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# Algebraic rotating-frame approach to electron-molecule scattering

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An approach to electron scattering from molecules is discussed, in which an algebraic description of the rovibrational states in the molecule (vibron model) is combined with a rotating-frame approximation. The latter was first introduced for atomic-molecule scattering under the name centrifugal sudden approximation. The coupled multichannel problem reduces to single-channel central potential scattering with a fluctuating potential. The method is applied to electron scattering from a rigid molecule with large dipole moment. Comparison with exact coupled-channel calculation shows that the approach works well for all partial waves except those with very low angular momentum. The method is also compared with the algebraic eikonal approach.

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## I. INTRODUCTION

The scattering of medium-energy electrons from polar molecules is a complex process, which involves the coupling of many channels [1–4]. Various methods were developed to solve the coupled-channel equations for electron-molecule scattering. However, for polyatomic molecules the number of channels becomes very large and the problem may become intractable.

Recently, an alternative method, the so-called algebraic eikonal approach, was introduced to describe the forward angle scattering of electrons from polar molecules [5,6]. In this method the rovibrational states of the molecule are described by an algebraic model [7] (the vibron model) and the scattering process is treated in a sudden eikonal approximation. The advantage of the approach is that the $S$ matrix is given in a closed form as a representation matrix of the group [8] associated with the internal structure of the molecule. Thus, the coupled-channel equations are solved effectively to all orders in the interaction by algebraic means. The approach describes well the forward angle scattering which is dominated by the long-range interactions, such as the dipole and quadrupole interactions [9,10].

To describe large-angle scattering, where short-range interactions dominate and the validity of the eikonal approach is questionable, one may use a hybrid approach [11]. The high-angular-momentum partial waves are calculated by the algebraic eikonal approach and the low-angular-momentum partial waves by a coupled-channel approach.

The algebraic eikonal approach requires the calculation of the representation matrices of the dynamical group of the molecule. Though such calculations are significantly simpler than a coupled-channel approach, they may still present a formidable task for polyatomic molecules whose dynamical group is of higher dimension and complexity. The purpose of this paper is to present an alternative approach to the eikonal which is based on a rotating-frame approximation. In this approach the molecule is still described algebraically by the vibron model, but the scattering process is treated in a frame which is rotating with the incoming electron. If the Coriolis coupling in the rotating frame is neglected, the number of coupled channels is greatly reduced. This approximation was first introduced in the early 1970s for atom-molecule scattering under the name centrifugal sudden [12–16] (CS) approximation. A more recent discussion of the success and validity of the approximation can be found in Ref. [17]. The approach was recently used for nuclear collisions [18,19].

The CS approximation was studied for various potentials in atom-molecule scattering and it was concluded that it is good for short-range or weakly anisotropic interactions but does not work well when a long-range interaction produces a significant fraction of the inelasticity or when strong polarization effects are present [17]. In electron scattering from polar molecules the dominating interaction is the long-range dipole interaction, so that the CS approximation is not expected to work. We shall show, however, that with a proper choice of a rotating-frame approximation and with a proper normalization of the interaction strength (which is found analytically), it is possible to apply the approximation successfully to electron scattering off polar molecules. For that purpose we compare the results of this approximation with an exact coupled-channel calculation [20] for an electron scattered off a rigid molecule with a large dipole moment. We remark that several versions of the CS approximation were suggested in the atom-molecule work which correspond to different choices of the effective centrifugal barrier but we will see that only one choice is the proper one for long-range interactions.

For medium-energy electron scattering the sudden approximation may also be used in analogy with the energy sudden (ES) approximation [14,16,20] in atom-molecule scattering. In this limit the problem is further reduced to a single-channel central potential scattering but with a fluctuating potential. One obtained the laboratory many-channel $S$ matrix by properly weighting the single-channel $S$-matrix elements.

The algebraic rotating-frame approach has two advantages over the algebraic eikonal approach as follows.

(i) The calculation of single-channel phase shifts is a simpler task than the calculation of the representation matrices of the group, in particular for polyatomic molecules. In the rotating-frame approach the algebraic structure still plays an important role, since the values of the fluctuating central potential are determined by diagonalizing a certain generator of the algebra.

(ii) The eikonal approximation is not assumed.

The outline of the paper is as follows: In Sec. II we introduce the algebraic rotating-frame approach to electron-molecule scattering. The approach is applied to polar diatomic molecules in Sec. III. An important conclusion is that only the time-reversal-preserving choice of the effective centrifugal barrier is suitable for electron-molecule scattering and that a normalization of the interaction strength is required. All partial cross sections except the very low ones are well reproduced. Finally in Sec. IV we compare the rotating-frame $S$ matrix with the eikonal $S$ matrix. For transitions to rotational states with low spin both methods are comparable, but for transitions to higher rotational states the rotating frame is a better approximation.

## II. ROTATING FRAME

### A. Rotating frame and sudden approximations

The electron-molecule system is described by the following Hamiltonian:

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

where $\mathbf{r}$ is the coordinate of the electron relative to the center of mass of the molecule, $\mathbf{p}$ is the conjugate momentum, and $\mu$ is the reduced mass. $H_0$ is the Hamiltonian of the molecule and $V$ is the electron-molecule interaction which is a rotational scalar. $V$ can be expanded in products of tensors in the orbital space and the molecular space

$$V(\mathbf{r},\xi)=\sum_{\lambda\mu}V_{\lambda\mu}(r,\xi)Y^{*}_{\lambda\mu}(\hat{\mathbf{r}})\ , \tag{2.2}$$

where $V_{\lambda\mu}$ is a tensor of rank $\lambda$ in the molecular space $\{\xi\}$.

We denote by $\mathbf{l}$ and $\mathbf{j}$ the electron orbital angular momentum and the molecules spin, respectively. The total angular momentum $\mathbf{J}=\mathbf{l}+\mathbf{j}$ is conserved so that it is possible to define a partial $S$ matrix $S^{J}_{l'j';lj}$ to scatter from initial $l,j$ to final $l',j'$ at total angular momentum $J$. The scattering amplitude for the electron to scatter from linear momentum $\mathbf{k}$ ($\|z$) to $\mathbf{k}'$ while the molecule is making a transition from a state $j,m$ to a state $j',m'$ ($m$ is the spin projection), is given by the partial-wave expansion

$$f_{j'm';jm}(\hat{\mathbf{k}}')=\frac{\sqrt{\pi}}{\sqrt{kk'}}\sum_{\substack{J,l,l'\\M,m_{l'}}}i^{l-l'-1}\sqrt{2l+1}(l0jm|Jm)(l'm_{l'}j'm'|JM)(S^{J}-1)_{l'j';lj}\mathcal{Y}_{l'm_{l'}}(\hat{\mathbf{k}})\ . \tag{2.3}$$

The rotating-frame (or centrifugal sudden) approximation was introduced in the early 1970s to reduce the number of coupled channels in atom-molecule collisions [12–17]. The rotating frame is defined such that its $z'$ axis is always along the direction $\hat{\mathbf{r}}$ of the projectile. It is possible to reformulate the scattering problem in this frame, in which the potential (2.2) assumes a particularly simple form

$$V=\sum_{\lambda}\left[\frac{2\lambda+1}{4\pi}\right]^{1/2}V_{\lambda 0}(r,\xi')\ , \tag{2.4}$$

which conserves the projection $\Omega$ of the spin $\mathbf{j}$ of the molecule on $z'$. However, the centrifugal potential $\mathbf{l}^2/2\mu r^2$ introduces coupling between $\Omega$ and $\Omega\pm1$. The rotating-frame approximation amounts to neglecting these couplings and introducing an average fixed barrier $\bar{l}(\bar{l}+1)/2\mu r^2$ with orbital angular momentum $\bar{l}$. In this approximation the original coupled-channel problem reduces to a set of spinless coupled-channel problems with an interaction (2.4) and channels $|j,\Omega\rangle$, where $\Omega$ is fixed at its initial value. If the $S$ matrix of the problem is denoted by $S^{\bar{l}[\Omega]}_{j'j}$, then the partial $S$ matrix of the original problem at total angular momentum $J$ ($\mathbf{J}=\mathbf{l}+\mathbf{j}$) is [12–15]

$$S^{J}_{l'j';lj}=i^{l+l'-2\bar{l}}\frac{\sqrt{(2l+1)(2l'+1)}}{2J+1}\times\sum_{\Omega}(l'0j'\Omega|J\Omega)S^{\bar{l}[\Omega]}_{j'j}(l0j\Omega|J\Omega)\ . \tag{2.5}$$

Various choices of $\bar{l}$ are discussed in the literature such as $\bar{l}=J$ [12,18,19], $\bar{l}=l$ or $\bar{l}=l'$ [15], $\bar{l}=(l+l')/2$, and others. The choice $\bar{l}=l'$ leads [15] to a simplified expression upon substitution in the partial-wave expansion (2.3), but violates time-reversal symmetry. The choices $\bar{l}(\bar{l}+1)=[l(l+1)+l'(l'+1)]/2$ and $\bar{l}=(l+l')/2$ lead to a time-reversal symmetric $S$ matrix. We shall show that only the latter two choices give the correct approximation for electron-molecule scattering.

If in addition the sudden approximation is assumed [16,21] (valid when the electron energy is much larger compared with the rovibrational excitation energies), a further simplification occurs. We calculate the partial $S$-matrix element $S^{\bar{l}}_{\xi}$ for a single-channel central potential scattering with a potential $\sum_{\lambda}\sqrt{(2\lambda+1)/4\pi}V_{\lambda 0}(r,\xi)$, where $\xi$ are arbitrary but fixed parameters. The $S$ matrix $S^{\bar{l}[\Omega]}_{j'j}$ is then given by

$$S^{\bar{l}[\Omega]}_{j'j}=\int D[\xi]\Phi^{*}_{j'\Omega}(\xi)S^{\bar{l}}_{\xi}\Phi_{j\Omega}(\xi)\ , \tag{2.6}$$

where $\Phi_{j\Omega}(\xi)$ are the molecule's eigenstates.

### B. The algebraic rotating-frame approach

In this section we explain how to apply the rotating-frame sudden approximation in the algebraic framework. In the vibron model [7] the molecule is described by a u(4) Hamiltonian. Most diatomic molecules have an o(4) dynamical symmetry, where

$$H_0 = aC_2(\,\mathrm{o}(4)) + b\mathbf{L}^2 \; . \tag{2.7}$$

The eigenstates of (2.8) are denoted by $|\sigma, j, m\rangle$, where $\sigma(\sigma+2)$ are the eigenvalues of $C_2(\mathrm{o}(4))$ and $j, m$ are the molecule's angular momentum and its projection. $\sigma$ is determined by the vibrational quantum number $v$ through $\sigma = (N-v)/2$, where $N$ is the total number of vibrons.

For a polar molecule, the dominating interaction at forward angle scattering is the long-range dipole interaction [1,2,5]

$$V(\mathbf{r}, \xi) = \alpha_1(r)\hat{\mathbf{r}}\cdot\mathbf{T} \; , \tag{2.8}$$

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

$$\alpha_1(r) = \frac{e^2}{r^2 + R_0^2} \; . \tag{2.9}$$

$R_0$ is a cutoff radius that crudely models the short-range electron-molecule interaction.

In the vibron model [7] the leading term in $\mathbf{T}$ is

$$\mathbf{T} = d_0\mathbf{D} \; , \tag{2.10}$$

where $\mathbf{D}$ is a dipole operator which together with the angular momentum $\mathbf{L}$ form an o(4) subalgebra of u(4). The applications in this paper will be for the dipole interaction (2.8). The methods, however, are general and can be applied to any interaction $V(\mathbf{r}, \xi)$.

In the frame which rotates with $\hat{\mathbf{r}}$, the incoming electron position is along $\hat{\mathbf{z}}$, and

$$V = \alpha_1(r)\hat{\mathbf{z}}'\cdot\mathbf{T} = d_0\alpha_1(r)D_{z'} \; . \tag{2.11}$$

Notice that this $V$ conserves the projection $\Omega$ of the molecular spin $\mathbf{L}$ along $\hat{\mathbf{z}}$. In the rotating-frame approximation, we solve the spinless coupled-channel problem with coupling

$$V_{j'j}^{[\Omega]}(r) \equiv d_0\alpha_1(r)\langle j'\Omega|D_{z'}|j\Omega\rangle \tag{2.12}$$

for each initial $\Omega$ ($|\Omega| \leq j$).

In the sudden approximation we can decouple the coupled-channel equations by transforming to the eigenstates of the interaction in the rotating frame. For (2.11) this amounts to finding the eigenstates of $D_z$ in the molecule's space. Exploiting the isomorphism of o(4) to su(2)×su(2), $D_z$ is diagonal in the latter basis. The su(2)×su(2) basis is $|\kappa m_1; \kappa m_2\rangle$ where $\kappa = \sigma/2$ is the su(2) quasispin and $m_1$, $m_2$ are the projection of the two su(2) quasispins. We have

$$D_z|\kappa m_1; \kappa m_2\rangle = (m_1 - m_2)|\kappa m_1; \kappa m_2\rangle \; . \tag{2.13}$$

The transformation which diagonalizes the spinless coupled-channel problem is

$$\begin{aligned} \phi_{m_1 m_2}^{\bar{l}}(r) &= \sum_{j'} \langle \kappa m_1; \kappa m_2 | j'\Omega\rangle \phi_{j'}^{\bar{l}}(r) \\ &= \sum_{j'} (\kappa m_1 \kappa m_2 | j'\Omega)\phi_{j'}^{\bar{l}}(r) \; , \end{aligned} \tag{2.14}$$

where we have used the fact that the transformation between the su(2)×su(2) basis and the o(4) basis is given by the Clebsch coefficients $(\kappa m_1 \kappa m_2 | j'\Omega)$.

The effective central potential scattering problem is

$$\left[ \frac{d^2}{dr^2} + k^2 - \frac{\bar{l}(\bar{l}+1)}{r^2} - \frac{2\mu}{\hbar^2} d_0(m_1 - m_2)\alpha_1(r) \right] \phi_{m_1,m_2}^{\bar{l}}(r) = 0 \; , \tag{2.15}$$

where $\alpha_1(r)$ is the dipole form factor (2.9). Equation (2.15) describes the scattering from an ordinary dipole potential with strength $d_0(m_1 - m_2)$. Denoting the corresponding partial wave $S$-matrix element by $S^{\bar{l}}[m_1, m_2]$, the $S$ matrix of the spinless coupled-channel problem is given by a suitable sum over $m_1$, $m_2$:

$$S_{j'j}^{\bar{l}[m]} = \sum_{m_1, m_2} (\kappa m_1 \kappa m_2 | j'm) S^{\bar{l}}[m_1, m_2] (\kappa m_1 \kappa m_2 | jm) \; . \tag{2.16}$$

The partial $S$ matrix of the original problem in which the spin of the molecule is taken into account is given by

$$S_{l'j';lj}^{J} \approx i^{l+l'-2\bar{l}} \frac{\sqrt{(2l+1)(2l'+1)}}{2J+1} \sum_{m_1, m_2, m} (l'0j'm|Jm)(\kappa m_1 \kappa m_2 | j'm) S^{\bar{l}}[m_1, m_2] (\kappa m_1 \kappa m_2 | jm)(l0jm|Jm) \; . \tag{2.17}$$

If the initial state is in the vibrational ground state $v=0$ then $\kappa = N/2$, where $N$ is the number of vibrons.

### C. Normalization of the coupling

In the rotating-frame approximation, a potential which may depend strongly on the relative orientation of the electron position and the molecule such as (2.8) is replaced by a central interaction. This results in overestimating the coupling between the electron and the molecule, in particular since the dipole interaction is long range. It is possible to compensate for this effect by reducing the dipole coupling strength. By doing so we shall see that we can extend the applicability of the CS approximation to such cases. The normalization constant can be found analytically by comparing the Born limit of the rotating-frame approximation with the Born approximation of the original problem. We note that the Born approximation for the $j=0 \rightarrow j'=1$ transition is exact in the limit of small momentum transfer. At small momentum transfer $\mathbf{q}$, the Born amplitude from an initial state $i$ to a final state $f$ can be written as

$$f_{fi} \approx -\frac{\mu}{2\pi\hbar^2} \int d^2\mathbf{b}\, e^{i\mathbf{q}\cdot\mathbf{b}} \int_{-\infty}^{\infty} dz \langle f|V(\mathbf{b}, z)|i\rangle \; , \tag{2.18}$$

where $\mathbf{b}$ is the impact parameter. For the dipole interaction (2.8) we find

$$f_{fi}^{(B)} \approx -\frac{\mu}{\hbar^2} i^{|m_f - m_i|} \left[ \int_0^\infty b\, db J_{|m_i - m_f|}(qb) \int_{-\infty}^{\infty} dz\, \alpha_1(r) \frac{b}{r} \right] \langle f | T_x | i \rangle \ . \tag{2.19}$$

For the rotating-frame interaction (2.11), the Born approximation gives

$$f_{fi}^{(R)} \approx -\frac{\mu}{\hbar^2} \delta_{m_f m_i} \left[ \int_0^\infty b\, db\, J_0(qb) \int_{-\infty}^{\infty} dz\, \alpha_1(r) \right] \langle f | T_z | i \rangle \ , \tag{2.20}$$

where $T_z$ conserves the spin projection $m$. The ratio between the cross sections for the transition $v=0$, $j=0 \rightarrow v'=0$, $j'=1$ obtained from (2.20) and (2.19) is then

$$\frac{(d\sigma/d\Omega)_{(R)}}{(d\sigma/d\Omega)_{(B)}} = \left| \frac{\int_0^\infty b\, db\, J_0(qb) \int_{-\infty}^{\infty} dz\, \alpha_1(r)}{\int_0^\infty b\, db\, J_1(qb) \int_{-\infty}^{\infty} dz\, \alpha_1(r) b/r} \right|^2 . \tag{2.21}$$

Using the form (2.9) for $\alpha_1(r)$ we find

$$\begin{aligned} \int_{-\infty}^{\infty} dz\, \alpha_1(r) \frac{b}{r} &= \frac{2}{(b^2+R_0^2)^{1/2}} \frac{b}{R_0} \ln \left\{ \frac{R_0}{b} + \left[ 1 + \left[ \frac{R_0}{b} \right]^2 \right]^{1/2} \right\} , \\ \int_{-\infty}^{\infty} dz\, \alpha_1(r) &= \pi \frac{1}{(b^2+R_0^2)^{1/2}} \ . \end{aligned} \tag{2.22}$$

Using in (2.21) the limiting expressions of (2.22) for $b \gg R_0$, we find

$$\frac{(d\sigma/d\Omega)_R}{(d\sigma/d\Omega)_B} \approx \left[ \frac{\pi}{2} \right]^2 . \tag{2.23}$$

After normalizing the strength of the dipole interaction

$$\bar{d}_0 = \frac{d_0}{\pi/2} \ , \tag{2.24}$$

the rotating-frame Born approximation will agree with the usual Born approximation. In the following we shall use this normalized value of the dipole strength.

## III. APPLICATIONS

To test the validity of the algebraic rotating-frame approach we apply it to electron scattering at $E=5$ eV from a molecule with $N=20$ vibrons and dipole moment of 6 D. $d_0$ is determined so as to reproduce the given dipole moment.

We compared the results with an exact coupled-channel calculation in the space-fixed frame [20]. In this calculation the molecule is assumed to be a rotor and convergence of the $S$ matrix associated with the $j'=0,1,2,3,4$ states of the molecule is achieved by including the first ten rotational states. The matrix $S^J$ is calculated for $0 \le J \le 20$. For $J > 20$ and $j'=0,1,2$ we use the eikonal $S$ matrix and for $j'=3,4$ the partial-wave expansion already converges with $J < 20$.

In the usual rotating-frame approach [18,19], one uses the spinless partial-wave expansion which corresponds to the choice $\bar{l}=l'$ [15]. Combining this expansion with the sudden approximation (2.16) for $S_{j'j}^{l}$, we obtain

$$f_{j'm';jm}(\hat{\mathbf{k}}') = \delta_{m'm} (-1)^{j+j'} \sum_{m_1, m_2} (\kappa m_1 \kappa m_2 | j' - m) f^{[m_1 m_2]}(\hat{\mathbf{k}}') (\kappa m_1 \kappa m_2 | j - m) \ , \tag{3.1}$$

where $f^{[m_1, m_2]}(\hat{\mathbf{k}})$ is the scattering amplitude for a one-channel dipole potential scattering (2.15)

$$f^{[m_1 m_2]}(\hat{\mathbf{k}}') = \frac{i}{\sqrt{2kk'}} \times \sum_{l'} (2l'+1)(S^{l'}[m_1 - m_2] - 1) P_{l'}(\cos\theta) \ . \tag{3.2}$$

The corresponding cross section $(d\sigma/d\Omega)_{j=0 \rightarrow j'=1}$ (for $v=0$) is shown in Fig. 1 and is compared with the exact result. There is a large discrepancy even at very forward angles where the Born approximation should be good. As discussed in Sec. II C, it is necessary to normalize the dipole coupling strength so we use $\bar{d}_0 = d_0/(\pi/2)$. The normalized rotating-frame approximation with $\bar{l}=l'$ is shown by the solid line in Fig. 1. While the agreement for $\theta \lesssim 10°$ (where the Born is valid) with the exact result is now better the above rotating-frame approximation fails even at forward angles. For example, the sharp minimum around $\theta \approx 70°$ in the exact cross section is shifted to $\theta \approx 30°$ in the normalized rotating-frame calculation.

The reason for the failure of the rotating-frame approximation is the particular choice $\bar{l}=l'$. It can be argued that the choice $\bar{l}(\bar{l}+1) = l(l+1)/2 + \bar{l}(l'+1)/2$ is the one that minimizes the first-order correction to the rotating frame. If $|l-l'| \ll (l+l')/2$, the latter $\bar{l}$ is approximated by $\bar{l} \approx (l+l')/2$. The choice $\bar{l}=(l+l')/2$ is simpler since $S^{\bar{l}}$ needs to be calculated only for integers and half integers $\bar{l}$. The (normalized) rotating-frame approximation for $\bar{l}=(l+l')/2$ is shown by the solid line of

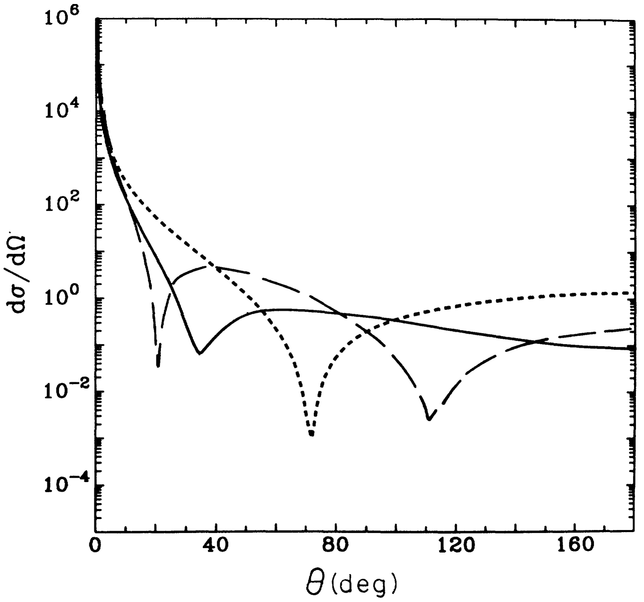

FIG. 1. Differential cross section for the transition $v=0$, $j=0\to v'=0$, $j'=1$ for electron scattering from a diatomic molecule with dipole moment of 6 D. The scattering energy is $E=5$ eV. The dashed line is the exact coupled-channel result [11,20]. The long-dashed line is the rotating-frame approximation using the spinless partial-wave expansion (3.1) and (3.2) (obtained for $\bar{l}=l'$). The solid line is the rotating-frame approximation with a normalized coupling $\bar{d}_0=d_0/(\pi/2)$. Notice the disagreement with the exact result even at forward angles.

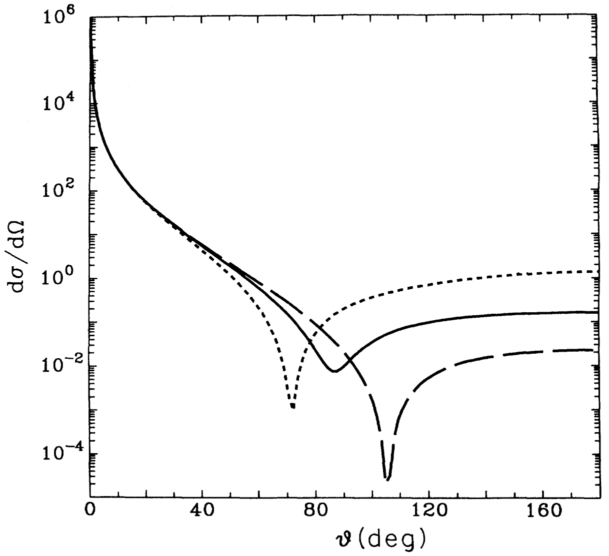

FIG. 2. Differential cross section for the transition $j=0\to j'=1$ in 5-eV electron scattering from a diatomic molecule with dipole moment of 6 D. The short-dashed line is the exact coupled-channel calculation, the long-dashed line is the eikonal approximation, and the solid line is the rotating-frame approximation with $\bar{l}=(l+l')/2$ and a normalized coupling. All three calculations agree at forward angles. The rotating frame is closer to the exact result than the eikonal.

Fig. 2, where we have used (2.17) and (2.3). The agreement with the exact result is now good, in particular at forward angles. In Fig. 2 we also show the algebraic eikonal approximation for the $j=0\to j'=1$ transition. All three curves agree well at forward angles. The rotating-frame approximation describes the cross section as well and even better than the eikonal approximation. Notice that the sharp minimum of the cross section in the rotating-frame calculation is between the ones for the eikonal and exact calculations. At large angles both the rotating-frame and the eikonal approximations do not work well but this can be taken care of in a hybrid approach [11].

To investigate in greater detail the validity of the rotating-frame approximation we examine its partial $S$ matrix. A quantity of interest is the partial cross section at a given total angular momentum $J$. The integrated cross section for a transition $j\to j'$ can be written as

$$\sigma_{j\to j'}=\frac{\pi}{kk'}\sum_J (2J+1)\sigma^J_{j\to j'} , \tag{3.3}$$

where the partial cross section $\sigma^J_{j\to j'}$ is

$$\sigma^J_{j\to j'}=\frac{1}{2j+1}\sum_{l,l'}|(S^J-1)_{l'j';lj}|^2 . \tag{3.4}$$

We have investigated the transitions $j=0\to j'$ where $j'=0,1,2,3,4$. Figure 3 shows $\sigma^J_{0\to j'}$ vs $J$ for the three possible choices of the rotating-frame approximation (corresponding to the various choices of $\bar{l}$) and for the exact coupled-channel calculation. As expected $\bar{l}=l'$ disagrees with the exact result while the other two choices (quadratic and average) agree very well for $J\geq 2$.

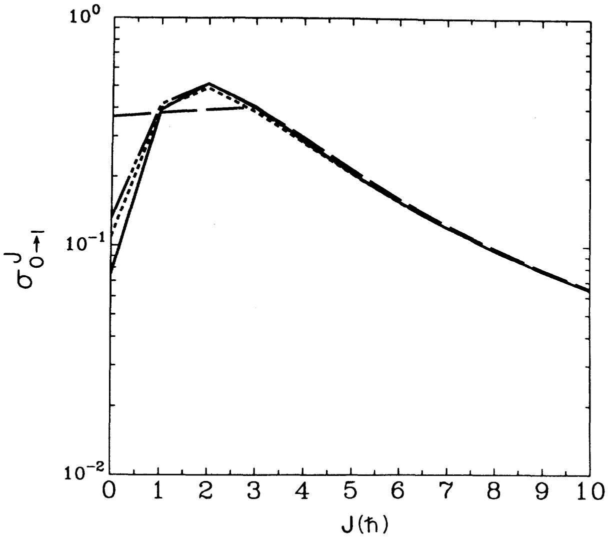

FIG. 3. The partial cross section $\sigma^J_{0\to1}$ vs $J$ for the $j=0\to j'=1$ transition in electron scattering ($E=5$ eV) from a diatomic molecule with dipole moment of 6 D. The short-dashed line is the exact coupled-channel result, while the other three lines are in the rotating-frame approximation with $\bar{l}=l'$ (long-dashed line), $\bar{l}(\bar{l}+1)=[l(l+1)+l'(l+1)]/2$ (long- and short-dashed line), and $\bar{l}=(l+l')/2$ (solid line).

Only for very low total angular momenta ($J=0$ and $J=1$) there is a discrepancy. The latter two choices for $\bar{l}$ which preserve time-reversal symmetry give similar results and in the following we shall discuss only the case $\bar{l}=(l+l')/2$.

The quantities $\sigma^J_{0\to j'}$ for $j'=0,2,3,4$ are shown in Fig. 4 vs $J$. Again we see that above a certain low angular momentum ($J=2$ or $J=3$) the agreement between the rotating-frame approach with $\bar{l}=(l+l')/2$ and the exact coupled-channel calculation is excellent. The rotating frame fails to reproduce only the very low angular momenta.

The quantity (3.4) does not give information on the individual magnetic transitions. To see how well the latter are reproduced in the rotating frame we define a partial cross section $\sigma^{l'}_{jm\to j'm'}$ through

$$\sigma_{jm\to j'm'}=\frac{\pi}{kk'}\sum_{l'}(2l'+1)\sigma^{l'}_{jm\to j'm'} \tag{3.5}$$

and

$$\sigma^{l'}_{jm\to j'm'}=\sum_{m_{l'}}\left|\sum_{J,l} i^{l-l'+1}\left[\frac{2l+1}{2J+1}\right]^{1/2}(l0jm|Jm)(l'm_{l'}j'm'|Jm)(S^J-1)_{l'j';lj}\right|^2 . \tag{3.6}$$

The quantity (3.6) offers a much more critical test of the rotating-frame approach. Figure 5 shows $\sigma^{l'}_{00\to 1m'}$ vs $l'$ for $m'=0$ and $m'=\pm1$. Here too the agreement is very good except for the very low $l'$. Notice that the partial cross section for $m'=0$ decreases much more rapidly than for $m'=\pm1$. This is well reproduced by the rotating-frame approximation.

A similar study for the $0,0\to 2m'$ transitions with $m'=0$, $\pm1$, and $\pm2$ is shown in Fig. 6.

## IV. COMPARISON WITH THE EIKONAL APPROXIMATION

The results of the previous section indicate that the rotating-frame approach is useful in bridging the low partial waves where an exact coupled-channel calculation is required, to the high partial waves where the Born approximation is valid. Other possible methods to use in a hybrid approach [22,23] are the algebraic eikonal [11] and the unitarized Born approximation (Born II) [24,25]. The latter two are compared in Ref. [11] for the same example discussed in Sec. III. It was concluded [11] that the unitarized Born works almost as well as the algebraic eikonal approach. However, it is in general much harder to calculate the $T$-matrix elements in a systematic way in the unitarized Born than in the algebraic eikonal approach. Also the algebraic eikonal seems to be a better starting point for a hybrid calculation. Since the algebraic eikonal was concluded to be preferable to Born II, we will compare the rotating frame directly to the algebraic eikonal approach.

### A. The eikonal approximation

The amplitude in the multichannel eikonal approximation is a function of the momentum transfer $\mathbf{q}=\mathbf{k}'-\mathbf{k}$ and is given by

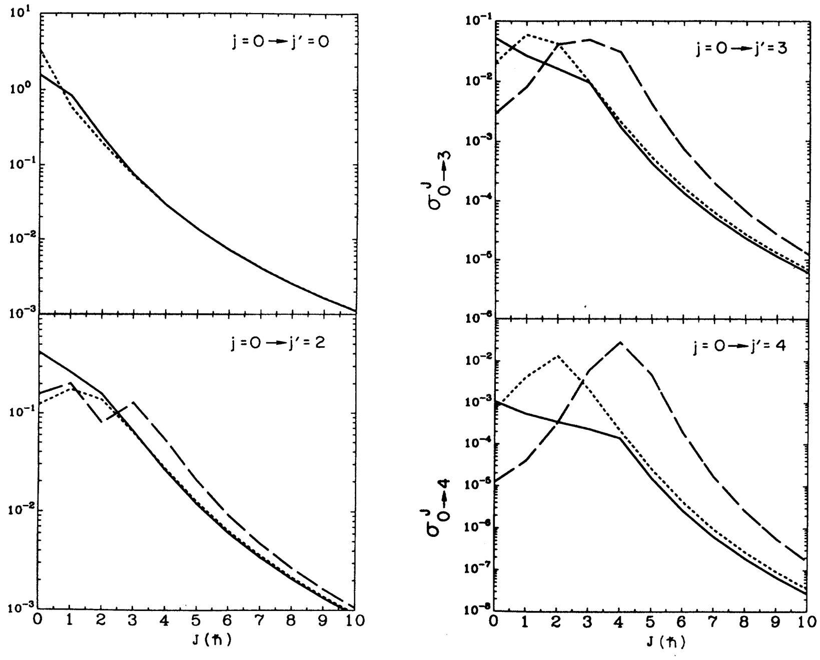

FIG. 4. Partial cross sections $\sigma^J_{0\to0}$, $\sigma^J_{0\to2}$ (left) and $\sigma^J_{0\to3}$, $\sigma^J_{0\to4}$ ( right ) vs $J$ for the same case as in Fig. 3. Short-dashed line: exact coupled-channel calculation. Long-dashed line: rotating-frame approximation with $\bar{l}=l'$. Solid line: rotating-frame approximation with $\bar{l}=(l+l')/2$.

$$f_{j'm';jm}(\mathbf{q})=ki^{|m-m'|-1}\int_0^{\infty}b\,db\,J_{|m-m'|}(qb)\langle j'm'|U(b)-1|jm\rangle\ , \tag{4.1}$$

where $U(b)$ is the propagator in the interaction picture for a straight-line trajectory at an impact parameter $\mathbf{b}$ parallel to $\mathbf{q}$ (which for convenience will be chosen as the $x'$ direction). If the sudden limit is also assumed then [5]

$$U(b)=\mathcal{T}_z\exp\left[-i\frac{\mu}{\hbar^2k}\int_{-\infty}^{\infty}dz'V(\mathbf{b},z')\right]\ . \tag{4.2}$$

To obtain an amplitude which satisfies time-reversal symmetry we choose [26] the $z'$ axis in (4.2) along the direction $(\mathbf{k}+\mathbf{k}')/|\mathbf{k}+\mathbf{k}'|$ which bisects $\hat{\mathbf{k}}$ and $\hat{\mathbf{k}}'$.

Neglecting the $z$ ordering in (4.2) (which is a $1/N$ effect [6]) we have (for $\mathbf{q}\|\hat{\mathbf{x}}$)

$$U(b)=\exp\left[-i\frac{\mu d_0}{\hbar^2k}\left[\int_{-\infty}^{\infty}dz\,\alpha_1(r)\frac{b}{r}\right]D_x\right]\ , \tag{4.3}$$

where we have used $\int_{-\infty}^{\infty}dz\,\alpha_1(r)/r=0$.

Notice that the interaction in (4.3) does not conserve $j_z$. It is possible [6] to rotate $D_x$ in (4.3) to $D_z$ so that

$$\langle j'm'|U(b)|jm\rangle=\sum_{m''}D^{j'*}_{m''m'}\left[\frac{\pi}{2}\right]\left\langle j'm''\left|\exp\left[-i\frac{\mu d_0}{\hbar^2k}\left[\int dz\,\alpha_1\frac{b}{r}\right]D_z\right]\right|jm''\right\rangle D^{j}_{m''m}\left[\frac{\pi}{2}\right]\ , \tag{4.4}$$

where $D(\pi/2)$ is the Wigner rotation matrix by $\pi/2$ around $\hat{\mathbf{y}}$. It is possible to calculate the matrix in (4.4) by transforming to eigenstates of $D_z$:

$$\begin{aligned}\langle j'm'|U(b)|jm\rangle=&\sum_{\substack{m''\\m_1,m_2}}D^{j'*}_{m''m'}\left[\frac{\pi}{2}\right](\kappa m_1\kappa m_2|j'm'')\\&\times\exp\left[-i\frac{\mu d_0}{\hbar^2k}\int_{-\infty}^{\infty}dz\,\alpha_1(b/r)(m_1-m_2)\right](\kappa m_1\kappa m_2|jm'')D^{j}_{m''m}\left[\frac{\pi}{2}\right]\ .\end{aligned} \tag{4.5}$$

Note that the exponential in (4.5) is the eikonal limit of $S^{\bar{l}}[m_1,m_2]$, so the expansion (4.5) has some similarities to (2.16). However, (4.5) contains an additional rotation with a Wigner function which is different from the transformation (2.5) to the rotating frame. Also, for a general interaction it is not possible to bring the interaction in the eikonal phase to the rotating-frame form (2.4) where only a $\mu=0$ component is present.

### B. Eikonal $S$ matrix

To make a detailed comparison between the eikonal and the rotating-frame approximations it is necessary to obtain a partial-wave expansion (2.3) for the eikonal amplitude. This is accomplished by an inversion of Eq. (2.3), as is done in Ref. [11]:

$$(S^J-1)_{l'j';lj}=\frac{\sqrt{kk'}}{2\pi}\frac{i^{l'-l+1}}{2J+1}\sum_{\substack{m,m'\\m_l,m_{l'}}}(lm_ljm|JM)(l'm_{l'}j'm'|JM)\int\int d\hat{\mathbf{k}}\,d\hat{\mathbf{k}}'\mathcal{Y}_{lm_l}(\hat{\mathbf{k}})\mathcal{Y}^{*}_{l'm_{l'}}(\hat{\mathbf{k}}')f_{j'm';jm}(\hat{\mathbf{k}}',\hat{\mathbf{k}})\ . \tag{4.6}$$

The eikonal partial $S$ matrix is obtained by using in Eq. (4.6) the eikonal amplitude $f_{j'm';jm}(\mathbf{q})$ [given by (4.1)]. Notice that the integral in (4.2) is calculated along a trajectory parallel to $(\mathbf{k}+\mathbf{k}')/|\mathbf{k}+\mathbf{k}'|$ while the quantization axis, with respect to which the projections $m$ and $m'$ are defined, is fixed in the laboratory frame. The four-dimensional integral over $\hat{\mathbf{k}}$ and $\hat{\mathbf{k}}'$ is evaluated in this fixed frame. It is, however, possible to reduce (4.6) to a one-dimensional integral as we shall now show. We define an $x'$-$y'$-$z'$ coordinate frame by a Euler rotation $(\Phi,\Theta,-\Phi)$, where $(\Theta,\Phi)$ are the spherical coordinates of $(\hat{\mathbf{k}}+\hat{\mathbf{k}}')/|\hat{\mathbf{k}}+\hat{\mathbf{k}}'|$ in the fixed $x$-$y$-$z$ laboratory frame. In this frame $z'$ is along $(\mathbf{k}+\mathbf{k}')/|\mathbf{k}+\mathbf{k}'|$. We define $\theta$ to be an angle between $\mathbf{k}$ and $\mathbf{k}'$, and $\phi$ the angle that the plane passing through $\hat{\mathbf{k}}$, $\hat{\mathbf{k}}'$ makes with the $x'$ axis. The polar angles of $\hat{\mathbf{k}}$ and $\hat{\mathbf{k}}'$ in the $x'$-$y'$-$z'$ frame are $(\theta/2,\phi+\pi)$ and $(\theta/2,\phi)$, respectively.

Denoting by $(\theta_1,\phi_1)$ and $(\theta_2,\phi_2)$ the polar angles of $\hat{\mathbf{k}}$ and $\hat{\mathbf{k}}'$ in the $x$-$y$-$z$ frame, we make the transformation

$$\theta_1,\phi_1;\theta_2,\phi_2\rightarrow\Theta,\Phi;\theta,\phi \tag{4.7}$$

in the double integral of Eq. (4.6). In Appendix B we show that the Jacobian of this transformation is such that

$$\sin\theta_1\sin\theta_2\,d\theta_1\,d\phi_1\,d\theta_2\,d\phi_2=\sin\theta\sin\Theta\,d\theta\,d\phi\,d\Theta\,d\Phi\ . \tag{4.8}$$

We first evaluate the $\Theta,\Phi$ integral. Denoting by $R$ the rotation operator associated with $(\Phi,\Theta,-\Phi)$ we have

$$|jm\rangle_{z'}=R\,|jm\rangle_z\ , \tag{4.9}$$

where the subscripts denote the axis with respect to which $m$ is calculated. Using the definition (4.1) of the eikonal amplitude we find

$$f_{j'm';jm}(\hat{\mathbf{k}}',\hat{\mathbf{k}})=\sum_{m_1m_1'} D^{j'}_{m'm_1'}(R)D^{j*}_{mm_1}(R)f_{j'm_1';jm_1}(\mathbf{q}) , \tag{4.10}$$

where $f_{j'm';jm}(\mathbf{q})$ is evaluated in the $x'$-$y'$-$z'$ frame, and depends only on $\theta,\phi$. The spherical harmonics $\mathcal{Y}_{lm_l}$ and $\mathcal{Y}_{l'm_{l'}}$ in the integral of (4.6) transform according to $D^l$ and $D^{l'}$, respectively. Recoupling of the various $D$'s using the orthogonality relations of the Wigner function we find

$$(S^J-1)_{l'j';lj}=\frac{2\sqrt{kk'}}{2J+1}i^{l'-l+1}\sum_{\substack{m,m',M\\ m_l,m_{l'}}}(lm_ljm|JM)(l'm_{l'}j'm'|JM)\int_0^{2\pi}d\phi\int_0^{\pi}\sin\theta\, d\theta\, \mathcal{Y}_{lm_l}(\hat{\boldsymbol{\kappa}})\mathcal{Y}_{l'm_{l'}}(\hat{\boldsymbol{\kappa}}')f_{j'm';jm}(\mathbf{q}) , \tag{4.11}$$

where $\hat{\boldsymbol{\kappa}}$ and $\hat{\boldsymbol{\kappa}}'$ are the vectors $\hat{\mathbf{k}}$ and $\hat{\mathbf{k}}'$ in the $x'$-$y'$-$z'$ frame. The $\phi$ dependence of $f_{j'm';jm}(\mathbf{q})$ is easily determined to be

$$f_{j'm';jm}(\mathbf{q})=e^{i(m-m')\phi}f_{j'm';jm}(q\hat{\mathbf{x}}') . \tag{4.12}$$

The $\phi$ integral in (4.11) can be done to give the final inversion formula

$$(S^J-1)_{l'j';lj}=\frac{\sqrt{kk'}}{4\pi}i^{l'-l+1}\frac{\sqrt{(2l+1)(2l'+1)}}{2J+1}\sum_{\substack{m,m',M\\ m_l,m_{l'}}}(lm_ljm|JM)$$
$$\times(l'm_{l'}j'm'|JM)\int_0^{\pi}\sin\theta\, d\theta\, d^l_{0m_l}\left[\frac{\theta}{2}\right]d^{l'}_{m_{l'}0}\left[\frac{\theta}{2}\right]f_{j'm';jm}(q\hat{\mathbf{x}}') . \tag{4.13}$$

$d^l$ in (4.13) are the Wigner functions. Notice that the eikonal amplitude in (4.13) depends only on the magnitude of $q$, $q=2k\sin(\theta/2)$.

### C. Comparison

We now compare the eikonal to the rotating-frame approximations for the same example discussed in Sec. III.

Figure 7 shows $\sigma^J_{0\to j'}$ vs $J$ for $j'=0$, 1, and 2. In each case we show the rotating-frame (solid line), eikonal (long dashed), and exact (dashed) calculations. Except for the very low waves ($J=0,1$) both the rotating-frame and eikonal results agree well with the exact results. Note, however, that for $j'=2$, the eikonal result shows some spurious oscillations while the rotating-frame result is smooth.

Figure 8 is similar to Fig. 7 but for $j'=3,4$. Here we see that the eikonal approximation fails even at large $J$. The rotating frame, however, works well for $J\gtrsim 3$. We conclude that the eikonal approximation is good for low spin excitations while the rotating frame is good for both low and high spins.

The differential unpolarized cross sections $(d\sigma/d\Omega)_{0\to 1}$ were already shown in Fig. 2. Both the rotating frame and the eikonal compare well with the exact calculation at forward angles. The discrepancy at large angles is due to the small partial waves ($J=0,1$) where the approximations do not work well. This can be corrected in a hybrid approach [11,27].

### D. A rotating-frame eikonal approximation

The basic quantity calculated in the rotating-frame approximation is the $S$-matrix element $S^{\bar{l}}[m_1,m_2]$ for the single-channel problem (2.15). It is possible to further simplify the calculation by taking the eikonal limit of $S^{\bar{l}}$

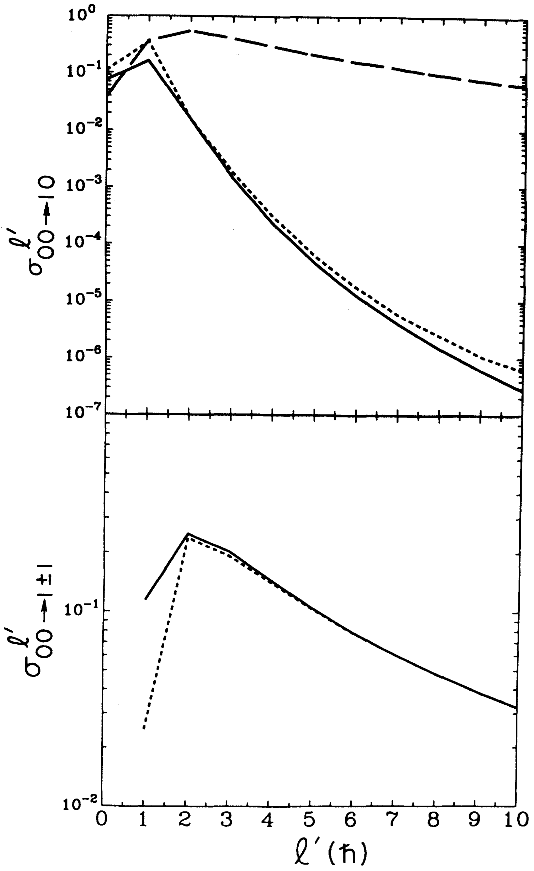

FIG. 5. The partial cross sections $\sigma^{l'}_{00\to j'm'}$ vs $l'$ for the transitions $0,0\to j'=1,m'=0$ (top) and $0,0\to j'=1,m'=\pm1$ (bottom). Lines are as in Fig. 4.

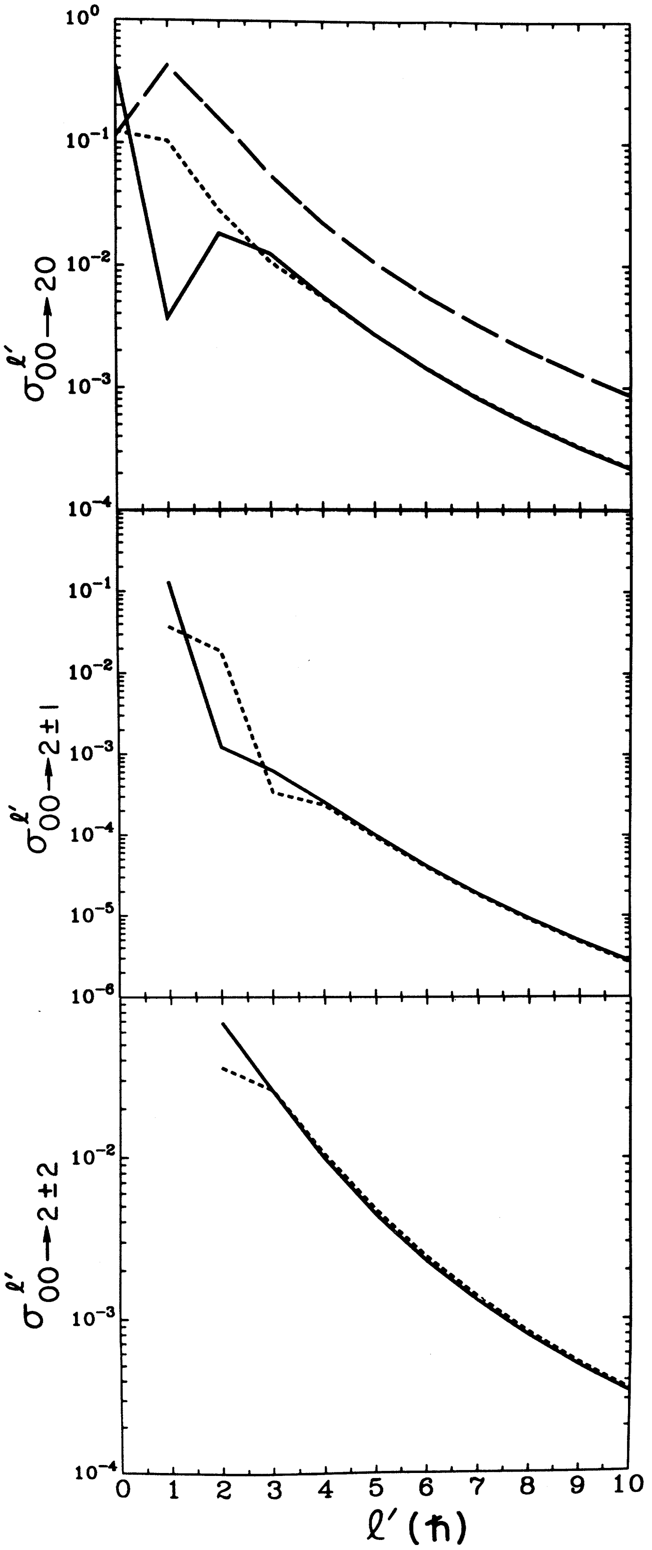

FIG. 6. As in Fig. 5 but for the transitions 0,0→2,0 (top), 0,0→2, ±1 (middle), and 0,0→2, ±2 (bottom).

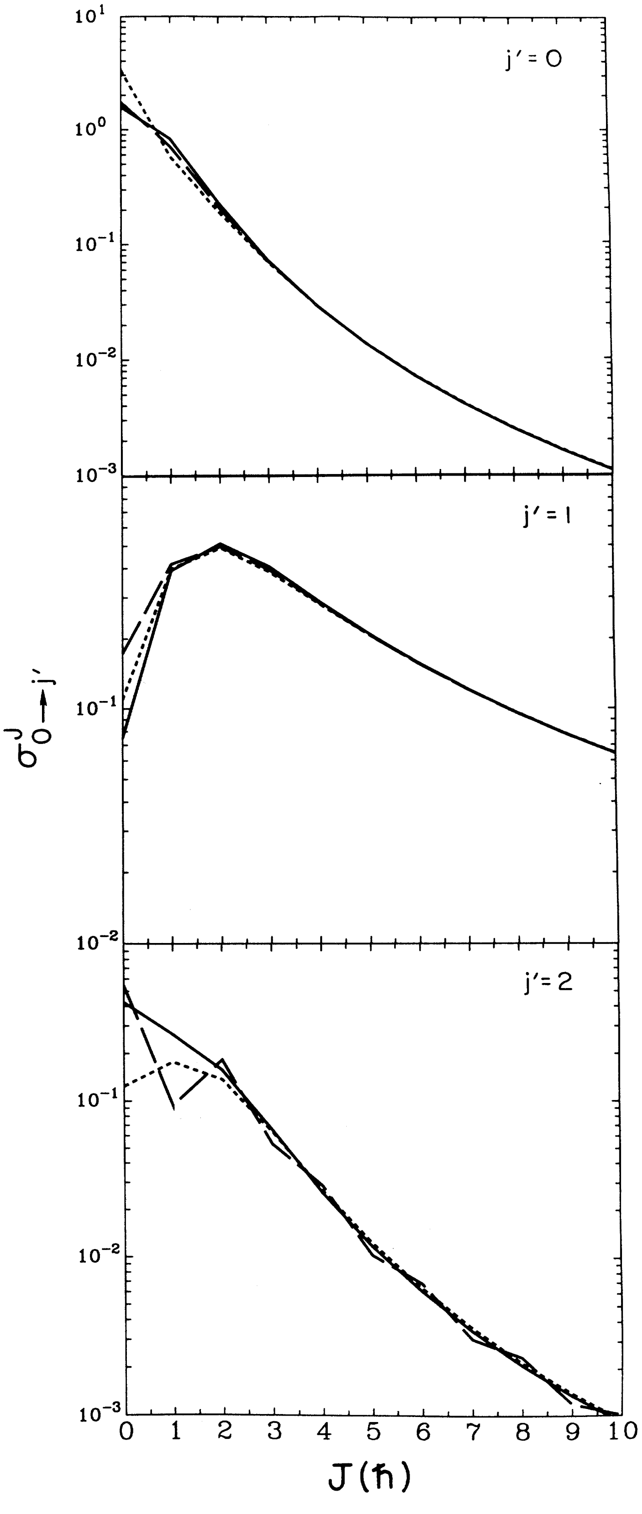

FIG. 7. The partial cross section $\sigma^{J}_{0\to j'}$ vs $J$ for the transition $j=0\to j'$ for 5-eV electrons scattered from a diatomic molecule with dipole moment of 6 D. Shown are the transitions 0→0 (top), 0→1 (middle), and 0→2 (bottom). Short-dashed lines: the exact coupled-channel [13,14] result. Long-dashed lines: the eikonal approximation using the inversion formula (4.13) with the eikonal amplitude (4.1). Solid lines: the rotating-frame approximation with $\bar{l}=(l+l')/2$.

$$
\begin{aligned}
S^{\bar{l}}[m_1,m_2] &\approx \exp\left[-\frac{i\mu}{\hbar^2 k}\bar{d}_0\int_{-\infty}^{\infty} dz\,\alpha_1(r)(m_1-m_2)\right] \\
&= \exp\left[-i\frac{\mu\bar{d}_0}{\hbar^2 k}\frac{\pi}{2}(b^2+R_0^2)^{-1/2}(m_1-m_2)\right]\Bigg|_{b=(\bar{l}+1/2)/k} . \qquad (4.14)
\end{aligned}
$$

Thus, for the above dipole interaction we even have an analytic result in that limit. We found that this rotating-frame eikonal approach also works quite well at forward angles. An example is shown in Fig. 9 for the cross section $j=0\rightarrow j'=1$. In general, the rotating-frame eikonal approximation is much simpler to calculate than the multichannel eikonal approximation.

## V. CONCLUSIONS

In this paper we have discussed and explored the validity of an algebraic rotating-frame approach to electron-molecule scattering. This approach, which is based on a centrifugal and energy sudden approximation introduced in atom-molecule scattering, is much simpler than the conventional coupled-channel approach since it reduces the problem to a family of single-channel potential scattering problems. When compared with the algebraic eikonal approach, it is found that both approximations work well for the transitions to low-lying rotational states except for the few low-$J$ partial waves. For transitions to higher rotational states, the $S$ matrix continues to be well reproduced in the rotating-frame approach but not in the eikonal approximation. Due to its simplicity the rotating-frame approach might be useful in treating electron scattering from complex polyatomic molecules. We remark that in realistic applications one should include short-range (such as exchange) interactions. These interactions affect mostly the low partial waves and can be dealt with in a hybrid calculation where the low partial amplitudes in the eikonal [11] or rotating-frame [27] approximations are replaced by the exact ones obtained from coupled-channel calculations.

## ACKNOWLEDGMENTS

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## APPENDIX A: DIPOLE POTENTIAL SCATTERING

The phase-shifts of the one-channel dipole potential scattering problem are found by solving the radial Schrödinger equation (2.15) using the Numerov algo-

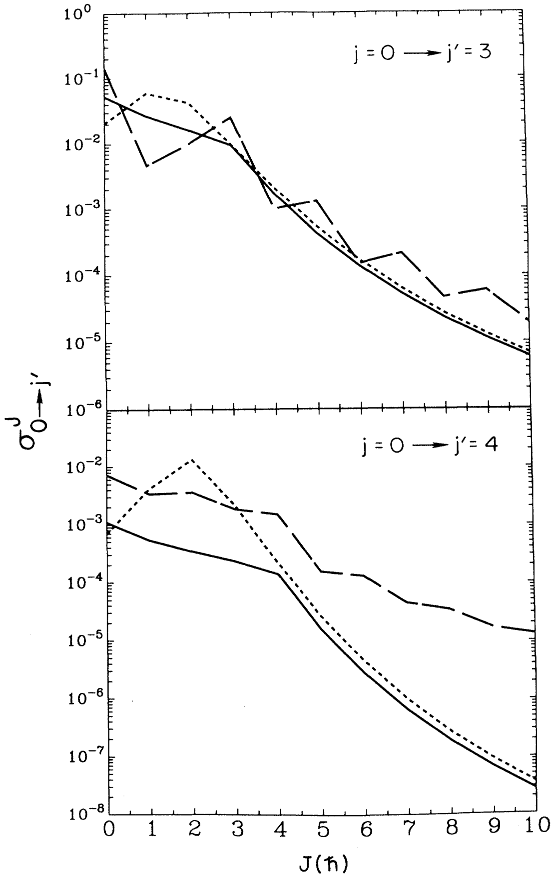

FIG. 8. As in Fig. 7 but for the transitions 0→3 and 0→4. Notice the oscillatory behavior in the eikonal result (for the 0→3 transition) and the disagreement between the eikonal and the exact result even at high $J$'s.

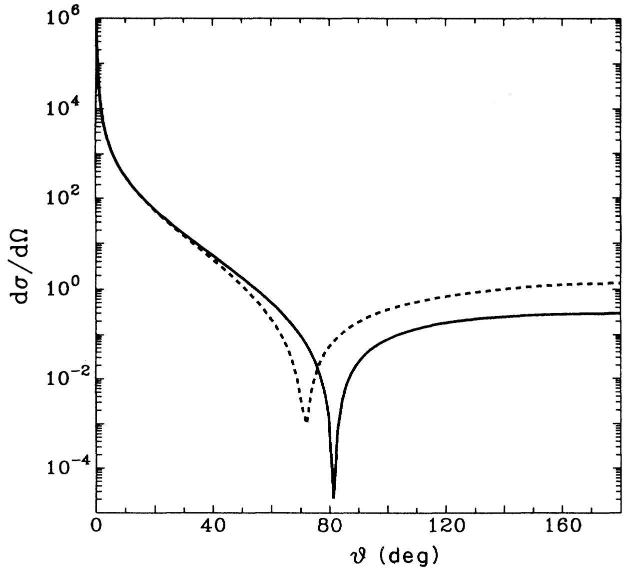

FIG. 9. Differential cross section $(d\sigma/d\Omega)_{0\rightarrow 1}$ for the same case as in Fig. 2. Dashed line: exact coupled-channel result. Solid line: the rotating-frame eikonal approximation.

rithm. Care should be taken since the dipole potential $d_0(m_1-m_2)e^2/(r^2+R_0^2)$ is a long-range potential, and in principle the equation has to be integrated to very large distances. To overcome this problem, notice that for $r \gg R_0$, Eq. (2.15) reduces to a Bessel equation for $\tilde{\phi}=\phi/\sqrt{x}$ $(x \equiv kr)$

$$\left[\frac{d^2}{dx^2}+\frac{1}{x}\frac{d}{dx}+\left[1-\frac{\nu^2}{x^2}\right]\right]\tilde{\phi}=0\ , \tag{A1}$$

where

$$\nu^2=\bar{l}(\bar{l}+1)+\tfrac{1}{4}-2\mu e^2 d_0(m_1-m_2)/\hbar^2\ . \tag{A2}$$

The general solution of (A1) is

$$\tilde{\phi}=AJ_\nu(x)+BN_\nu(x)\ , \tag{A3}$$

where $J_\nu,N_\nu$ are Bessel functions of order $\nu$. By solving (2.15) to distance $r \gg R_0$, we can determine $B/A$ in (A3). Using the asymptotic expansion of $J_\nu$, $N_\nu$ at yet longer distances we find the $S$-matrix element $S^{\bar{l}}$ from

$$S^{\bar{l}}=-\frac{1-iB/A}{1+iB/A}e^{i(\bar{l}-\nu-1/2)\pi}\ . \tag{A4}$$

## APPENDIX B: JACOBIAN OF EQ. (4.7)

In this Appendix we show that the transformation (4.7) preserves the Jacobian (4.8).

The transformation $\theta_1,\phi_1;\theta_2,\phi_2 \to \Theta,\Phi;\theta,\phi$ is defined by the rotation $\mathcal{R}(\Phi,\Theta,-\Phi)$ from the $x$-$y$-$z$ to $x'$-$y'$-$z'$ frame

$$\begin{aligned}\hat{\mathbf{k}}&=\mathcal{R}(\Phi,\Theta,-\Phi)\hat{\boldsymbol{\kappa}}\ ,\\ \hat{\mathbf{k}}'&=\mathcal{R}(\Phi,\Theta,-\Phi)\hat{\boldsymbol{\kappa}}'\ ,\end{aligned} \tag{B1}$$

where $\mathcal{R}$ is the Cartesian rotation matrix and $\hat{\boldsymbol{\kappa}}$, $\hat{\boldsymbol{\kappa}}'$ are the vectors $\hat{\mathbf{k}}$, $\hat{\mathbf{k}}'$ in the $x'$-$y'$-$z'$ frame

$$\hat{\boldsymbol{\kappa}}=\begin{bmatrix}\sin\frac{\theta}{2}\cos(\pi+\phi)\\ \sin\frac{\theta}{2}\sin(\pi+\phi)\\ \cos\frac{\theta}{2}\end{bmatrix}\ ,\quad \hat{\boldsymbol{\kappa}}'=\begin{bmatrix}\sin\frac{\theta}{2}\cos\phi\\ \sin\frac{\theta}{2}\sin\phi\\ \cos\frac{\theta}{2}\end{bmatrix}\ . \tag{B2}$$

The metric in the $x$-$y$-$z$ frame is given by

$$\begin{aligned}(ds^2)=(d\hat{\mathbf{k}})^2+(d\hat{\mathbf{k}}')^2&=(d\theta_1)^2+\sin^2\theta_1(d\phi_1)^2\\ &\quad+(d\theta_2)^2+\sin^2\theta_2(d\phi_2)^2\ .\end{aligned} \tag{B3}$$

An infinitesimal rotation $d\mathcal{R}$ is parametrized by

$$d\mathcal{R}=\mathcal{R}(-id\boldsymbol{\omega}'\cdot\boldsymbol{\mathcal{J}})\ , \tag{B4}$$

where $d\boldsymbol{\omega}'$ are the components of the rotation vector along the $x'$-$y'$-$z'$ frame and $\boldsymbol{\mathcal{J}}$ is the spin-1 representation of the angular momentum. Using (B1) and (B2) we can express $(d\hat{\mathbf{k}})^2$ in the rotated frame as

$$(d\hat{\mathbf{k}})^2=(d\hat{\boldsymbol{\kappa}})^2-\hat{\boldsymbol{\kappa}}^T(-id\boldsymbol{\omega}'\cdot\boldsymbol{\mathcal{J}})^2\hat{\boldsymbol{\kappa}}+2\,d\hat{\boldsymbol{\kappa}}^T(-id\boldsymbol{\omega}\cdot\boldsymbol{\mathcal{J}})\hat{\boldsymbol{\kappa}}\ . \tag{B5}$$

Using a similar expression for $(d\hat{\mathbf{k}}')^2$ and $k_{x'}=-\kappa_x$, $k_{y'}=-\kappa_y$, $k_{z'}=\kappa_z$ we find

$$\begin{aligned}(ds)^2&=2(1-\kappa_{x'}^2)d\omega_{x'}^2+2(1-\kappa_{y'}^2)d\omega_{y'}^2+2(1-\kappa_{z'}^2)d\omega_{z'}^2\\ &\quad-4\kappa_{x'}\kappa_{y'}d\omega_{x'}d\omega_{y'}+4\sin^2(\theta/2)d\phi\,d\omega_{z'}\ .\end{aligned} \tag{B6}$$

In terms of the Euler angles,

$$\begin{bmatrix}d\omega_{x'}\\ d\omega_{y'}\\ d\omega_{z'}\end{bmatrix}=\begin{bmatrix}-\cos\Phi\sin\Theta & -\sin\Phi & 0\\ -\sin\Phi\sin\Theta & -\cos\Phi & 0\\ \cos\Theta & 0 & 1\end{bmatrix}\begin{bmatrix}\dot{\Phi}\\ \dot{\Theta}\\ -\dot{\Phi}\end{bmatrix}\ . \tag{B7}$$

Using (B6) and (B7) we find the metric tensor $g$ in the coordinates $\Theta,\Phi;\theta,\phi$

$$g=2\begin{bmatrix}g_{\Phi\Phi} & g_{\Phi\Theta} & g_{\Phi\phi} & 0\\ g_{\Phi\Theta} & g_{\Theta\Theta} & 0 & 0\\ g_{\Phi\phi} & 0 & g_{\phi\phi} & 0\\ 0 & 0 & 0 & g_{\theta\theta}\end{bmatrix}\ , \tag{B8}$$

where

$$\begin{aligned}g_{\Phi\Phi}&=[1-(\kappa_{x'}\cos\Phi+\kappa_{y'}\sin\Phi)^2]\sin^2\Theta\\ &\quad+(1-\kappa_{z'}^2)(\cos\Theta-1)^2\ ,\\ g_{\Theta\Theta}&=1-(\kappa_{x'}\sin\Phi-\kappa_{y'}\cos\Phi)^2\ ,\\ g_{\phi\phi}&=\sin^2\theta\ ,\quad g_{\theta\theta}=\tfrac{1}{4}\ ,\\ g_{\Phi\Theta}&=[\kappa_{x'}\kappa_{y'}\cos2\Phi-\tfrac{1}{2}(\kappa_{x'}^2-\kappa_{y'}^2)\sin2\Phi]\sin\Theta\ ,\\ g_{\Phi\phi}&=(\cos\Theta-1)\sin^2\frac{\theta}{2}\ .\end{aligned} \tag{B9}$$

The volume element is then found to be

$$\sqrt{\det g}\ d\Phi\,d\Theta\,d\phi\,d\theta=\sin\Theta\,d\Theta\,d\Phi\,\sin\theta\,d\theta\,d\phi\ . \tag{B10}$$

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