}{r^{\lambda+1}} \right|^2 , \qquad (3.33)$$

and $\hat{\mathbf{r}}=(b/r,0,z/r)$. The factor $F_\lambda(q)$ is geometrical and determines the angular dependence of $d\sigma/d\Omega$, while the strength $|(v',j'\|Q_\lambda\|v,j)|^2$ determines a global scale for $d\sigma/d\Omega$. The Born cross section for the dipole interaction ($\lambda=1$) was evaluated in paper I. For the quadrupole interaction ($\lambda=2$), we find

$$F_2(q) = 2\left|\int_{-\infty}^{\infty} db\, bJ_2(qb)G_2(b)\right|^2 + \left|\int_0^\infty db\, bJ_0(qb)G_0(b)\right|^2 , \qquad (3.34)$$

where

$$\begin{aligned} G_0(b) &= \int_{-\infty}^{\infty} \frac{dz}{(r^2+R_0^2)^{3/2}} \mathcal{Y}_{20} \\ &= \left[\frac{5}{16\pi}\right]^{1/2} \left[\frac{4R_0^2+6b^2}{R_0^2(b^2+R_0^2)} - \frac{6b}{R_0^3} \arctan\left[\frac{R_0}{b}\right]\right] , \\ G_2(b) &= \int_{-\infty}^{\infty} \frac{dz}{(r^2+R_0^2)^{3/2}} \mathcal{Y}_{22} \\ &= \left[\frac{15}{32\pi}\right]^{1/2} \left[-\frac{2b^2}{R_0^2(b^2+R_0^2)} + \frac{2b}{R_0^3} \arctan\left[\frac{R_0}{b}\right]\right] . \end{aligned} \qquad (3.35)$$

For $b \gg R_0$ we have the following approximation for G_0 and G_2:

$$\begin{aligned} G_0(b) &\approx \frac{1}{\sqrt{5\pi}} \frac{R_0^2}{b^4} , \\ G_2(b) &\approx \left[\frac{5}{6\pi}\right]^{1/2} \frac{1}{b^2} - \left[\frac{6}{5\pi}\right]^{1/2} \frac{R_0^2}{b^4} . \end{aligned} \qquad (3.36)$$

The magnitude of the cross section is determined by the reduced matrix elements of Q_λ. For the quadrupole ($\lambda=2$) interaction we have from (3.27)

$$(v',j'\|Q_2\|v,j) = -\frac{q_0}{2}\sqrt{5(2j+1)(2j'+1)} \begin{Bmatrix} N/2-v' & N/2-v' & j' \\ N/2-v & N/2-v & j \\ 1 & 1 & 2 \end{Bmatrix} \times \begin{cases} (N+2)(N-2v+1) & \text{for } v'=v \\ \sqrt{4(N-2v+1)(N-2v-1)(N-v+1)(v+1)} & \text{for } v'=v+1 . \end{cases} \qquad (3.37)$$

IV. ELECTRON-MOLECULE SCATTERING

The scattering amplitude in the Glauber approximation has been calculated in paper I for a dipole interaction. The calculation was done to all orders in d_0 and to first order in d_1 (which is weak compared to d_0). Since the quadrupole and quadrupole polarization interactions are relatively weak, we shall expand $U(b)$ to first order in these interactions. Thus only the strongest dipole d_0 term is dealt with to all orders. Since $\mathbf{D}$ is in the o(4) algebra, the corresponding propagator $U_0(b)$ is an element of O(4) for which the calculation of the representation matrices is much easier than for U(4). One could include the quadrupole to all orders but this will require the evaluation of U(4) matrix elements.

The sudden propagator $U_0(b,z)$ between $-\infty$ and z and at impact parameter b was parametrized in paper I as

$$U_0(b,z) = \exp[2i(\theta_b D_b + \theta_z D_z + \theta_\phi L_\phi)] , \qquad (4.1)$$

with $\boldsymbol{\theta}=\boldsymbol{\theta}(b,z)$, and is easily written as an SU(2)×SU(2) element

$$\begin{aligned} U_0(b,z) &= U_0^{(1)}(b,z) U_0^{(2)}(b,z) , \\ U_0^{(i)}(b,z) &= \exp(2i\boldsymbol{\theta}_i \cdot \mathbf{K}_i) . \end{aligned} \qquad (4.2)$$

$\mathbf{K}_1$ and $\mathbf{K}_2$ are the su(2)×su(2) generators, $\boldsymbol{\theta}_1=\boldsymbol{\theta}$ and $\theta_{2b}=-\theta_{1b}$, $\theta_{2\phi}=\theta_{1\phi}$, $\theta_{2z}=-\theta_{1z}$. Due to time reversal symmetry $\theta_z=0$.

A. Dipole interaction

This case was already discussed in Paper I, where we refer the reader for details. We found

$$U(b) = U_0(b)[1+\delta U_d] , \qquad (4.3)$$

where δU_d is given by Eq. (4.38) of paper I.

B. Quadrupole interaction

The vibrational elastic cross section (summed over final rotational states) for electron scattering from a polar molecule is dominated by the dipole interaction. However, the cross sections to individual rotational states in the vibrational elastic channel may be strongly affected by higher-order interactions. In this section we discuss the quadrupole interaction.

The quadrupole interaction (3.5) with Q_2 given by (3.18) is

$$V_q = q_0\alpha_2(r)\sum_{\mu} \mathcal{Y}^*_{2\mu}(\hat{\mathbf{r}})(p^\dagger \times \tilde{p})^{(2)}_\mu . \tag{4.4}$$

This V_q is in the u(4) algebra and therefore the corresponding evolution operator $U(b)$ is a U(4) group element. However, since the quadrupole interaction is weak relative to the d_0 dipole interaction, it is simpler to treat it also as a perturbation similar to the d_1 dipole term. Including V_q in addition to V_d, we find

$$U(b) = U_0(b)[1+\delta U_d+\delta U_q] , \tag{4.5}$$

where δU_q is given by

$$\delta U_q = -i\frac{m}{\hbar^2 k}\int_{-\infty}^{\infty} dz\, U_0^{-1}(b,z)V_q(\mathbf{r})U_0(b,z) . \tag{4.6}$$

Expressing $(p^\dagger\times\tilde{p})^{(2)}$ in terms of the tensors $T_{(s,t)}$ (see Sec. III C), we obtain

$$U_0^{-1}(p^\dagger\times\tilde{p})^{(2)}_\mu U_0 = \sum_{M,M'} h^{(2)}_{MM',\mu}(\theta)T_{(1,M)(1,M')} , \tag{4.7}$$

where

$$h^{(2)}_{MM'\mu}(\theta) = \sum_{M,M'}(1m1m'|2\mu)D_{M,m}(\theta)D^*_{M',m'}(\theta) . \tag{4.8}$$

Therefore δU_q in Eq. (4.5) is

$$\delta U_q = i\frac{4\pi}{5}\frac{meq_0}{\hbar^2 k}\sum_{M,M'}\epsilon_{MM'}(b)T_{(1,M)(1,M')} , \tag{4.9}$$

where

$$\epsilon_{MM'}(b) = \int_{-\infty}^{\infty} dz \sum_{\mu}\frac{\mathcal{Y}^*_{2\mu}(r)}{(r^2+R_0^2)^{3/2}}h^{(2)}_{MM'\mu}(\theta) . \tag{4.10}$$

Notice that the operator (4.9) is a combination of rotational tensors with rank 0, 1, and 2. If we neglect the noncommutation of $U_0(b)$ and Q_2 in Eq. (4.6), then only a second-rank tensor (Q_2) is present. Since in (2.2) we take $\mathbf{r}=(b/r,0,z/r)$, we have in (4.10)

$$\begin{aligned}
\mathcal{Y}_{2,0}(\hat{\mathbf{r}}) &= \left[\frac{5}{16\pi}\right]^{1/2}\left[3\frac{z^2}{r^2}-1\right] ,\\
\mathcal{Y}_{2,\pm1}(\hat{\mathbf{r}}) &= \mp\left[\frac{15}{8\pi}\right]^{1/2}\frac{bz}{r^2} , \\
\mathcal{Y}_{2,\pm2}(\hat{\mathbf{r}}) &= \left[\frac{15}{32\pi}\right]^{1/2}\frac{b^2}{r^2} .
\end{aligned} \tag{4.11}$$

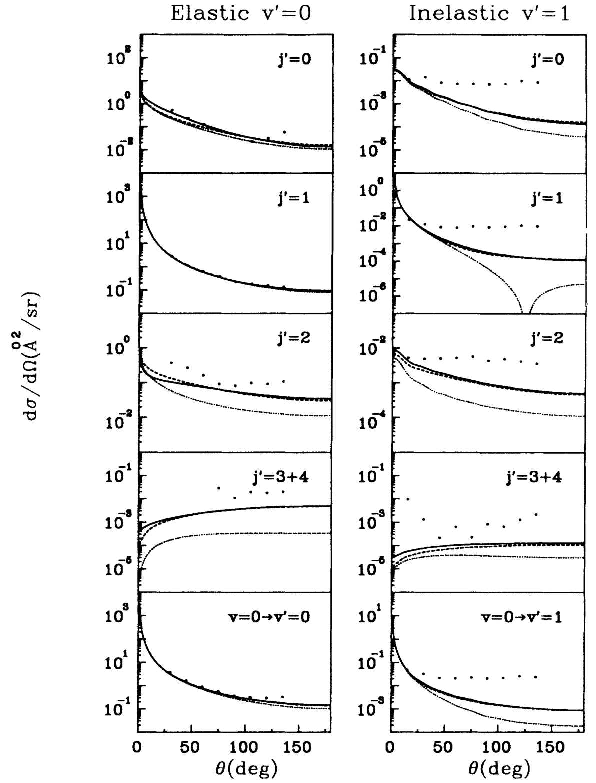

FIG. 1. The differential cross sections for the scattering of electrons from HF at $E=3$ eV. Left column: $v'=0$ channel. Right column: $v'=1$. Shown separately are the cross sections to excite the $j'=0,1,2$ and $3+4$ states and the summed cross section over all rotational states (bottom row). Dotted lines: with the dipole interaction. Dashed lines: with the addition of the quadrupole interaction. The solid lines are obtained with the inclusion of the quadrupole and monopole polarization interactions, so that the full interaction (3.16) is considered. The data points (dots) are taken from Ref. [9].

To illustrate the importance of the quadrupole interaction we compare in Fig. 1 the cross sections for e +HF at $E=3$ eV with both quadrupole and dipole interactions (dashed lines) against the corresponding cross sections computed with only a dipole interaction (dotted lines). The parameters used are determined as explained below in Sec. V. In the vibrational elastic channels, we see that the inclusion of the quadrupole interaction affects strongly the $j'=2$ and $j'=3+4$ channels (where the cross sections are increased between one and two orders of magnitudes), while the $j'=0$ and $j'=1$ channels are much less affected. The change in the summed elastic cross section ($v=0\rightarrow v'=0$) is rather small, but in agreement with the data. In the vibrationally inelastic channels ($v'=1$), there is a significant effect also for $j'=0$ and $j'=1$ at backward angles. The summed inelastic cross section ($v=0\rightarrow v'=1$) increases significantly, especially at backward angles.

C. Polarization potential

The quadrupole polarization interaction

$$V_P^{(2)} = \frac{4\pi}{5}\alpha_0(r)\sum_{\mu}\mathcal{Y}^*_{2\mu}(\hat{\mathbf{r}})\alpha'\frac{q_0}{\Theta_v}(p^\dagger\times\tilde{p})^{(2)}_\mu \tag{4.12}$$

is proportional to the anisotropic polarizability α' and has a form similar to the quadrupole interaction (4.4), except that $\alpha_2(r)$ is replaced by $(4\pi/5)\alpha_0(r)(\alpha'/\theta_v)$. The inclusion of $V_p^{(2)}$ is thus straightforward and leads to

$$U(b)=U_0(b)[1+\delta U_d+\delta U_q+\delta U_p^{(2)}] , \tag{4.13}$$

with

$$\delta U_p^{(2)}=i\frac{4\pi}{5}\frac{me^2}{\hbar^2 k}\alpha'\frac{q_0}{\theta_v}\sum \chi_{MM'}(b)T_{(1,M)(1,M')} , \tag{4.14}$$

and

$$\chi_{MM'}(b)=\int_{-\infty}^{\infty} dz \sum_{\mu} \frac{\mathcal{Y}_{2\mu}^{*}(\hat{\mathbf{r}})}{2(r^2+R_{0p}^2)^2} h_{MM'\mu}^{(2)}(\theta) . \tag{4.15}$$

The monopole polarization potential is too strong to treat in an eikonal approximation. We therefore use a distorted-wave eikonal approximation developed in Ref. [6], where the monopole polarization is treated exactly but the other interactions are treated in the eikonal approximation. In this approximation

$$\not{f}_{fi}(\mathbf{q})=ki^{|m_f-m_i|-1}\int_0^{\infty} b\, db\, J_{|m_f-m_i|}(qb) \times\langle f|S(b)U(b)-|i\rangle . \tag{4.16}$$

Here $U(b)$ is the propogator due to all interactions except the monopole polarization, while $S(b)$ is the impact-parameter representation S matrix of the polarization potential alone. For $U(b)$ we use (4.13). To find $S(b)$ notice that the exact scattering amplitude $f(\theta)$ due to a monopole polarization potential

$$V_p^{(0)}=\alpha_0(r)\alpha , \tag{4.17}$$

can be written in the impact-parameter representation [18] as

$$f(\theta)=-ik\int_0^{\infty} b\, db\, J_0(qb)[S(b)-1] . \tag{4.18}$$

The amplitude $f(\theta)$ can be calculated from the partial-wave expansion

$$f(\theta)=\sum_l (2l+1)f_l P_l(\cos\theta) , \tag{4.19}$$

where $f_l \equiv (e^{2i\delta l}-1)/2ik$ are the partial-wave amplitudes. The phase shifts δ_l can be calculated numerically using the Numerov method [19]. The relation of f_l to $S(b)$ is

$$f_l=-i\int_0^{\infty} db\, J_{2l+1}(2kb)(S(b)-1) . \tag{4.20}$$

It is possible to invert (4.18) in order to express $S(b)$ in terms of $f(\theta)$. For that purpose we use the orthogonality relation [20] of the Bessel functions of odd order

$$\int_0^{\infty}\frac{dx}{x}J_{2m+1}(x)J_{2n+1}(x)=\frac{1}{2(2m+1)}\delta_{mn} . \tag{4.21}$$

Expanding

$$b[S(b)-1]=\sum_l c_l(k)J_{2l+1}(2kb) , \tag{4.22}$$

we obtain, using Eqs. (4.21) and (4.20),

$$c_l=2i(2l+1)f_l . \tag{4.23}$$

Thus

$$S(b)-1=2\frac{i}{b}\sum_l (2l+1)f_l J_{2l+1}(2kb) . \tag{4.24}$$

We note that $\{J_{2l+1}(x)\}$ is not a complete set and it is *a priori* not clear that (4.22) is possible. We can instead use (4.24) as the definition of $S(b)$. Equation (4.20) follows then from the orthogonality relation (4.21). Expanding $J_0(qb)$ in the Legendre polynomials

$$J_0(qb)=\sum_l \frac{2l+1}{kb}J_{2l+1}(kb)P_l(\cos\theta) , \tag{4.25}$$

we can derive (4.18) from (4.20) and (4.19). For large b, the potential is weak and we expect $S(b)$ to approach the eikonal limit

$$S_{\text{eik}}(b)=\exp\left[-i\frac{m}{\hbar^2 k}\int_{-\infty}^{\infty} dz\, V_p^{(0)}(b,z)\right] . \tag{4.26}$$

The inversion of (4.18) is not unique and unfortunately the solution (4.24) does not approach (4.26) for large b. It

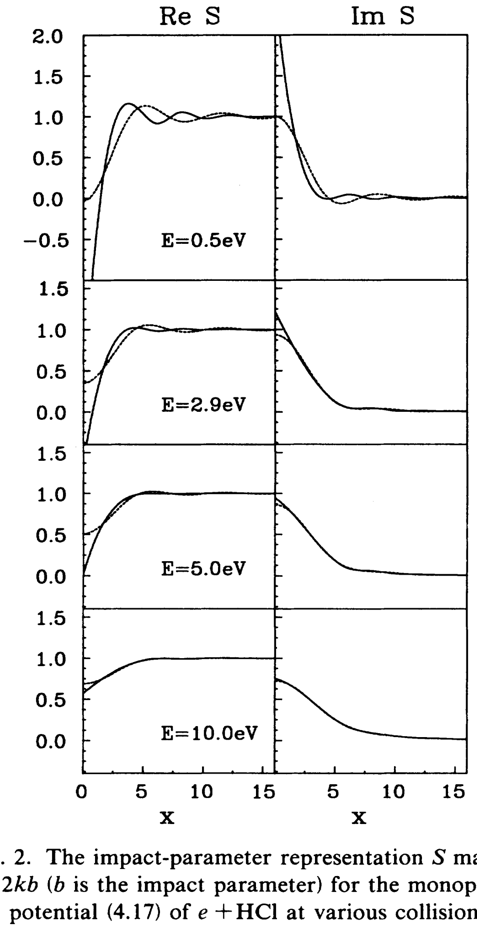

FIG. 2. The impact-parameter representation S matrix $S(b)$ vs $x=2kb$ (b is the impact parameter) for the monopole polarization potential (4.17) of $e+\text{HCl}$ at various collision energies. Left column: real part of $S(b)$. Right column: imaginary part of $S(b)$. The dashed lines are the analytic inversion (4.24), while the solid lines are the numerical inversion that has the correct eikonal limit at large b.

TABLE II. Dipole moment (μ_e), dipole transition matrix element ($R_{0,1}$), quadrupole moment (Θ_v), and polarizabilities (α and α') for the molecules LiF, HF, and HCl. In brackets next to each value is the reference from which it is taken. We have used experimental values if known. Otherwise we have used *ab initio* calculations (denoted by $*$). † denotes references where theoretical calculations are combined with experimental values to infer the quoted quantity.

Molecule	μ_e (D)	$R_{0,1}$ (D)	Θ_v (e Å^2)	α (Å^3)	α' (Å^3)
LiF	6.58 [21]†	0.2718 [21]†	1.207 [17]	1.57 [24]*	−0.01 [24]*
HF	1.827 [25]	9.85×10^{-2} [22]	0.491 [17]	0.8 [26]	0.16 [26]
HCl	1.108 [25]	7.12×10^{-2} [23]	0.786 [17]	2.15 [27]	0.19 [27]†

is, however, possible to construct a solution to (4.18) that does approach the eikonal limit by using a numerical technique described in Ref. [6].

Solving (4.18) for $S(b)$ is equivalent to solving (4.20), using the known partial amplitudes f_l. Choosing $\bar{b}$ to be such that the eikonal approximation (4.26) is good for $b > \bar{b}$, we rewrite (4.20) as

$$f_l = \bar{f}_l - i \int_{\bar{b}}^{\infty} db\, J_{2l+1}(2kb)[S_{\text{eik}}(b) - 1] \,, \tag{4.27}$$

where

$$\bar{f}_l = -i \int_0^{\bar{b}} db\, J_{2l+1}(2kb)[S(b) - 1] \,. \tag{4.28}$$

$\bar{f}_l$ can be calculated from the known f_l and $S_{\text{eik}}(b)$ given by (4.26). It then remains to solve (4.28) for $S(b)$. We have done this by iterations as described in Ref. [6], except that we have used a cubic spline interpolation rather than a Lagrange interpolation.

Figure 2 shows the impact-parameter representation $S(b)$ for the polarization monopole potential of HCl at different collision energies. The dashed lines are the analytic inversion (4.24) and the solid lines represent the numerical inversion that satisfies the eikonal limit (4.26). Notice the oscillatory behavior of the analytic $S(b)$ at large b's (in particular for $E = 0.5$ eV). The two different solutions for $S(b)$ get closer at higher energies.

The solid lines in Fig. 1 are the results of the calculations when the polarization potential is included in addition to the dipole and quadrupole interactions. A enhancement is observed in the elastic $v'=0$, $j'=0$ channel in agreement with the data. The effect in all other channels is small.

V. APPLICATIONS

In this section we compare the results of our calculations with experimental data for electron scattering off LiF, HF, and HCl. We describe these molecules by an O(4) Hamiltonian where the number of bosons N is given in Table III. The molecule dipole parameters d_0 and d_1 are determined from the measured dipole moment μ_e and the infrared transition matrix element $R_{0,1}$, using Eqs. (3.32) of paper I. Since only $R_{0,1}^2$ is measured, we know $|R_{0,1}|$ but not its sign. The sign is determined by comparing with *ab initio* calculations [28]. When $R_{0,1}$ is not measured we determined it from a calculation. The quadrupole parameters q_0 in (3.18) are determined from (3.24) and (3.29) using the measured quadrupole moment Θ_v. Table II provides the experimental dipole and quadrupole parameters μ_e, $R_{0,1}$, and Θ_v while Table III provides the model parameters d_0, d_1, and q_0.

A. e + LiF

Here the number of bosons is relatively large, $N = 113$. The total vibrational elastic and inelastic cross sections due to the dipole interaction were already discussed in paper I (see Figs. 3 and 4 of I). In Fig. 3 we show the cross sections to individual rotational states ($j'=0,1,2$ and $3+4$) for $E = 5.44$ eV. We show the cross sections with the dipole interaction (dotted lines); with dipole and quadrupole interactions (dashed lines); and with dipole, quadrupole, and polarization interactions (solid lines). The quadrupole moment of LiF is quite large so the correction due to the quadrupole interaction is substantial even in the $j'=0$ and $j'=1$ channels (in particular at backward angles). The effect of the polarization potential is small even in the $j'=0$ elastic channel.

B. e + HF

Figures 1 and 4–6 show the e+HF elastic ($v=0 \to v'=0$) and inelastic ($v=0 \to v'=1$) scattering cross sections for a series of energies between 0.63 and 10 eV. In each vibrational (v') channel we show separately the cross section for $j'=0,1,2$ and $3+4$ as well as the

TABLE III. Vibron model parameters used in the electron scattering off LiF, HF, and HCl. N is the number of bosons, d_0 and d_1 are the dipole operator parameters [see Eq. (3.17)], and q_0 is the quadrupole operator parameter [Eq. (3.18)]. R_0 is the cutoff parameter for the dipole and quadrupole interactions, while R_{0p} is the cutoff parameter of the polarization potential.

Molecule	N	d_0 (e Å)	d_1(e Å)	q_0 (e Å^2)	R_0 (Å)	R_{0p} (Å)
LiF	113	1.73×10^{-2}	-0.469×10^{-4}	1.62×10^{-2}	0.5	1.8
HF	44	1.14×10^{-2}	-0.694×10^{-4}	1.65×10^{-2}	0.5	1.0
HCl	55	0.606×10^{-2}	-0.360×10^{-4}	2.13×10^{-2}	0.5	1.3

summed cross section. The dotted lines are results with only a dipole interaction, while the dashed lines include the quadrupole interaction. In the vibrational elastic channels ($v'=0$) the quadrupole interaction affects mostly $j'=2$ and $j'=3+4$. The corresponding increase in their cross sections due to the inclusion of a quadrupole interaction is larger at higher energies. The solid lines show the calculations that include the polarization interaction. The quadrupole part of the polarization is weak and is responsible for small corrections. The monopole part, however, is strong and affects mostly the elastic $j'=0$ channel. The cutoff parameter $R_{0p_0}=1$ Å is close to the internuclear separation $R_e=0.9168$ Å. We expect to obtain good results at forward angles that are not much affected by the particular choice of the cutoff. Various cutoff models have been suggested in the literature and they may lead to different results at larger and backward angles (dominated by smaller impact parameter).

At higher energies and at backward angles the calculation underestimates the data. The difference should be accounted for by the exchange interaction, which is not

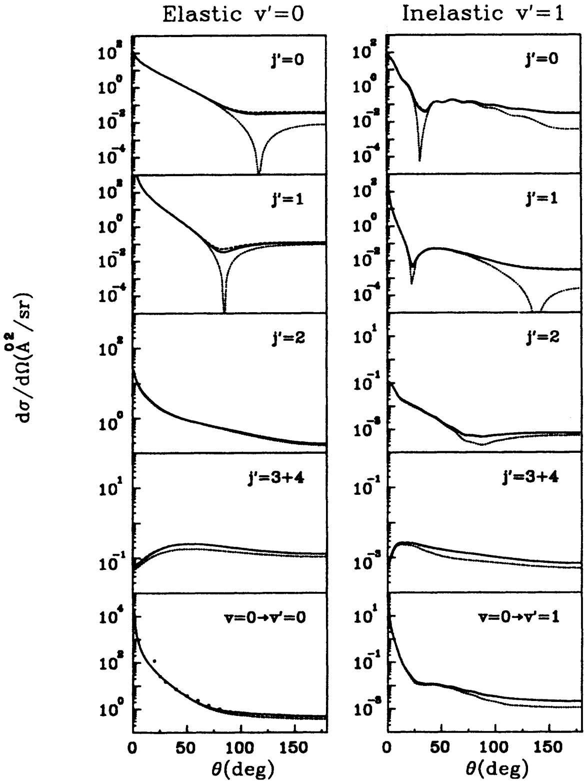

FIG. 3. The differential cross sections for $e+\mathrm{LiF}$ at $E=5.44$ eV. Shown are the cross sections to individual rotational states $j'=0,1,2$ and $3+4$ in the vibrational elastic ($v'=0$, left column) and the inelastic ($v'=1$, right column) channels. In the bottom row are the summed cross sections. Dotted lines: with only a dipole interaction. Dashed lines: with dipole and quadrupole interactions. The solid lines correspond to the inclusion of the polarization potential in addition to the dipole and quadrupole. The various interaction parameters are given in Table III. The data (dots) is taken from Ref. [14].

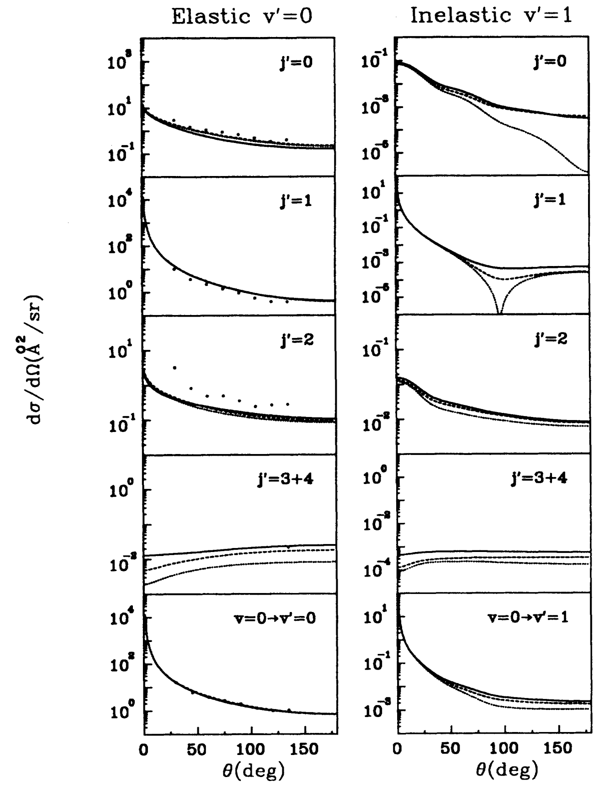

FIG. 4. The differential cross sections for $e+\mathrm{HF}$ at $E=0.63$ eV. The data is taken from Ref. [9]. See Fig. 1 for details.

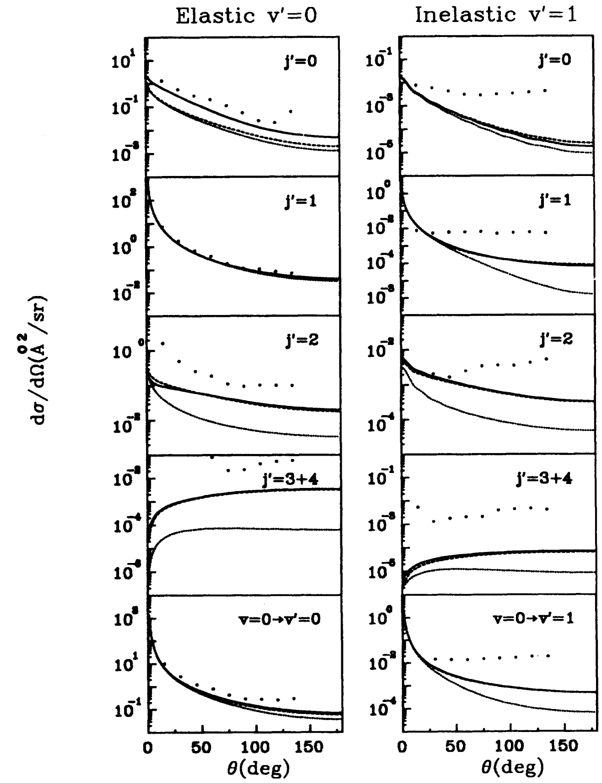

FIG. 5. As in Fig. 4, but for a collision energy of $E=6$ eV.

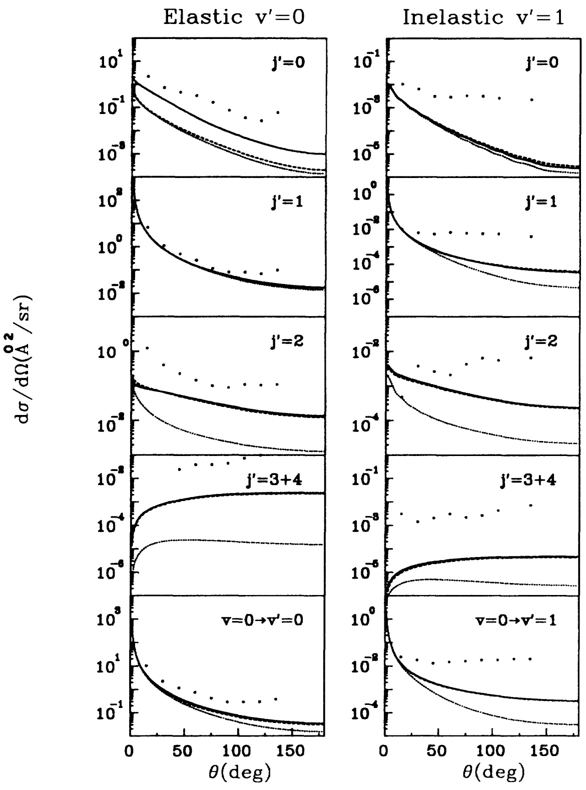

FIG. 6. As in Fig. 4, but for $E = 10$ eV.

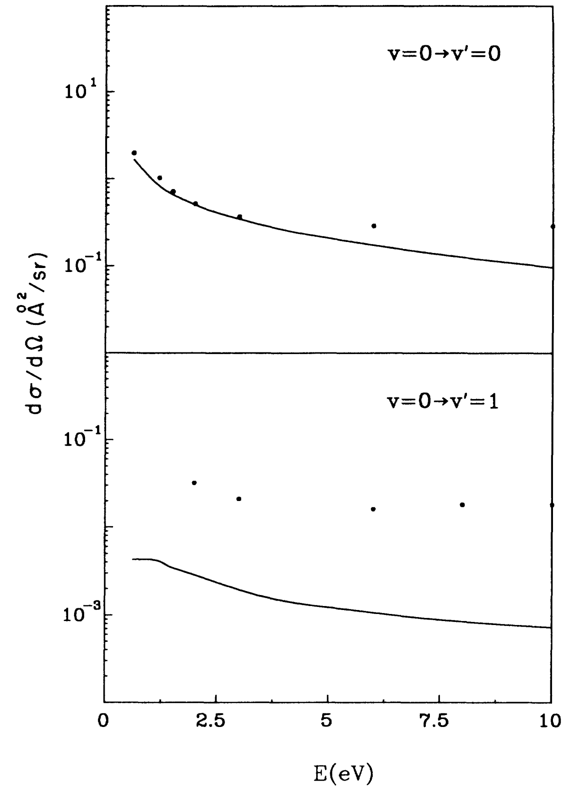

FIG. 7. The vibrational elastic ($v'=0$) and inelastic ($v'=1$) differential cross sections for $e+\mathrm{HF}$ at $\theta=90°$ vs the energy of the electron. The solid lines are the algebraic eikonal calculations and the dots are the data [9].

included in the present calculations.

Figure 7 shows the energy dependence of the vibrationally elastic ($v'=0$) and inelastic ($v'=1$) differential cross sections at $\theta=90°$. While our calculations in the vibrational elastic channels ($v=0, j=0 \rightarrow v'=0, j'$) agree fairly well with the data, the calculated inelastic vibrational cross sections underestimate significantly the data. This again reflects the larger importance of the exchange interaction in the inelastic channel. Thus though the inclusion of more realistic dipole and quadrupole interactions increases the inelastic cross section by one or two orders of magnitude, it is still not sufficient to account for the experimental data.

An interesting experimental observation [29] in the scattering of electrons from hydrogen halides (such as HF and HCl) is the existence of sharp threshold peaks in the vibrational excitation cross sections. This observation was followed by extensive theoretical studies [1(b),30]. The peaks were reproduced by solving the coupled-channel equations for a model potential [31] and in an *ab initio* adiabatic calculation [32] when short-range exchange interactions are included. A more detailed *ab initio* calculation [33], in which the vibrational motion is treated nonadiabatically, led to an interpretation of the peaks in terms of nuclear Feshbach resonances.

Since the present model calculation excludes the electronic degrees of freedom of the molecule and does not include short range and exchange interactions, it cannot reproduce the threshold peaks.

C. $e+\mathrm{HCl}$

We have carried a study similar to that of $e+\mathrm{HF}$ but for the $e+\mathrm{HCl}$ system. Figures 8–11 show the $e+\mathrm{HCl}$ elastic and inelastic scattering for several collision energies between 0.5 and 7 eV. The relevant parameters are tabulated in Tables II and III. It is interesting to compare the two systems. The HCl molecule is bigger ($R_e=1.274$ Å) than the HF molecule, so that $R_{0p}=1.3$ Å is also chosen to be larger accordingly. The polarizability of HCl is relatively large compared with HF. The monopole polarization interaction is thus stronger and affects much more the $j'=0$ channel of HCl. This agrees nicely with the data. The quadrupole moment of HCl is larger than that of HF and is indeed seen to have a stronger effect in the $j'=2$ and $j'=3+4$ channels. The cross section in the $j'=3+4$ channel is underestimated, probably since higher multipoles are neglected.

To compare the HF and HCl systems, notice that a relevant dimensionless scale is kR_e, with R_e the internuclear separation. Since $k \propto \sqrt{E}$, we find that in order to have the same value of kR_e, the energy for the $e+\mathrm{HCl}$ system should be smaller by about a factor of 2 than the energy for $e+\mathrm{HF}$. When comparing the $e+\mathrm{HF}$ and $e+\mathrm{HCl}$ systems at such respective energies, we indeed see a similar quality of the fit to the data.

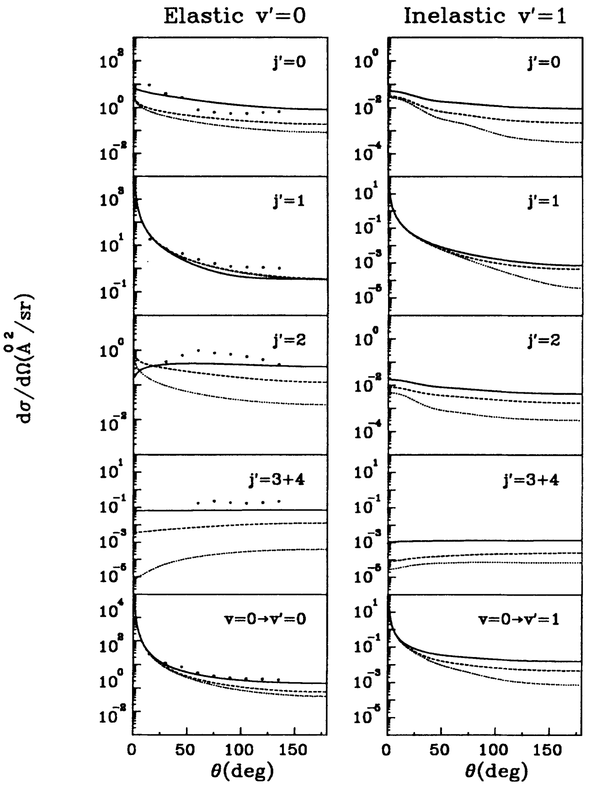

FIG. 8. The differential cross sections for vibrational elastic and inelastic scattering of $e+\mathrm{HCl}$ at $E=0.5$ eV. The data is taken from Ref. [9]. See Fig. 1 for details.

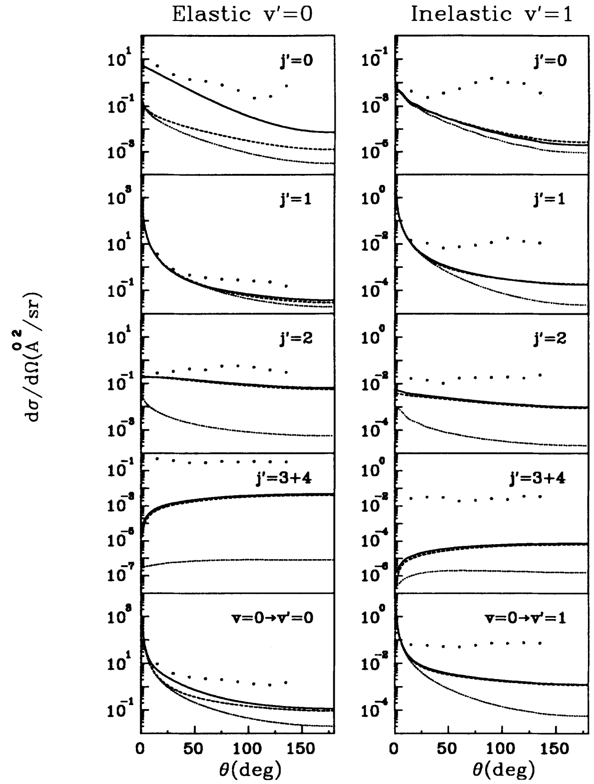

FIG. 10. As in Fig. 8, but for $E=5$ eV.

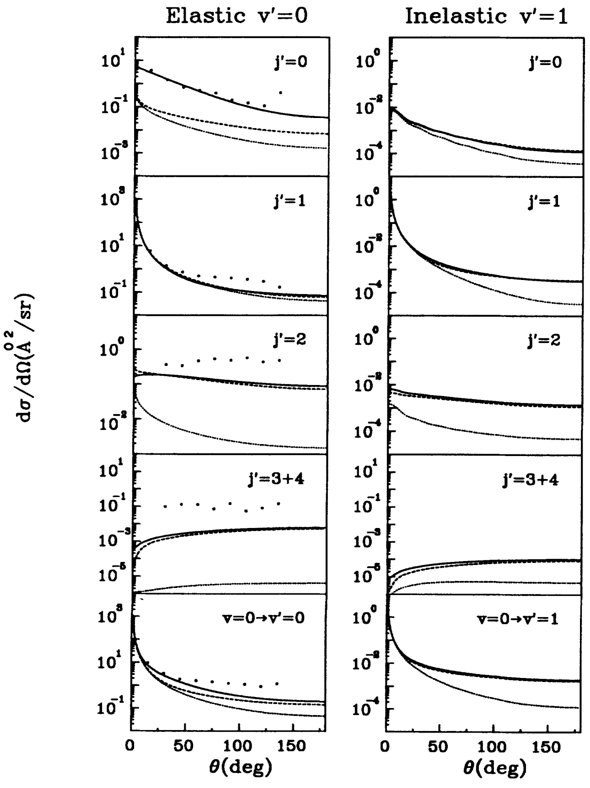

FIG. 9. As in Fig. 8, but for $E=2.9$ eV.

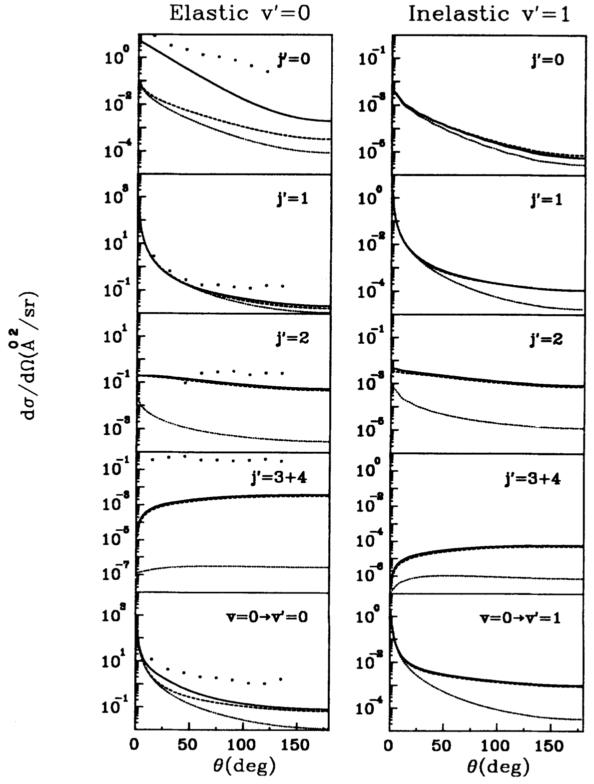

FIG. 11. As in Fig. 8, but for $E=7$ eV.

Detailed coupled-channel calculations [2] for e +HCl, which include exchange in addition to static and polarization interactions, reproduce well the energy dependence of the vibrationally elastic cross sections even at higher energies. The inclusion of an exchange interaction also results in an order-of-magnitude increase of the cross section for the vibrationally inelastic channels [10]. The failure of our calculations at higher energies and in the vibrationally inelastic scattering is because we have not yet included the exchange interaction in the algebraic approach.

VI. CONCLUSIONS

We have applied the generalized algebraic eikonal framework of paper I to electron-molecule scattering with more realistic interactions than previously included in this approach [5]. Our calculations, which use an improved dipole, a quadrupole, and polarization interactions are compared with data of electron scattering from LiF, HF, and HCl. The agreement with the experiment in the vibrational elastic channels (for different rotational states) is good. In the vibrational inelastic channels there is a strong enhancement when compared with the calculations of Ref. [5], but we still underestimate the data, in particular at backward angles. This is mainly because we have not yet included the short-range exchange interaction [2,8,12,13] in our algebraic formulation. The inclusion of such an interaction can be done in a phenomenological way using the local free-electron gas exchange interaction [10]. A better way will be to use an algebraic extension [34] of the vibron model, which includes the electronic degrees of freedom. A secondary reason for the discrepancy at large angles may be due to the sudden approximation. Our generalized framework allows the algebraic evaluation of corrections to the sudden approximation (to all orders in the coupling). For the dipole interaction these corrections diverge, but for other interactions (e.g., quadrupole) they are convergent. It will be interesting to investigate these corrections.

ACKNOWLEDGMENTS

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