LETTER TO THE EDITOR

A first-order non-degenerate adiabatic theory for calculating near-threshold cross sections for rovibrational excitation of molecules by electron impact

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Abstract. An approximate expression is derived for the inelastic K-matrix elements for rotational excitation of molecules by electron impact. This expression incorporates a Born–Oppenheimer separation of the projectile and nuclear coordinates in the continuum wavefunction but allows for different energies in the entrance and exit channels. Hence it is particularly suited to near-threshold collisions. The method is applied to pure rotational excitation of H_2 by comparing approximate cross sections with those from laboratory frame close-coupling calculations.

The calculation of cross sections for near-threshold rotational and vibrational excitation of molecules by electrons is plagued by practical problems. Beyond the need to include in the electron–molecule interaction potential accurate terms representing non-local effects such as exchange and correlation, difficulties beset the implementation of the collision theory itself. These difficulties essentially stem from the question: how accurately must one account for the influences on the scattering function of the nuclear dynamics?

These influences are (in principle) treated exactly in rovibrational laboratory frame close-coupling (LFCC) theory (Arthurs and Dalgarno 1960, Henry 1970). The resulting computational scheme is, however, intractable for all but the simplest systems (see reviews by Lane (1980), Norcross and Collins (1982), and Morrison (1983)). For most molecules, a huge number of target states must be included in the target-state expansion even at low scattering energies, and extensive partial-wave coupling is induced by the highly non-spherical interaction potential.

These difficulties are alleviated by the adiabatic-nuclei (AN) approximation (Chase 1956, Hara 1969), which is predicated on the assumption of separability (in the Born–Oppenheimer sense) of the projectile and nuclear motion (Shugard and Hazi 1975). Since the AN scattering function depends only parametrically on the nuclear geometry, the effects of the nuclear Hamiltonian are absent from the scattering equations. The resulting computational and conceptual simplifications have made possible the study of low-energy rovibrational excitation for a large and diverse range of molecules (Rescigno *et al* 1982, Jain and Thompson 1983; see also Norcross and Collins (1982) and references therein).

In addition to the Born–Oppenheimer separation of the continuum function, the AN method entails a further assumption: neglect of the separation between the initial- and final-state energies of the target. This is the assumption of target-state degeneracy. At the very least, this assumption will be invalid near the threshold for a given excitation.

Breakdown of the AN approximation has been anticipated since its introduction to electron–molecule scattering (Chang and Temkin 1970), and recent research on electron–H_2 scattering has confirmed and quantified this expectation, showing that the AN approximation introduces errors of the order of 30% in cross sections for pure rotational excitation (Morrison *et al* 1984a), and of the order of hundreds of per cent in cross sections for pure vibrational and rovibrational excitation (Morrison *et al* 1984b).

These findings have lent urgency to the need for new scattering theories for near-threshold electron–molecule scattering—theories that preserve as many of the simplifying features of the AN method as possible without suffering its deficiencies near threshold.

Shugard and Hazi (1975) first proposed that one might achieve this goal by venturing off the energy–momentum shell (see chapter 18 of Taylor (1972)). They suggested retaining the Born–Oppenheimer separation of the AN method but calculating an off-shell transition matrix, thereby avoiding the assumption of target-state degeneracy in the entrance and exit channels. The particular method proposed by Shugard and Hazi has not, to date, been implemented; but several theories that go beyond the AN approximation have recently been introduced. These include the off-shell adiabatic theory of Varracchio and Lamanna (1984), which in lowest order leads to an integral equation for the off-shell T matrix; the multipole-extracted AN method of Norcross and Padial (1982), which is especially useful for scattering from polar molecules; the non-adiabatic theory of Domcke *et al* (1979), which has been extensively and successfully applied to resonant scattering (another energy regime where the assumptions of the AN approximation are prone to break down); the scaled AN rotation theory of Feldt and Morrison (1984), which applies only to rotational excitation; the energy-modified adiabatic (EMA) approximation of Nesbet (1977); and the vibrational frame-transformation theory of Greene and Jungen (1985).

In this paper we present the formalism and first implementation of a first-order non-degenerate adiabatic (FONDA) theory for rotational and vibrational excitation. The idea behind the FONDA method can be found in Chase's original paper on the AN approximation, in which he first derives an approximate inelastic scattering amplitude which is accurate to first order in the perturbing Hamiltonian, by making an adiabatic separation of variables, and then obtains the usual AN scattering amplitude, which is accurate to second order, by imposing the assumption of target-state degeneracy. The FONDA method is essentially an adaptation of Chase's first-order theory to the electron–molecule problem.

A primary goal in developing the FONDA method was that the resulting expressions be computationally convenient, easily extensible to complicated systems and calculable in terms of the radial scattering functions of body frame fixed-nuclei theory. In the past two decades a vast amount of effort has gone into the study of these functions, their relation to the 'physical' scattering function in the laboratory frame (Chang and Fano 1972) and their numerical calculation via a variety of numerical methods (see the review by Buckley *et al* (1984)). The FONDA laboratory frame K matrix is calculated from these radial functions and other familiar coupling transformation matrices. It can then be fed into standard computer programs that compute differential and integral inelastic cross sections. In the first part of this letter we sketch the derivation of the FONDA K matrix.

In the latter part we describe the application of this method to the comparatively simple and exhaustively studied problem of rotational excitation of H_2 in the rigid-rotator approximation (see Lane (1980) and Shimamura (1984)). In particular, we

compare FONDA cross sections for this process with those from comparable LFCC calculations.

We shall begin in the (space fixed) laboratory reference frame (LF), denoting the spatial coordinates of the projectile by primes (r'), and will make the rigid-rotator approximation, fixing the internuclear separation R at its equilibrium value, $R_e = 1.402\, a_0$ for H_2. Furthermore, we shall consider only electronically elastic scattering, within the ground (Born-Oppenheimer) electronic state of the target, $X\,{}^1\Sigma_g^+$ for H_2. After the electronic wavefunction for this state has been projected out of the time-independent Schrödinger equation of the system, there remains a 'reduced' equation for the scattering of an electron with initial momentum k_0 from a molecule in an initial rotational state $\nu_0 \equiv (j_0, m_{j_0})$, i.e.

$$(\hat{T}_e + \hat{V}_{int} + \hat{\mathcal{H}}^{(r)})\Psi_{k_0,\nu_0}(r', \hat{R}) = E\Psi_{k_0,\nu_0}(r', \hat{R}) \tag{1}$$

where $\hat{T}_e$ is the kinetic energy of the projectile, the nuclear Hamiltonian is just the rotational kinetic energy operator $\hat{\mathcal{H}}^{(r)}$, and $\hat{V}_{int}$ is the electron–molecule interaction potential averaged over the $X\,{}^1\Sigma_g^+$ wavefunction. In general, $\hat{V}_{int}$ includes static (non-local) exchange, and polarisation terms, the latter to compensate for our jettisoning of the closed electronic channels from the Hilbert space of the problem. (We have suppressed the dependence on R throughout.) In equation (1) E is the total energy:

$$E = \tfrac{1}{2}k_0^2 + \varepsilon_{j_0} = \tfrac{1}{2}k_j^2 + \varepsilon_j \tag{2}$$

where ε_j is the Born–Oppenheimer energy of the target in state ν. In terms of the rotational constant of the ground state, $B_{X\,{}^1\Sigma_g^+} = 60.80\ \mathrm{cm}^{-1}$ for H_2 (Herzberg 1950), this energy is simply

$$\varepsilon_j = B_{X\,{}^1\Sigma_g^+}\, j(j+1). \tag{3}$$

Equation (3) also defines the channel energies $\tfrac{1}{2}k_j^2$.

The wavefunction $\Psi_{k_0,\nu_0}(r', \hat{R})$ of (1) satisfies plane-wave boundary conditions with initial momentum k_0. It is convenient to introduce a function that identifies with the entrance channel a particular orbital angular momentum state of the projectile $|l_0, m_0\rangle$, where l_0 corresponds to the square of the orbital angular momentum operator l, and m_0 to its projection on the space fixed z axis $\hat{e}_{z'}$. This wavefunction is related to $\Psi_{k_0,\nu_0}(r', \hat{R})$ by the transformation matrix between plane-wave and angular momentum eigenfunctions†, i.e.

$$\Psi_{k_0,\nu_0}(r', \hat{R}) = \frac{1}{(2\pi)^{1/2}}\sum_{l_0 m_0}\frac{i^{l_0+1}}{k_0}Y_{l_0}^{m_0*}(\hat{k}_0')\Psi_{E,\nu_0,l_0,m_0}(r', \hat{R}). \tag{4}$$

Ultimately we shall couple the orbital and rotational angular momenta, l and j, to derive a scattering matrix in the coupled-angular-momentum representation. However, the derivation of the FONDA equations is considerably clearer in the uncoupled angular momentum (UCAM) representation of equation (4). In this representation asymptotic channels will be labelled by the index $\gamma \equiv (j, m_j, l, m)$.

We begin with the integral equation for the reactance matrix K in the UCAM representation. This matrix is derived (Taylor 1972) by transforming into integral form

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† The transformation matrix used in this equation corresponds to plane waves that obey Dirac delta function normalisation but to angular momentum free waves that are not energy normalised. See equation (8) and chapter 11 of Taylor (1972).

the coupled radial differential scattering equations that result from expanding first the wavefunction $\Psi_{E,\nu_0,l_0,m_0}(r', \hat{R})$ in target (rotational) states $|jm_j\rangle$:

$$\Psi_{E,\nu_0,l_0,m_0}(r', \hat{R}) = \sum_{j,m_j} \eta_{\nu,\nu_0}(r') Y_j^{m_j}(\hat{R}) \tag{5a}$$

and then the scattering functions $\eta_{\nu,\nu_0}(r')$ in partial waves $|lm\rangle$:

$$\eta_{\nu,\nu_0}(r') = \frac{1}{r} \sum_{l,m} u_{\gamma,\gamma_0}(r) Y_l^m(\hat{r}'). \tag{5b}$$

The LF UCAM radial functions $u_{\gamma,\gamma_0}(r)$ are coupled by the matrix elements

$$V_{\gamma,\gamma'}(r) = \langle jm_jlm| \hat{V}_{\text{int}}|j'm'_jl'm'\rangle \tag{6}$$

where the implied integration is over $d\hat{r}'$ and $d\hat{R}$. Thus our starting point is

$$K_{\gamma,\gamma_0} = -\frac{2}{(k_jk_0)^{1/2}} \sum_{\gamma'} \int_0^\infty \hat{j}_l(k_jr) V_{\gamma,\gamma'}(r) u_{\gamma',\gamma_0}(r)\, dr \tag{7}$$

where $\hat{j}_l(k_jr)$ is the Ricatti–Bessel function.

Formally, we want to approximate the system wavefunction $\Psi_{E,\nu_0,l_0,m_0}(r', \hat{R})$, in which the projectile and target coordinates are rigorously non-separable, by the product of an adiabatic electronic function $\beta_{l_0m_0}(r'; \hat{R})$, which depends on the internuclear orientation $\hat{R}$ only parametrically, and a target function for the initial rotational state $Y_{j_0}^{m_{j_0}}(\hat{R})$. To clarify how this replacement is implemented in equation (7) we first rewrite this equation in terms of the asymptotic free wavefunctions

$$\phi_{l,m}^{(s)}(r'; k_j) \equiv r^{-1}\hat{j}_l(k_jr) Y_l^m(\hat{r}') \tag{8}$$

and then evaluate the sums over l' and m' implied by $\Sigma_{\gamma'}$ in equation (7), obtaining

$$K_{\gamma,\gamma_0} = -\frac{2}{(k_jk_0)^{1/2}} \int dr' \int d\hat{R} Y_j^{m_j*}(\hat{R})\phi_{l,m}^{(s)*}(r'; k_j) \hat{V}_{\text{int}}(r', \hat{R})\left(\sum_{\nu'} \eta_{\nu',\nu_0}(r') Y_j^{m_j}(\hat{R})\right). \tag{9}$$

Now, the summation in brackets in (9) is, according to equation (5a), the system wavefunction $\Psi_{E,\nu_0,l_0,m_0}(r', \hat{R}_0)$; this sum explicitly exhibits the coupling of the nuclear dynamics to the motion of the projectile. So we replace this summation with the product of the laboratory frame, fixed-nuclei (LF-FN) scattering function $\beta_{l_0m_0}(r'; \hat{R})$ and the initial target-state wavefunction $Y_{j_0}^{m_{j_0}}(\hat{R})$, i.e.

$$\sum_{\nu'} \eta_{\nu',\nu_0}(r') Y_j^{m_{j'}}(\hat{R}) \to \beta_{l_0m_0}(r'; \hat{R}) Y_{j_0}^{m_{j_0}}(\hat{R}). \tag{10}$$

Making this substitution in the integral equation (7) and expanding $\beta_{l_0m_0}(r'; \hat{R})$ in partial waves, we obtain the UCAM K matrix in the FONDA approximation, i.e.

$$\mathcal{K}_{\gamma\gamma_0}^{(1)} = -\frac{2}{(k_jk_0)^{1/2}} \int d\hat{R}\, Y_j^{m_j*}(\hat{R})$$

$$\times \left(\sum_{l'm'} \int dr\, d\hat{r}'\, \hat{j}_l(k_jr) Y_l^{m*}(\hat{r}') \hat{V}_{\text{int}}(r', \hat{R})\tilde{u}_{l'm',l_0m_0}(r, k_0) Y_{l'}^{m'}(\hat{r}') Y_{j_0}^{m_{j_0}}(\hat{R})\right). \tag{11}$$

We have appended a label k_0 to the (adiabatic) LF-FN radial functions $\tilde{u}_{l'm',l_0m_0}(r, k_0)$ to emphasise that they are to be evaluated at the entrance channel energy $\frac{1}{2}k_0^2$. The superscript (1) on the K matrix (11) connotes that this expresion is valid to first order in $\hat{\mathcal{K}}^{(r)}$.

Were we to impose on $\mathcal{H}^{(1)}_{\gamma\gamma_0}$ the additional assumption that the entrance and exit channel energies are equal, setting $k_j = k_0$, equation (11) would reduce to the usual AN K matrix in the LF-UCAM representation (Lane 1980), which is accurate to second order in $\hat{\mathcal{H}}^{(r)}$ (Chase 1956). We shall not, however, do this.

Instead, we shall express the FONDA K matrix (11) in a form convenient for computation by transforming to the coupled angular momentum (CAM) representation and writing the resulting matrix in terms of FN radial scattering functions in the body frame. The body frame (BF), in which coordinates will be unprimed (r), is obtained from the LF by a rotation through Euler angles chosen to align the body polar axis $\hat{e}_z$ with the internuclear axis $\hat{R}$. In the body representation, with the nuclear geometry frozen, channels are labelled by the quantum numbers l and Λ, the latter corresponding to the projection $l \cdot \hat{R}$. (Because $\hat{\mathcal{H}}^{(r)}$ has been 'frozen out' of the BF scattering equations by the FN approximation in this derivation, these channels are not coupled in Λ.)

The BF-FN radial scattering equations are solutions of the coupled equations

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + k_b^2\right) w^\Lambda_{l,l_0}(r, k_b) = 2 \sum_{l'} V^\Lambda_{l,l'}(r) w^\Lambda_{l',l_0}(r, k_b). \tag{12}$$

The coupling matrix elements are

$$V^\Lambda_{l,l'}(r) = \langle l, \Lambda | \hat{V}_{int} | l', \Lambda \rangle = \sum_\lambda g_\lambda(ll'; \Lambda) v_\lambda(r) \tag{13}$$

where $v_\lambda(r)$ is the expansion coefficient of $\hat{V}_{int}$ in Legendre polynomials and the coupling coefficient $g_\lambda(ll'; \Lambda)$ is given by

$$g_\lambda(ll'; \Lambda) = \left(\frac{2l'+1}{2l+1}\right)^{1/2} C(l'\lambda l; \Lambda 0) C(l'\lambda l; 00) \tag{14}$$

where $C(j_1 j_2 j_3; m_1 m_2)$ is a Clebsch–Gordan coefficient.

In equation (12), $\frac{1}{2}k_b^2$ is the body energy—the energy at which the BF-FN scattering equations are solved. The essential ambiguity of the AN procedure is that once the target states have been divorced from the scattering function, through the assumption of target-state degeneracy, the definition of the body energy becomes ambiguous. Various choices for this energy have been suggested, e.g. the entrance- or exit-channel energies (Chase (1956) and Chang and Temkin (1970), respectively) and their geometric mean (Nesbet 1977, Norcross and Padial 1982). The FONDA method, like other off-shell theories, prescribes an unambiguous definition of the body energy: according to (11), we choose $k_b = k_0$.

The BF-FN radial functions $w^\Lambda_{l,l_0}(r, k_0)$ are related to the LF-FN functions $\tilde{u}_{l'm',l_0 m_0}(r, k_0)$ in (11) via the Wigner rotation matrices, i.e.

$$\tilde{u}_{l'm',l_0 m_0}(r, k_0) = \sum_\Lambda \mathcal{D}^{l'}_{m',\Lambda}(\hat{R}) w^\Lambda_{l',l_0}(r, k_0) \mathcal{D}^{l_0*}_{m_0,\Lambda}(\hat{R}). \tag{15}$$

To derive the desired simple form for the FONDA K matrix in the CAM representation, we insert (15) into the integral equation (11) and then couple the rotational orbital angular momenta via the unitary transformation

$$\mathcal{H}^J_{jl,j_0 l_0} = \sum_{m_j m} \sum_{m_{j_0} m_0} C(jlJ; m_j m) \mathcal{H}^{(1)}_{\gamma\gamma_0} C(j_0 l_0 J; m_{j_0} m_0) \tag{16}$$

where, of course, $m_j + m = m_{j_0} + m_0$.

There remains only to express the resulting K-matrix elements in as simple a form as possible. These final steps consist of tedious but straightforward applications of

standard angular momentum coupling theory (Rose 1957) and will not be reproduced here. The final result can be written in terms of the coupling coefficient $g_\lambda(ll'; \Lambda)$ of equation (14), the matrix element of the rotational frame transformation (Chang and Fano 1972, Lane 1980)

$$A_{j\Lambda}^{Jl} = \left(\frac{2j+1}{2J+1}\right)^{1/2} C(jlJ; 0\Lambda) \tag{17}$$

and radial integrals

$$I_{l'\Lambda}^{\Lambda}(ll_0; k_j) \equiv \int_0^\infty dr\, \hat{j}_l(k_j r) v_\lambda(r) w_{l',l_0}^{\Lambda}(r, k_0) \tag{18}$$

i.e.

$$\mathcal{K}_{jl,j_0l_0}^J = -\frac{2}{(k_j k_0)^{1/2}} \sum_\Lambda A_{j\Lambda}^{Jl} \left(\sum_{l'\lambda} g_\lambda(ll'; \Lambda) I_{l'\Lambda}^{\Lambda}(ll_0; k_j)\right) A_{j_0\Lambda}^{Jl_0}. \tag{19}$$

From this K matrix we calculate the FONDA approximation to the LF CAM T matrix and then, using the standard formulae of LFCC theory (Arthurs and Dalgarno 1960, Lane 1980), evaluate the integral and differential cross sections for rotational excitation.

Several points about equation (19) are worth noting. Firstly, the FONDA approximation ensures that the scattering wavefunction in the entrance channel is evaluated at the incident (initial-state) energy $\frac{1}{2}k_0^2$ and the free wave in the exit channel at the final-state energy $\frac{1}{2}k_j^2$. Secondly, as a check on the algebra leading to this equation, we can apply the further approximation of target-state degeneracy, $k_j = k_0 = k_b$, whereupon equation (19) reduces to

$$\mathcal{K}_{jl,j_0l_0}^J = \sum_\Lambda A_{j\Lambda}^{Jl} K_{ll_0}^{\Lambda} A_{j_0\Lambda}^{Jl_0} \tag{20}$$

where $K_{ll_0}^{\Lambda}$ is

$$K_{ll_0}^{\Lambda} = -\frac{2}{k_b} \sum_{l'} \int_0^\infty dr\, \hat{j}_l(k_b r) V_{ll'}^{\Lambda}(r) w_{l',l_0}^{\Lambda}(r, k_b) \tag{21a}$$

$$= -\frac{2}{k_b} \sum_{l'\lambda} g_\lambda(ll'; \Lambda) I_{l'\Lambda}^{\Lambda}(ll_0; k_b). \tag{21b}$$

Equation (21) is just the integral equation for the BF–FN K matrix evaluated at the body energy $\frac{1}{2}k_b^2$, so (20) is the usual adiabatic nuclear rotation (ANR) result that is obtained (Lane 1980) when this matrix is expressed in the laboratory CAM representation via the rotational frame transformation (17).

The static, exchange and polarisation components of the e–H_2 interaction potential are identical to those used in our earlier study of the ANR theory for this system (Morrison *et al* 1984a). The static potential is calculated using standard computer programs (Morrison 1980, Collins *et al* 1980) that average the bound–free Coulomb interactions over the ground electronic state of the target. The wavefunction for this state was calculated in the Hartree–Fock approximation using a (5s2p/3s2p) basis (Huzinaga 1965) of contracted nucleus-centred Gaussian type orbitals.

The resulting equilibrium X $^1\Sigma_g^+$ charge density was used to calculate the exchange potential, which is modelled by a local, energy-dependent 'tuned' free electron gas exchange potential (Weitzel *et al* 1983) that was optimised for the study of rotational and vibrational excitation (Morrison *et al* 1984b).

The aforementioned basis is augmented by diffuse functions to obtain the basis for calculation of the polarisation potential used in this work. A detailed description of

this potential has been given by Gibson and Morrison (1984). Suffice it to say here that this model potential is based on a variational calculation of the energy lowering of the molecule due to the electric field of the projectile. This potential incorporates non-adiabatic effects using the non-penetrating approximation of Temkin (1957).

The integrals $I_{l'\lambda}^{\Lambda}(ll_0; k_j)$ were evaluated using a Numerov integrator (Hartree 1957) out to 50.0 a_0 with a mesh chosen to guarantee convergence to better than 1%. The remainder of this integral, from 50.0 a_0 to infinity, was calculated using the Born approximation, as described in § IV.A of Morrison *et al* (1984a). In equation (19) the maximum values of the summation indices were: $\Lambda = 2$, $l' = 6(5)$ for gerade (ungerade) symmetries, and $\lambda = 8$. In calculating cross sections $\sigma_{j_0 \to j}$ the maximum value of the total angular momentum quantum number was $J = 3$.

Integral FONDA cross sections for $j_0 = 0 \to j = 2$ and $j_0 = 1 \to j = 3$ are shown in figure 1, where they are compared with their LFCC counterparts and with cross sections determined using the ANR method. The sharp decrease in $\sigma_{j_0 \to j}$ as threshold is approached makes it difficult to appraise the FONDA cross sections in this critical region. Hence in figure 2 we show the percentage difference of approximate cross sections from LFCC results. In addition to the FONDA and ANR percentages, these figures include comparisons with an implementation of the energy modified adiabatic (EMA) approximation†. Unlike the ANR cross sections in figure 1, those used to calculate the percentages in figure 2 have been 'corrected'—i.e., forced to go to zero at threshold— via the *ad hoc* strategy of multiplying by the ratio k_j/k_0 (Chang and Temkin 1969). Adiabatic-nuclei cross sections calculated without this correction (figure 1) deviate from LFCC cross sections by far more than is indicated in figure 2. For example, at 47 meV the 'pure' ANR $\sigma_{0 \to 2}$ is in error by 414%, while the 'corrected' cross section is in error by 28%.

Figures 1 and 2 show that the FONDA is capable of producing accurate integrated cross sections even very near threshold (e.g., the FONDA cross section for $0 \to 2$ at 3 meV
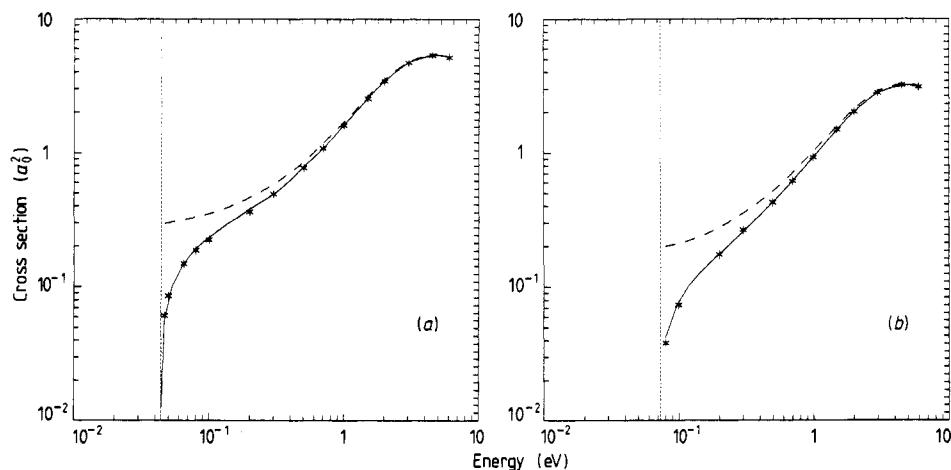
Figure 1. Integral cross sections for rotational excitations (*a*) $j_0 = 0 \to j = 2$ and (*b*) $j_0 = 1 \to j = 3$ of H_2. ——, LFCC; – – –, ANR; *, FONDA. On each graph the thresholds for these excitations, (*a*) 44.1 meV and (*b*) 73.5 meV, are shown as broken lines.

† Our implementation of the EMA method entails simply calculating $w_{l,l_0}^{\Lambda}(r, k_b)$ at $k_b = (k_j k_0)^{1/2}$; this is not a full implementation of Nesbet's proposed theory (Nesbet 1977).
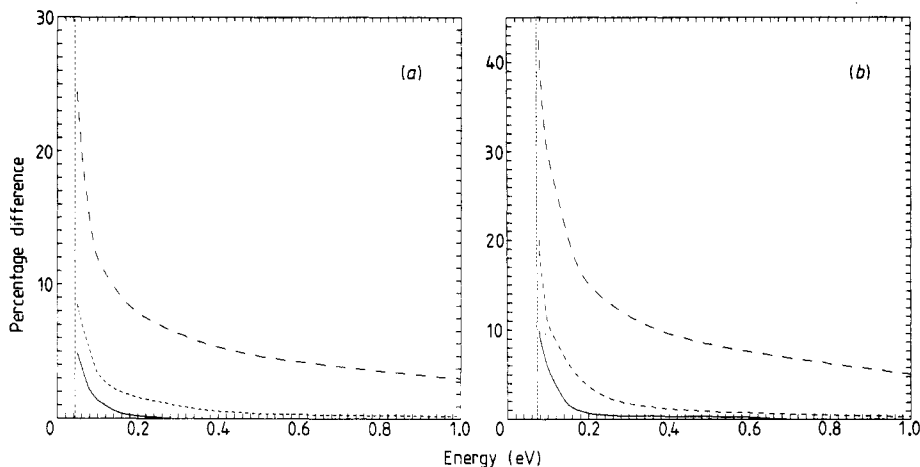
Figure 2. Percentage differences of cross sections from LFCC results for (a) $j_0 = 0 \rightarrow j = 2$ and (b) $j_0 = 1 \rightarrow j = 3$. ———, FONDA; – – –, ANR; - - - -, EMA. As in figure 1, thresholds for these excitations are shown as broken lines.

above threshold differs from the LFCC result by 4.9%; the ANR and EMA cross sections at this energy are in error by 28% and 9% respectively). The percentage error introduced into $\sigma_{j_0 \rightarrow j}$ by the FONDA approximation drops to less than 1% by 0.1 eV; that introduced by the ANR remains greater than 1% until the energy is larger than 3.0 eV.

More extensive comparisons, including differential cross sections, an examination of important K-matrix elements and results of other theories, will appear in a forthcoming report on the FONDA method. The most important next stage in the development of this theory is its implementation for vibrational excitation. For rotational excitation, several theories, such as the scaled ANR theory (Feldt and Morrison 1984) can produce sufficiently accurate cross sections. However, for vibrational excitation the situation is far more acute; the scaled ANR method, for example, is not applicable to this scattering process. The extension of the FONDA method to vibrational excitation and its generalisation to allow an exact treatment of exchange are presently under way.

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