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Vibrational excitation of molecules in electron scattering

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We derive the summed and averaged differential cross section for vibrational excitation of molecules in electron scattering in the framework of the algebraic-eikonal approach. The additional ingredient is that the T-matrix elements are derived in the mean-field approximation using intrinsic wave functions for the vibrational excitations.

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I. INTRODUCTION

In most electron-molecule scattering processes at intermediate energy (2–50 eV), the rotational final state of the molecule is not resolved, and in many cases the initial state of the molecule is distributed over many rotational states as well. In these cases it is only the cross section summed over final states and averaged over initial states that is of interest. By contrast, typically the vibrational states can be resolved. The job of theory is to calculate this rotationally summed and averaged cross section. This can be done by first calculating each individual rotational state cross section and then summing and averaging, but this is not just time consuming, it also is wasteful since it first introduces a great amount of detailed information, and then averages most of that detail away.

In this note we want to reemphasize [1, 2] that in order to calculate the summed and averaged differential cross section it is not necessary to first calculate the individual rotational transitions separately. This cross section can be calculated directly using intrinsic wave functions. No detailed knowledge about the various rotational states is needed. For vibrationally inelastic scattering, we use a generalized dipole operator and show that its effects are easily calculated using mean-field methods. These two steps—using only intrinsic states and exploiting the mean field—can be generalized to a wide class of problems where they give promise of great simplification.

In Sec. II we show how the intrinsic state formalism simplifies the calculation of the summed and averaged cross section. In Sec. III we introduce the vibron model and show how the eikonal T-matrix elements can be derived in the mean-field approximation. In Sec. IV we apply the formalism in a simple illustrative case. Section V presents some conclusions. Some technical details are presented in the Appendix.

II. DIFFERENTIAL CROSS SECTION

The intrinsic state formalism assumes that a molecule has an internal equilibrium state or shape. That state can be a real geometric shape as in the fixed dipole shape of a diatomic molecule, or it can be an "algebraic" state found in the mean-field approximation. The intrinsic state usually breaks the rotational invariance of the Hamiltonian. The individual rotational states can then be obtained by projecting the intrinsic states onto states of good angular momentum and parity.

The basic assumption made in medium energy electron-molecule scattering is that the electron goes by the molecule in a time short compared with the rotational time. This is equivalent to the assumption that the scattering is diagonal in the intrinsic state. Assuming that the rotational motion is independent of the vibrational state, the completeness of the rotational states allows the sums involved in the final-state summing and initial-state averaging to be done by closure. In this case the summed and averaged cross section is particularly simple. It is the cross section in a certain intrinsic state averaged over its orientation. For a diatomic molecule that orientation is specified by two angles, which we denote by Ω.

As a result one finds that the rotationally summed and averaged differential cross section for electron scattering from a diatomic molecule from vibrational state v to v' is given by [1, 2]

$$\frac{d\sigma(v \to v'|q)}{d\Omega} = \frac{1}{4\pi} \int d\Omega | < \mathbf{k}', v', \Omega \, |T| \, \mathbf{k}, v, \Omega > |^2 \; , \tag{1}$$

where $q = |\mathbf{k} - \mathbf{k}'|$ is the momentum transfer. This form is quite general. It depends only on the completeness of the rotational states, and on the assumption that an intrinsic state formalism exists in which vibrational excitation does not change the orientation Ω.

It is particularly simple to calculate the T-matrix element in the eikonal approximation. The eikonal approximation is a short-wavelength approximation and thus it shares the same domain of validity as the approximation that makes the T-matrix element diagonal in Ω. The T-matrix element for vibrational transitions $v \to v'$ in the eikonal approximation is given by

$$
\begin{aligned}
T_{v'v}(\mathbf{q},\Omega) &= < \mathbf{k}', v', \Omega | T | \mathbf{k}, v, \Omega > \\
&= \frac{k}{2\pi i} \int d^2b \; e^{i\mathbf{q}\cdot\mathbf{b}} < v', \Omega | e^{ig(b)\hat{\mathbf{b}}\cdot\hat{\mathbf{T}}} - 1 | v, \Omega > ,
\end{aligned}
\tag{2}
$$

where we have taken a dipole coupling between the incoming electron and the molecule

$$
V(\mathbf{r}) = -\frac{e}{r^2 + R_0^2} \hat{\mathbf{r}} \cdot \hat{\mathbf{T}} \; . \tag{3}
$$

Here $\hat{\mathbf{T}}$ is the dipole operator in the molecular space, and R_0 a parameter introduced to crudely model the short-range electron-molecule interaction that cuts off the dipole interaction at short distance. The eikonal profile function is then

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

To calculate the matrix elements of the dipole operator between intrinsic molecular states it is convenient, but not essential, to use an algebraic description of the rotational and vibrational excitations of the molecule in terms of the vibron model [3]. The combination of the eikonal approximation for the scattering and the vibron model for the molecular dynamics is usually referred to as the algebraic-eikonal approach. In the next section we discuss the derivation of the T-matrix elements in the vibron model.

III. VIBRON MODEL

The vibron model [3] describes the molecular states of a diatomic molecule in terms of a dipole boson $p_\mu^\dagger$ ($\mu = 1, 0, -1$) and a scalar boson $s^\dagger$. The total number of vibrons N is conserved by interactions in the model. The vibrational wave functions in the intrinsic frame can be parametrized in terms of three geometric variables, a coordinate β, and two Euler angles $\Omega = (\phi, \theta, 0)$ [4],

$$
|N, v, \beta, \Omega >= R(\Omega) |N, v, \beta > , \tag{5}
$$

with

$$
\begin{aligned}
|N, v, \beta >= & \frac{1}{\sqrt{v!(N-v)!}} \left(-\beta s^\dagger + \sqrt{1-\beta^2}\, p_0^\dagger \right)^v \\
& \times \left(\sqrt{1-\beta^2}\, s^\dagger + \beta p_0^\dagger \right)^{N-v} |0> ,
\end{aligned}
\tag{6}
$$

where $R(\Omega)$ is a rotation given by

$$
R(\Omega) = e^{-i\phi L_z} e^{-i\theta L_y} \; . \tag{7}
$$

The value of β can be determined by minimizing the expectation value of the Hamiltonian in the ground state $|N, v = 0, \beta >$, or equivalently, by solving the Hamiltonian in the Hartree approximation. The intrinsic ground state is easily seen to be a condensate of a dynamically appropriate linear combination (depending on β) of $s^\dagger$ and $p_0^\dagger$ bosons, while vibrational excitations are created by promoting v bosons from the condensate to the orthogonal combination.

In our previous work [2] we used a simple form for the dipole operator in the molecular space

$$
\hat{D}_\mu = (p^\dagger s - s^\dagger \tilde{p})^{(1)}_\mu , \tag{8}
$$

where $\tilde{p}_\mu = (-1)^{1-\mu} p_\mu$. Since this operator is a generator of U(4), the matrix elements of the exponentiated dipole operator between molecular states can be interpreted as representation matrix elements of the symmetry group. With the exception of the rotation group for which the representation matrix elements are the familiar Wigner $\mathcal{D}$ functions, the use of representation matrix elements of other groups is not very common in physics applications. There is therefore much interest in the group theoretical technology required to calculate them. In Ref. [5] we showed how to derive them for the U(3) and SO(4) limits of the vibron model.

The $\hat{D}$ form of the dipole operator gives a good account of dipole transitions within a rotational band, but a study of infrared intensities in hydrogen halide molecules [6] showed that the dipole operator

$$
\hat{T}_\mu = d_0 \hat{D}_\mu + \tfrac{1}{2} d_1 \left(e^{\lambda \hat{n}_p} \hat{D}_\mu + \hat{D}_\mu e^{\lambda \hat{n}_p} \right) , \tag{9}
$$

where $\hat{n}_p$ is the p-boson number operator, provides a much better description of the available data for vibrationally inelastic transitions. The same operator $\hat{T}_\mu$ was used to describe vibrational excitation in electron scattering [7].

The calculation of the matrix elements of the eikonal operator with this more complicated form for $\hat{T}$ is a formidable challenge, since the dipole operator is no longer linear in the generators of the symmetry group. There is one feature of the algebraic description of molecules that can simplify the calculation greatly. For most molecules the number of bosons N is large. This means that one can calculate matrix elements to a good approximation in mean-field by replacing the boson operators by their expectation values in the mean field. The corrections to this approximation are of order $1/N$. We illustrate this method in a study of electron-molecule scattering with vibrational excitation. The method is illustrated for vibrational excitation of diatomic molecules, but we would like to stress once again that it can easily be extended to more complicated molecules and to any other dynamical scheme.

In this note, however, we only want to introduce the method, and illustrate it with some simple examples. The extension to vibrational excitation of larger (triatomic and polyatomic) molecules and to treatments beyond the eikonal approximation will be the subject of a future publication.

A. Vibrationally elastic scattering

The matrix element appearing in the integrand of the expression for the T-matrix element, Eq. (2), can be evaluated simply in the mean-field approximation. For vibrationally elastic transitions it is given by

$$
\begin{aligned}
& < N, v = 0, \beta, \Omega | e^{ig(b)\hat{\mathbf{b}}\cdot\hat{\mathbf{T}}} - 1 | N, v = 0, \beta, \Omega > \\
& \qquad = < N, v = 0, \beta | \mathcal{R} e^{ig(b) T_z} \mathcal{R}^{-1} - 1 | N, v = 0, \beta > ,
\end{aligned}
\tag{10}
$$

where $\mathcal{R}$ is the product of the orientation rotation and a rotation, $(\hat{\mathbf{b}}) = (\phi_b, \pi/2, 0)$, of the transition operator to the z axis

$$\mathcal{R} = R^{-1}(\Omega)R(\hat{\mathbf{b}}) = e^{i\theta L_y} e^{i(\phi-\phi_b)L_z} e^{-i\frac{\pi}{2}L_y} \ . \tag{11}$$

The vibron operators appearing in the z component of the dipole operator are transformed into

$$\begin{aligned}
\mathcal{R}s^\dagger\mathcal{R}^{-1} &= s^\dagger \ , \\
\mathcal{R}p_x^\dagger\mathcal{R}^{-1} &= (\sin\theta)p_x^\dagger - (\cos\theta)p_z^\dagger \ , \\
\mathcal{R}p_y^\dagger\mathcal{R}^{-1} &= \cos(\phi_b - \phi)p_y^\dagger \\
&\quad - \sin(\phi_b - \phi)[(\cos\theta)p_x^\dagger + (\sin\theta)p_z^\dagger] \ , \\
\mathcal{R}p_z^\dagger\mathcal{R}^{-1} &= \sin(\phi_b - \phi)p_y^\dagger \\
&\quad + \cos(\phi_b - \phi)[(\cos\theta)p_x^\dagger + (\sin\theta)p_z^\dagger] \ .
\end{aligned} \tag{12}$$

We now evaluate the matrix element in the mean-field approximation, in which the boson operators are replaced by their expectation values in the condensate, namely

$$\begin{aligned}
s^\dagger &\rightarrow \sqrt{N(1-\beta^2)} \ , \\
p_x^\dagger &\rightarrow 0 \ , \\
p_y^\dagger &\rightarrow 0 \ , \\
p_z^\dagger &\rightarrow \sqrt{N\beta^2} \ .
\end{aligned} \tag{13}$$

As a result we find that the T-matrix element for vibrationally elastic scattering for $v = 0 \rightarrow v' = 0$ is given by

$$T_{00}(\mathbf{q},\Omega) = \frac{k}{2\pi i}\int d^2b \ e^{i\mathbf{q}\cdot\mathbf{b}} \times \left(e^{i\xi_0 g(b)\cos(\phi_b-\phi)\sin\theta} - 1\right) \ . \tag{14}$$

The coefficient ξ_0 is the intrinsic matrix element of the dipole operator of Eq. (9) in the mean-field approximation

$$\begin{aligned}
\xi_0 &= < N, v=0, \beta|\hat{T}|N, v=0, \beta > \\
&= 2N\beta\sqrt{1-\beta^2}\left(d_0 + d_1 e^{\lambda N\beta^2}\right) \ ,
\end{aligned} \tag{15}$$

and can be normalized to the static dipole moment of the molecule by $\xi_0 = d_{\rm expt}$. The angular part of the integral over the two-dimensional impact parameter, $\mathbf{b} = (b, \phi_b)$, can be evaluated analytically by expanding the exponentials in terms of Bessel functions. As a result the T-matrix element simplifies to a one-dimensional integral over the impact parameter

$$T_{00}(\mathbf{q},\Omega) = \frac{k}{i}\int_0^\infty b \ db\left[J_0(qb)\{J_0(\xi_0 g(b)\sin\theta) - 1\} + 2\sum_{n=1}^{\infty}(-1)^n J_n(qb)J_n(\xi_0 g(b)\sin\theta)\cos[n(\phi_q - \phi)]\right] \ . \tag{16}$$

The convergence of the integral over the impact parameter is very slow due to the dipole nature of the interaction potential. Numerically it is very efficient to first subtract the leading-order contribution from the integrand and then add back in again the correction integral. We show in detail how this is done in the Appendix.

B. Vibrationally inelastic scattering

Using the same mean-field arguments as above, the T matrix for vibrationally inelastic scattering for $v = 0 \rightarrow v' = 1$ is given by

$$\begin{aligned}
T_{10}(\mathbf{q},\Omega) = \frac{k}{2\pi i}\int d^2b \ e^{i\mathbf{q}\cdot\mathbf{b}} \ i\xi_1 g(b)\cos(\phi_b - \phi)\sin\theta \\
\times e^{i\xi_0 g(b)\cos(\phi_b-\phi)\sin\theta} \ ,
\end{aligned} \tag{17}$$

where ξ_1 denotes the intrinsic transition matrix element of the dipole operator

$$\begin{aligned}
\xi_1 &= < N, v=1, \beta|\hat{T}|N, v=0, \beta > \\
&= (1-2\beta^2)\sqrt{N}(d_0 + d_1 e^{\lambda N\beta^2}) \\
&\quad + 2\beta^2(1-\beta^2)N\sqrt{N} \ \lambda d_1 e^{\lambda N\beta^2} \ .
\end{aligned} \tag{18}$$

The first term in ξ_1 comes from the linear term in the transition operator and contributes only if the SO(4) dynamical symmetry is broken (for $\beta^2 \neq 0.5$), whereas the second term arises from the exponential part of the dipole operator. ξ_1 can be normalized to the dipole transition matrix element $\xi_1 = R_{01}$ [8], either taken from experiment or from *ab initio* calculations. In deriving this equation we have used the fact that all parameters (d_0, d_1, and λ) in the dipole operator scale with $1/N$.

Note that the elastic T-matrix element $T_{00} \sim 1$, whereas the inelastic one $T_{10} \sim 1/\sqrt{N}$. This indicates that in leading order in N there are only $\Delta v = 0$ transitions, in first order $\Delta v = 1$ transitions, etc.

Also in this case the angular part of the integral can be evaluated in closed form

$$\begin{aligned}
T_{10}(\mathbf{q},\Omega) = -\frac{k}{i}\int_0^\infty b \ db \ \xi_1 g(b)\sin\theta \\
\times \sum_{n=-\infty}^{\infty} J_n(\xi_0 g(b)\sin\theta)J_{1-n}(qb) \\
\times \cos[(1-n)(\phi_q - \phi)] \ .
\end{aligned} \tag{19}$$

The convergence of the integral in Eq. (19) can be improved using similar methods as for vibrationally elastic scattering. Details are given in the Appendix.

IV. APPLICATIONS

To apply these methods in a sample calculation we have to determine the parameters in this approach. Those in the vibron Hamiltonian and the total number of vibrons N can be determined by studying the rotational and vibrational excitations of the molecule [2]. Once the Hamiltonian is specified the value of β that characterizes the structure of the intrinsic states can be obtained by minimizing the energy surface. In the vibron model for diatomic molecules the equilibrium value of β can be obtained analytically for the most general one- and two-body Hamiltonian. In the notation of [2], the energy surface is written as

$$\begin{aligned} H_{\rm mol} &= A\hat{P}_4 + B\hat{L}\cdot\hat{L} + \epsilon\hat{n}_p + \delta\hat{n}_p^2 \ , \\ E(\beta) &= < N, v = 0, \beta | H_{\rm mol} | N, v = 0, \beta > \qquad (20) \\ &= x\,\beta^4 + y\,\beta^2 + z, \end{aligned}$$

with

$$\begin{aligned} x &= (A+\delta)N(N-1) \ , \\ y &= N[\epsilon + \delta + 2B - A(N-1)] \ , \qquad (21) \\ z &= AN(N-1)/4 \ . \end{aligned}$$

The energy surface has minima at $\beta = 0$ for $y > 0$, and at $\beta^2 = -y/2x$ for $y < 0$ and $x > 0$. In the exact SO(4) limit, one has $y = -x$ or $\beta^2 = 0.50$. An examination of typical vibron fits to diatomic molecules [2] yields values of β near the SO(4) limiting value (for example, $\beta^2 = 0.57$ for LiF and $\beta^2 = 0.54$ for KI).

The parameters in the dipole operator, d_0, d_1, and λ, can in principle be determined by studying the infrared transitions [6]. However, as we have seen in Eqs. (14) and (17) the vibrational excitations $v = 0 \to v' = 0, 1$ only depend on ξ_0 and ξ_1. These intrinsic matrix elements can either be calculated by inserting the appropriate values of the parameters in Eqs. (15) and (18), or be determined directly from the static dipole moment, $\xi_0 = d_{\rm expt}$, and the transition matrix element, $\xi_1 = R_{01}$.

As an illustration of the methods developed in the previous sections we apply our approach to electron scattering from LiF. The parameters in the vibron Hamiltonian are taken from [2]: $A = 7.929$ cm^{-1}, $B = 1.898$ cm^{-1}, $\epsilon = -127.268$ cm^{-1}, and $\delta = 0$ cm^{-1}. The number of vibrons is $N = 113$. The coefficients ξ appearing in Eqs. (14) and (17) are determined by the experimental dipole moment of LiF $\xi_0 = d_{\rm expt} = 6.58$ D and the dipole transition matrix element $\xi_1 = R_{01} = 0.2718$ D, which was obtained from an *ab initio* calculation [8]. Finally, the dipole cutoff radius we take is $R_0 = 0.5$ Å.

In Fig. 1 we show the summed and averaged differential cross section for vibrationally elastic excitation ($v = 0 \to v' = 0$) of LiF by 5.44-eV electrons. We compare the results obtained in the intrinsic mean-field approximation by integrating over the orientation of the molecule (solid line) with those obtained by explicitly summing and averaging the contributions from the individual rotational transitions (dashed line). The results of these two methods are identical to the accuracy of the plot. This agreement is no surprise, it is really a test of completeness. We present it here since so many molecular scattering calculations, even when they begin with the amplitudes in the intrinsic state, first project and then sum and average. We want to stress that is not necessary.

Even though we used different dipole operators in the two calculations, Eqs. (9) and (8), respectively, the final results are virtually identical, since in both cases the strength of the dipole operator is normalized as to reproduce the static dipole moment of LiF. Equation (14) shows explicitly that the vibrationally elastic scattering is determined completely by $\xi_0 = d_{\rm expt}$.

In Fig. 1 we also plot the cross section for excitation of the first vibrational excitation ($v = 0 \to v' = 1$). The linear term in the dipole operator $\hat{D}$ cannot induce vibrational excitations in the SO(4) limit. In previous work [2] we calculated inelastic excitation using $\hat{D}$, but introducing a symmetry-breaking term in the Hamiltonian. Using only the linear term we find cross sections

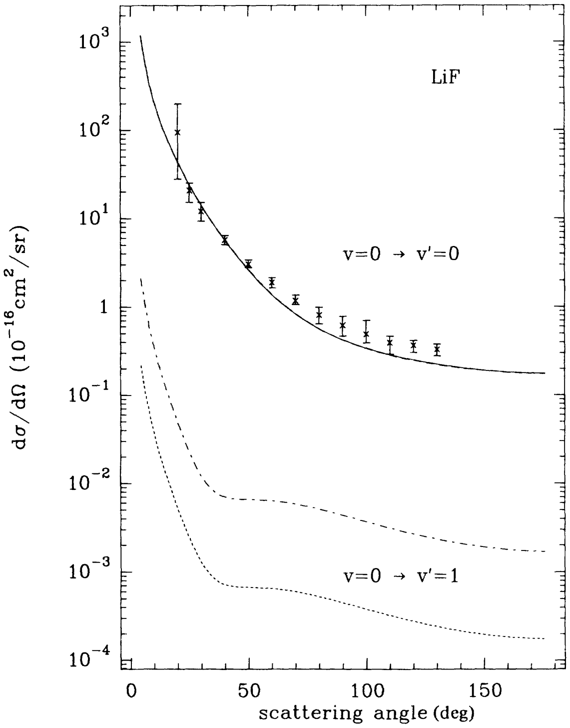

FIG. 1. Differential cross section in Å^2/sr for vibrationally elastic $v = 0 \to v' = 0$ and inelastic $v = 0 \to v' = 1$ excitation of LiF by 5.44-eV electrons. For elastic scattering the averaged mean-field calculation (solid line) and summed cross section from individual rotational transitions (dashed line) are virtually identical. For excitation of the first vibrational state, we show the cross section calculated with a simple dipole operator (dotted line) and with a generalized dipole operator (dashed-dotted line). The experimental data [9] are normalized to our results at 40°.

that are three orders of magnitude smaller than the elastic (dotted line). A study of infrared intensities showed [6] that for vibrationally inelastic transitions it is important to use the generalized dipole operator of Eq. (9). Figure 1 shows that the cross sections calculated with this operator (dashed-dotted line) are only two orders of magnitude smaller than the elastic one, just as we expect from $1/N$ counting. Similar results for inelastic scattering have been obtained by Mengoni and Shirai [7] and independently by Alhassid and Shao [8].

In contrast to the elastic case which only depends on the static dipole moment of the molecule, Eq. (17) shows that the vibrationally inelastic scattering ($v = 0 \rightarrow v' = 1$) is determined both by the static dipole moment $\xi_0 = d_{\mathrm{expt}}$ and a transition matrix element $\xi_1 = R_{01}$.

V. SUMMARY AND CONCLUSIONS

We reemphasized that in order to calculate the summed and averaged differential cross section, it is not necessary to first calculate the individual rotational transitions separately and then sum them. This cross section can be calculated directly using intrinsic wave functions. No detailed knowledge about the various rotational states is needed.

The method was applied to vibrational excitation of diatomic molecules using a dipole interaction only. It is straightforward to generalize this treatment to larger molecules and to include other multipole interactions, such as, for example, a quadrupole interaction.

For those more complex operators, even for a more complex form of the dipole operator, algebraic evaluation of matrix elements is difficult. However, semiclassical (large N) expansions are very appropriate for the cases considered here. They make it possible to evaluate the matrix element of any operator that is an arbitrary function of the algebraic operators. This greatly simplifies our eikonal treatment, but similar ideas can be applied in other more accurate dynamic schemes where they hold promise of great simplification. These include direct calculation of scattering in the intrinsic (body-fixed) frame for vibrational excitation of both diatomic and more complex molecules.

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APPENDIX

In Sec. III we showed that the eikonal T-matrix element can be expressed in terms of a one-dimensional integral over the impact parameter, see Eqs. (16) and (19). The convergence of the integral can be improved by using that for large values of the impact parameter ($b \geq b_0$) the eikonal phase approaches the point dipole form $\xi_0 g(b) \rightarrow 2\alpha/b$ with $\alpha = med_{\mathrm{expt}}/\hbar^2 k$. The Bessel functions appearing in the integrand can then be approximated by $J_n(\xi_0 g(b)\sin\theta) \rightarrow (\alpha\sin\theta/b)^n/n!$. As a result, for $b \leq b_0$ the integral can be calculated numerically using Eqs. (16) and (19), while for $b \geq b_0$ we rewrite the T-matrix element as

$$T_{v'v}(\mathbf{q},\Omega) = T^{(1)}_{v'v}(\mathbf{q},\Omega) + T^{(2)}_{v'v}(\mathbf{q},\Omega)\ . \tag{A1}$$

The first term has a rapidly converging integrand (as a function of the impact parameter), as we have subtracted the leading-order contribution from the integrand. The second term represents the remainder, which in case of a dipole interaction can be derived analytically.

For vibrationally elastic scattering ($v = 0 \rightarrow v' = 0$) the contribution to the eikonal T-matrix element for $b \geq b_0$ is given by

$$\begin{aligned} T^{(1)}_{00}(\mathbf{q},\Omega) = \frac{k}{i}\int_{b_0}^{\infty} b\,db\Bigg[& J_0(qb)\left\{J_0(\xi_0 g(b)\sin\theta) - 1\right\} \\ & + 2\sum_{n=1}^{\infty}(-1)^n J_n(qb)\left\{J_n(\xi_0 g(b)\sin\theta) - \frac{1}{n!}\left(\frac{\alpha\sin\theta}{b}\right)^n\right\}\cos[n(\phi_q-\phi)]\Bigg]\ , \end{aligned} \tag{A2}$$

and

$$T^{(2)}_{00}(\mathbf{q},\Omega) = \frac{k}{i}\sum_{n=1}^{\infty}(-1)^n\frac{2}{n!}(\alpha\sin\theta)^n\frac{J_{n-1}(qb_0)}{qb_0^{n-1}}\cos[n(\phi_q-\phi)]\ . \tag{A3}$$

Similarly, for the vibrationally inelastic scattering ($v = 0 \rightarrow v' = 1$) the integral is calculated numerically for $b \leq b_0$ using Eq. (18), while for $b \geq b_0$ we first subtract the leading-order contribution from the integrand and then add back a correction integral. As a result we have for $b \geq b_0$,

$$\begin{aligned} T^{(1)}_{10}(\mathbf{q},\Omega) = -\frac{k}{i}\int_{b_0}^{\infty} b\,db\,\xi_1\sum_{n=0}^{\infty}(-1)^n\Bigg[& J_n(qb)\cos[n(\phi_q-\phi)]J_{n+1}(\xi_0 g(b)\sin\theta)g(b)\sin\theta \\ & + J_{n+1}(qb)\cos[(n+1)(\phi_q-\phi)] \\ & \times\left\{J_n(\xi_0 g(b)\sin\theta)g(b)\sin\theta - \frac{2}{\xi_0 n!}\left(\frac{\alpha\sin\theta}{b}\right)^{n+1}\right\}\Bigg]\ , \end{aligned} \tag{A4}$$

and

$$T_{10}^{(2)}(\mathbf{q},\Omega) = -\frac{k}{i}\frac{2\xi_1}{\xi_0}\sum_{n=0}^{\infty}(-1)^n\frac{1}{n!}(\alpha\sin\theta)^{n+1}\frac{J_n(qb_0)}{qb_0^n}\cos[(n+1)(\phi_q-\phi)]\ . \tag{A5}$$

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