Analytic Born completion in the calculation of electron-molecule differential cross sections

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In calculating the elastic differential cross section for electron scattering from linear nonpolar molecules, one must include elements of the transition matrix corresponding to a large number of partial waves in order to obtain convergence at small angles. We present an analytic correction to the widely used expression for the differential cross section in terms of body-frame T-matrix elements calculated in the fixed-nuclear-orientation approximation. This correction incorporates contributions from all high-order partial waves via the Born approximation. It efficiently produces accurate differential cross sections and shows rapid convergence even at small angles. We illustrate the importance and accuracy of this procedure for low-energy (less than 10 eV) collisions of electrons with H_2 and N_2. [S1050-2947(96)08906-8]

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I. INTRODUCTION

One of the standard methods for calculating the differential cross section (DCS) is expansion of the scattering amplitude in partial waves [1]. For spherical potentials, the orbital angular momentum of the projectile is conserved and the partial-wave scattering amplitudes (or phase shifts) are labeled by the quantum number l. For a nonspherical potential, as in electron-molecule scattering, the projectile orbital angular momenta are coupled in both the entrance and exit channels, so the amplitudes—and elements of the transition (T) matrix—are labeled by both l and l_0. The partial-wave expression for the DCS involves infinite sums over these angular momenta, which, unless evaluated analytically, must obviously be truncated. Convergence of the DCS in these sums can be slow, especially at small angles (e.g., $\theta \leqslant 30°$), and the effort required increases as the square of the number of terms included in the original partial-wave expansion.

Recent advances in crossed-beam experiments [2] have significantly improved the accuracy of measurements of small-angle electron-molecule DCS's. For example, the measurements reported by Sun *et al.* [2] of the e-N_2 DCS at and above 4.0 eV show clear small-angle structures which had not been previously resolved. Such measurements highlight the need for accurate theoretical e-N_2 DCS's. At angles below about 30°, many partial waves are required to converge these DCS's [2]. One could easily generate the large number of T-matrix elements necessary for convergence in the first Born approximation (FBA) [3,4], but such a brute-force approach to this problem is certainly inefficient and potentially inaccurate, especially for strongly nonspherical systems.

The partial-wave convergence problem also arises in calculating small-angle electron-atom DCS's. For electron-rare-gas scattering, Thompson [5] has provided an alternative to brute-force numerical convergence: an *analytic* expression that includes contributions from all partial waves l greater than some $l_{\max}$. These contributions are approximated in the FBA using only the long-range part of the potential $V(r) \sim -\alpha_0/2r^4$, where α_0 is the spherical polarizability of the atom. (Wadehra and Nahar [6] give expressions for the long-range contribution to the scattering amplitude for spherical potentials that fall off as r^{-n} for n ranging from 3 to 8.) We will refer to such a procedure as analytic Born completion.

The electron-molecule problem is complicated by the nonspherical interaction potential and the need to account for rotation and vibration. Use of the FBA to approximate high-order elements of the electron-molecule T matrix dates back to studies of electron–polar-molecule scattering by Crawford and Dalgarno [7,8]. Most such implementations of this idea focus on the expansion of the DCS in Legendre polynomials with respect to the lab-frame scattering angle θ,

$$\frac{d\sigma}{d\Omega}(\theta,k_0) = \frac{1}{k_0^2}\sum_{L=0}^{\infty} A_L(k_0) P_L(\cos\theta), \tag{1}$$

where the coefficients $A_L(k_0^2)$ contain all the dynamical information, embedded in T-matrix elements. Thus, for example, Norcross and Padial, in a study of electron–polar-molecule scattering [3], introduced a procedure that includes high-order partial-wave contributions to the DCS by exploiting the simple closed form of the lab-frame DCS in the FBA [9]. To correct this form, they add a finite sum of terms that in effect replaces low-order *Born* Legendre contributions by their close-coupling counterparts. In addition to its first application to e-CO and vibrationally elastic e-HCl scattering [3], their method was subsequently applied to vibrationally inelastic e-HCl collisions [10,11], and to e-HCN collisions [12]. Numerical Born completion of the DCS is applicable to any long-range potential and has been used extensively in electron-molecule scattering [13–16].

The approach we adopt is to apply Born completion analytically not to the DCS, but to the electron-molecule scattering amplitude. Rescigno *et al.* [17] have summarized recently the advantages of completing the scattering amplitude for electron–polar-molecule scattering; and Fliflet and McKoy [18] have successfully implemented an analytic amplitude-based Born completion for electronic excitation in the distorted-wave approximation, presenting closed forms for the Born terms.

In Sec. II we derive an analytic correction to the scattering amplitude for elastic electron scattering from a nonpolar molecule in the ground state. Using this correction, we obtain an expression for the FBA-corrected elastic DCS in

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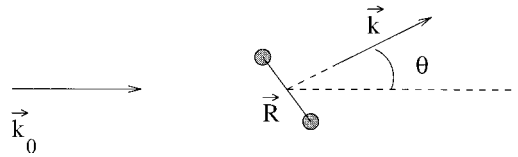

FIG. 1. Geometry for fixed-nuclear-orientation scattering in a space-fixed (laboratory) reference frame.

which low-order partial-wave T-matrix elements are included from body-frame scattering calculations in the fixed-nuclear-orientation approximation. In Sec. III we use this result to generate DCS's for e-H_2 and e-N_2 scattering. By comparing these cross sections with those obtained by brute-force numerical convergence, we illustrate the advantages of the analytic Born completion. We use atomic units throughout.

II. THEORY

The idea of Born completion is simple. Since we expect the Born approximation to accurately represent contributions to the scattering amplitude from elements of the T matrix corresponding to high-order partial waves (large l) [4,19], we can evaluate the amplitude by computing the Born amplitude, then replacing the Born partial-wave amplitudes for low partial waves with amplitudes from a more accurate treatment.

The implementation of this idea is complicated in the case of electron-molecule scattering because of the nonsphericity of the interaction potential. If we consider scattering energies that are large compared to the molecule's rotational constant, we can treat the direction $\hat{R}$ of the internuclear axis as fixed for the duration of the collision, as illustrated in Fig. 1; here $\vec{k}_0$ and $\vec{k}$ are the incoming and outgoing wave vectors, respectively, in a space-fixed (laboratory) reference frame [20]. This is the fixed-nuclear-orientation (FNO) approximation [21]. The FNO scattering amplitude therefore depends on $\hat{R}$, and the measured elastic DCS is the average over orientations of the squared modulus of this amplitude [22],

$$\frac{d\sigma}{d\Omega}(\vec{k},\vec{k}_0)=\frac{1}{4\pi}\int |f(\vec{k},\vec{k}_0;\hat{R})|^2 d\hat{R}. \tag{2}$$

Using Born completion, we can write the elastic FNO amplitude as

$$f(\vec{k},\vec{k}_0;\hat{R})=f^B(\vec{k},\vec{k}_0;\hat{R})-\sum_{l,l_0=0}^{l_{\max}}\sum_{m,m_0}\langle\vec{k}|klm\rangle \times[f^B_{lm,l_0m_0}(k_0;\hat{R})-f_{lm,l_0m_0}(k_0;\hat{R})] \times\langle k_0 l_0 m_0|\vec{k}_0\rangle, \tag{3}$$

where $f^B(\vec{k},\vec{k}_0;\hat{R})$ is the first Born approximate to $f(\vec{k},\vec{k}_0;\hat{R})$, and $f^B_{lm,l_0m_0}(k_0;\hat{R})$ are Born partial-wave amplitudes (see below). The coefficient

$$\langle\vec{k}|klm\rangle=\frac{(2\pi)^{3/2}}{k}\,i^{-l}Y_{lm}(\hat{k}) \tag{4}$$

effects the transformation from the plane-wave representation of the asymptotic free states to the partial-wave representation. The expression (3) is structurally similar to that used by Thompson [5] for electron-atom scattering.

For the electron-molecule interaction potential $V(\vec{r};\hat{R})$, the Born amplitude is [23]

$$f^B(\vec{k},\vec{k}_0;\hat{R})=-\frac{1}{2\pi}\int e^{i\vec{q}\cdot\vec{r}}V(\vec{r};\hat{R})\vec{d}r, \tag{5}$$

where $\vec{q}=\vec{k}_0-\vec{k}$ is the momentum transfer. For elastic scattering, the magnitude of q is related to the scattering angle by $q=2k\sin\theta$. Since we will use the Born approximation for high-order partial waves, we also need the partial-wave amplitudes

$$f^B_{lm,l_0m_0}(k_0;\hat{R})=-\frac{k_0^2}{\pi^2}\int j_l(k_0r)Y^*_{lm}(\hat{r})V(\vec{r};\hat{R})j_{l_0}(k_0r) \times Y_{l_0m_0}(\hat{r})\vec{d}r, \tag{6}$$

where the $j_l(x)$ are spherical Bessel functions. For large l, the centrifugal barrier term in the coupled radial scattering equations will dominate the potential in the small-r region, so scattering in those partial waves is due to the long-range form of the electron-molecule potential,

$$V_{\rm LR}(\vec{r};\hat{R})=-\frac{\alpha_0}{2r^4}-\left(\frac{\alpha_2}{2r^4}+\frac{Q}{r^3}\right)P_2(\hat{r}\cdot\hat{R}). \tag{7}$$

Replacing $V(\vec{r};\hat{R})$ by this potential allows us to evaluate Eqs. (5) and (6) analytically. In particular, from Eq. (5) we obtain

$$f^B(\vec{k},\vec{k}_0;\hat{R})=\alpha_0 M_0^4(q)-P_2(\hat{q}\cdot\hat{R})\left(\frac{\alpha_2\pi q}{16}+\frac{2}{3}Q\right), \tag{8}$$

and from Eq. (6),

$$f^B_{lm,l_0m_0}(k_0;\hat{R})=k_0^2\Bigg\{\frac{\alpha_0}{2\pi^2}M^4_{ll}(k_0)\delta_{ll_0}\delta_{mm_0} +\pi^{-3/2}A^{mm_0}_{ll_02}Y^*_{2,m-m_0}(\hat{R})[\alpha_2 M^4_{ll_0}(k_0) +2QM^3_{ll_0}(k_0)]\Bigg\}. \tag{9}$$

The coefficients $M^\nu_{ll_0}$ are integrals over Bessel functions [24],

$$M^\nu_l(q)=\int_0^\infty dr\; r^{2-\nu}j_l(qr), \tag{10}$$

$$M^\nu_{ll_0}(k_0)=\int_0^\infty dr\; r^{2-\nu}j_l(k_0r)j_{l_0}(k_0r). \tag{11}$$

The coefficients $A^{mm_0}_{ll_0\lambda}$ arise from the angular momentum coupling and are given by

$$A^{mm_0}_{ll_0\lambda}=(-1)^m(2l+1)^{1/2}(2l_0+1)^{1/2}(2\lambda+1)^{-1/2}\times\begin{pmatrix} l & l_0 & \lambda\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l & l_0 & \lambda\\ -m & m_0 & m-m_0\end{pmatrix}. \quad (12)$$

The remaining step in obtaining the analytic Born completion expression for the amplitude (3) is to evaluate the partial-wave amplitudes $f_{lm,l_0m_0}(k_0;\hat{R})$ for low-order partial waves. In the FNO approximation, the projection of the electron's orbital angular momentum on the internuclear axis, denoted by the quantum number Λ, is a constant of the motion. So additional simplifications obtain if we transform into the body-fixed (BF) reference frame, where the z axis is coincident with the internuclear axis $\hat{R}$. The amplitudes $f_{lm,l_0m_0}(k_0;\hat{R})$ are then related to elements of the BF FNO T-matrix elements by a simple rotation [25], effected by the Wigner rotation matrices [26]

$$f_{lm,l_0m_0}(k_0;\hat{R})=\frac{ik_0}{4\pi^2}\sum_{\Lambda} D^{l*}_{\Lambda m}(\hat{R})T^{\Lambda}_{ll_0}D^{l_0}_{\Lambda m_0}(\hat{R}). \quad (13)$$

Using the amplitudes (8) and (9) along with the rotation (13) in (3) and performing the average over orientations (2), we obtain the DCS

$$\frac{d\sigma}{d\Omega}(\theta,k_0)=\frac{1}{4k_0^2}\sum_{ll_0=0}^{l_{\max}}\sum_{l'l_0'=0}^{l_{\max}}\sum_{\Lambda\Lambda'}\sum_{L} d_L(ll_0\Lambda,l'l_0'\Lambda')\times T^{\Lambda}_{ll_0}T^{\Lambda'*}_{l'l_0'}P_L(\cos\theta)+[F_0(\theta)]^2+\tfrac{1}{5}\sum_{m=-2}^{2}[F_2^m(\theta)]^2+\frac{1}{k_0}\sum_{ll_0=0}^{l_{\max}}\sum_{\Lambda}[F_0(\theta)\delta_{ll_0}+F_2^0(\theta)c(ll_0\Lambda)]\mathrm{Im}(T^{\Lambda}_{ll_0})P_l(\cos\theta). \quad (14)$$

The sums over l, l_0, l', and l_0' in Eq. (14) include all partial waves from 0 to $l_{\max}$; the sums over Λ, Λ', and L include all values allowed by projection and triangle rules implied in the three-j symbols in $d_L(ll_0\Lambda,l'l_0'\Lambda')$ (see below). The factor $F_0(\theta)$ reflects the spherical long-range potential and depends on α_0, while $F_2^m(\theta)$ is due to α_2 and Q:

$$F_0(\theta)=\frac{\alpha_0\pi q}{4}+\alpha_0\pi k_0\sum_{l=0}^{l_{\max}}\frac{1}{(2l+1)(2l+3)}P_l(\cos\theta), \quad (15a)$$

$$F_2^m(\theta)=\frac{1}{\sqrt{5}}\left(\frac{\alpha_2\pi q}{16}+\frac{2Q}{3}\right)Y_{2m}(\hat{q})+\sum_{ll_0=0}^{l_{\max}} i^{l_0-l}(-1)^m\times(2l+1)^{1/2}(2l_0+1)\begin{pmatrix} l & l_0 & 2\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l & l_0 & 2\\ m & 0 & -m\end{pmatrix}\times[\alpha_2M^4_{ll_0}(k_0)+2QM^3_{ll_0}(k_0)]Y_{lm}(\hat{k}). \quad (15b)$$

The coefficients $d_L(ll_0\Lambda,l'l_0'\Lambda')$ and $c(ll_0\Lambda)$ contain angular momentum coupling information resulting from the frame transformation and the average over orientations and are given by

$$d_L(ll_0\Lambda,l'l_0'\Lambda')=i^{l_0-l+l'-l_0'}[(2l_0+1)(2l+1)(2l'+1)\times(2l_0'+1)]^{1/2}(2L+1)\begin{pmatrix} l & l' & L\\ 0 & 0 & 0\end{pmatrix}\times\begin{pmatrix} l_0 & l_0' & L\\ 0 & 0 & 0\end{pmatrix}\begin{pmatrix} l & l' & L\\ \Lambda & -\Lambda' & \Lambda'-\Lambda\end{pmatrix}\times\begin{pmatrix} l_0 & l_0' & L\\ \Lambda & -\Lambda' & \Lambda'-\Lambda\end{pmatrix}, \quad (16)$$

$$c(ll_0\Lambda)=(-1)^{\Lambda}i^{l_0-l}[(2l_0+1)(2l+1)]^{1/2}\begin{pmatrix} l & l_0 & 2\\ 0 & 0 & 0\end{pmatrix}\times\begin{pmatrix} l & l_0 & 2\\ \Lambda & -\Lambda & 0\end{pmatrix}. \quad (17)$$

The first term in Eq. (14) is the usual expression for the DCS in terms of BF T-matrix elements; Malegat [27] has published a code for computation of numerically converged DCS's for electronic excitation of diatomic molecules. The other terms are the analytic Born completion corrections. In the limit $l_{\max}\to\infty$, these correction terms should tend to zero; we have verified numerically that they do so. Note that these terms involve only the imaginary parts of the T-matrix elements; this is consistent with the fact that in the FBA the T matrix is purely imaginary. When we set $Q=0$ and $\alpha_2=0$ in Eqs. (14)–(17), returning the potential to a purely spherical form, we regain Thompson's expression for the electron–rare-gas DCS.

Although we have written the equations for analytic Born completion of the DCS without reference to vibrational states, their extension to vibrational excitation is straightforward. To obtain this extension, we would include in Eq. (2) a factor k_v/k_0, use the proper relation between the momentum transfer q and the incoming and outgoing wave numbers k_v and k_0, replace the moments in Eq. (7) by vibrational matrix elements (e.g., Q is replaced by $\langle v_0|Q|v\rangle$), and insert T-matrix elements from the proper vibrational block T^{Λ}_{vl,v_0l_0}.

III. RESULTS

In this section we compare two methods for obtaining DCS's from BF FNO T-matrix elements: the usual method of truncating sums over angular momentum quantum numbers and the analytic Born completion method described in the previous section. We will show that analytic Born completion generates more accurate results more efficiently than the truncated sum expression.

As noted above, by setting $l_{\max}=\infty$ in the first term in Eq. (14), we regain the familiar expression for the DCS in terms of BF FNO T-matrix elements [22,27]. In the absence of some sort of completion procedure, these sums must be truncated. Since the BF FNO T matrix is block diagonal in the projection quantum number Λ, we choose to truncate the sums at some $\Lambda_{\max}$,

$$\frac{d\sigma}{d\Omega}(\theta,k_0)=\frac{1}{4k_0^2}\sum_{\Lambda\Lambda'=-\Lambda_{\max}}^{\Lambda_{\max}}\sum_{ll_0l'l_0'}\sum_{L} d_L(ll_0\Lambda,l'l_0'\Lambda') \times T^{\Lambda}_{ll_0}T^{\Lambda'*}_{l'l_0'}P_L(\cos\theta). \quad (18)$$

For each Λ and Λ', we truncate the sums on l, l_0, l', and l_0', including enough partial waves to numerically converge the DCS (typically, from 3 to 8), and include all Legendre terms L allowed by the triangle and projection rules implied by (16). We will show that the computationally efficient choice of a small $\Lambda_{\max}$ introduces significant error in the DCS, especially at small angles. One purpose of the analytic Born completion procedure is to eliminate this error without incurring significant additional computational demands.

It is important to note that in contrast to Eq. (18), the Born completion expression (14) involves only one parameter $l_{\max}$, which in this equation represents *the maximum-order partial wave of the included BF FNO T-matrix elements*. The infinity of additional elements with l or $l_0>l_{\max}$ is included analytically.

A. e-H_2 scattering

Electron-H_2 scattering provides a good verification of the analytic Born completion method because the truncated expression (18) is relatively easy to converge. The e-H_2 interaction potential is very nearly spherical, with a weak short-range potential; contributions from higher-order partial waves are small because the centrifugal barrier dominates the short-range interaction. We base our comparisons here on Σ ($\Lambda=0$) and Π ($|\Lambda|=1$) T matrices from the body-frame-vibrational close-coupling (BFVCC) calculations of Trail and Morrison [28]. These authors solved the integro-differential e-H_2 scattering equations using the linear algebraic method [29], including exchange effects exactly and approximating the correlation-polarization potential with a local, parameter-free model potential [30].

Figures 2 and 3 show elastic DCS's at two representative energies, 1 and 10 eV, respectively, calculated with and without Born completion. For these DCS's, the truncated sum expression (18) converges by $\Lambda_{\max}=1$ with six partial waves for each symmetry. Results from the analytic Born completion calculations are labeled by $l_{\max}$, the maximum order partial wave of the included body-frame-vibrational close-coupling (BFVCC) T matrices. At both energies, $l_{\max}=1$ is sufficient to converge the analytically Born completed DCS's; contributions from $l\geqslant 2$ are easily and accurately represented by the correction terms in (14). We have verified these conclusions for e-H_2 at several other energies below 10 eV (not shown).

B. e-N_2 scattering

The e-N_2 interaction potential is stronger and more nonspherical than the e-H_2 potential, so we expect the e-N_2 DCS to require T-matrix elements from higher-order symmetries and partial waves (i.e., to converge more slowly), and the effect and value of the analytic Born completion to be greater for this system. These expectations are borne out by the DCS's in Figs. 4–6.

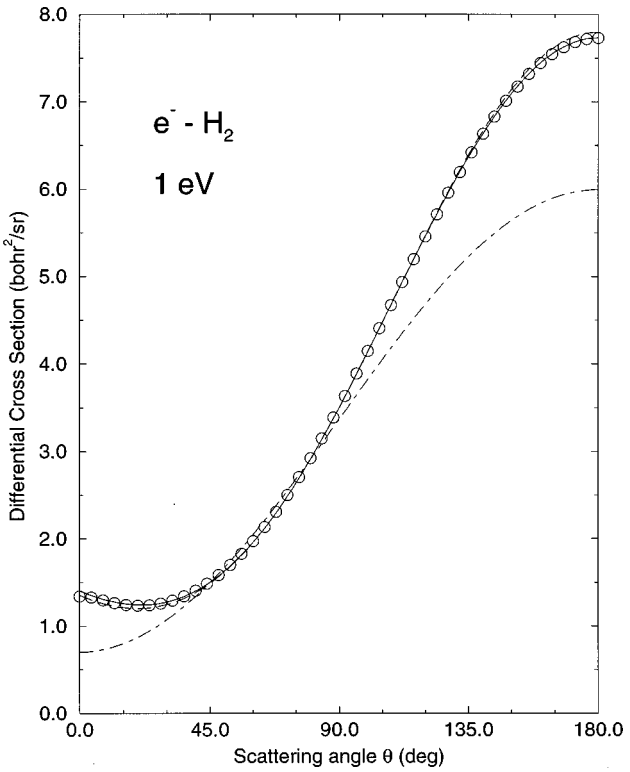

FIG. 2. DCS for e-H_2 scattering at 1.0 eV, calculated by the truncated sum (18) with $\Lambda_{\max}=1$ (open circles), and by analytic Born completion (14) with $l_{\max}=0$ (dot-dash line), $l_{\max}=1$ (dashed line), and $l_{\max}=2$ (solid line).

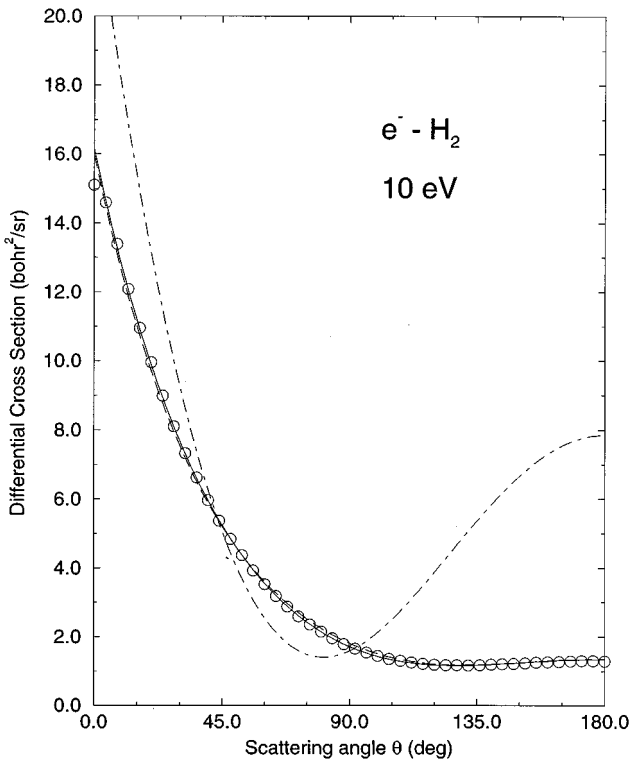

FIG. 3. DCS for e-H_2 scattering at 10.0 eV. Symbols and lines as in Fig. 2.

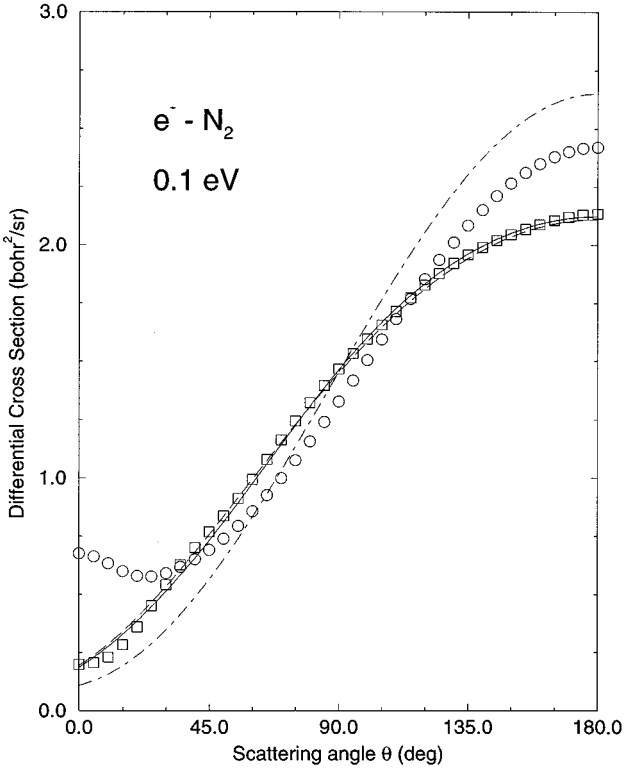

FIG. 4. DCS for e-N_2 scattering at 0.1 eV, calculated by the truncated sum (18) with $\Lambda_{max}=1$ (open circles) and $\Lambda_{max}=7$ (open squares), and by analytic Born completion (14) with $l_{max}=0$ (dot-dash line), $l_{max}=1$ (dashed line), and $l_{max}=2$ (solid line).

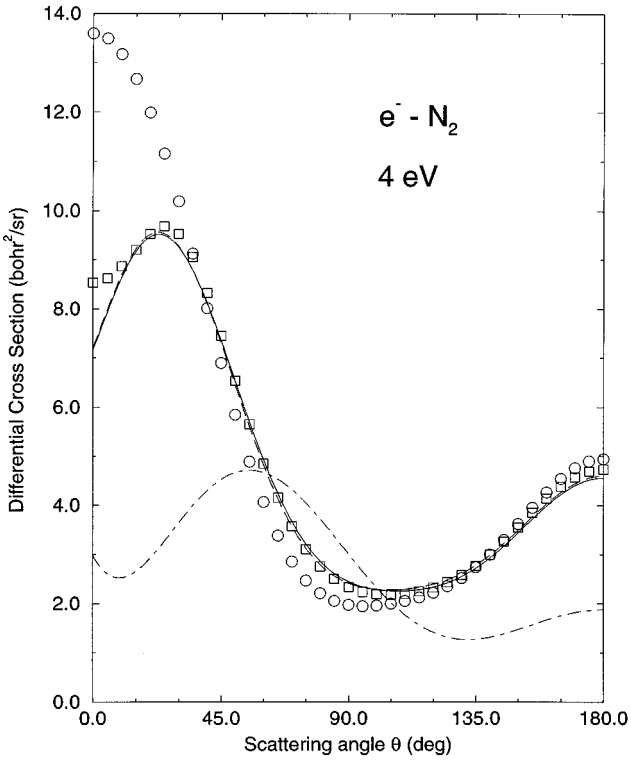

FIG. 5. DCS for e-N_2 scattering at 4.0 eV, calculated by the truncated sum (18) with $\Lambda_{max}=1$ (open circles) and $\Lambda_{max}=7$ (open squares), and by analytic Born completion (14) with $l_{max}=1$ (dot-dash line), $l_{max}=2$ (dashed line), and $l_{max}=3$ (solid line).

We have used T matrices with $|\Lambda|=0,1,2$ from the BFVCC calculations of Sun *et al.* [2], in which exchange effects were approximated by a tuned free-electron-gas model and correlation-polarization effects by the extension to e-N_2 of the parameter-free model used by Trail and Morrison [28] for e-H_2 scattering. In the truncated DCS calculations, T-matrix elements from symmetries with $\Lambda \geqslant 3$ required for convergence of the DCS (18) were calculated in the FBA [4].

As shown in Fig. 4, the DCS's at 0.1 eV calculated from the truncated expression with $\Lambda_{max}=1$ are not converged. To converge Eq. (18) requires $\Lambda_{max}=7$. At this low energy much of the scattering is due to the long-range potential (7), so these higher-order partial waves and symmetries are important to the DCS's. By contrast, with the analytic Born completion we obtain convergence by $l_{max}=2$. That is, we must include only BFVCC T-matrix elements $T^{\Lambda}_{ll_0}$ with both partial-wave labels l and l_0 less than or equal to 2; analytic Born completion correctly includes all higher-order contributions.

One point of theoretical interest is that the truncated sum (18) cannot produce the proper behavior of the DCS at $\theta=0°$. In general, the slope of the DCS at zero degrees is nonzero [31]. But because Eq. (18) is the sum of a finite number of Legendre polynomials this truncated sum always produces a DCS whose slope at zero degrees is zero. This distinction explains the remaining discrepancy between the analytic Born completed DCS's and the truncated DCS's at small angles in Fig. 4.

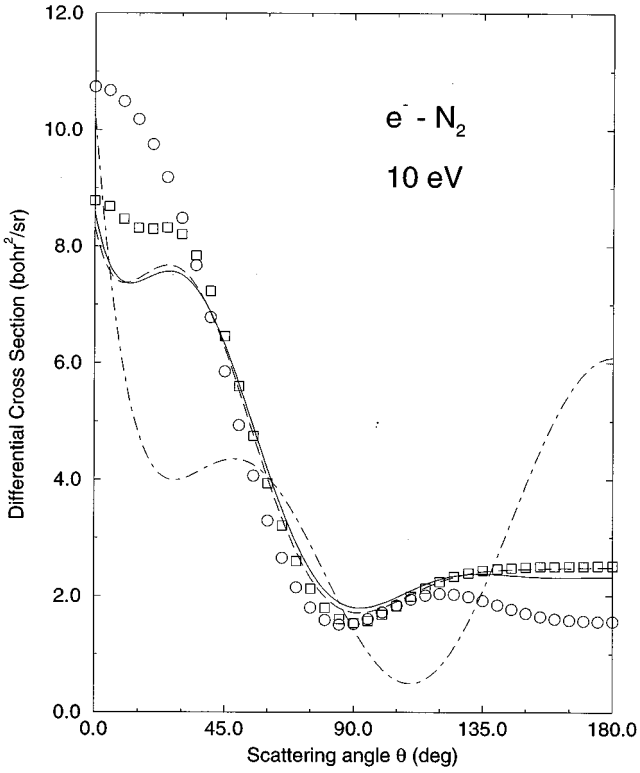

FIG. 6. DCS for e-N_2 scattering at 10.0 eV. Symbols and lines as in Fig. 5.

The shape of the elastic DCS's at energies above the 2.4 eV resonance differs strikingly from that of low-energy DCS's such as the one in Fig. 4. Measurements by Buckman and collaborators [2] show a characteristic structural feature at $\theta \leqslant 30°$ that persists from 4 to 10 eV. Because small-angle e-N_2 DCS's at these energies vary rapidly with angle and involve contributions from a large number of partial waves, they offer a stringent test of analytic Born completion.

This feature is evident in the elastic DCS at 4.0 eV in Fig. 5. The convergence behavior of this DCS is similar that of the 0.1 eV case. Even with $\Lambda_{max}=7$, the truncated sum DCS is not converged at small angles ($\theta \leqslant 20°$); the analytic Born completion expression, however, converges by $l_{max}=2$. This behavior indicates that scattering by the long-range potential makes a significant contribution to the DCS at all angles and is especially important at small angles.

The small-angle feature in the 4 eV DCS persists at energies up to 10 eV, though as illustrated in Fig. 6 it changes character somewhat. The truncated sum (18) is poorly converged for $\theta \leqslant 45°$ even by $\Lambda_{max}=7$. Convergence of the analytic Born completed DCS, however, is both rapid and smooth, requiring only $l_{max}=3$ in Eq. (14). This figure also vividly illustrates that a DCS calculated from the truncated sum, no matter how large a value of Λ_{max} is used, will not have a nonzero slope at zero degrees, while the analytic Born completed DCS, which includes all partial waves, behaves properly in this limit.

The convergence behavior of these e-N_2 DCS's demonstrates the computational advantages of the analytic Born completion equation (14). Using this equation with $l_{max}=2$ requires only nine BFVCC T-matrix elements; the truncated expression (18) with $\Lambda_{max}=7$ requires several hundred T-matrix elements. Although the completion procedure incurs a small overhead in calculating the correction terms, it is uniformly faster than converging the truncated sum. Most importantly, the analytic Born completion shows clear convergence at all angles.

IV. CONCLUSIONS

We have presented an analytic correction to the widely used truncated sums expression for calculating the elastic DCS from BF FNO T-matrix elements. For scattering from a linear nonpolar target, this term efficiently includes contributions from all high-order partial waves. This method, which is implemented in Eqs. (14)–(17), is much more efficient than converging the truncated sum expression (18) for the DCS. The sums in (14) involve only one parameter l_{max}, so determining convergence is straightforward. Moreover, this method ensures the correct behavior of the slope of the DCS as θ approaches 0°.

The importance of correctly evaluating small-angle DCS's is emphasized by recent e-N_2 DCS measurements of Buckman and collaborators [2]. These authors have reported similar distinctive small-angle features in DCS's for electron scattering from NO [32], O_2 [33], and CO [34]. The present analysis of e-N_2 DCS's, along with the theoretical results of Sun *et al.* [2], show the central role of the long-range potential in determining such structures. The similarity of the most important permanent and induced moments for other systems where this small-angle structure appears further suggests that it may be a generic feature arising from long-range scattering.

The extension of this method to vibrational excitation was noted in Sec. II. Its general extension to other molecules should also be straightforward. One could include the effects of higher-multipole terms in the long-range potential by a procedure analogous to that of Sec. II. The case of a permanent-dipole term, which causes the BF FNO DCS to diverge in the forward direction, can be treated with procedures developed by Norcross and Padial [3].

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