PHYSICAL REVIEW A VOLUME 42, NUMBER 11 1 DECEMBER 1990

Hybrid approach to electron scattering from polar molecules

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(Received 19 July 1990)

Electron scattering from polar molecules is studied in a hybrid approach that uses the recently introduced algebraic-eikonal approach to describe the forward-angle scattering and the results of, for example, a close-coupling calculation for larger angles. The two calculations are matched by making a partial-wave expansion and combining the high partial waves of the algebraic-eikonal approach with the low partial waves obtained in a full close-coupling calculation. The method is illustrated by applying it to electron scattering from a rigid-rotor molecule with a large dipole moment.

I. INTRODUCTION AND MOTIVATION

The scattering of medium energy (5–50 eV) electrons from polar molecules is a complicated process involving many partial waves and the virtual excitation of many intermediate states.[1] For forward angles ($\theta < 60^\circ$) the scattering process is largely dominated by the long-range dipole interaction between the incoming electron and the molecule. For large angles the scattering is sensitive to short-range features of the molecular dynamics such as exchange correlations. For relatively small values of the dipole moment (≈ 1 D) and for small scattering angles the Born approximation already gives a good description of the experimental cross section. For larger angles and for strongly polar molecules the channel coupling between the rotational and vibrational degrees of freedom becomes increasingly important. The standard approach to treat these multistep processes is that of a coupled-channel or close-coupling calculation. In practice the number of channels becomes, except for some very simple systems, prohibitively large and various different methods and approximation schemes have been developed to solve the scattering equations. For projectile energies well above the rotational and vibrational energies one can use the adiabatic or fixed nucleus approximation, which becomes particularly useful for electron collisions with polar molecules. However, even in the adiabatic limit, a standard coupled-channel calculation presents a complicated problem involving the coupling of many different channels especially for larger (triatomic and polyatomic) molecules. Therefore it is of great interest to find a simple prescription that both exploits the simplifications that arise from the dominance of the dipole interaction at forward angles, and, at the same time, incorporates the rotational-vibrational structure and internal molecular dynamics at a level sufficient to calculate the cross sections of interest at all angles.

Recently, in a series of three papers[2–4] an alternative method to calculate cross sections for electron scattering from polar molecules has been proposed. This method, called the algebraic-eikonal approach, is a combination of an algebraic description[5] of rotational and vibrational excitation in molecules (the vibron model) and the eikonal approximation[6] in the adiabatic limit. It was inspired by recent developments in nuclear physics,[7] in which a similar method was used to calculate the effects of multistep processes in medium energy (≈ 500 MeV) proton scattering from collective nuclei. The algebraic-eikonal approach is very well suited to describe the forward angle scattering of electrons from strongly polar molecules. This process is dominated by the long-range dipole coupling between the projectile electron and the target molecule. In order to extend the calculations to larger angles the short-range dynamics, which up to now have been treated rather crudely by introducing a cutoff parameter in the dipole interaction, have to be taken into account in a more complete way.

There are several ways in which the effects of short-range correlations, such as the exchange and polarization potentials, and exchange correlations can be included in the algebraic-eikonal approach. A straightforward way would be to express these interactions explicitly in terms of the vibron operators. However, this will lead to many complications and will destroy the simplicity and elegance of the method. Among other things it will give rise to nonlinear terms in the eikonal phase which are very hard to calculate. One may also question the validity of the eikonal approximation at larger angles, even though in practice it seems to work for much larger angles than expected.

Instead, in this paper we propose a hybrid procedure, in which the results of the algebraic-eikonal approach for the high partial waves are combined with, for example, the methods used in Ref. 8, in which all the relevant short-range correlations and channel couplings are included from the outset, for the low partial waves. In this way we hope to combine the best parts of two different methods, one which is better suited to the low partial waves and another which is more efficient for the high partial waves, into one single theoretical framework, that will be numerically efficient and at the same time presents a physically clear and accurate treatment of the scattering problem.

In Sec. II we briefly review the main features of the algebraic-eikonal approach to electron-molecule scattering. In Sec. III we discuss the hybrid approach both for the eikonal and the Born approximation. The method is illustrated in Sec. IV by applying it to electron scattering from a rigid rotor. In Sec. V we present some concluding remarks.

II. ALGEBRAIC-EIKONAL APPROACH

The algebraic-eikonal approach was originally proposed[2,3] to describe electron scattering from diatomic molecules. In a subsequent paper[4] it was generalized to triatomic molecules as well. In this section we will discuss briefly the main features of this approach. A more detailed account can be found in Refs. 2–4.

For medium and high energy scattering the eikonal approximation is a good approximation for elastic and inelastic scattering. The Hamiltonian is in general given by

$$H = \frac{\hbar^2 k^2}{2\mu_e} + H_{\rm mol}(\xi) + V(\mathbf{r},\xi), \tag{1}$$

where $H_{\rm mol}(\xi)$ is the vibron Hamiltonian describing the molecular dynamics, and $V(\mathbf{r},\xi)$ represents the coupling between the incoming electron and the molecule. For small-angle scattering (peripheral collisions) the long-range dipole interaction is by far the dominant term in $V(\mathbf{r},\xi)$. We therefore take

$$V(\mathbf{r},\xi) = V(r)\,\hat{\mathbf{r}}\cdot\mathbf{D}(\xi) = -\frac{ed}{r^2+R_0^2}\,\hat{\mathbf{r}}\cdot\mathbf{D}(\xi), \tag{2}$$

where $\mathbf{r}$ is the projectile coordinate measured with respect to the center of mass of the molecule and $\mathbf{D}(\xi)$ is the molecular dipole operator. d is the static dipole moment of the molecule. The cutoff radius R_0 in Eq.(2) is introduced to remove the singularity at the origin ($r=0$), thus crudely modeling the short-range part of the electron-molecule interaction. For scattering processes in which the projectile energy is much larger than the coupling potential and in which the projectile wavelength is small compared to the range of variation of the potential, one may use the eikonal approximation to describe the scattering. If, in addition, the molecular motion is slow (adiabatic) compared to the interaction time of the projectile electron with the molecule, one can neglect $H_{\rm mol}(\xi)$ in Eq.(1). Under these approximations the scattering amplitude for scattering an electron with initial momentum $\mathbf{k}$ from an initial molecular state $|i\rangle = |v,l,m\rangle$ to final momentum $\mathbf{k}'$ and a final state $|f\rangle = |v',l',m'\rangle$ can be expressed in terms of a one-dimensional integral over the impact parameter b,

$$\begin{aligned} F(i\rightarrow f|\mathbf{q}) &= \frac{k}{2\pi i}\int d\mathbf{b}\; e^{i\mathbf{q}\cdot\mathbf{b}}\langle f \mid e^{i\chi(\mathbf{b})}-1 \mid i\rangle \\ &= \frac{k}{i}\, i^{m-m'}\int_0^\infty b\,db\, J_{m-m'}(qb)\sum_{L,M}\sqrt{\frac{4\pi}{2L+1}}\,Y^*_{L,M}(\hat{\mathbf{q}})\frac{2L+1}{2l'+1}\langle L,M,l,m|l',m'\rangle\sum_{m''}\langle L,0,l,m''|l',m''\rangle \\ &\quad\times\langle v',l',m'' \mid e^{ig(b)D_z(\xi)}-1 \mid v,l,m''\rangle \end{aligned} \tag{3}$$

where $\mathbf{q} = \mathbf{k}-\mathbf{k}'$ is the momentum transfer and $g(b)$ is the eikonal phase, that the projectile acquires as it goes by the target

$$g(b) = -\frac{\mu_e}{\hbar^2 k}\int_{-\infty}^{\infty} dz\,\frac{-ed}{r^2+R_0^2}\,\frac{b}{r}. \tag{4}$$

In the derivation of Eq.(3) we have written the projectile coordinate as $\mathbf{r} = \mathbf{b}+\mathbf{z}$, where the impact parameter $\mathbf{b}$ is perpendicular to the z axis, which is chosen along $\mathbf{z} = (\mathbf{k}+\mathbf{k}')/|\mathbf{k}+\mathbf{k}'|$. Note that we use a somewhat different set of molecular state labels from the standard ones in Ref. 1. We use l instead of j to label the rotational state and L for the total angular momentum, in place of J.

The transition matrix element appearing in the integrand of the scattering amplitude has a very simple form since it only depends on the z component of the molecular dipole operator, $D_z(\xi)$. It contains the coupling between molecular eigenstates to *all* orders in the coupling strength $g(b)$ and can be calculated *exactly* in the framework of the vibron model. The vibron model is similar in spirit to the interacting boson model[9] of nuclear physics and provides an algebraic description of the rotational and vibrational excitations in molecules. Although it cannot match the high accuracy for the energy spectrum obtained in more conventional *ab initio* calculations, the vibron model gives a good global description of the properties of rotational and vibrational excitations. It becomes particularly useful in the calculation of transition probabilities, which in general involve a complicated sum over intermediate states. Using the algebraic properties of the vibron model these matrix elements can be expressed in terms of the representation matrices of the group O(4), which are a generalization of the well-known Wigner D functions for SU(2). Another attractive feature of the algebraic-eikonal approach is that the elastic and inelastic excitation of both rotational and vibrational states are treated on the same footing. Moreover, it can easily be generalized to more complex systems, such as triatomic and polyatomic molecules.

Previous studies, in which this approach was applied to electron scattering from both diatomic [LiF, KI (Ref. 3), and HCl (Ref. 10)] and triatomic [HCN (Ref. 4)] molecules, show that, in general, there is good agreement with the available experimental data for forward angles. To describe the scattering to larger angles more accurately, a more sophisticated treatment of short-range correlations, such as exchange and polarization potentials, is required. In Sec. III we propose a method to incorporate these effects.

III. HYBRID APPROACH

The proposed hybrid approach is similar in spirit to the procedure outlined in Refs. 11 and 12, in which the low partial waves obtained from solving the coupled-channel equations were matched with the high partial waves calculated in the Born approximation. In the present paper we use instead the algebraic-eikonal approach to calculate the high partial waves. To do the matching we first have to calculate the partial-wave T-matrix elements. We expand the eikonal scattering amplitude of Eq.(3) into partial waves according to

$$F(i \rightarrow f|\mathbf{q}) = \frac{2\pi i}{\sqrt{kk'}} \sum_{\lambda,\mu} Y^{*}_{\lambda,\mu}(\hat{\mathbf{k}}) \sum_{\lambda',\mu'} Y_{\lambda',\mu'}(\hat{\mathbf{k}}') i^{\lambda-\lambda'} \sum_{L,M} T^{L}(l'\lambda'|l\lambda) \langle l,m,\lambda,\mu|L,M\rangle \langle l',m',\lambda',\mu'|L,M\rangle, \tag{5}$$

where $k'^2 = k^2 + 2\mu_e(E_{vl} - E_{v'l'})/\hbar^2$. The T-matrix elements appearing in the right-hand side can be obtained simply by inverting the above equation

$$T^{L}(l'\lambda'|l\lambda) = \frac{\sqrt{kk'}}{2\pi i} \sum_{m,\mu} \langle l,m,\lambda,\mu|L,M\rangle \sum_{m',\mu'} \langle l',m',\lambda',\mu'|L,M\rangle \frac{i^{\lambda'-\lambda}}{2L+1} \int d\hat{\mathbf{k}}\, Y_{\lambda,\mu}(\hat{\mathbf{k}}) \int d\hat{\mathbf{k}}'\, Y^{*}_{\lambda',\mu'}(\hat{\mathbf{k}}')\, F(i \rightarrow f|\mathbf{q}). \tag{6}$$

The quantity of interest is the differential cross section, summed over the final magnetic substates and averaged over the initial ones. It can be expressed explicitly in terms of the T-matrix elements as[13,14]

$$\begin{aligned} \frac{d\sigma(i \rightarrow f|\mathbf{q})}{d\Omega} &= \frac{2}{2l+1} \frac{k'}{k} \sum_{m,m'} |F(i \rightarrow f|\mathbf{q})|^2 \\ &= 2 \sum_{\nu=0}^{\infty} A_\nu P_\nu(\cos\theta), \end{aligned} \tag{7}$$

where θ is the scattering angle with $\cos\theta = \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}'$ and

$$A_\nu = \frac{(-1)^{l'-l}}{4(2l+1)k^2} \sum_{L_1,L_2} \sum_{\lambda_1,\lambda_2} \sum_{\lambda'_1,\lambda'_2} T^{L_1}(l'\lambda'_1|l\lambda_1)^{*} Z(\lambda_1 L_1 \lambda_2 L_2; l\nu) Z(\lambda'_1 L_1 \lambda'_2 L_2; l'\nu) T^{L_2}(l'\lambda'_2|l\lambda_2), \tag{8}$$

where Z is a geometric coefficient

$$\begin{aligned} Z(abcd;ef) = {} & (-1)^{(f-a+c)/2} \\ & \times \sqrt{(2a+1)(2b+1)(2c+1)(2d+1)} \\ & \times \langle a0c0|f0\rangle W(abcd;ef). \end{aligned} \tag{9}$$

Next we combine the eikonal approach for the high partial waves with the coupled-channel approach for the low partial waves, by replacing the T^L's in A_ν by the close-coupling T-matrix elements[14] for $L < L_0$, while keeping the eikonal T-matrix elements of Eq.(7) for $L \geq L_0$. Calling these new coefficients $B_\nu(L_0)$, the summed and averaged differential cross section can be written as[12]

$$\begin{aligned} \frac{d\sigma(i \rightarrow f|\mathbf{q})}{d\Omega} = {} & \left.\frac{d\sigma(i \rightarrow f|\mathbf{q})}{d\Omega}\right|_{\text{eik}} \\ & + 2\sum_{\nu=0}^{\nu_0} \left[B_\nu(L_0) - A_\nu^{\text{eik}}\right] P_\nu(\cos\theta), \end{aligned} \tag{10}$$

with $B_\nu(0) = A_\nu^{\text{eik}}$. The values of L_0 and ν_0 are determined such that the differential cross section of Eq.(10) is in good agreement with that obtained by solving the full coupled-channel equations. The total cross section and momentum-transfer cross section can be obtained by integrating the differential cross section,

$$\begin{aligned}\sigma_t(i \rightarrow f) &= \int \frac{d\sigma(i \rightarrow f|\mathbf{q})}{d\Omega}\, d\Omega \\ &= \sigma_t(i \rightarrow f)|_{\rm eik} + 8\pi\ \left[B_0(L_0) - A_0^{\rm eik}\right] \qquad (11)\end{aligned}$$

and

$$\begin{aligned}\sigma_m(i \rightarrow f) &= \int \frac{d\sigma(i \rightarrow f|\mathbf{q})}{d\Omega}(1-\cos\theta)\, d\Omega \\ &= \sigma_m(i \rightarrow f)|_{\rm eik} + 8\pi[B_0(L_0) - A_0^{\rm eik}] \\ &\quad -\frac{8\pi}{3}[B_1(L_0) - A_1^{\rm eik}]. \qquad (12)\end{aligned}$$

A similar hybrid method has been employed by many authors using the Born approximation for the high partial waves.[11,12] In order to compare the different methods for the high partial waves we also present in the following the relevant expressions for the T-matrix elements in the first Born and the unitarized Born approximation. Again we use the vibron model to describe the rotational and vibrational excitations of the molecule. In analogy with Sec. II one could call this method the "algebraic-Born" approach. The scattering amplitude in first Born approximation (B1) can be obtained from that in the eikonal approximation by expanding the exponential in the transition matrix element and keeping only the leading-order term,

$$\begin{aligned}&F(i \rightarrow f|\mathbf{q}) \\ &\quad = -\frac{\mu_e}{2\pi\hbar^2}\int d\mathbf{r}\, e^{i\mathbf{q}\cdot\mathbf{r}}\, \langle v', l', m' \mid V(\mathbf{r},\xi) \mid v, l, m\rangle. \qquad (13)\end{aligned}$$

Using Eq.(6) one can easily derive the expression for the T-matrix elements

$$\begin{aligned}[T^L(l'\lambda'|l\lambda)]_{\rm B1} = 4i\sqrt{kk'}\,\frac{\mu_e}{\hbar^2}\int_0^\infty r^2 dr j_\lambda(kr) j_{\lambda'}(k'r) V(r)(-1)^{l'-L}\sqrt{(2\lambda+1)(2\lambda'+1)/3}\,\langle \lambda, 0, \lambda', 0|1, 0\rangle \\ \times \left\{\begin{matrix} l & l' & 1 \\ \lambda' & \lambda & L\end{matrix}\right\}\langle v', l'||D(\xi)||v, l\rangle. \qquad (14)\end{aligned}$$

The matrix element of the dipole operator $D(\xi)$ can be derived simply in the vibron model, especially in the SO(4) limit, which in the limit of a large number of vibrons, N, reduces to a three-dimensional Morse oscillator.[15] In this case the dipole operator is diagonal in the vibrational quantum number and the reduced matrix elements of the rescaled[2] dipole operator in the SO(4) basis are given by

$$\begin{aligned}\langle v', l'||D(\xi)||v, l\rangle = \delta_{v,v'}\Bigg(&\sqrt{\frac{(N-2v-l)(N-2v+l+2)}{N(N+2)}}\,\sqrt{l+1}\,\delta_{l',l+1} \\ &-\sqrt{\frac{(N-2v-l+1)(N-2v+l+1)}{N(N+2)}}\,\sqrt{l}\,\delta_{l',l-1}\Bigg). \qquad (15)\end{aligned}$$

For $N \rightarrow \infty$ the expression for the T-matrix element reduces to the one derived in the classical rotor model.[11]

Since for transitions with $|\Delta l| \neq 1$ the first Born approximation vanishes, we use instead the unitarized Born approximation (B2).[16] In this case the reactance matrix is treated in the first Born approximation, $R^L = iT_{\rm B1}^L/2$. As a result the T-matrix elements can be expressed in terms of those in the first Born approximation as

$$(T_{\rm B2}^L)_{ij} = \left(\frac{-2iR^L}{1-iR^L}\right)_{ij} = [2T_{\rm B1}^L(2+T_{\rm B1}^L)^{-1}]_{ij}, \qquad (16)$$

where the subscript ij is a shorthand notation for the channel $\{l\lambda\}$. Unlike the first Born approximation the unitarized Born approximation satisfies the unitarity constraints. In Ref. 17 it was shown that for large partial waves the (body fixed) B2 T-matrix elements are a good approximation to those obtained exactly in a close-coupling calculation. It is, however, important to note, that in general it is much harder to calculate the T-matrix elements in a systematic way in the unitarized Born approximation than it is in the (algebraic-) eikonal approach. In Sec. IV we will show that, especially for strongly polar molecules, the algebraic-eikonal approach offers in many cases a better starting point for a hybrid calculation than the (unitarized) Born approximation.

IV. APPLICATIONS

In this section we investigate the scope and applicability of the hybrid approach by presenting a set of model calculations for electron scattering from a rigid-rotor molecule. We introduce a cutoff for the short-distance electron-rotor coupling of the form given in Eq.(2) with $R_0 = 0.5$ Å. All calculations are performed in the laboratory frame. We consider two values of the rotor dipole moment, 1 D, a relatively small value, and 6 D, a large value typical of a molecule like LiF. We calculate the scattering at four projectile energies, 1, 5, 10, and 50 eV. The exact scattering calculations[18] taken from a full coupled-channel calculation are compared with calculations using the algebraic-eikonal method, the unitarized Born approximation, the first Born approximation (where appropriate), and with hybrid calculations where each of these approximate schemes is mixed with low partial waves from the exact calculation. We are particularly interested in how many exact waves we need to take into account before the cross sections converge to the exact answers. Since the exact waves are more difficult to calculate, the utility of the method depends on the crossover partial wave being relatively small. In the following we only study rotational transitions from the ground state. It is easy to show that for realistic values of the dipole coupling the scattering amplitude, Eq.(3), depends on $\Delta l = |l - l'|$, rather than on the initial and final rotational states separately. We can therefore without loss of generality take $l^\pi = 0^+$ and thus reduce the calculational effort considerably.

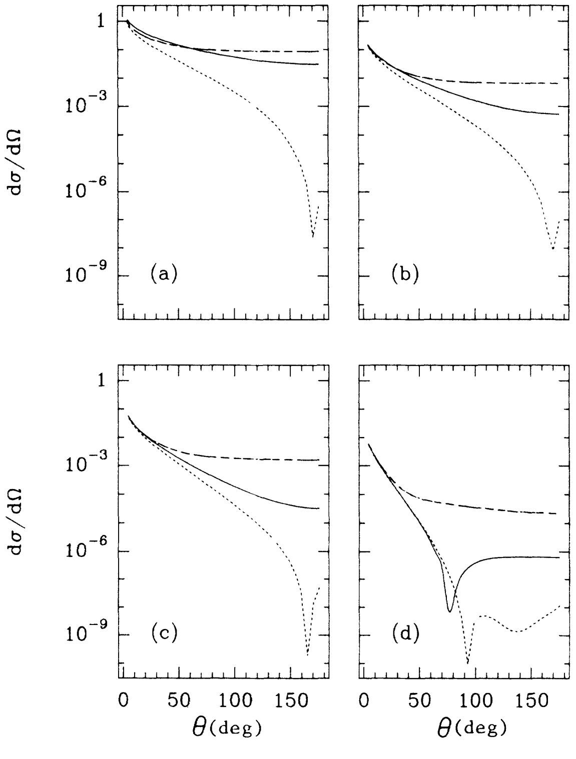

FIG. 1. Differential cross sections for electron scattering from a rigid-rotor molecule with a dipole moment of 1 D for the $0^+ \rightarrow 0^+$ transition. The scattering energies are (a) 1 eV, (b) 5 eV, (c) 10 eV, and (d) 50 eV. The solid line is the algebraic-eikonal calculation, and the dotted line the unitarized Born approximation. The third line is a superposition of two curves, the hybrid algebraic-eikonal (short-dashed) and the hybrid unitarized Born (short-dash-dotted), each mixed with the exact amplitudes up to $L = 10$.

The first calculation we present is that for elastic scattering from the ground state of a molecule ($0^+ \rightarrow 0^+$) with a dipole moment of 1 D for projectile energies of 1, 5, 10, and 50 eV. In Fig. 1 we show the differential cross section calculated in the algebraic-eikonal (AE) (solid line) and the unitarized Born approximation (B2) (dotted line) for the four scattering energies. Since in our simple model the electron-molecule coupling is pure dipole, the first Born approximation does not contribute to elastic scattering. The short-dashed and the short-dash-dotted lines are the result of hybrid calculations where the exact coupled-channel (CC) waves are mixed with either the AE or the B2 waves, respectively, with $L_0 = 10$. For such a large value of the matching L_0 these two cases give identical cross sections, which are in turn identical with the exact coupled-channel result. Figure 1 shows that AE is a better approximation than B2 for forward-angle scattering. For larger angles, in particular for backward angles, neither approximation is very good. When used in a hybrid calculation to complete the high partial waves for sufficiently large values of L_0 both converge to the exact results.

In Fig. 2 we repeat the calculation of the elastic differential cross section for a dipole moment of 6 D. Now there is much more structure in the cross sections. Although AE is somewhat better than B2, neither is adequate ex-

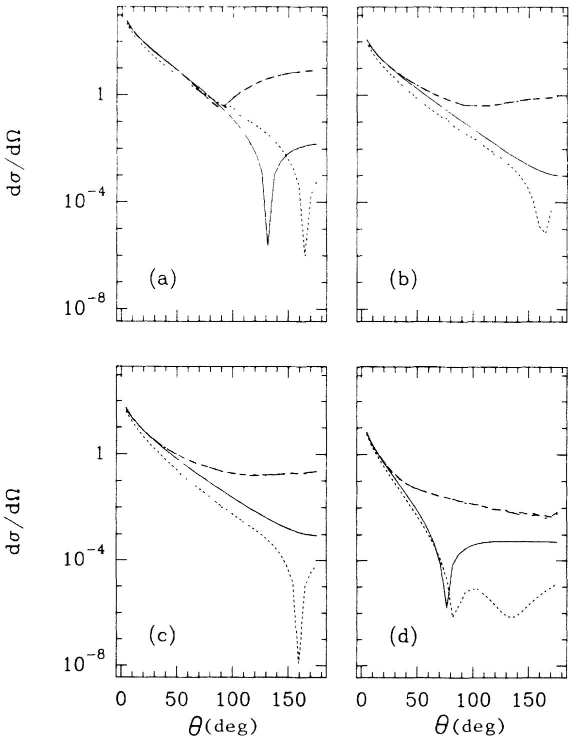

FIG. 2. Same as Fig. 1 but with a dipole moment of 6 D.

cept at the smallest momentum transfers. Again both methods converge to the exact cross sections when combined with the exact coupled-channel T-matrix elements with $L_0 \leq 10$. We next study the differential cross section for scattering to the first rotational excited state of the rotor, $0^+ \rightarrow 1^-$. In this case there is also a contribution from the first Born approximation (B1). For this transition we only discuss the result for 6 D, since in the 1 D case B1 dominates at all energies. In Fig. 3 we show the angular distribution for the $0^+ \rightarrow 1^-$ transition at the same four projectile energies and for a dipole moment of 6 D. We show separately the AE, B2, and B1 calculations and each of these crossed with the exact amplitudes with $L_0 = 10$. Except in the minimum, where the hybrid B2 shows a deviation, the three hybrid calculations give the same results. In Fig. 4 we show the calculation for the $0^+ \rightarrow 2^+$ transition with a dipole moment of 6 D. In this case there is no B1 and AE and B2 are very similar. They both converge to the exact value when matched at $L_0 = 10$.

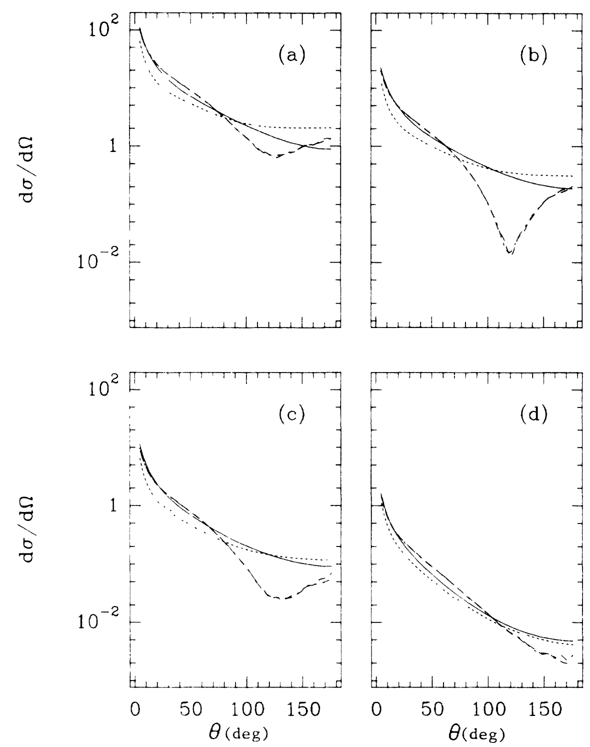

FIG. 4. Same as Fig. 2 but for the $0^+ \rightarrow 2^+$ transition.

We now turn to a study of the rate of convergence of the hybrid approach. We want to study convergence as a function of the matching partial wave L_0. We chose to make the detailed comparison at 5 eV since at 1 eV there are too few partial waves to be interesting, while for 10 or 50 eV, the simple approximation schemes begin to work "too well." Figure 5 shows the results for elastic scattering of 5-eV electrons from a molecule with a dipole moment of 6 D. The short-dashed line in Fig. 5(a) is

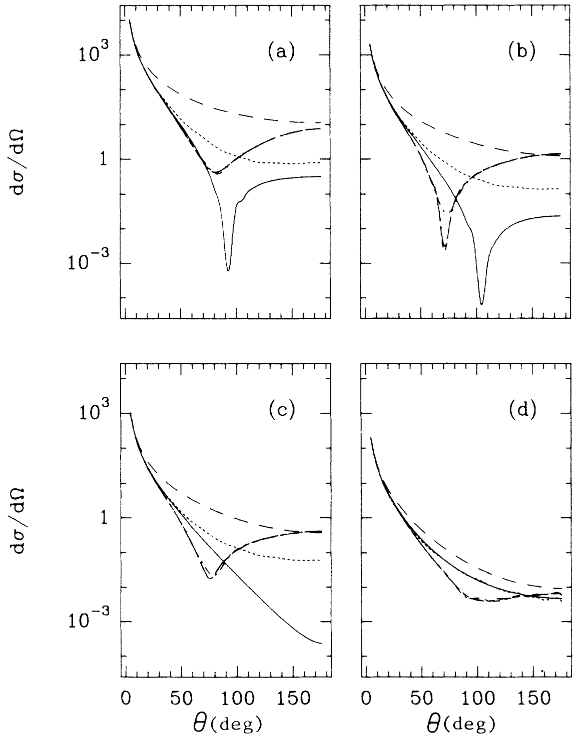

FIG. 3. Same as Fig. 2 but for the $0^+ \rightarrow 1^-$ transition. Now there is also a contribution from the first-order Born approximation (long-dashed line). The long-dash-dotted line represents the hybrid first-order Born and coincides with the hybrid algebraic-eikonal and unitarized Born curves.

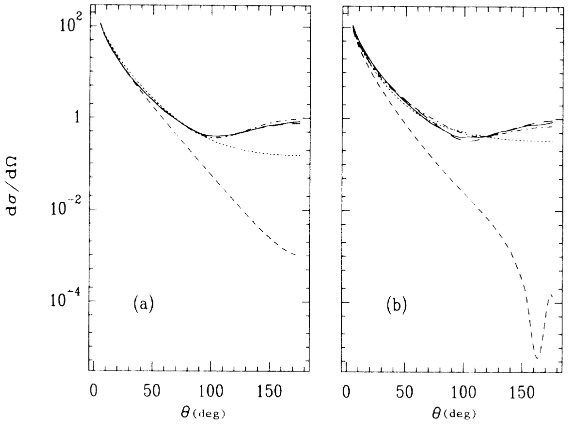

FIG. 5. The differential cross section for electron energy of 5 eV and dipole moment of 6 D for the $0^+ \rightarrow 0^+$ transition. In (a) we show the results for the algebraic-eikonal approach (short-dashed line) and the corresponding hybrid calculations with $L_0 = 0$ (dotted), $L_0 = 1$ (short-dash-dotted), $L_0 = 2$ (long-dashed) and the exact result with $L_0 = 10$ (solid line). In (b) we present the same set of calculations for the unitarized Born approximation.

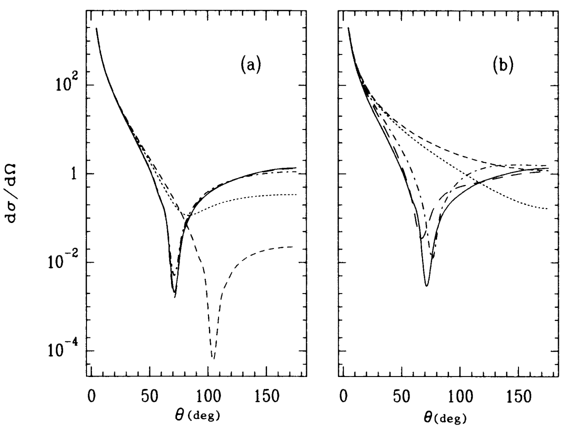

FIG. 6. Same as Fig. 5 but for the $0^+ \longrightarrow 1^-$ transition. In (b) we show the results for the first-order Born approximation.

pure AE, whereas the other curves represent the results of a hybrid calculation in which the low partial waves are replaced by the exact ones from a coupled-channel calculation, with the matching successively at $L_0 = 0, 1, 2$, and 10. We see that already for $L_0 = 2$, the result is essentially exact, a remarkably rapid convergence. Figure 5(b) shows the same thing but starting from B2. Again by $L_0 = 2$ the convergence is complete even though the starting point of B2 is not nearly as satisfactory as that of AE. In Fig. 6(a) we show the convergence for the $0^+ \longrightarrow 1^-$ transition for the AE case. Again for $L_0 = 1, 2$ we are there, even in the minimum. Figure 6(b) shows the same calculation for the B1. In this case we have to match at a much higher value of L_0 to obtain a similar convergence ($L_0 = 7, 8$). Figures 7(a) and 7(b) show the convergence for the $0^+ \longrightarrow 2^+$ transition in the AE and B2 cases, respectively. Although AE converges much more rapidly than B2 in the forward angles, and it is these angles that dominate, getting the correct answer in the vicinity of the deep backward minimum requires matching at $L_0 = 4, 5$ in either case.

For all three transitions studied with $\Delta l = 0, 1$, and 2 the hybrid approach offers a great advantage over an exact calculation in the coupled-channel approach, since one only has to calculate a few T-matrix elements exactly to get a good convergence. In a full coupled-channel calculation of the differential cross section according to Eqs.(7) and (8), one has to sum over many T-matrix elements to obtain a similar convergence. For the $\Delta l = 0$ and 2 transitions the differential cross section summed to $L = 20$ still shows an oscillatory behavior, while for the $\Delta l = 1$ transitions the differential cross section diverges at forward angles. For the $\Delta l = 3$ and 4 transitions the high partial waves do not contribute very much to the differential cross section. The coupled-channel calculation is already converged when summed to $L = 4, 5$. In this case there is not much to be gained from a hybrid calculation with either the eikonal or the unitarized Born approximation.

Finally we study convergence in a global way. We consider the momentum-transfer cross section of Eq.(12) as a function of matching wave L_0. This cross section is a more stringent test than the regular integrated cross

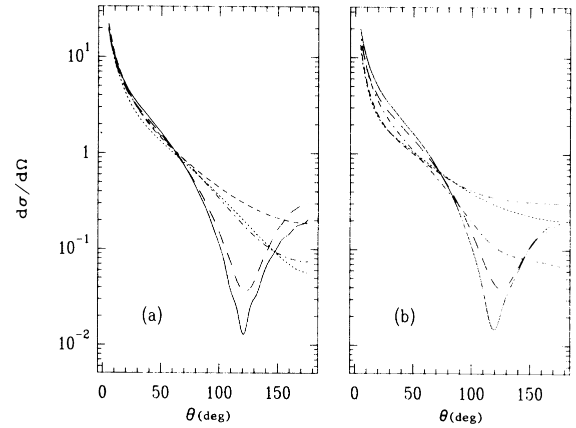

FIG. 7. Same as Fig. 5 but for the $0^+ \longrightarrow 2^+$ transition.

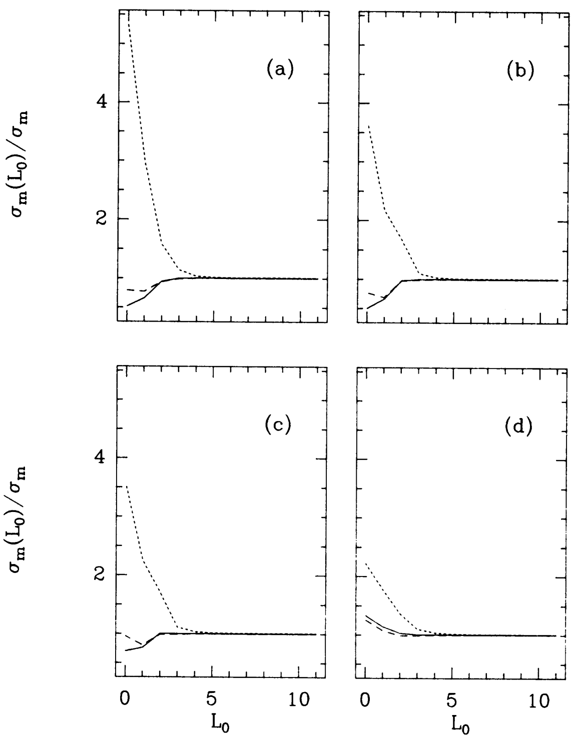

FIG. 8. The momentum-transfer cross section as a function of the matching parameter L_0 relative to the exact value for the $0^+ \longrightarrow 1^-$ transition. We show the four energies, (a) 1 eV, (b) 5 eV, (c) 10 eV, and (d) 50 eV all for a dipole moment of 6 D. The solid line is AE, the short-dashed line is B1, and the long-dashed line B2.

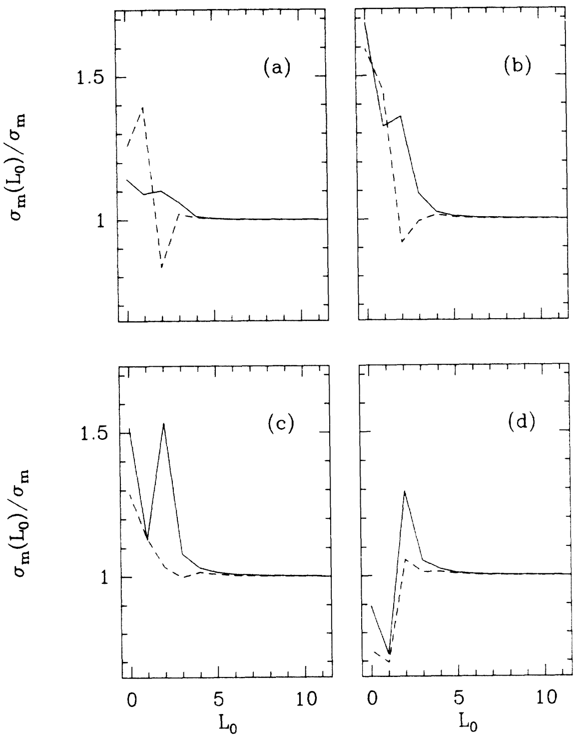

FIG. 9. Same as Fig. 8 but for the transition $0^+ \rightarrow 2^+$. In this case there is no B1.

section, since in the former the forward angles are suppressed. All approximations seem to work well at forward angles, where the cross sections tend to be largest. In Fig. 8 we show the ratio of the momentum-transfer cross section matched at L_0 to the exact momentum-transfer cross section as a function of L_0. We consider the $0^+ \rightarrow 1^-$ transition with 6 D and study the same four energies as before for the three approximations, AE, B1, and B2. We see that at all energies convergence is achieved for AE and B2 at $L_0 = 2, 3$, while for B1 one needs to go to about $L_0 = 5$. This slower convergence for B1 is also seen in Fig. 6(b). Figure 9 shows the convergence of the momentum-transfer cross section for the $0^+ \rightarrow 2^+$ transition. Now there is no B1. The convergence is "noisy" but essentially complete by $L_0 = 5$ for both AE and B2. The erratic convergence reflects the fact that as a function of L_0, the AE T-matrix elements oscillate when compared with the exact value. The B2 T-matrix elements do so as well, but less. This oscillation is particularly marked in the $0^+ \rightarrow 2^+$ case.

Finally we note that for each transition, convergence seems to occur for the same value of L_0 independent of energy. This is surprising if we think in terms of some scattering radius R and believe that it is kR that governs the matching point. Note that kR changes by a factor of 7 between 1 and 50 eV. We have no explanation of the relative constancy of the optimal L_0 with energy.

V. SUMMARY AND CONCLUSIONS

We have discussed here an extension of the algebraic-eikonal approach, combining it with the results of a coupled-channel calculation for the low partial waves. The approach not only corrects the improper use of an eikonal-based approximation for large angles, but more importantly permits the introduction of new short-range interactions such as exchange correlations in the electron-molecule dynamics. Such a mixed scheme exploits the simplicity of the algebraic-eikonal technique for correctly summing the full effect of channel coupling in the peripheral waves, while still allowing complete freedom for introducing dynamical details in the low waves that sense the molecular interior. In our model calculation we find that very few exact interior waves are required to give convergence. Our simple model, involving just a rigid rotor, does not have any interesting interior dynamics. But the success of our method suggests that the interior dynamics can be easily introduced, and we plan to turn our method to some real molecular examples in subsequent work.

We find that the hybrid scheme works almost as well for the unitarized Born approximation as for the algebraic-eikonal approach (but much less so for the first Born approximation). However, the unitarized Born approximation amplitudes are far more difficult to calculate in a systematic way than those of the algebraic-eikonal, even in the simple case of the rigid rotor. In extensions to more complicated cases, for example triatomic and polyatomic molecules, the comparison will be even more stark. We do plan to extend our hybrid method to polyatomic molecules where it may only be necessary to include the overall molecular dipole moment to model the peripheral waves. This may further enhance the scope and applicability of this approach.

In summary, the first results are very encouraging and indicate that the proposed hybrid approach may provide a powerful framework to study electron scattering from polar molecules.

ACKNOWLEDGMENTS

We would like to thank F. Iachello and B. Schneider for many encouraging conversations. This work was performed as part of the research program of the Stichting voor Fundamenteel Onderzoek der Materie (FOM) with financial support from the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO) and was also supported in part by a grant of the National Science Foundation and by the U.S. Department of Energy through the Theoretical Division of the Los Alamos National Laboratory.

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