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Algebraic-eikonal approach to the electron-molecule-collision process: Vibrational excitation and quadrupole interaction

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The vibrational excitation mechanism has been included in the algebraic-eikonal approach to the electron–polar-molecule collision process. A dipole operator that can induce vibrational transitions has been used, and a technique for the evaluation of the matrix elements required for the calculation of the scattering amplitude in the Glauber approximation has been developed. In addition to the long-range dipole interaction, the quadrupole interaction has been included in the same framework in order to improve the potential description of the collision process. Numerical calculations are shown for electron-induced rotational-vibrational excitation through the dipole and dipole-plus-quadrupole interactions.

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I. INTRODUCTION

Among the variety of processes that occur in an electron-molecule collision, the rotational and vibrational excitation of polar molecules by the scattered electrons plays a fundamental role. Because of its possible application in a variety of fields, many theoretical studies [1–5] have been devoted to its understanding.

Following the development of computational methods, *ab initio* calculations became feasible in the past several years and much effort has been put in the inclusion of various types of interactions into the calculations of scattering cross section, at least for simple molecules. In the standard *ab initio* techniques, both the scattering process and the molecular dynamic problems are treated starting from first principles. However, in the case of electron energies of several electron volts and of strong dipolar targets, the channel coupling between the rotational and vibrational degrees of freedom, even in the adiabatic approximation, can be a prohibitive problem from the computational point of view, particularly for polyatomic molecular targets.

On the other hand, perturbative methods such as the Born approximation, or the diffractive theories (Glauber approximation), even though restricted in their range of applicability, provide very simple, closed-form expressions for the calculation of scattering cross sections. Moreover, they can be used as starting points on which more elaborated approaches can be developed [5].

Recently, some attention has been gained by a novel approach to the calculation of the differential cross section within the Glauber approximation: the algebraic-eikonal approach [6]. This method makes use of an algebraic description of the molecular rovibrational degrees of freedom, the vibron model [7,8], in conjunction with the Glauber diffractive theory in the adiabatic approximation. This theory, originally developed for the calculation of the scattering cross section of protons by deformed nuclei [9], has been applied so far to the calculation of rotational excitation of diatomic [10,11] and linear triatomic [12] polar molecules.

In the algebraic-eikonal approach, the description of molecular degrees of freedom, and of the interaction to a certain extent, using algebraic techniques, allows for a treatment of the rotational and vibrational coupling without recurring to the standard coupled-channels calculation.

More recently [13], the algebraic-eikonal approach has been used *in conjunction* with close-coupling calculations in order to include the effect of the short-range interactions. In this approach, the hybrid approach, long-range dipole interaction, responsible for the scattering at forward angles, has been accounted for by the algebraic-eikonal technique whereas the short-range interaction has been included through full close-coupling calculations.

However, the vibrational excitation process was left out up to now from the algebraic-eikonal formalism, except for a first-order perturbation theory proposed in Ref. [10], where the possible vibrational excitation mechanism was introduced asuming a so-called broken O(4) symmetry in the description of the diatomic target. This approach leads to vibrational excitation cross sections several orders of magnitude smaller than the vibrationally elastic one and, moreover, the calculation of dipole transition moments using this approach lead to infrared intensities at variance with experimental values [14].

In this work we will follow a different line. We will remain within the O(4) dynamical symmetry of the vibron model and we will make use of a different dipole operator which can induce vibrational transitions unlike the dipole operator first proposed in Ref. [6]. This transition operator has been recently introduced [15] and successfully applied [15–17] to the calculation of infrared transition intensities in diatomic as well as in several polyatomic molecules.

In addition to the vibrational excitation, we will also include the quadrupole interaction in the same algebraic-eikonal framework in order to improve the potential description of the collision process.

After a general introduction of the basic quantities of the Glauber approximation in Sec. II, we will introduce the dipole transition operator and show a technique to calculate analytically the matrix elements required for the evaluation of the scattering amplitude in Sec. III. In Sec. III E we will include the quadrupole interaction in the model and give a technique to approximate the scattering amplitude. In Sec. IV we will give an illustrative example of the proposed methodology for calculation of the scattering cross section, and finally give the conclusions.

II. GENERAL FORMULATION

In the Glauber approximation, the scattering amplitude for a collision process in which the electron momentum transferred from an initial wave vector $\mathbf{k}$ to the final one $\mathbf{k}'$ is $\mathbf{q}=\mathbf{k}-\mathbf{k}'$ and the molecule goes from an initial state i to a final state f is given by

$$F_{fi}(\mathbf{q})=\frac{ik}{2\pi}\int d^2\mathbf{b}\,e^{i\mathbf{q}\cdot\mathbf{b}}\langle f|1-e^{i\chi(\mathbf{b})}|i\rangle \;, \tag{2.1}$$

where $\mathbf{b}$ is the vector lying on the plane through the origin perpendicular to the $\hat{\mathbf{z}}$ axis, chosen to be in the direction of the incident electron wave vector $\mathbf{k}=k\hat{\mathbf{z}}$.

For the rotational excitation of a polar molecule from an initial state with total angular momentum J and third component M to a final state with J' and M', the matrix elements appearing in Eq. (2.1) are explicitly given by

$$\langle f|1-e^{i\chi(\mathbf{b})}|i\rangle=\int Y^{*}_{J'M'}(\Omega_s)(1-e^{i\chi(\mathbf{b},\Omega_s)}) \times Y_{JM}(\Omega_s)d\Omega_s \;, \tag{2.2}$$

where the spherical harmonics $Y_{JM}(\Omega_s)$ are taken as molecular eigenfunctions.

In Eq. (2.2), the dependence on the molecular symmetry axis orientation Ω_s is shown explicitly in both the molecular eigenfunctions as well as in the eikonal phase $\chi(\mathbf{b},\Omega_s)$.

The explicit form of the eikonal phase acquired by the electron, while interacting with the molecule, depends on the interaction potential. In fact the eikonal phase is defined by

$$\chi(\mathbf{b},\Omega_s)=-\frac{m_e}{\hbar^2 k}\int V(\mathbf{r},\Omega_s)dz \;, \tag{2.3}$$

where m_e is the electron mass and $\mathbf{r}$ is the position vector of the electron as measured from the center of mass of the molecule.

In general, the interaction potential can be written as

$$V(\mathbf{r},\Omega_s)=\sum_{\lambda} v_{\lambda}(r)\left[\frac{4\pi}{2\lambda+1}\right]^{1/2} \times\sum_{\nu}(-1)^{\nu}Y_{\lambda,\nu}(\Omega_e)Y_{\lambda,-\nu}(\Omega_s) \;, \tag{2.4}$$

where Ω_e defines the orientation of $\mathbf{r}$ and the functions $v_{\lambda}(r)$ depend only on the magnitude of $\mathbf{r}$.

As an example, for the dipole interaction we have ($\lambda=1$)

$$v_1(r)=-\left[\frac{4\pi}{3}\right]^{1/2}\frac{eD}{r^2} \;, \tag{2.5}$$

where D is the dipole moment of the molecule and e the electron charge. Eventually, $v_1(r)$ can be cutoff [dipole-cutoff (DCO) models] in order to remove the singularity at $r=0$,

$$v_1(r)=-\left[\frac{4\pi}{3}\right]^{1/2}\frac{eD}{r^2+R_1^2} \;, \tag{2.6}$$

where R_1 is the dipole cutoff radius.

The problem of calculating the scattering amplitude in the Glauber approximation for rotational excitation has been solved so far in the assumption that the molecular eigenfunctions are spherical harmonics in the case of dipole interaction [18] and for the more general case $\lambda=0,1,2$ [19].

A number of complications arise when trying to extend this kind of approach to vibrational excitation process. In order to keep the problem manageable, usually the assumptions are made that: (i) the molecular vibrational and rotational degrees of freedom are decoupled and (ii) the interaction potential is expanded in power series of the internuclear distance R around the equilibrium position R_e,

$$V(\mathbf{r},\Omega_s,R)=V(\mathbf{r},\Omega_s,R=R_e)+\left.\frac{\partial V(\mathbf{r},\Omega_s,R)}{\partial R}\right|_{R=R_e} \times(R-R_e)+\cdots \;. \tag{2.7}$$

Within these approximations, the problem has been solved so far only for the case in which

$$1-e^{i\chi(\mathbf{b},\Omega_s)}\simeq -i\chi(\mathbf{b},\Omega_s) \;, \tag{2.8}$$

that is, in the first Born approximation (FBA).

For the allowed rotational transitions $J'=J\pm1\leftarrow J$, the FBA cross section is given by the well-known relation [20]

$$\frac{d\sigma}{d\Omega}(\theta)=\frac{4}{3}\frac{k'}{k}D^2\frac{J_{>}}{2J+1}\frac{1}{q^2} \;, \tag{2.9}$$

where $q^2=k'^2+k^2-2kk'\cos(\theta)$ and $J_{>}=\max(J',J)$.

When the expansion (2.7) is adopted, this relation holds for the general transition $v'J'\leftarrow vJ$ if D^2 is replaced by the matrix elements $\langle v'J'|\hat{D}|vJ\rangle^2$ of the dipole operator $\hat{D}$ between the vibrational states v' and v.

In order to extend to rovibrational transition the general expression for the Glauber amplitude (2.1), we will adopt the algebraic-eikonal approach which allows for a unified description of the molecular rovibrational degrees of freedom and at the mean time for a general dipole interaction, bypassing therefore the commonly adopted approximations described above.

III. THE ALGEBRAIC APPROACH

A. The vibron model

In the algebraic approach, the molecular operators are replaced by the elements of a Lie algebra. The realization of this algebra is made through the use of creation and annihilation operators for two types of vibrons, called σ

and π vibrons. Products of these operators, which transform as spherical tensors, are the elements of the algebra.

It has been proposed [7] that the appropriate algebra which describes the rotation-vibration degrees of freedom of a diatomic molecular bound is the U(4) algebra. It hasd $4^2=16$ elements. However, only a subset of these elements is needed to describe the spectrum accurately. They are the elements of the O(4) algebra in the chain $U(4)\supset O(4)\supset O(3)$ and therefore the molecular states are referred to as O(4) states.

The operators that we will use here are

$$\hat{n}_\pi=-\sqrt{3}(\pi^\dagger\tilde{\pi})_0^{(0)} , \tag{3.1a}$$

$$\hat{J}_\mu=\sqrt{2}(\pi^\dagger\tilde{\pi})_\mu^{(1)} , \tag{3.1b}$$

$$\hat{D}_\mu=(\pi^\dagger\tilde{\sigma}+\sigma^\dagger\tilde{\pi})_\mu^{(1)} , \tag{3.1c}$$

$$\hat{Q}_\mu=(\pi^\dagger\tilde{\pi})_\mu^{(2)} , \tag{3.1d}$$

where the creation and annihilation operators for σ and π vibrons are used explicitly. A detailed account of definitions and properties of these operators can be found in Refs. [8,21].

The algebraic Hamiltonian is of the type

$$\hat{H}=h_0+A\hat{D}\cdot\hat{D}+B\hat{J}\cdot\hat{J} , \tag{3.2}$$

with h_0, A, and B constants. This Hamiltonian has analytical eigenvalues that can be arranged into the form

$$\begin{aligned}E(v,J)=h_0&-4A(N+2)(v+\tfrac{1}{2})\\&+4A(v+\tfrac{1}{2})^2+(B-A)J(J+1) ,\end{aligned} \tag{3.3}$$

where N is the total number of vibrons, to be determined together with h_0, A, and B from the molecular constants. We have

$$\begin{gathered}T_e=h_0,\quad \omega_e=-4A(N+2),\quad \omega_e\chi_e=-4A ,\\ \text{and}\\ B_e=B-A .\end{gathered} \tag{3.4}$$

When calculating the scattering amplitude in this framework we have to proceed as follows: (i) replace the molecular eigenfunctions, usually spherical harmonics, by the algebraic eigenstates; (ii) replace the $Y_{\lambda\nu}(\Omega)$ in the interaction potential by the appropriate algebraic operators; (iii) replace the dependence on the internuclear distance in Eq. (2.7) in order to allow for vibrational transitions; (iv) calculate the relative matrix elements.

The basis for this procedure [except for point (iii)] has been developed for the calculation of rotational excitation cross sections of diatomic [6] and triatomic [12] molecules by the long-range dipole interaction potential.

B. Transition operator for vibrational excitation

A dipole operator of type

$$\hat{T}_\mu=d_0\hat{D}_\mu \tag{3.5}$$

has been previously used [6]. The constant d_0 is fixed by the condition $\langle v'=0J'=1\|\hat{T}\|v=J=0\rangle=D$ (dipole moment). When the O(4) eigenstates are used, this operator has selection rules $\Delta v=0$ and $\Delta J=\pm 1$.

An appropriate operator that can describe accurately infrared intensities has been recently suggested [15] to be of type

$$\hat{T}_\mu=\sum_{k=0}^{\infty} d_k\tfrac{1}{2}(e^{\lambda_k\hat{n}_\pi}\hat{D}_\mu+\hat{D}_\mu e^{\lambda_k\hat{n}_\pi})_\mu . \tag{3.6}$$

The summation in this expression is very quickly convergent indeed and only very few terms are sufficient to reproduce the experimental intensities [15–17].

The factor $e^{\lambda_k\hat{n}_\pi}$ in Eq. (3.6) breaks the selection rules $\Delta v=0$ making the dipole operator capable of inducing vibrational transitions. This, in turn, modifies the interaction potential. The dependence of the interaction potential on the internuclear distance, Eq. (2.7), is achieved in the algebraic formalism through the presence of the operator $\hat{n}_\pi$ in Eq. (3.6). In fact, it has been suggested [22] that the operator $\hat{n}_\pi$ might be asssociated with the bond length in a diatomic molecule.

In order to make the calculation of the matrix elements feasible for obtaining the transition rates in a certain accuracy, we will retain here only two terms in the expansion (3.6),

$$\hat{T}_\mu=d_0\hat{D}_\mu+d_1\tfrac{1}{2}(e^{\lambda\hat{n}_\pi}\hat{D}_\mu+\hat{D}_\mu e^{\lambda\hat{n}_\pi})_\mu\equiv\hat{G}_\mu+\hat{E}_\mu . \tag{3.7}$$

In this case, in addition to the total number of vibrons N, there are three constants d_0, d_1, and λ to be determined from the experimental dipole moment and infrared intensities. The matrix elements of the operator $\hat{T}_\mu$ in Eq. (3.7) can be calculated analytically and their expressions are given in Appendix A.

C. Matrix elements for the scattering amplitude

We will use now the operator in Eq. (3.7) for the calculation of the scattering amplitude in the Glauber approximation. The dipole interaction potential, expressed in terms of algebraic operators, is

$$V_1(\mathbf{r},\hat{a})=v_1(r)\left[\frac{4\pi}{3}\right]^{1/2}Y^{(1)}\cdot\hat{T} , \tag{3.8}$$

where we have generally indicated with $\hat{a}$ the algebraic variables. The corresponding eikonal phase is expressed as follows:

$$\chi_D(\mathbf{b},\hat{a})=\eta_1(b)\hat{\mathbf{b}}\cdot\hat{T} , \tag{3.9}$$

with

$$\eta_1(b)=\frac{em_e}{\hbar^2k}\int\frac{b}{(r^2+R_1^2)r}dz \tag{3.10}$$

and $r=(b^2+z^2)^{1/2}$.

The matrix elements of the exponential function in Eq. (2.1) have the property [6]

$$\begin{aligned}\langle v'J'M'|e^{i\chi_D(\mathbf{b})}|vJM\rangle&\\=e^{i(M-M')\phi_b}&\sum_m d_{M'm}^{(J')}[\pi/2]d_{Mm}^{(J)}[\pi/2]\\&\times\langle v'J'm|e^{i\eta_1(b)\hat{T}_0}|vJm\rangle ,\end{aligned} \tag{3.11}$$

where $d^{(l)}_{mn}[\pi/2]$ are the Wigner d functions [23] and $\hat{T}_0$ is the $\mu=0$ component of the operator defined in Eq. (3.7).

For the case $\hat{T}_0=d_0\hat{D}_0=\hat{G}_0$ the matrix elements are given by [10]

$$\langle v'J'm|e^{i\eta_1(b)\hat{G}_0}|vJm\rangle$$
$$=\delta_{v',v}\sum_{\sigma}\left(\frac{\omega}{2}\sigma\frac{\omega}{2}m-\sigma\middle|J'm\right)\left(\frac{\omega}{2}\sigma\frac{\omega}{2}m-\sigma\middle|Jm\right)$$
$$\times e^{i\eta_1(b)(2\sigma-m)}, \tag{3.12}$$

where $\omega\equiv N-2v$ and the $(\ldots\ldots|\ldots)$ are Clebsch-Gordan coefficients.

Essentially, the inclusion of vibrational excitation is reduced to the calculation of the matrix elements

$$\langle v'J'm|e^{i\eta_1(b)\hat{T}_0}|vJm\rangle \tag{3.13}$$

for the general opeator $\hat{T}_{\mu=0}$ of Eq. (3.7).

One way to solve the problem is to calculate these matrix elements numerically, that is, find a basis diagonalizing the operator $\hat{T}_{\mu=0}$, calculate the matrix elements of $e^{i\eta\hat{T}_0}$, and then rotate back to the O(4) basis.

Another way to proceed is to consider the second term in Eq. (3.7) as a correction to the leading first term. Then

$$e^{i\eta(\hat{G}_0+\hat{E}_0)}\sim 1+i\eta(\hat{G}_0+\hat{E}_0)-\tfrac{1}{2}\eta^2(\hat{G}_0+\hat{E}_0)^2+\cdots$$
$$=1+i\eta\hat{G}_0-\tfrac{1}{2}\eta^2\hat{G}_0^2+i\eta\hat{E}_0$$
$$-\tfrac{1}{2}\eta^2(\hat{G}_0\hat{E}_0+\hat{E}_0\hat{G}_0)-\tfrac{1}{2}\eta^2\hat{E}_0^2\,. \tag{3.14}$$

The first three terms in the last expression are well approximated by $e^{i\eta\hat{G}_0}$. Now consider

$$e^{i\eta\hat{G}_0}\hat{E}_0+\hat{E}_0e^{i\eta\hat{G}_0}\sim(1+i\eta\hat{G}_0)\hat{E}_0+\hat{E}_0(1+i\eta\hat{G}_0)$$
$$=\hat{E}_0+i\eta\hat{G}_0\hat{E}_0+\hat{E}_0+i\eta\hat{E}_0\hat{G}_0$$
$$=2\hat{E}_0+i\eta(\hat{G}_0\hat{E}_0+\hat{E}_0\hat{G}_0)\,.$$

Therefore

$$\tfrac{1}{2}i\eta(e^{i\eta\hat{G}_0}\hat{E}_0+\hat{E}_0e^{i\eta\hat{G}_0})=i\eta\hat{E}_0-\tfrac{1}{2}\eta^2(\hat{G}_0\hat{E}_0+\hat{E}_0\hat{G}_0)$$

and

$$e^{i\eta(\hat{G}_0+\hat{E}_0)}\sim e^{i\eta\hat{G}_0}+\tfrac{1}{2}i\eta(e^{i\eta\hat{G}_0}\hat{E}_0+\hat{E}_0e^{i\eta\hat{G}_0})-\tfrac{1}{2}\eta^2\hat{E}_0^2\,. \tag{3.15}$$

The matrix elements of the first term in Eq. (3.15) were given above in Eq. (3.12). The calculation of the matrix elements of the second term requires some algebra. The results are

$$\langle v'J'm|e^{i\eta_1(b)\hat{G}_0}\hat{E}_0|vJm\rangle=\frac{(10Jm|J+1m)}{\sqrt{2J+3}}\langle v'J+1\|\hat{E}\|vJ\rangle\langle v'J'm|e^{i\eta_1(b)\hat{G}_0}|v'J+1m\rangle$$
$$+\frac{(10Jm|J-1m)}{\sqrt{2J-1}}\langle v'J-1\|\hat{E}\|vJ\rangle\langle v'J'm|e^{i\eta_1(b)\hat{G}_0}|v'J-1m\rangle \tag{3.16a}$$

and

$$\langle v'J'm|\hat{E}_0e^{i\eta_1(b)\hat{G}_0}|vJm\rangle=\frac{(10J'+1m|J'm)}{\sqrt{2J'+1}}\langle v'J'\|\hat{E}\|vJ'+1\rangle\langle vJ'+1m|e^{i\eta_1(b)\hat{G}_0}|vJm\rangle$$
$$+\frac{(10J'-1m|J'm)}{\sqrt{2J'+1}}\langle v'J'\|\hat{E}\|vJ'-1\rangle\langle vJ'-1m|e^{i\eta_1(b)\hat{G}_0}|vJm\rangle\,. \tag{3.16b}$$

The last term in Eq. (3.15) is in η^2 and can be neglected in practical cases since $\eta\ll 1$ (see below), though the calculation of its matrix elements do not present any difficulty.

We can therefore evaluate analytically all the matrix elements required for the calculation of the scattering amplitude.

In order to check the validity of the approximation given in Eq. (3.14), we have performed a number of calculations and found a very good agreement between the results obtained through a numerical diagonalization and those obtained using the analytical expressions (3.12), (3.16a), and (3.16b).

As an example, in Table I we report the values of the matrix elements, Eq. (3.13), for the initial state $v=0$, $J=0$, and the final states $v'=0,1,2,$, $J'=0,1,2$, and $m=0$ as a function of the impact parameter b (column 1). The parameters used in these calculations are those given below in Table II for the HF molecule.

In column 2 we report the values of $\eta_1(b)$, Eq. (3.10), calculated at $E_e=6$ eV. In columns 3 and 4, the real and imaginary parts of the matrix elements calculated using Eqs. (3.15), (3.16a), and (3.16b) are given, respectively. In columns 5 and 6 the same quantities are shown as calculated using the numerical diagonalization technique.

Due to the good agreement obtained using the exact (numerical) technique as compared with the analytical one, we will adopt the approximation of Eq. (3.14) in all the subsequent calculations.

D. Scattering amplitude and differential cross section

In order to calculate the scattering amplitude Eq. (2.1), we will make use of the expansion

$$e^{\mathbf{q}\cdot\mathbf{b}}=\sum_{\lambda}i^{\lambda}J_{\lambda}(qb)e^{i\lambda(\phi_b-\phi_q)}, \tag{3.17}$$

TABLE I. Comparison of the analytical and numerical matrix element calculations of Eq. (3.13). See the text (Sec. III C) for the explanation of the entries in this table. ($x\,[y]=x\times 10^{y}$).

		Analytical		Numerical	
$b(A)$	$\eta_1(b)$	Re	Im	Re	Im
$v'=0,\ J'=0\leftarrow v=0,\ J=0$					
0.01	0.1155	0.993 19	0.0	0.992 62	0.0
0.10	0.5687	0.838 46	0.0	0.830 11	0.0
1.00	0.5398	0.854 14	0.0	0.846 15	0.0
10.00	0.0626	0.998 00	0.0	0.997 83	0.0
100.00	0.0063	0.999 98	0.0	0.999 98	0.0
1000.00	0.0006	0.100 00[1]	0.0	0.100 00[1]	0.0
$v'=0,\ J'=1\leftarrow v=0,\ J=0$					
0.01		0.0	0.121 04	0.0	0.120 89
0.10		0.0	0.550 80	0.0	0.536 05
1.00		0.0	0.527 23	0.0	0.514 39
10.00		0.0	0.657 61[−1]	0.0	0.657 38[−1]
100.00		0.0	0.659 31[−2]	0.0	0.659 31[−2]
1000.00		0.0	0.659 33[−3]	0.0	0.659 33[−3]
$v'=0,\ J'=2\leftarrow v=0,\ J=0$					
0.01		−0.605 62[−2]	0.0	−0.655 87[−2]	0.0
0.10		−0.142 28	0.0	−0.147 69	0.0
1.00		−0.128 61	0.0	−0.134 06	0.0
10.00		−0.178 11[−2]	0.0	−0.193 15[−2]	0.0
100.00		−0.178 76[−4]	0.0	−0.193 96[−4]	0.0
1000.00		−0.178 76[−6]	0.0	−0.193 97[−6]	0.0
$v'=1,\ J'=0\leftarrow v=0,\ J=0$					
0.01	0.1155	−0.950 04[−3]	0.0	−0.743 34[−3]	0.0
0.10	0.5687	−0.197 81[−1]	0.0	−0.164 39[−1]	0.0
1.00	0.5398	−0.181 07[−1]	0.0	−0.149 51[−1]	0.0
10.00	0.0626	−0.280 42[−3]	0.0	−0.219 02[−3]	0.0
100.00	0.0063	−0.281 87[−5]	0.0	−0.220 00[−5]	0.0
1000.00	0.0006	−0.281 88[−7]	0.0	−0.220 10[−7]	0.0
$v'=1,\ J'=1\leftarrow v=0,\ J=0$					
0.01		0.0	0.643 82[−2]	0.0	0.648 68[−2]
0.10		0.0	0.187 00[−1]	0.0	0.237 08[−1]
1.00		0.0	0.189 22[−1]	0.0	0.232 70[−1]
10.00		0.0	0.353 76[−2]	0.0	0.354 54[−2]
100.00		0.0	0.356 32[−3]	0.0	0.356 32[−3]
1000.00		0.0	0.356 34[−4]	0.0	0.356 34[−4]
$v'=1,\ J'=2\leftarrow v=0,\ J=0$					
0.01		−0.842 13[−3]	0.0	−0.659 61[−3]	0.0
0.10		−0.163 56[−1]	0.0	−0.140 08[−1]	0.0
1.00		−0.150 90[−1]	0.0	−0.127 97[−1]	0.0
10.00		−0.249 04[−3]	0.0	−0.194 57[−3]	0.0
100.00		−0.250 52[−5]	0.0	−0.195 53[−5]	0.0
1000.00		−0.250 54[−7]	0.0	−0.195 54[−7]	0.0
$v'=2,\ J'=0\leftarrow v=0,\ J=0$					
0.01	0.1155	0.119 37[−3]	0.0	0.670 82[−4]	0.0
0.10	0.5687	0.251 99[−2]	0.0	0.159 30[−2]	0.0
1.00	0.5398	0.230 31[−2]	0.0	0.143 82[−2]	0.0
10.00	0.0626	0.352 21[−4]	0.0	0.197 23[−4]	0.0
100.00	0.0063	0.353 98[−6]	0.0	0.197 93[−6]	0.0
1000.00	0.0006	0.353 99[−8]	0.0	0.197 93[−8]	0.0

TABLE I. (*Continued*).

		Analytical		Numerical	
$b(A)$	$\eta_1(b)$	Re	Im	Re	Im
$v'=2, J'=1 \leftarrow v=0, J=0$					
0.01		0.0	−0.864 52[−3]	0.0	−0.875 42[−3]
0.10		0.0	−0.269 70[−2]	0.0	−0.385 25[−2]
1.00		0.0	−0.270 14[−2]	0.0	−0.370 16[−2]
10.00		0.0	−0.474 31[−3]	0.0	−0.476 05[−3]
100.00		0.0	−0.477 45[−4]	0.0	−0.477 46[−4]
1000.00		0.0	−0.477 48[−5]	0.0	−0.477 48[−5]
$v'=2, J'=2 \leftarrow v=0, J=0$					
0.01		0.105 68[−3]	0.0	0.595 14[−4]	0.0
0.10		0.209 57[−2]	0.0	0.140 05[−2]	0.0
1.00		0.192 89[−2]	0.0	0.126 57[−2]	0.0
10.00		0.312 36[−4]	0.0	0.175 02[−4]	0.0
100.00		0.314 15[−6]	0.0	0.175 66[−6]	0.0
1000.00		0.314 61[−8]	0.0	0.175 66[−8]	0.0

where $J_\lambda(x)$ are Bessel functions of integer order.

Then, after integrating over azumithal orientation of **b** we obtain, for an initial state $i=(vJM)$ and a final state $f=(v'J'M')$,

$$F_{fi}^{(D)}(\mathbf{q})=iki^{(M'-M)}\int b\,db\,J_{(M'-M)}(qb)\times\left[\delta_{fi}-\sum_m d_{M'm}^{(J')}[\pi/2]d_{Mm}^{(J)}[\pi/2]\times\langle v'J'm|e^{i\eta_1(b)\hat{T}_0}|vJm\rangle\right]\times e^{i(M-M')\phi_q}\,. \tag{3.18}$$

The scattering cross section for a transition $v'J'\leftarrow vJ$ is obtained by summing up over all the final M' and averaging over M,

$$\frac{d\sigma}{d\Omega}(v'J'\leftarrow vJ|\theta)=\frac{1}{2J+1}\sum_{M',M}\frac{k'}{k}|F_{fi}^{D}(\mathbf{q})|^2\,. \tag{3.19}$$

We note here that for given M',M, the exponential factor $e^{i(M-M')\phi_q}$ in Eq. (3.18) does not effect the calculation of the scattering cross section, making it essentially dependent only on $|\mathbf{q}|$ or on the scattering angle θ. Also, it is easy to verify that for large b, using the approximation in Eq. (2.8), the expression (3.18) leads to the FBA value Eq. (2.9). Therefore, as it should be, in the limit of small scattering angle the Glauber amplitude in the algebraic approach converges to the FBA result.

TABLE II. Parameters used in the calculations of the e^-+HF and e^-+HCl differential cross sections.

	HF	HCl
N	44	55
h_0 (cm^{-1})	0.0	0.0
A (cm^{-1})	−22.475	−13.19
B (cm^{-1})	−1.515	−2.597
D (D)	1.826	1.109
δD^{a}	0.054	0.064
δD^{b}	−0.007	−0.007
Q (10^{-26} esu cm^2)	2.36	3.8
δQ^{c}	−0.136	−0.124
d_0 (D)	0.052 5	0.027 9
d_1 (D)	−0.003 34	−0.002 45
λ	0.056 9	0.043 1
R_1 (Å)	0.5	0.5
R_2 (Å)	0.1	0.1

[a] $\langle v'=1,J'=1\|\hat{T}\|v=0,J=0\rangle\langle v'=0,J'=1\|\hat{T}\|v=0,J=0\rangle^{-1}$.
[b] $\langle v'=2,J'=1\|\hat{T}\|v=0,J=0\rangle\langle v'=0,J'=1\|\hat{T}\|v=0,J=0\rangle^{-1}$.
[c] $\langle v'=1,J'=2\|\hat{Q}\|v=0,J=0\rangle\langle v'=0,J'=2\|\hat{Q}\|v=0,J=0\rangle^{-1}$.

E. The quadrupole interaction

The quadrupole interaction potential is given by

$$V_2(\mathbf{r},\Omega_s)=v_2(r)\left[\frac{4\pi}{5}\right]^{1/2}\sum_{v}(-1)^{v}Y_{2v}(\Omega_e)Y_{2-v}(\Omega_s)\,, \tag{3.20}$$

with

$$v_2(r)=-\left[\frac{4\pi}{5}\right]^{1/2}\frac{eQ}{r^3}\,, \tag{3.21}$$

where Q is the quadrupole moment of the molecule. From this potential the eikonal phase can be easily rewritten into the form

$$\chi_Q(\mathbf{b},\Omega_S)=\eta_2(b)Q\,[\,Y_{22}(\Omega_S)e^{-2i\phi_b}+Y_{2-2}(\Omega_S)e^{2i\phi_b}],\tag{3.22}$$

with

$$\eta_2(b)=\frac{m_e eQ}{\hbar^2 k}\frac{1}{b^2+R_2^2}\,, \tag{3.23}$$

where, in analogy with the dipole case, R_2 is a quadrupole cutoff radius.

In terms of algebraic operators, we will express the eikonal phase as

$$\chi_Q(\mathbf{b},\hat{a})=\eta_2(b)q_0(\hat{Q}_2e^{-2i\phi_b}+\hat{Q}_{-2}e^{-2i\phi_b}) , \qquad (3.24)$$

where the operator $\hat{Q}$ has been defined in Eq. (3.1d) and the constant q_0 is fixed in order to have

$$\langle v=0J'=2\|q_0\hat{Q}\|v=J=0\rangle=Q$$

(quadrupole moment).

When the quadrupole interaction is included, the eikonal phase is given as

$$\chi(\mathbf{b},\hat{a})=\chi_D(\mathbf{b},\hat{a})+\chi_Q(\mathbf{b},\hat{a}) . \qquad (3.25)$$

In order to calculate the matrix elements of $e^{i\chi(\mathbf{b},\hat{a})}$, we will make the assumption that

$$e^{i\chi(\mathbf{b},\hat{a})}=e^{i\chi_D(\mathbf{b},\hat{a})}+\tfrac{1}{2}i[e^{i\chi_D(\mathbf{b},\hat{a})}\chi_Q(\mathbf{b},\hat{a}) + \chi_Q(\mathbf{b},\hat{a})e^{i\chi_D(\mathbf{b},\hat{a})}] . \qquad (3.26)$$

The derivation of this expression follows the one given above in Eqs. (3.14) and (3.15). The calculation of the matrix elements of this operator is rather technical and is given in Appendix B.

The inclusion of quadrupole interaction introduces an additional term to the scattering amplitude Eq. (3.18), namely

$$F_{fi}(\mathbf{q})=F^D_{fi}(\mathbf{q})+F^Q_{fi}(\mathbf{q}) , \qquad (3.27)$$

where

$$F^Q_{fi}(\mathbf{q})=\frac{k}{4\pi}i^{(M'-M)}\int b\,dbJ_{M'-M}(qb)e^{i(M-M')\phi_q} \times\int_0^{2\pi}\langle v'J'M'|e^{i\chi_D(\mathbf{b})}\chi_Q(\mathbf{b}) +\chi_Q(\mathbf{b})e^{i\chi_D(\mathbf{b})}|vJM\rangle \times e^{i(M'-M)\phi_b}d\phi_b , \qquad (3.28)$$

where the calculation of the integral in $d\phi_b$ can be performed analytically and the result is given in Appendix B. It can be noted from Eq. (3.28) that the calculation of the scattering amplitude is reduced to the calculation of a single integral over the impact parameter b.

At this point, the differential cross section can be calculated with Eq. (3.19), replacing $F^D_{fi}(\mathbf{q})$ with $F_{fi}(\mathbf{q})$.

IV. A NUMERICAL EXAMPLE

In order to check the formulation proposed in the preceding section we will show the calculation of the scattering cross section for electron collision with two diatomic targets. These are supposed to be schematic calculations even though, in order to have a realistic set of parameters to use in the computation, two actual molecules, HF and HCl, have been chosen as molecular targets.

The differential cross section for the e^-+HF and e^-+HCl scattering has been calculated at a collision energy $E_e=20$ eV. The parameters used are given in Table II. The Hamiltonian constants of Eq. (3.4) are derived from molecular constants [24]. The whole set of parameters is given, namely h_0, A, B, and N, even though only the total number of vibrons, N plays an important role in the calculation of all the matrix elements given above. The dipole and quadrupole moments are from Ref. [24] and the constants d_0, d_1, and λ are derived according to Ref. [15]. The dipole cutoff radii have been arbitrarily set to the values given in Table II. This limitation is common to all the DCO models and is the main drawback of the phenomenological approaches as compared with the more sophisticated *ab initio* calculations.

The differential cross section for the various rotational transitions in e^-+HF and in e^-+HCl collisions are given in Figs. 1 and 2, respectively, for the vibrational elastic channel.

In Figs. 3 and 4, and 5 and 6, the same quantities are shown for the excitation of the first and the second vibrational bands through the long-range dipole interaction. The FBA results, calculated using the same dipole matrix elements (see Table II), as those resulting from our calculations made with the operator in Eq. (3.7), are also shown in the figures for comparison. One can realize that, as should be expected, the FBA and the algebraic-eikonal calculations approach a common value at very small scattering angle. However, due to the higher-order approximation, the algebraic-eikonal approach leads to different selection rules for the excitation of the various rotational states, more realistic if compared to the simple FBA. This was already evident from the calculations of Ref. [18], made with the Glauber approximation.

It can be noted from Figs. 3–6 that, as comapred with the vibrationally elastic channel, the excitation of the $J'=2$ states contributes differently to the differential cross section. In fact at large angles, the excitation of

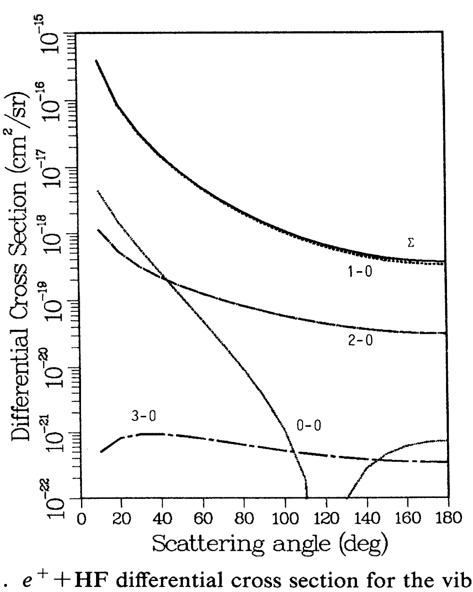

FIG. 1. e^++HF differential cross section for the vibrational elastic scattering at $E_e=20$ eV. The various rotational contributions are shown separately. Σ denotes the cross section summed over the rotational states J'.

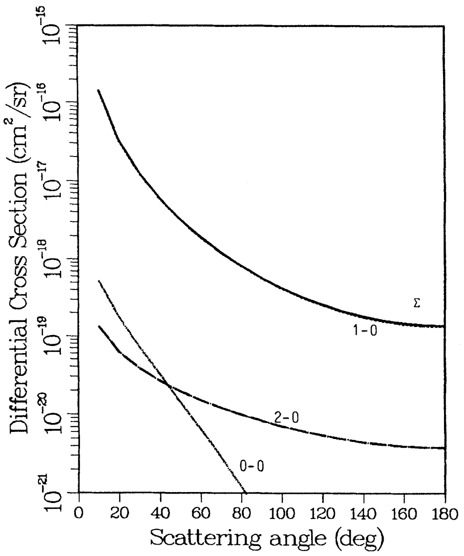

FIG. 2. $e^- + \mathrm{HCl}$ differential cross section for the vibrational elastic scattering at $E_e = 20$ eV. The various rotational contributions are shown separately. Σ denotes the cross section summed over the rotational states J'.

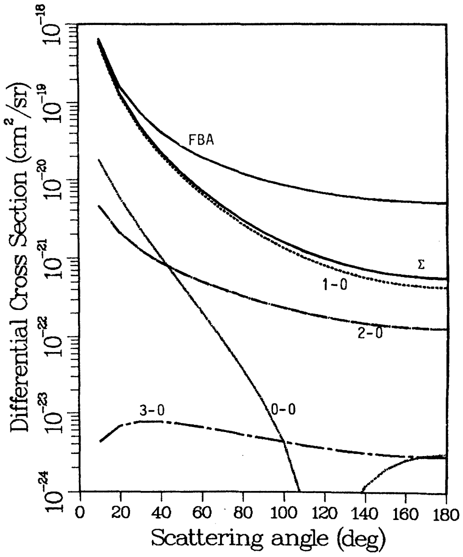

FIG. 4. $e^- + \mathrm{HCl}$ differential cross section for excitation of the $v' = 1$ vibrational band at $E_e = 20$ eV. The various rotational contributions are shown separately. Σ denotes the cross section summed over the rotational states J', whereas FBA denotes the calculation made using Eq. (2.9).

this channel is comparable with the $J' = 1$ channel which is instead overall dominant in the vibrational elastic case. This result induced us to pursue the inclusion of the quadrupole interaction which should favor even more than $J' = 2$ state.

In fact, this is already evident from Figs. 7 and 8 where the differential cross section for the vibrational elastic channel is shown in the case of dipole-plus-quadrupole interactions. Even more pronounced is the same effect on the vibrational excitation cross sections shown in Figs. 9 and 10.

The main effect of the inclusion of the quadrupole interaction is on the $J' = 2$ and on the $J' = 0$ channels. This is due to the quadrupole operator selection rules. How-

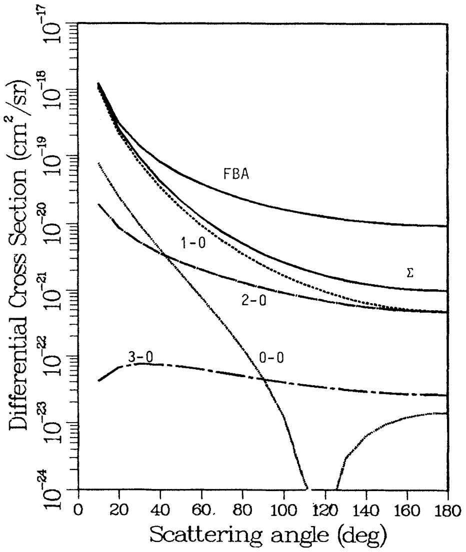

FIG. 3. $e^- + \mathrm{HF}$ differential cross section for excitation of the $v' = 1$ vibrational band at $E_e = 20$ eV. The various rotational contributions are shown separately. Σ denotes the cross section summed over the rotational states J', whereas FBA denotes the calculation made using Eq. (2.9).

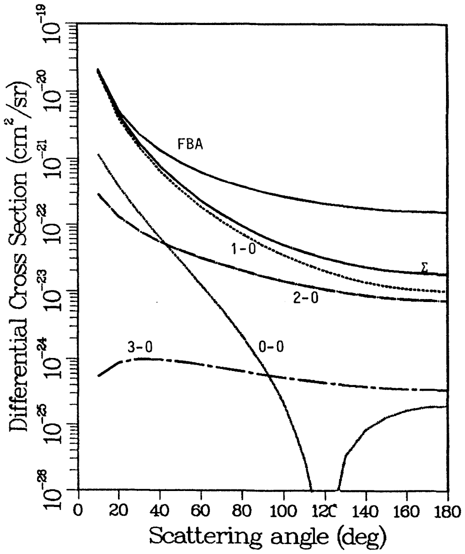

FIG. 5. The same as in Fig. 3 for the $v' = 2$ band.

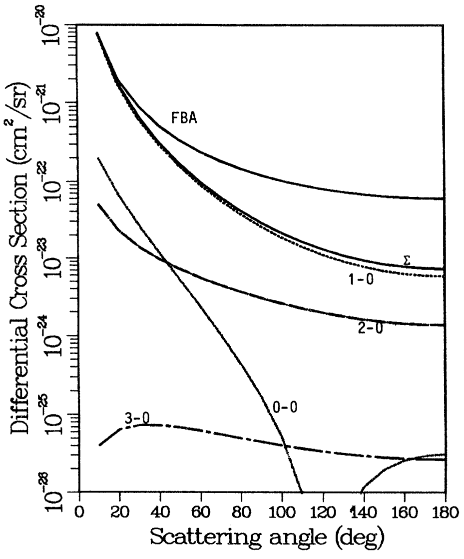

FIG. 6. The same as in Fig. 4 for the $v'=2$ band.

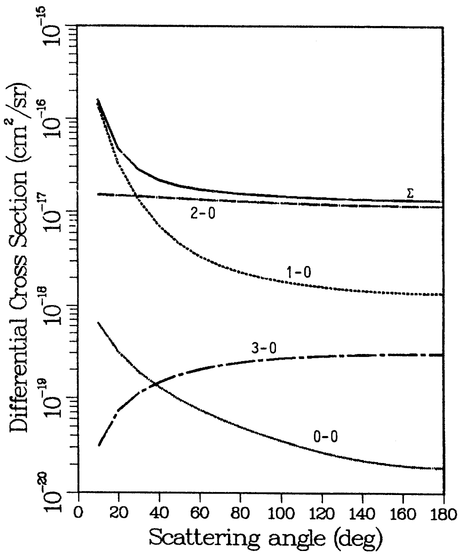

FIG. 8. e^-+HCl differential cross section for the vibrational elastic scattering at $E_e=20$ eV. Dipole-plus-quadrupole interaction is included simultaneously.

ever, from our experience it came out that also the cutoff radius R_2 affects the results particularly at large angles, even though the relative contributions of the various J' channels remain practically independent on the cutoff procedure. The values of R_2 used in the present calculations were such that in the case of pure quadrupole interaction we were able to obtain a cross section for the $J'=2$ channels convergent to the FBA values for this interaction.

Moreover, it should be noted that at large angles the Glauber approximation is questionable and it has to be born in mind that other short-range types of interactions should be included into the model. In fact, exchange and correlation-polarization interactions play an important role, particularly for vibrational excitation as shown, for instance, by the coupled-channel calculations of Refs. [25,26]. As already mentioned, the inclusion of short-range interactions through combined algebraic and close-coupling methods has been recently achieved for the case of rotational excitation by the hybrid approach [13].

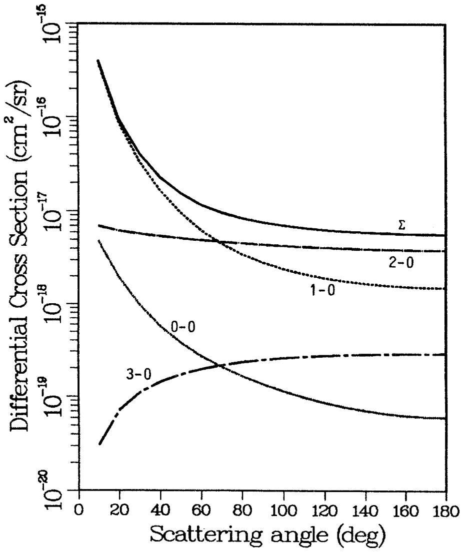

FIG. 7. e^-+HF differential cross section for the vibrational elastic scattering at $E_e=20$ eV. Dipole-plus-quadrupole interaction is included simultaneously.

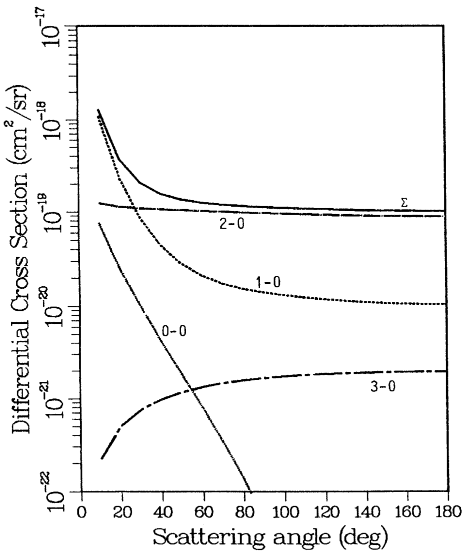

FIG. 9. The same as in Fig. 7 for the $v'=1$ band.

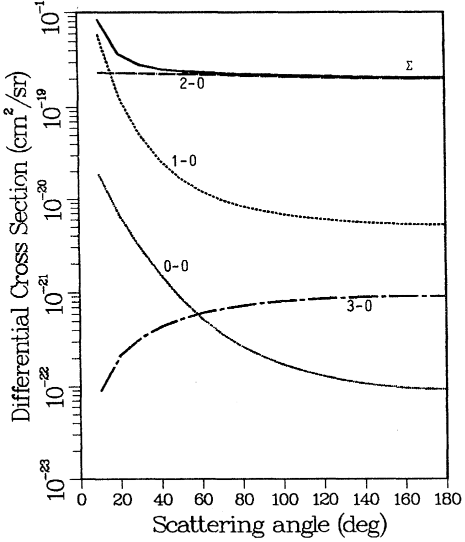

FIG. 10. The same as in Fig. 8 for the $v'=1$ band.

V. CONCLUSIONS

Two main targets have been achieved in the present work. The first is the inclusion of vibrational excitation in the algebraic approach to the calculation of the scattering cross section for the $e^- +$ molecule collision process in the Glauber approximation. This has been done introducing into the algebraic-eikonal formalism an appropriate dipole transition operator which can induce vibrational excitation. The second is the inclusion of the quadrupole interaction potential into the same framework.

As far as the vibrational excitation for dipole interaction is concerned, a simple analytical expression for the matrix elements involved in the calculation has been derived, making the calculation feasible without recurring to numerical diagonalizations. This can be considered particularly useful for the generalization of the algebraic approach to the collision process of electrons with polyatomic molecules.

The inclusion of quadrupole interaction improve the potential description of the scattering process even though the drawback of DCO models could not be avoided at the present status of the theory.

Finally, we would like to remark that the inclusion of the vibrational excitation as well as of the quadrupole interaction could be easily introduced into the framework of the hybrid approach in order to make the algebraic techniques suitable for more realistic calculations of the scattering cross section for the vibrational excitation in the electron-molecule collision process.

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APPENDIX A: MATRIX ELEMENTS FOR DIPOLE TRANSITIONS

The reduced matrix elements of the operators given in the text, necessary for the calculation of the scattering amplitude, are

$$\langle v'J+1\|\hat{D}\|vJ\rangle=\delta_{v',v}[(J+1)(N+2v+J+2)\times(N-2v-J)]^{1/2}\,, \tag{A1}$$

$$\langle v'J\|e^{\lambda\hat{n}_\pi}\hat{D}+\hat{D}e^{\lambda\hat{n}_\pi}\|vJ\rangle =(\langle vJ'\|\hat{D}\|vJ\rangle+\langle v'J'\|\hat{D}\|v'J\rangle)\times\langle v'|e^{\lambda\hat{n}_\pi}|v\rangle\,, \tag{A2}$$

where

$$v'>v,\quad \Delta v=v'-v\,,$$
$$\langle v'|e^{\lambda\hat{n}_\pi}|v\rangle=(-1)^{\Delta v}\langle\Delta v|e^{\lambda\hat{n}_\pi}|0\rangle\left[\frac{v'!}{v!\Delta v!}\right]^{1/2}, \tag{A3}$$

$$v'<v,\quad \Delta v=v-v'\,,$$
$$\langle v'|e^{\lambda\hat{n}_\pi}|v\rangle=(-1)^{\Delta v}\langle\Delta v|e^{\lambda\hat{n}_\pi}|0\rangle\left[\frac{v!}{v'!\Delta v!}\right]^{1/2}, \tag{A4}$$

and

$$\langle v|e^{\lambda\hat{n}_\pi}|0\rangle=\left[\frac{N!}{v!(N-v)!}\right]^{1/2}\left[\frac{e^{\lambda}-1}{e^{\lambda}+1}\right]^{v}\left[\frac{e^{\lambda}+1}{2}\right]^{N}. \tag{A5}$$

The matrix elements of the two terms of the dipole transition operator given in Eq. (3.7) can be calculated from relations (A1) and (A2).

APPENDIX B: SCATTERING AMPLITUDES FOR QUADRUPOLE INTERACTION

The matrix elements of the first term in Eq. (3.26) already given above in Eq. (3.11), with Eqs. (3.16a) and (3.16b). Those of the second term can be calculated as follows. We first note that

$$\langle v'J'M'|e^{i\chi_D(\mathbf{b})}\chi_Q(\mathbf{b})|vJM\rangle = \sum_{v'',J'',M''}\langle v'J'M'|e^{i\chi_D(\mathbf{b})}|v''J''M''\rangle \times\langle v''J''M''|\chi_Q(\mathbf{b})|vJM\rangle\,, \tag{B1}$$

where we have dropped $\hat{a}$ in the notation because it is inessential here. It is convenient at this point to calculate the quantity

$$\int_0^{2\pi}\langle v'J'M'|e^{i\chi_D(\mathbf{b})}\chi_Q(\mathbf{b})|vJM\rangle e^{i\lambda\phi_b}d\phi_b\,,$$

because some selection rules can be applied in this case. The result of the integration, using (B1), is

$$2\pi\delta_{\lambda,M'-M}\eta_2(b)q_0 \sum_{v''J''M''} \langle v'J'M'|e^{i\chi_D(\mathbf{b})}|v''J''M''\rangle \times \langle v''J''M''|\hat{Q}_{M''-M}|vJM\rangle \ , \tag{B2}$$

with $v''=v-1,v,v+1$, $J''=J-2,J,J+2$, and $M''=M-2,M+2$. The matrix elements of $\hat{Q}$ are given below. Analogously,

$$\begin{aligned}\int_0^{2\pi}\langle v'J'M'|\chi_Q(\mathbf{b})e^{i\chi_D(\mathbf{b})}|vJM\rangle e^{i\lambda\phi_b}d\phi_b &= 2\pi\delta_{\lambda,M'-M}\eta_2(b)q_0 \\ &\quad\times\sum_{v''J''M'}\langle v'J'M'|\hat{Q}_{M'-M''}|v''J''M''\rangle \\ &\quad\times\langle v''J''M''|e^{i\chi_D(\mathbf{b})}|vJM\rangle \ ,\end{aligned} \tag{B3}$$

with $v''=v'-1,v',v'+1$, $J''=J'-1,J',J'+1$, and $M''=M'-2,M'+2$.

It is worth nothing here that, even though the summations in Eqs. (B2) and (B3) run over three indices, the selection rules of $\hat{Q}$ keep the calculation easily manageable. Moreover, in actual situations the calculation has to be performed for the initial molecular state with $v=0$, $J=0$, and $M=0$. In this case, only the values $v''=0,1$, $J''=0,2$, and $M''=-2,2$ are to be included in the summations.

We finally give here the reduced matrix elements of the quadrupole operator defined in Eq. (3.1d) appearing above in Eqs. (B2) and (B3):

$$\langle\omega'J'\|\hat{Q}\|\omega J\rangle = -\sqrt{5(2J'+1)(2J+1)}\,X \ , \tag{B4}$$

where

$$\omega'=\omega-2,\quad X=\begin{Bmatrix}\frac{\omega-1}{2} & \frac{\omega-1}{2} & J' \\ \frac{\omega-1}{2} & \frac{\omega-1}{2} & J \\ 1 & 1 & 2\end{Bmatrix} \times\left[\frac{(\omega+1)(N-\omega+2)(N+\omega+2)}{4(\omega-1)}\right]^{1/2},$$

$$\omega'=\omega,\quad X=\begin{Bmatrix}\frac{\omega}{2} & \frac{\omega}{2} & J' \\ \frac{\omega}{2} & \frac{\omega}{2} & J \\ 1 & 1 & 2\end{Bmatrix}(\omega+1)\frac{(N+2)}{2},$$

$$\omega'=\omega+2,\quad X=\begin{Bmatrix}\frac{\omega+1}{2} & \frac{\omega+1}{2} & J' \\ \frac{\omega+1}{2} & \frac{\omega+1}{2} & J \\ 1 & 1 & 2\end{Bmatrix} \times\left[\frac{(\omega+1)(N-\omega)(N+\omega+4)}{4(\omega+3)}\right]^{1/2},$$

where $\omega\equiv N-2v$ and $\{\ \cdots\ \}$ denote $9j$ symbols.

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