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Discrete momentum representation method for polar molecules: Calculation of the elastic electron scattering on the H_2O molecule

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We present an extension of the method of discrete momentum representation to the calculation of elastic electron scattering from polar molecules. The essence of this method is the subtraction of the first Born term from the Lippmann-Schwinger equation, which is solved for a modified interaction potential from which the long-range part is removed. Forward scattering is described in the first Born approximation. The use of this method is demonstrated for electron scattering from the H_2O molecule in the static-exchange approximation. The results are in good agreement with former calculations as well as with experiments.

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I. INTRODUCTION

The method of discrete momentum representation (DMR) was originally developed by Polášek *et al.* [1] for calculating the differential and integral cross sections of the nonresonant elastic electron-molecule scattering. It belongs to the group of methods based on the solution of the Lippmann-Schwinger equation in momentum space. A similar, but numerically different approach was used by McCarthy and Stelbovics [2] and Bray and Stelbovics [3] for atoms and by McCarthy and Rossi [4,5] for diatomic molecules. In Ref. [1], as well as in this paper, larger molecules are treated. The Hartree-Fock wave function was used for the molecule, and the scattered electron wave function was composed of plane waves, which are the natural basis of scattering processes. The static-exchange approximation was employed to evaluate the **T** matrix. Although this method is quite simple, it provided good results for the elastic electron scattering on hydrogen and methane molecules. However, the straightforward extension of this theory to polar targets is not possible because the dipole potential influences the incoming electron even at a long distance from the target. This long-range potential causes infinite values for the diagonal matrix elements of the Coulomb terms, i.e., those corresponding to the zero-momentum-transfer vector, making any further treatment of the interaction potential matrix impossible. Moreover, the problem with the dipole moment complicates not only the calculation of the elastic scattering of polar molecules, but also the calculation of inelastic scattering processes. Electronically excited states are often polar, even for molecules with a nonpolar ground state, and some vibrational modes give rise to polar molecular structures even when the target molecule has a zero dipole moment at its equilibrium geometry. This means that the original version of DMR cannot be applied to inelastic-scattering calculations.

Several papers describe methods for calculating elastic scattering by dipole potentials analytically [6,7]. Unfortunately, analytical methods cannot be employed in calculations of scattering on molecular potentials; their short-range parts are too complicated. Similarly, even the two-potential formalism (see, e.g., Joachain [8]), where the dipole scattering is solved analytically and the rest is calculated in the basis of dipole-scattering eigenfunctions, seems to be too complicated for our case. To avoid these problems, we have developed a simpler formalism, one that is easier to apply computationally. It is based on the fact that differential cross sections as well as scattering amplitudes tend to their first Born approximations in the limit of forward scattering. This limit was recognized by Mittleman and von Holdt [6] and later used by other authors in the development of Born closure methods [9–15]. In these methods, the partial-wave expansion is truncated at some certain quantum number, and the contribution of higher partial waves is expressed in terms of the first Born approximation. In the older studies [9–13], this approach was applied directly to the differential cross section, while in the more recent ones [14,15] it is the scattering amplitude that is expressed in this way. Similarly, in our method this approximation is also applied to the scattering amplitude, but in a different way. Since no partial-wave expansion is used in this method, the scattering amplitude for low angles can be directly replaced by its first Born counterpart, and we can concentrate on calculating large-angle scattering only. Since large-angle scattering is controlled by the short-range part of the interaction potential, we may use a truncated potential, one in which the long-range part is cut off by a rapidly decreasing function (e.g., by an exponential function with a negative exponent). Thus the truncation of the partial-wave expansion is replaced by the truncation of the interaction potential. Altogether, it means that we can calculate the scattering amplitude with the subtracted first Born term and the truncated potential, and then we can simply add back the first Born amplitude.

The theoretical background of the proposed method is given in Sec. II, and Sec. III describes computational details. Section IV continues with results for our calculations of the differential and momentum-transfer cross sections for H_2O,

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*Corresponding author. Email address: carsky@jh-inst.cas.cz followed by a comparison of these results with some other theoretical results and with experimental data.

II. THEORY

A. Overview of the DMR method

The DMR method is discussed in detail in Ref. [1] and only a brief summary is given here. An extension of the treatment to polar molecules is described below. As in Ref. [1], all the quantities in the following equations are in atomic units.

The basic equation of the scattering problem is the Lippmann-Schwinger (LS) equation:

$$|\Psi^{(+)}\rangle=|\mathbf{k}_0\rangle=\int d^3\mathbf{k}\,\frac{|\mathbf{k}\rangle\langle\mathbf{k}|}{k_0^2-k^2+i\varepsilon}\,U|\Psi^{(+)}\rangle. \tag{1}$$

In the DMR method, Eq. (1) is solved to obtain matrix elements of the T operator for all combinations of wave vectors of the incoming and outgoing waves with magnitude

$$k_0=\sqrt{2E}, \tag{2}$$

where E is the energy of the incident electron. To perform this, we transform the equation to the form

$$\langle\mathbf{k}'|T|\mathbf{k}_0\rangle=\langle\mathbf{k}'|U|\mathbf{k}_0\rangle+\int d^3\mathbf{k}\,\frac{\langle\mathbf{k}'|U|\mathbf{k}\rangle\langle\mathbf{k}|T|\mathbf{k}_0\rangle}{k_0^2-k^2+i\varepsilon}. \tag{3}$$

The integral on the right-hand side of Eq. (3) can be formally evaluated in the form of its principal value and a residue:

$$\begin{aligned}\int d^3\mathbf{k}\,&\frac{\langle\mathbf{k}'|U|\mathbf{k}\rangle\langle\mathbf{k}|T|\mathbf{k}_0\rangle}{k_0^2-k^2+i\varepsilon}\\ &=P\int_0^\infty dk\int_{\Omega_k}d\Omega_k\frac{k^2\langle\mathbf{k}'|U|\mathbf{k}\rangle\langle\mathbf{k}|T|\mathbf{k}_0\rangle}{k_0^2-k^2+i\varepsilon}\\ &\quad-\frac{i\pi k_0}{2}\int_{\Omega_k}d\Omega_k\langle\mathbf{k}'|U|\mathbf{k}_0\rangle\langle\mathbf{k}_0|T|\mathbf{k}_0\rangle.\end{aligned} \tag{4}$$

In this equation, Ω_k is a solid angle in $\mathbf{k}$ space. From Eq. (4) we can obtain the $\mathbf{T}$-matrix element for any pair of incoming and outgoing wave vectors from the continuous momentum space, but we must know all the corresponding U elements, defined as twice the interaction potential $V(U=2V)$ elements. The analytical solution of Eq. (4) is not accessible. Therefore we transformed it into matrix form, discretizing the integral by means of quadrature in both the radial and angular subspaces. The former is composed of the abscissas of Gauss-Legendre integration quadrature after transformation of the integration interval ($k_{\min}$,$k_{\max}$) onto the interval (-1, 1) ($k_{\min}$ is a number close to zero and $k_{\max}$ is a cutoff value; see Ref. [1]) by the following substitution

$$x=\frac{a(k-k_0)}{b(k+k_0)}, \tag{5}$$

where a and b are constants. The latter is a Lebedev integration quadrature [16] of a given order. Radial quadrature also contains the residue point, which corresponds to the energy of the incident electron.

This discretization provides the LS equation in the matrix form

$$\mathbf{T}=\mathbf{U}+\mathbf{U}\mathbf{G}_0^+\mathbf{T}, \tag{6}$$

where $\mathbf{G}_0^+$ is the matrix of the Green's function in the discrete-momentum representation. Because of a typographical error in Ref. [1], we repeat the definition of its elements in this paper:

$$(\mathbf{G}_0^+)_{qj,pi}=-\delta_{qp}\delta_{ji}i\pi w_i k_0/2 \quad \text{for} \quad p=0, \tag{7a}$$

$$(\mathbf{G}_0^+)_{qj,pi}=\delta_{qp}\delta_{ji}\frac{2abw_pw_ik_p^2k_0}{(a-bx_p)^2(k_0^2-k_p^2)} \quad \text{for} \quad p\neq 0. \tag{7b}$$

In these equations, $p=0$ when $k_p=k_0$, and x_p is defined by Eq. (5). Equation (6) can be easily solved for the $\mathbf{T}$ matrix

$$\mathbf{T}=(\mathbf{1}-\mathbf{U}\mathbf{G}_0^+)^{-1}\mathbf{U}. \tag{8}$$

Once the $\mathbf{T}$ matrix is known, we can calculate the scattering amplitude and differential cross section for those pairs of $\mathbf{k}$ vectors that are present in the angular quadrature,

$$A_{fi}=-\frac{1}{2\pi}\langle\mathbf{k}_f|T|\mathbf{k}_i\rangle, \tag{9}$$

$$\sigma_{fi}=\frac{|\mathbf{k}_f|}{|\mathbf{k}_i|}|A_{fi}|^2. \tag{10}$$

The determination of the scattering amplitudes for different pairs of vectors as well as the averaging over the molecular orientation is described in detail in Sec. II D.

Once the differential cross section is calculated, we can calculate the integral and momentum-transfer cross sections:

$$\sigma_{\text{inf}}=\int_\Omega\sigma(\Omega)d\Omega, \tag{11}$$

$$\sigma_{\text{mt}}=\int_\Omega\sigma(\Omega)[1-\cos(\theta)]d\Omega, \tag{12}$$

where θ is the scattering angle and Ω represents the integration angles.

B. Construction of the optical potential

The optical potential represents the interaction between the incident electron and the target molecule. Its construction allows us to describe the electron-molecule collision as a one-electron process. Its form for the DMR method [1] in the static-exchange approximation consists of the static part (in

Ref. [1], the factor $4\pi/K^2$ is also erroneously applied to the Coulombic term, but the computer code is free of this error)

$$\langle \mathbf{k}_1|V_S|\mathbf{k}_2\rangle = -\frac{4\pi}{K^2}\sum_A Z_A \exp(i\mathbf{K}\cdot\mathbf{R}_A) + \sum_{\alpha,\beta} P_{\alpha\beta}\left\langle \mathbf{k}_1\alpha\left|\frac{1}{r_{12}}\right|\mathbf{k}_2\beta\right\rangle, \tag{13}$$

and the exchange part

$$\langle \mathbf{k}_1|V_X|\mathbf{k}_2\rangle = -\frac{1}{2}\sum_{\alpha,\beta} P_{\alpha\beta}\left\langle \mathbf{k}_1\alpha\left|\frac{1}{r_{12}}\right|\beta\mathbf{k}_2\right\rangle. \tag{14}$$

Here α and β denote the basis-set functions, $P_{\alpha\beta}$ are the density-matrix elements, $\mathbf{K}=\mathbf{k}_2-\mathbf{k}_1$ is the momentum-transfer vector, Z_A is the nuclear charge of the nucleus A, and $\mathbf{R}_A$ is its position vector. Methods for calculating the Coulomb and exchange integrals that occur in Eqs. (13) and (14) are described in detail in [17].

C. Modification of DMR for polar targets

The problem of the dipole singularity originates from the static potential. As we showed in Ref. [1], by integration over $\mathbf{r}_1$, the matrix element can be expressed as

$$\langle \mathbf{k}_1|V_S|\mathbf{k}_2\rangle = \frac{4\pi}{K^2}\int e^{i\mathbf{K}\cdot\mathbf{r}}\rho(\mathbf{r})d\mathbf{r}, \tag{15}$$

where the total charge density (nuclear plus electronic) is defined as

$$\rho(\mathbf{r}) = -\sum_A Z_A\delta(\mathbf{r}-\mathbf{R}_A) + 2\sum_i |\varphi_i(\mathbf{r})|^2. \tag{16}$$

The symbol φ_i stands for all occupied spatial orbitals. Using the Taylor expansion for the exponential in Eq. (15) we obtain

$$\langle \mathbf{k}_1|V_S|\mathbf{k}_2\rangle = \frac{4\pi}{K^2}\int\left[1 + i\mathbf{K}\cdot\mathbf{r} - \frac{(\mathbf{K}\cdot\mathbf{r})^2}{2} - i\frac{(\mathbf{K}\cdot\mathbf{r})^3}{6} + \cdots\right]\rho(\mathbf{r})d^3\mathbf{r}. \tag{17}$$

The first term on the right-hand side of Eq. (17) represents integration over the total charge density, and it therefore vanishes for neutral molecules. The second term corresponds to the electron-permanent dipole interaction. It is obvious that this term tends to infinity in the forward direction, i.e., when $\mathbf{K}\rightarrow\mathbf{0}$. All other terms of the static part of the U element in Eq. (17) are finite. Therefore the dipole term is a leading term in the forward direction. As we mentioned above, this singularity is caused by the long-range part of the interaction potential and does not influence significantly scattering to larger angles. Moreover, the scattering amplitude tends to its first Born approximation in the forward direction (see, e.g., Ref. [6]). For these reasons, we introduce an approximate theory involving a modified potential from which the long-range part is removed.

Consequently, we propose a method for the solution of the LS equation in which the first Born term is subtracted. It is derived from Eq. (6) in the following simple way:

$$\mathbf{T} = \mathbf{U} + \mathbf{U}\mathbf{G}_0^+\mathbf{T},$$

$$\mathbf{T}-\mathbf{U} = \mathbf{U}\mathbf{G}_0^+\mathbf{T} = \mathbf{U}\mathbf{G}_0^+(\mathbf{T}-\mathbf{U}+\mathbf{U}) = \mathbf{U}\mathbf{G}_0^+\mathbf{U} + \mathbf{U}\mathbf{G}_0^+(\mathbf{T}-\mathbf{U}),$$

$$\mathbf{T}-\mathbf{U} = (\mathbf{1}-\mathbf{U}\mathbf{G}_0^+)^{-1}\mathbf{U}\mathbf{G}_0^+\mathbf{U}. \tag{18}$$

In general, we can derive a whole class of such equations, subtracting more than one Born term:

$$\mathbf{T}-\mathbf{B}_1-\cdots-\mathbf{B}_n = (\mathbf{1}-\mathbf{U}\mathbf{G}_0^+)^{-1}\mathbf{B}_{n+1}, \tag{19}$$

where $\mathbf{B}_n$ denotes the nth Born term. For our practical purpose, however, Eq. (18) is the most suitable. The potential of a polar molecule consists of the dipole part U_D and the short-range part. For the purpose of the solution of Eq. (18), we construct a modified dipole potential U_m of the form

$$U_m(\mathbf{r}) = U_D(\mathbf{r})e^{-cr} = 2\frac{\mathbf{D}\cdot\mathbf{r}}{r^3}e^{-cr}, \tag{20}$$

and use it instead of the dipole potential U_D ($\mathbf{D}$ is the dipole moment). The factor 2 arises from the difference between U and V potentials ($U=2V$). Whereas the U_D element of the unmodified dipole potential is

$$\langle \mathbf{k}_1|U_D|\mathbf{k}_2\rangle = \frac{8\pi i\mathbf{K}\cdot\mathbf{D}}{K^2}, \tag{21}$$

the element of U_m is

$$\langle \mathbf{k}_1|U_m|\mathbf{k}_2\rangle = \frac{8\pi i\mathbf{K}\cdot\mathbf{D}}{K^2}\left[1-\frac{c}{K}\arctan\left(\frac{K}{c}\right)\right]. \tag{22}$$

Obviously, this element is analytical over the whole momentum space, including the origin of the coordinate system, for which its limit as $\mathbf{K}\rightarrow\mathbf{0}$ is vanishing. Having obtained U_m, we substitute it for the dipole potential U_D, which may be identified with the second term on the right-hand side of Eq. (17). The U potential so prepared is then used for the ''subtracted'' LS equation (18). Its solution may be viewed as integration of singular functions ignoring the singularity [18]. Although this method must be used with caution in some cases, it can provide reasonable results. Then, for the elements with nonzero $\mathbf{K}$, we evaluate the first Born term as it is done for nonpolar targets [1], and we add them to the solution of Eq. (18) to obtain the complete $\mathbf{T}$ matrix.

This approach is similar to the method of Rescigno *et al.* [14] and Gianturco and Scialla [19]. They also divided the scattering amplitude into the first Born term and the rest. The latter part is expressed in the form of a truncated partial-wave expansion in which the short-range potential plays the dominant role. This part is especially important in the larger-angle directions. The long-range part, on the other hand, is described by the first Born term and is dominant in the low-angle directions. We do not truncate the partial-wave series, but the potential itself.

Next, we comment on the form of the U_m potential. The smaller the constant c, the more accurate the result we can obtain because the modified potential U_m approximates better the dipole potential. However, our grid consists of a finite number of $\mathbf{k}$ vectors. Hence for a sufficiently small value of the constant c, the U_m elements are practically indistinguishable from the U_D elements for all pairs of $\mathbf{k}$ vectors present in our grid that have a nonzero difference. Differences between U_m and U_D elements occur only for $\mathbf{K}$ vectors too small to be resolved by our grid vectors. Therefore we use U_D elements instead of U_m elements for all pairs of grid vectors with $\mathbf{K}$ different from zero, and for $\mathbf{K}=\mathbf{0}$ we set the element to zero. Potential elements evaluated in this way correspond to elements of the U_m potential with an extremely small c. (It should be mentioned that the function e^{-cr} is not the only possibility for the cutoff function. Many functions that decrease rapidly at large distances and are equal to 1 at the origin might be used. The present choice was done mainly for mathematical convenience.)

When the conclusions of the preceding paragraph are applied, the computational procedure can be simplified considerably. The U_S elements are evaluated by means of Eq. (17) for all pairs of $\mathbf{k}$ vectors with $\mathbf{K}\neq\mathbf{0}$, just as they are done for nonpolar targets. Thus the second (dipole) term in Eq. (17) is kept without change. For $\mathbf{K}=\mathbf{0}$, however, only the third (quadrupole) term in Eq. (17) is kept, since the dipole term is omitted (as explained in the preceding paragraph) and the other terms are equal to zero. Thus the singularity in the forward scattering is eliminated by this construction of the potential elements. Equation (18) can be rearranged back to the form of Eq. (8), as it is no longer necessary to subtract the singular part of the potential elements. Physically meaningful scattering amplitudes are obtained for nonzero scattering angles. The results for the water molecule were obtained in this way.

D. Averaging over the molecular orientation

A basic method of molecular-orientation averaging was described in [1]. In this technique, many pairs of $\mathbf{k}$ vectors are constructed for every scattering angle, distributing their endpoints on a circle of a given radius around each quadrature point. Although this method provides reliable results, its disadvantage is that it requires a large computational effort and therefore enormous demands on computer time. To cope with this problem we suggest an alternative method based on the same principle but using the calculated matrix elements more efficiently.

In this alternative method, a set of randomly oriented vectors of magnitude $|\mathbf{k}_0|$ is generated using a random-number generator. New T elements are calculated for every pair of the vectors using the following equations:

$$T_{i,n}=\sum_j \,[(\mathbf{1}-\mathbf{U}\mathbf{G}_0^+)^{-1}]_{i,j}U_{j,n}\,, \tag{23}$$

$$T_{m,n}=U_{m,n}+\sum_j \,U_{mj}(G_0^+)_jT_{j,n}\,. \tag{24}$$

In these equations, the indices i,j correspond to the original quadrature vectors, while m,n denote the newly generated random vectors. Hence we need to evaluate the rectangle matrix $\mathbf{U}_{j,n}$ (and its complex conjugate $\mathbf{U}_{m,j}$) and the square matrix $\mathbf{U}_{m,n}$. After the evaluation of the additional T elements, all the pairs of the new vectors are sorted according to the angle between them into the intervals of a given length, e.g., 1°. Scattering amplitudes and corresponding differential cross sections are determined for these pairs and averaged within every interval. The averaged value is then considered as the value of the differential cross section at the middle point of the given interval.

Thus the values of the differential cross sections are obtained for many points over the interval [0°, 180°]. The more random vectors we generate, the smoother is the curve formed by the calculated points. Its smoothness can be further improved by expanding the individual averaging intervals, since more vectors are averaged in each interval. However, when the differential cross section changes rapidly over a short range of angles, structure can be lost in the averaging procedure if the intervals are too long. Although it is possible in principle to use a large number of random vectors and so produce very smooth curves, this technique would be very costly. Therefore it is more efficient to use only some of the vectors, e.g., one in ten, and to construct the curve by fitting with cubic splines.

Another problem with this method arises from the fact that the number of pairs of random vectors in every interval is proportional to the sine of the angle corresponding to the interval (e.g., its middle point). Due to this proportionality, the highest number of pairs occurs in the intervals around 90°, while in the intervals around 0° and 180° the number of pairs is markedly smaller. Therefore in these sparse areas the cross section must be extrapolated from the adjoining intervals. Nevertheless, when calculating polar molecules there are no problems with the region close to 0°, because here the cross section diverges, and we do not calculate values in this region at all. A different and more efficient averaging method based on the decomposition of the T element in the basis of spherical harmonic functions is presently being developed in our group.

III. COMPUTATIONAL DETAILS

All calculations for the water molecule were performed in its optimized geometry at the Hartree-Fock level using Sadlej's TZV basis set [20]. The value of the dipole moment for the SCF-optimized geometry in this basis set is 0.8060 a.u., which is slightly overestimated in comparison with the experimental value of 0.724 a.u. [21]. The basis set and the obtained molecular-orbital density matrix were transferred into the DMR program to compute Coulomb and exchange integrals by means of Eqs. (13) and (14). The numerical quadrature used for the integration of the Lippmann-Schwinger equation consisted of a radial part formed by a Gauss-Legendre quadrature transformed to the integration

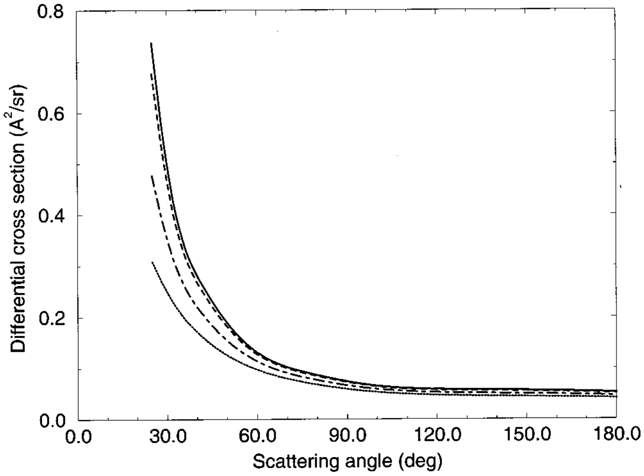

FIG. 1. Differential cross sections for the pure dipole potential (1 a.u.) for different values of the constant c. Dotted line, $c=0.1$; dot-dashed line, $c=0.05$; dashed line, $c=0.01$; solid line, $c=0$.

interval (see Sec. II A) and an angular part consisting of the points of Lebedev quadrature [16]. Radial quadratures with 19, 21, and 23 points and angular quadratures with 50, 86, and 110 points were used in individual calculations to demonstrate the convergence in both dimensions. In the averaging procedure, 1000 random vectors were generated and the averaging-interval length was set to 1°.

IV. RESULTS AND DISCUSSION

As the results of our method depend on the constant c [see Eqs. (20) and (22)], we first tested the convergence of the cross section with respect to this constant. For this purpose, the elastic electron scattering on the dipole potential (dipole moment of 1 a.u.) was calculated. The differential cross sections for several values of c are presented in Fig. 1. The values apparently converge to the limiting value $c=0$, as was explained in Sec. II C. Hence in practice it is not necessary to restrict the long-range potential by the exponential function since it is done automatically by the discrete integration grid in the **k** space.

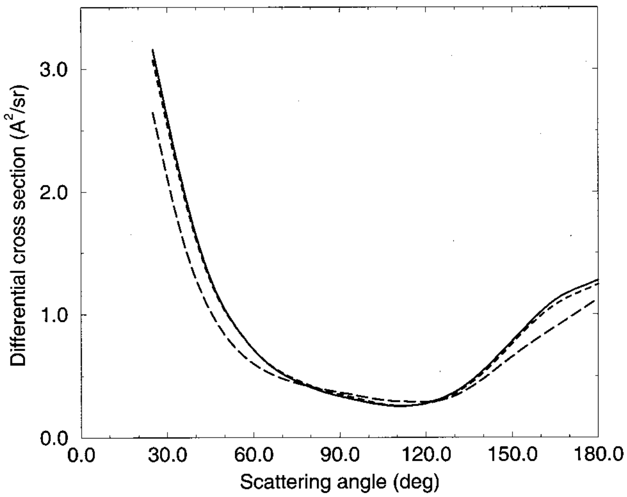

FIG. 3. Differential cross sections of the elastic electron scattering on H_2O for 20 eV (convergence with respect to the angular quadrature, the number of radial points in all calculations is 23). Long-dashed line, 50 angular points; dashed line, 86 angular points; solid line, 110 angular points.

Making use of this fact, we developed a remarkably simple method of using the modified dipole potential. For each pair of **k** vectors with $\mathbf{K}\neq\mathbf{0}$ the value of the unmodified interaction potential is used, and for $\mathbf{K}=\mathbf{0}$ its dipole part in Eq. (17) is set to zero. We used this method to calculate differential and momentum-transfer cross sections of elastic electron scattering from the H_2O molecule in the static-

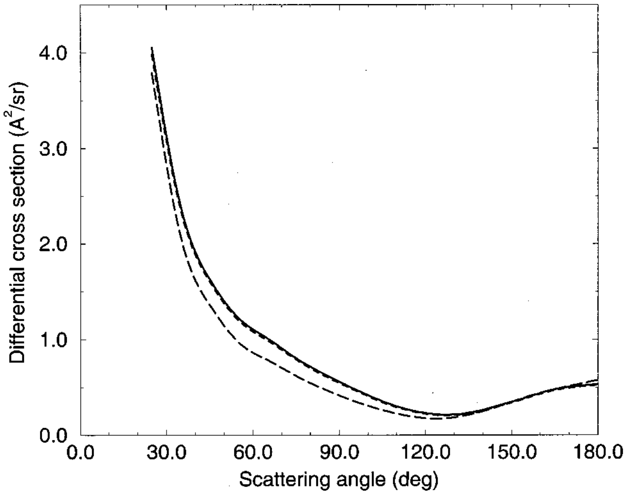

FIG. 2. Differential cross sections of the elastic electron scattering on H_2O for 6 eV (convergence with respect to the angular quadrature, the number of radial points in all calculations is 23). Long-dashed line, 50 angular points; dashed line, 86 angular points; solid line, 110 angular points.

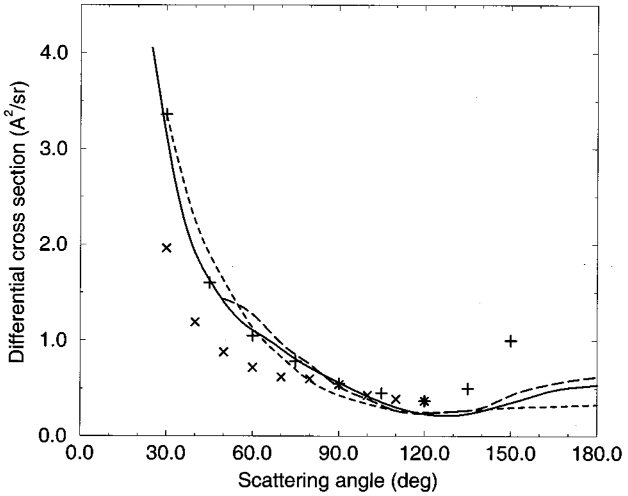

FIG. 4. Differential cross sections of the elastic electron scattering on H_2O for 6 eV. Solid line, present results; long-dashed line, calculations by Brescansin *et al.* [22]; dashed line, calculations by Gianturco and Scialla [19]; +, experiment by Shyn and Cho [23]; ×, experiment by Danjo and Nishimura [24].

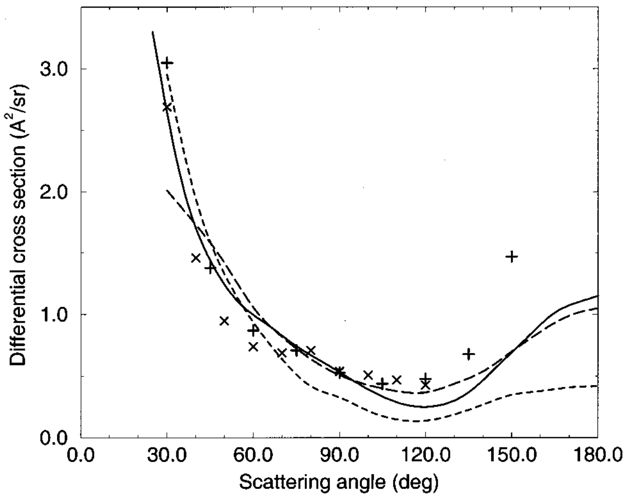

FIG. 5. Differential cross sections of the elastic electron scattering on H_2O for 10 eV. For the description of the individual curves see Fig. 4.

exchange approximation for incident electron energies from 2 to 20 eV. The convergence studies were performed for all combinations of three radial (19, 21, 23 points) and three angular Lebedev quadratures (50, 86, 110 points). The calculation is remarkably stable with respect to the change in the radial quadrature. The corresponding curves are, in fact, identical, and therefore not shown. The angular convergence is demonstrated in Figs. 2 and 3 for 6 and 20 eV, respectively. The angular quadrature with 50 points is apparently insufficient, but the two higher ones provide good convergence. Identical convergence tests were also performed for energies of 10 and 15 eV with analogous results (not shown). Differential cross sections for 6, 10, 15, and 20 eV are shown in Figs. 4–7 together with the results of Brescansin *et al.* [22] and Gianturco and Scialla [19], also performed in the static-exchange approximation, and with two sets of experimental values by Shyn and Cho [23] and Danjo and Nishimura [24]. These results are also tabulated in Table I. The agreement with previous theoretical results seems to be satisfactory. Our results are closer to those of Brescansin *et al.* [22], which may be explained by the rather different approach that was used in the calculations of Gianturco and Scialla [19]. The experimental data are also reproduced relatively well, although only the static-exchange approximation is used. Calculations for energies lower than 2 eV were not attempted since the use of the static-exchange approximation is not justifiable in this region.

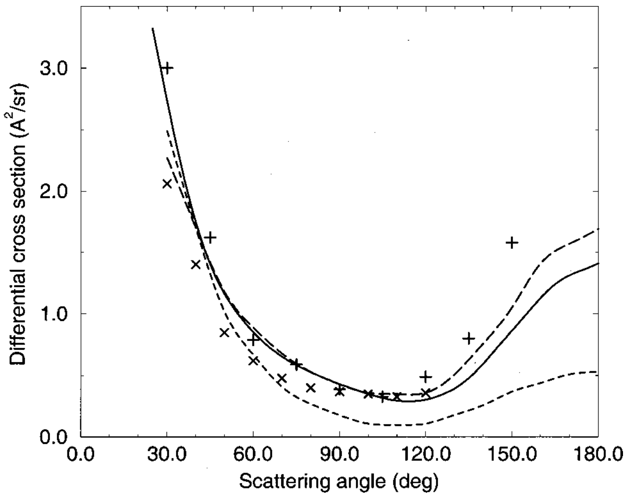

FIG. 6. Differential cross sections of the elastic electron scattering on H_2O for 15 eV. For the description of the individual curves see Fig. 4.

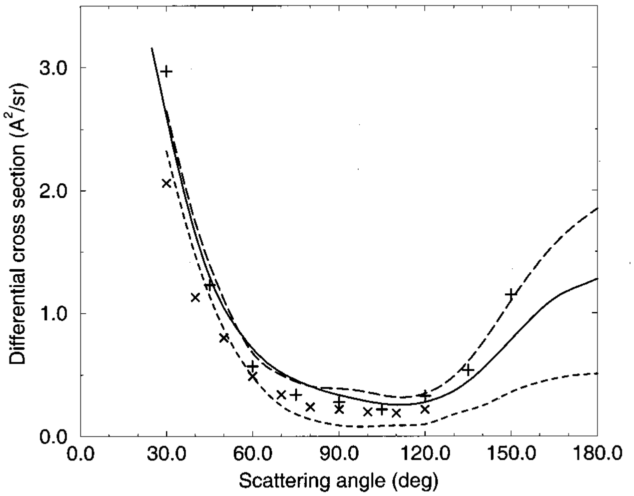

FIG. 7. Differential cross sections of the elastic electron scattering on H_2O for 20 eV. For the description of the individual curves see Fig. 4.

Momentum-transfer cross sections were calculated using Eq. (12). Only the values of differential cross sections from

TABLE I. Differential cross sections for elastic electron scattering on H_2O for electron energies of 6, 10, 15, and 20 eV.

Scattering angle (deg)	DCS (Å^2/sr)			
	6 eV	10 eV	15 eV	20 eV
25	4.05	3.30	3.32	3.16
30	3.14	2.64	2.73	2.61
40	1.91	1.70	1.75	1.65
50	1.40	1.24	1.16	1.04
60	1.11	1.00	0.85	0.72
70	0.91	0.83	0.65	0.52
80	0.72	0.67	0.53	0.41
90	0.56	0.53	0.43	0.34
100	0.42	0.40	0.35	0.29
110	0.30	0.29	0.30	0.26
120	0.23	0.25	0.31	0.28
130	0.22	0.30	0.40	0.37
140	0.27	0.47	0.60	0.55
150	0.35	0.69	0.86	0.78
160	0.44	0.92	1.13	1.02
170	0.51	1.07	1.31	1.18
180	0.54	1.15	1.41	1.28

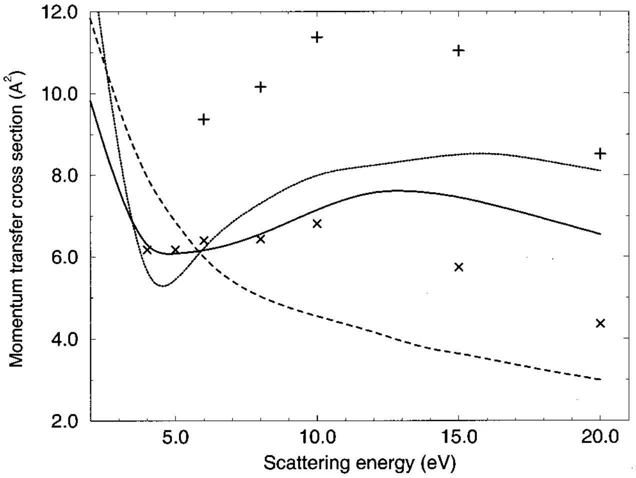

FIG. 8. Integral cross sections for the elastic electron scattering on H_2O. Solid line, present results; dotted line, calculation by Brescansin *et al.* [22]; dashed line, calculation by Gianturco and Scialla [19]; +, experiment by Shyn and Cho [23]; ×, experiment by Danjo and Nishimura [24].

25° to 180° are taken into account for two reasons. The data for lower angles are not reliable, and they contribute negligibly to the integral. The result is plotted in Fig. 8 together with other theoretical [19,22] and experimental [23,24] results, and it is tabulated in Table II. Our curve agrees better with the one from Ref. [22] than with that from Ref. [19] for the reasons discussed above. Both experimental results [23,24] show the maximum in the energy range of 10–15 eV. A more precise statement cannot be given because only a few experimental points are available in both studies (see Fig. 8). However, this feature is qualitatively reproduced by our calculation; the absolute values lie between the two experiments. We can conclude that both the calculations of differential and integral cross sections provide reliable results in the investigated energy region.

TABLE II. Integral cross sections for elastic electron scattering on H_2O.

Energy (eV)	ICS (Å^2)	Energy (eV)	ICS (Å^2)
2	9.82	12	7.57
3	7.68	13	7.61
4	6.30	14	7.56
5	6.08	15	7.45
6	6.16	16	7.30
7	6.32	17	7.12
8	6.56	18	6.93
9	6.85	19	6.74
10	7.15	20	6.55
11	7.40		

V. CONCLUSIONS

We have extended the original DMR method [1] to the calculation of elastic electron-molecule-scattering cross sections for polar targets. Although the method is remarkably simple, it provides good results for intermediate scattering energies, as was demonstrated by the example of the H_2O molecule. Moreover, this method is not excessively time consuming, so it may be applied to scattering calculations for larger molecules. An alternative algorithm for averaging the result over the molecular orientation was introduced, which is based on the same principle as the former one [1] but is more efficient. With the planned addition of polarization terms to the optical potential, the DMR method seems to have the potential to be very promising as a powerful tool in the field of scattering calculations.

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