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# On irregular oscillatory structures in resonant vibrational excitation cross-sections in diatomic molecules

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This paper is dedicated to the 60th birthday of Wolfgang Domcke our friend and collaborator who influenced significantly our scientific career.

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**Abstract**

We examine in detail the origin of irregular oscillatory structures in the cross-sections of low-energy resonant vibrational excitation of several diatomic molecules by electron impact. We show that these irregularities are caused by a combination of two phenomena: enhancing of the magnitude of the nuclear wave function in the vicinity of poles in the complex energy plane corresponding to quasi-bound vibrational states of the molecular anion, and energy variations of the phase of the nuclear wave function which corresponds to the reflection in the potential well of the molecular anion and which are sometimes called boomerang oscillations. These two phenomena are usually both involved in the nuclear dynamics. The former one is usually dominant at lower energies (NO molecule) and in systems where the potential energy of the molecular anion ($H_2$ in high rotational states) possesses an outer potential well. The latter one dominates if the width of the quasi-bound vibrational states of the molecular anion is relatively large (e.g. at higher energies for NO and $N_2$ molecule, $H_2$ in ground state).

*Keywords:* Electron–molecule collisions; Resonances; Vibrational excitation; Negative molecular ions

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## 1. Introduction

While the treatment of the vibrational dynamics of small molecules in the electronically bound states is becoming more and more routine, the treatment of the systems involving electrons in continuum still presents a challenge for theory. An important example in terms of both applications and interesting basic phenomena to be comprehended by theory, is the treatment of low-energy electron collisions with diatomic molecules $e^- + AB$ (treatment of polyatomic molecules is even more challenging but beyond the scope of the present paper). One of the additional difficulties in the theoretical treatment of low-energy electron–molecule collisions is the frequent presence of resonances (metastable $AB^-$ states) which enhance the coupling of the electronic and nuclear degrees of freedom. This coupling is responsible for large size of inelastic cross-sections and for number of interesting phenomena including threshold peaks, cusps at the opening of new channels, sharp vibrational resonances and oscillations below dissociative attachment $A + B^-$ threshold.

It would be difficult to comprehend all these phenomena with brute-force methods like vibrational close coupling expansions. On the other hand powerful approach capable to describe all these phenomena has been proposed long time ago in pioneering works of Chen [1], O'Malley [2,3], Bardsley [4] and Nakamura [5,6]. It is based on projection-operator separation of the electronic space to a discrete electronic state and an electronic continuum and is often described with the term "non-local resonance model" (NRM). Common understanding of the role of the discrete

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state is, that it should approximate the resonance state $AB^-$ as close as possible with a square-integrable function. While this may be good for some cases, it has been known for long time [7] that more important is that the discrete state is weakly dependent on the internuclear distance $R$ and that orthogonalization of the electronic continuum to this state restores the validity of Born–Oppenheimer approximation for the nuclear motion. Recently it has even been demonstrated explicitly, for exactly solvable model [8] that the choice of the discrete state is, in fact, to a large degree arbitrary as long as it describes the correct asymptotic bound state $A + B^-$ for large $R$ and it depends weakly on $R$ for all distances.

Following the initial development of the theory [1,2,7,4–6] the theory has been used for the semiempirical determination of model parameters within the local complex potential (LCP) approximation. The theory was further refined and its use for calculation of cross-sections for inelastic low-energy electron–molecule processes from the first principles has been pioneered by Wolfgang Domcke and collaborators [9] for number of systems and a very good agreement of the theory with scattering experiments has been reached.

One of the key advantages of the non-local resonance model is its interpretation power due to enormous simplification of the complicated many-body problem. The key quantity of the theory, the discrete state component of the full wave function of the system, is a function of one coordinate $R$ only and is thus easily plotted and interpreted.

To our best knowledge, nobody systematically studied the origin of the irregularities (asymmetric peaks) in the oscillatory structures which often occur in the vibrational excitation cross-sections for energies below the dissociative attachment threshold. A main goal of this paper is, to take the advantage of the interpretation power of the non-local resonance theory, and to explain these irregularities using several well-studied diatomic resonance systems. We also show that the qualitative explanation of these structures is more or less independent of the level of approximation used for the description of nuclear dynamics.

After a general theoretical discussion of the origin of these irregularities in the next section we present results for the $N_2$ and NO molecules for which we used the local complex potential approximation [10,11] and for the $H_2$ molecule for which we employed the latest non-local resonance model [12].

## 2. Description of nuclear dynamics and interpretation of projected wave function

The non-local resonance model and the solution of the dynamics within its framework has been described in detail elsewhere [9]. In this section we only briefly review the formulae needed as a basis for subsequent discussion. We also give a preliminary quantitative discussion of the phenomena occurring below dissociative attachment threshold. The subsequent chapters support these qualitative arguments with quantitative results for different systems.

Nuclear dynamics involved in resonance electron–molecule collisions can be described by the effective Schrödinger equation with the non-local, energy-dependent, and complex potential $V_{\rm eff}(E,R,R')$ which can sometimes be approximated by a local complex potential (like in the $N_2$ case). In general, a discrete state component $\psi_E(R)$ of the full wave function of the $e^- + AB$ system satisfies the equation

$$(E - T_N)\psi_E(R) - \int dR' V_{\rm eff}(E,R,R')\psi_E(R') = V_{d\epsilon_i}(R)\chi_{v_i}(R), \tag{1}$$

where $T_N$ is the kinetic energy operator of the nuclei, $V_{d\epsilon_i}$ is the coupling matrix element of the electronic hamiltonian between the discrete state and the continuum state with the energy $\epsilon_i$ of the incoming electron and $\chi_{v_i}(R)$ is the vibrational wave function of the target molecule in the Born–Oppenheimer approximation. The energy conservation requires $E = E_{v_i} + \epsilon_i$. This equation does not fix the normalization of the wave function $\psi_E(R)$ since any solution of the homogeneous equation can be added. This problem is removed by rewriting Schrödinger equation into the integral form of Lippmann-Schwinger equation

$$\psi_E = G_0(E)V_{d\epsilon_i}\chi_{v_i} + G_0(E)V_{\rm eff}\psi_E, \tag{2}$$

where $G_0(E) = [E + i\varepsilon - T_N]^{-1}$ is the retarded free-particle Green's function. Both $G_0(E)$ and $V_{\rm eff}$ act as integral operators on $\psi_E(R)$ in coordinate representation. In this formulation the normalization of the wave function $\psi_E(R)$ is fixed with the incoming flux of electrons, with spatial distribution determined by the target vibrational wave function $\chi_{v_i}(R)$ and the size of the flux is controlled by the coupling element $V_{d\epsilon_i}$ between the discrete state $AB^-$ and the initial continuum state $e^- + AB$ with electron energy $\epsilon_i$. One would therefore expect that the magnitude of the wave function $\psi_E(R)$ is mainly determined by $V_{d\epsilon_i}$. As we will see later the dependence is in general much more complicated.

To understand this we will first look on the form of the effective potential

$$V_{\rm eff}(E,R,R') = V_d(R)\delta(R-R') + \int V_{d\epsilon}(R) \times [E - T_N - V_0(R) - \epsilon + i\varepsilon]^{-1} V^*_{d\epsilon}(R')d\epsilon. \tag{3}$$

The first term is the local discrete state potential $V_d(R)$. The second term is the non-local non-hermitian part resulting from the coupling with the electron continuum. While this term is both computationally and interpretationally more difficult, it has usually limited range in $R$. For large $R$ we can fully comprehend the dynamics as motion in the local potential $V_d(R)$.

Now let us return to the magnitude of the wave function $\psi_E(R)$. If the coupling $V_{d\epsilon}$ is small, than the second term on the right hand side in Eq. (3) is also small and the dynamics of $\psi_E(R)$ can be understood as an oscillatory motion in $V_{\mathrm{d}}(R)$ with small leaking for small $R$ due to the non-local term. In the time-dependent picture we would see this oscillatory motion with a small absorption at the small $R$. The smallness of the absorption (the consequence of the small magnitude of $V_{\mathrm{d}\epsilon}$) leads to the long residence time which will manifest in the time-independent picture as a dramatic increase of the magnitude of the wave function. However this is possible only for certain energies, where the positive interference of the wave travelling one cycle in $V_{\mathrm{d}}$ with itself is happening. The energy dependence of the magnitude of the wave function will thus show peaks for energies where this condition is met, coinciding with the energies of the bound states in $V_{\mathrm{d}}(R)$ with precision controlled by the uncertainty principle between the energy width and the residence lifetime, controlled in turn with the magnitude of $V_{\mathrm{d}\epsilon}$. This gives the picture of vibrational anion resonances $AB^-$. The peaks in the wave function magnitude lead to the peaks in the vibrational excitation cross-section

$$\sigma_{i\to f} = \frac{4\pi^3}{k_{\mathrm{i}}^2}\left|\langle\chi_{v_{\mathrm{f}}}|V_{\mathrm{d}\epsilon_{\mathrm{f}}}|\psi_E\rangle\right|^2. \tag{4}$$

For the large coupling $V_{\mathrm{d}\epsilon}$ the dynamics could be understood as follows: the source term (the first term on the right hand side) in (2) describes the capture of the electron in the discrete state. This is followed by immediate (direct) decay, but some of the flux escapes into region of larger $R$ where the dynamics is governed by purely local potential $V_{\mathrm{d}}(R)$. For the energies below dissociation attachment threshold the flux is reflected back into region of small $R$ where the electron leaves by autodetachment (decay after reflection), with probability controlled again by $V_{\mathrm{d}\epsilon}$. For large $V_{\mathrm{d}\epsilon}$, all the flux is thus absorbed, but the direct decay and the decay after reflection interfere giving interference oscillations in the cross-section. The frequency of the oscillations is controlled by the energy dependence of the phase for travelling in the potential $V_{\mathrm{d}}$ from the capture point (close to the equilibrium distance $R_0$) to the outer turning point for given energy $E$ and back again. This gives the picture of the boomerang oscillations.

The magnitude of the quantity $V_{\mathrm{d}\epsilon}$ depends both on energy $E$ and the internuclear distance $R$. There is thus smooth transition between both the above mentioned mechanisms and they can mix in a complicated way. It is furthermore difficult to distinguish between them from the cross-section, because the phase determining the separation of the vibrational anion resonances $AB^-$ and the phase controlling boomerang oscillations differ only by phase attained by travelling in $V_{\mathrm{d}}$ from the point $R_0$ to the inner turning point in $V_{\mathrm{d}}$ which are usually close. But the two phases can differ noticeably. In the subsequent sections we will show how to separate the two effects and how the interplay of both with noticeably different phase can lead to irregularities in the shape of the structures in the vibrational excitation cross-section. The separation is based on the observation that *the first mechanism* involves the change of *the magnitude of the wave function* $\psi_E$, while *the phase* is important for *the second mechanism*. We will also show the cases that can be understood as purely boomerang oscillations or purely as vibrational anion resonances.

The analysis performed above remains fully valid also for the local complex potential approximation, where the non-local part of the potential is replaced with the local quantity $\delta(R-R')\left[\Delta(R)-\frac{i}{2}\Gamma(R)\right]$ and the discrete state-continuum coupling with $\sqrt{(\Gamma(R)/2\pi)}$.

## 3. Discussion of specific systems

In this section we analyse the structure of vibrational excitation cross-sections for several systems. Calculations were performed using both local complex potential approximation (for molecules $N_2$ and NO) and non-local resonance model (for $H_2$) to demonstrate universality of the suggested explanation of observed structures.

### 3.1. $N_2$ – *almost pure boomerang oscillations*

Though vibrationally inelastic electron scattering off the $N_2$ molecule was discussed by many authors (see e.g. [10,13–16]), no detailed explanation of the irregular oscillatory structure was provided yet. Therefore we have chosen this classical example of the so-called *boomerang oscillations* to discuss first, although it is not an example of pure boomerang oscillations but rather both mechanism described above play an important role.

The cross-sections of vibrational excitation of $N_2$ from ground vibrational state to several final states calculated in the LCP approximation are shown in Fig. 1, solid lines. Oscillatory structures in these cross-sections are compared with the energy dependence of the square of the norm, $N(E)$ (short dashed lines), of the nuclear wave function $\psi_E(R)$ (see Eq. (1)) multiplied by the exit amplitude $V_{\mathrm{d}E_{\mathrm{f}}}(R)$ which is in this case independent of the final channel and given by the square root of the width $\Gamma(R)$ divided by $2\pi$, hence

$$N(E) = \langle\psi_E|\Gamma(R)/2\pi|\psi_E\rangle. \tag{5}$$

The peaks in the energy dependence of the norm $N(E)$ of the wave function provide information how the dynamics of the electron–molecule system is influenced by the poles in the complex-energy plane corresponding to quasi-bound vibrational states of the molecular anion. The smaller is the width $\Gamma(E,R)$, the closer these poles lie to the real axis and the more pronounced is the effect of these states. Note that in the limit of zero width the vibrational states of the molecular anion would be bound and the norm would become infinite at the corresponding energies. Note also that the decrease of the norm for lower and higher energies is due to the lower probability of creation of $N_2^-$ (proportional to $|V_{\mathrm{d}\epsilon}|^2$) for these energies.

The most striking characteristics of the vibrational excitation cross-section in Fig. 1, clearly visible for the transition 0 → 1, is the difference between the spacing of peaks

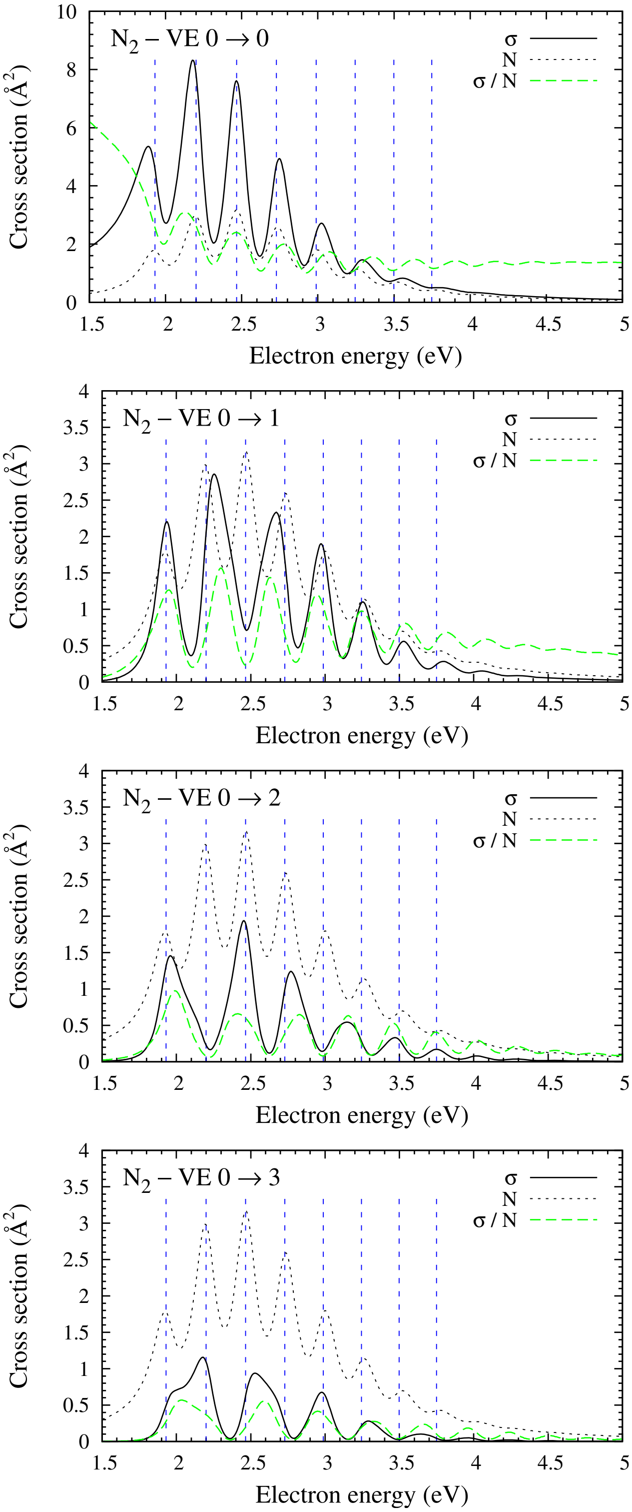

Fig. 1. Vibrational excitation cross-sections (solid lines) for transitions from the ground vibrational state of $N_2$ to the final states $0, \ldots, 4$ are plotted together with the square of the norm of the wave function $\psi_E(R)$ (short dashed lines, see Eq. (1)) and the cross-section divided by this quantity which should exhibit boomerang oscillations (long dashed curve). Vertical lines indicate positions of vibrational levels in the real part of the local complex potential of $N_2^-$. Notice that spacing between peaks of the boomerang oscillations is different (larger) than that of vibrational levels in the molecular anion potential (see text for details).

in the cross-section and the spacing of quasi-bound vibrational levels of $N_2^-$ (depicted by vertical lines) or the spacing between peaks in the norm $N(E)$. We see that there is no clear assignment of the cross-section peaks to vibrational levels of the molecular anion, not even for the elastic cross-section (top panel).

To understand fully the positions of the peaks in the cross-sections we can ask whether one would see any structure in the cross-section if there would be no enhancement of the magnitude of the nuclear wave functions for energies close to the quasi-bound vibrational states of the molecular anion. To answer this question we *renormalized* the expression $V_{dk_f}(R)\psi_E(R)$ to have a unit norm (i.e. $N(E) = 1$) before we calculate the cross-section using the formula (4). This renormalization is equivalent to division of the cross-section by $N(E)$. In other words we factorise the cross-section into the product of the term (5), *independent of the phase of the wave function* and the renormalized term *independent of the magnitude of the wave function* $\psi_E$. By this procedure we suppress the influence of the enhancement of the magnitude of the wave function on the cross-section and what is left are pure oscillations resulting from energy variation of the relative phase of the nuclear wave function with respect to the final vibrational state.

To demonstrate this we plotted in Fig. 1 also the cross-sections divided by $N(E)$. In these functions we can observe rather regular oscillations of similar frequency as in the cross-sections. Positions of minima in the cross-sections are almost exactly determined by minima of these functions (note that some peaks which are pronounced in the norm $N(E)$, completely disappear in the cross-sections) but positions of peaks in the cross-section are clearly influenced by positions of maxima of both $N(E)$ and the boomerang oscillations. Therefore we can conclude that both mechanism are important for explanation of the oscillatory structure for $N_2$ molecule.

To finish our discussion of the vibrational excitation cross-sections for $N_2$ we plotted in Fig. 2 the cross-sections for transitions 1 → 2 and 2 → 3. We can see that for higher initial vibrational states some peaks in the norm of the wave function disappear (e.g. the third peak for $v_i = 1$) and that the rest is not so regular as for $v_i = 0$; as a consequence some peaks are more pronounced than the others. This behaviour can be understood if we write a formal solution of Eq. (1) as

$$|\psi_E\rangle = \lim_{\eta \to 0} \sum_n \frac{|\phi_n\rangle\langle\phi_n|\sqrt{\Gamma(R)/2\pi}|\chi_{v_i}\rangle}{E - E_n + i\eta}, \qquad (6)$$

where $|\phi_n\rangle$ are quasi-bound vibrational states with complex energies $E_n$ (the finite lifetime of these state is determined by the resonance width $\Gamma(R)$). We can see that the effect of the pole at energy $E_n$ on the dynamics of the system can be suppressed if the overlap $\langle\phi_n|\sqrt{\Gamma(R)/2\pi}|\chi_{v_i}\rangle$ is zero or very small. This was not the case of $v_i = 0$ but it happens for higher initial vibrational states.

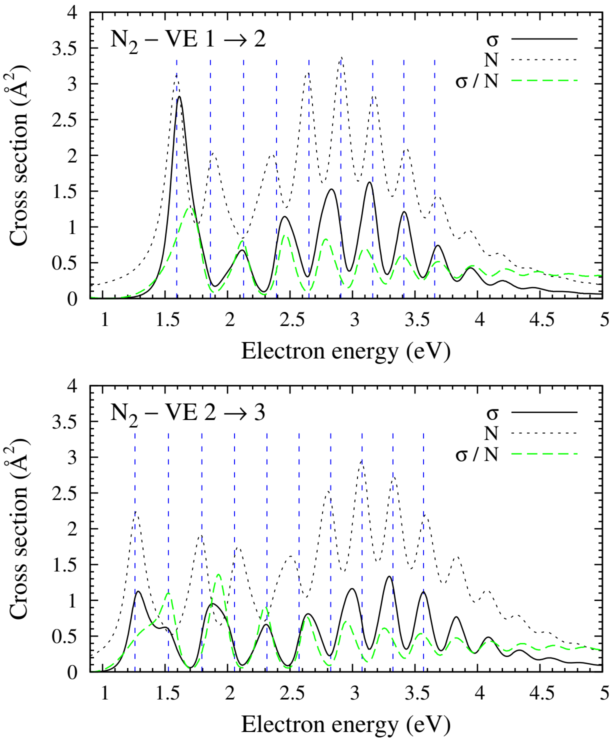

Fig. 2. The same as in Fig. 1 but for transitions 1 → 2 and 2 → 3. Notice that there are vibrational levels in the molecular anion potential to which no peak in the energy dependence of the norm corresponds (see text for details).

### 3.2. *NO – boomerang oscillations strongly influenced by existence of quasi-bound vibrational state of* NO$^-$

In the case of NO molecule the situation is more complicated than in N$_2$ case because of the existence of three resonances of NO$^-$ ($^3\Sigma^-$, $^1\Delta$, and $^1\Sigma^+$ electronic states) which all contribute significantly to the vibrational excitation cross-sections. For simplicity we limit ourself to the discussion of the irregularities in the cross-section which result from the contribution of the $^3\Sigma^-$ negative ion state. Other irregularities which come into play because of adding the three contribution together are discussed in other papers (see e.g. [11,17]).

Because the non-local resonance model for electron collisions with NO molecule is not yet available we have calculated the contribution of $^3\Sigma^-$ state to the vibrational excitation (0 → 1 and 0 → 2) cross-sections using the local complex potential approximation as given by Trevisan et al. [11]. In Fig. 3 we show the results obtained by the standard local complex potential (LCP) approximation in which the entry and exit amplitudes are energy-independent. The cross-sections in Fig. 3 have incorrect behaviour for energies close to the threshold (the cross-section is overestimated by the standard LCP approximation), therefore somewhat arbitrary barrier penetration factor was introduced in [11] to get more realistic energy dependence of the cross-sections at the threshold. The resulting cross-sections for the same transitions as in Fig. 3 are plotted in Fig. 4.

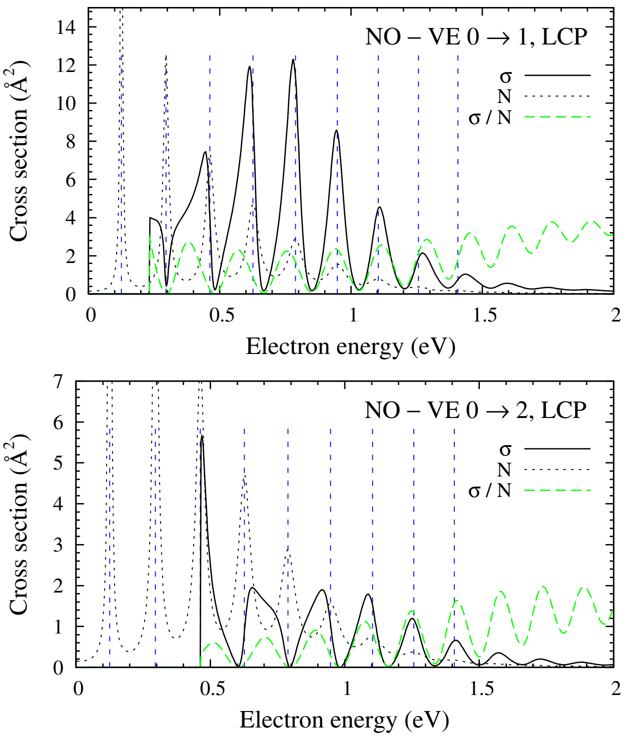

Fig. 3. The same as in Fig. 1 but for the NO molecule and the transition 0 → 1 and 0 → 2 only. Results of the standard LCP approximation calculation.

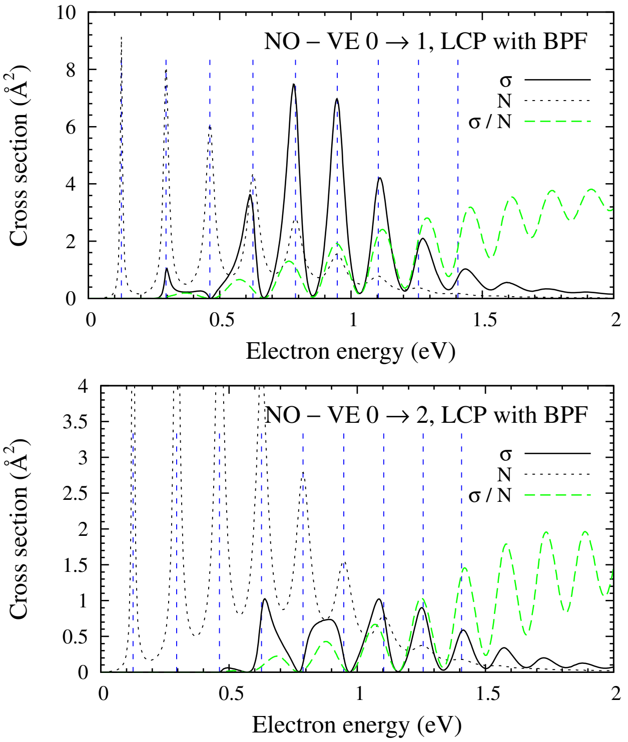

Fig. 4. The same as in Fig. 3 but results obtained using the LCP approximation with the energy-dependent barrier penetration factor. Notice that appearance or disappearance of some peaks corresponding to quasi-bound vibrational levels of the molecular anion strongly depend on the used model.

As in the $N_2$ case we observe irregularities in the oscillatory structure, especially for energies near the threshold, and some peaks which are profound in the norm $N(E)$ are suppressed in the cross-section. Thus the positions of the peaks result again from the interplay of the two mechanisms described above. Both contributions give a nice regular structures and only in combination the irregularities appear. What should be stressed is that appearance or disappearance of some peaks corresponding to vibrational levels of $NO^-$ is strongly dependent on the model which it is used for calculations. For example the second peak in the norm $N(E)$ is suppressed if the standard LCP approximation is used (Fig. 3, upper panel), but it appears in the cross-section if the barrier penetration factor is included. Thus it would be worthy to study this process in detail using a non-local resonance model constructed with a correct energy dependence of the resonance width and entry and exit amplitudes.

### 3.3. $H_2$ *molecule – pure boomerang oscillations for ground state, narrow resonances for high rotational states*

The origin of the oscillatory structure in the cross-sections of vibrational excitation of hydrogen molecule was a conundrum since its existence was predicted by Mündel et al. [18] and confirmed experimentally by Allan [19]. Gertitschke and Domcke [20] used a time-dependent description of resonant electron–molecule collisions to study this process and claimed that the oscillatory structure is “a consequence of the dramatic broadening of the wave packet” rather than its quasiperiodic movement in the potential well of negative anion. This was in contrast to the previous explanations of similar structures in the vibrational excitation cross-sections for $N_2$ based on the boomerang model [13,14,16] and provoked to search for an alternative explanations. We mention at least two papers by Narevicius and Moiseyev [21,22] in which the authors proposed that the oscillatory structure is “a fingerprint of broad overlapping resonances” supporting their statement by a non-Hermitian properties of the effective Hamiltonian of $H_2^-$ within the local complex potential approximation. Although their results are mathematically correct we do not think they provide a better physical insight into the dynamics of the studied process. They found a solution of the problem in a non-standard, but complete basis of the non-physical vibrational states of $H_2^-$ with complex energies but scattering solutions at real energies which are needed for calculation of the cross-sections do not show a fingerprint of these states, not even for energies close to the energies of these states because corresponding poles lie far from the real axis due to the large resonance width of $H_2^-$ and many poles contribute and interfere in a complicated way.

Finally the authors of this paper in collaboration with Domcke [23] returned to the original ideas of the boomerang model [13] and suggested that the oscillatory structure in the vibrational excitation cross-sections has indeed its origin in the reflection of the wave packet in the long-range potential of $H_2^-$ and that these oscillations are even *pure boomerang oscillations* if the molecule $H_2$ is initially non-rotating. This result was supported by inspection of the properties of the oscillations which were explained completely on the basis of the boomerang model (see [23] for details).

Following the general discussion of the previous section we demonstrated explicitly in Fig. 5 that the structures (for angular momentum $J = 0$ and the vibrational transition $v_i = 0 \rightarrow 4$) are pure boomerang oscillations for the norm does not show any enhancement in the vicinity of the quasi-bound vibrational levels of $H_2^-$ (indicated again by vertical lines). Note that in this case the oscillations are very regular apart from the rapid decrease of spacing between subsequent peaks towards the dissociative attachment threshold at 3.72 eV which is caused by the profound anharmonicity of the long-range potential energy curve of $H_2^-$.

The situation changes if the initial rotational state of the hydrogen molecule with higher $J$ is considered. Then the oscillations become more irregular (see Fig. 6) and again the two effects discussed above play important role. The reason is that for $J \gtrsim 20$ an inner barrier in the effective potential of $H_2^-$ appears (see [24], Fig. 1) which prevents the system to return into the autodetachment region where the captured electron can again escape and thus the width of the quasi-bound vibrational states of $H_2^-$ is considerably smaller having much more profound effect on the dynamics of the $H_2^-$ system. (see [25,24] for details on these long-lived states of $H_2^-$). In Fig. 6 we plot an example of an irregular oscillatory structure for higher rotational state of $H_2, J = 20$. We can see that in this case the energy dependence of the norm $N(E)$ is very dramatic about the first

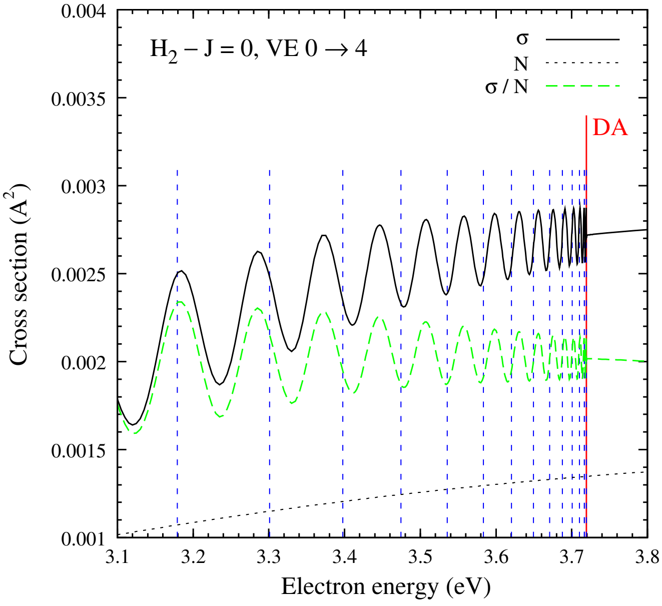

Fig. 5. The same as in Fig. 1 but for the $H_2$ molecule with $J = 0$ and the vibrational transition $0 \rightarrow 4$. Results of the NRM calculation based on the model of [12]. Notice that the norm $N(E)$ does not show any structure.

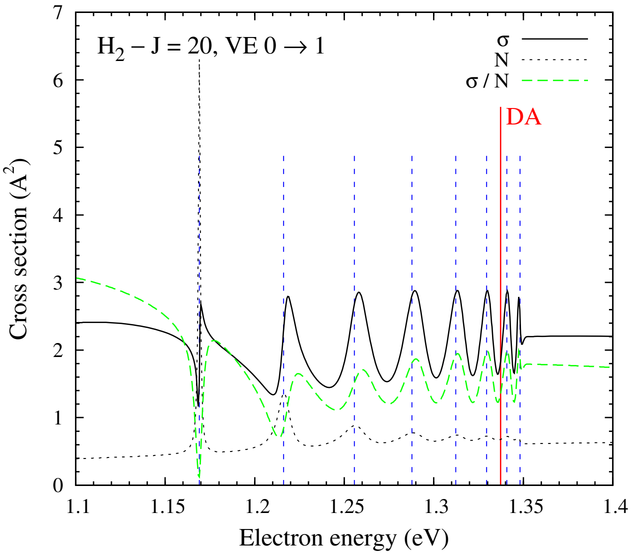

Fig. 6. The same as in Fig. 1 but for the $H_2$ molecule with $J = 20$ and the vibrational transition $0 \to 1$. Results of the NRM calculation based on the model of [12]. Notice a narrow resonance around the first quasi-bound vibrational state of $H_2^-$ and other, not so narrow, around other states. The last two oscillations in cross-section are located above dissociative attachment (DA) threshold protected from dissociation by 15 meV high centrifugal barrier.

three vibrational states of $H_2^-$ but much less for states closer to the dissociative attachment threshold. Thus we deal here again with both mechanisms described above.

## 4. Conclusions

We have used the interpretation power of the simple and accurate description of the low-energy resonant collisions of electrons with the diatomic molecules developed by Domcke and others to study irregularities in the oscillatory structure of the vibrational excitation cross-sections. We have shown by comparing the cross-section functions with the energy dependence of the norm of the resonant part of the nuclear wave function that these structures are very often a combination of two effects, enhancement of this norm in the vicinity of vibrational levels of the negative molecular ion and the interference due to phase changes of this wave function with energy.

The resulting boomerang oscillations in the cross-sections can have peaks displaced from the positions of the vibrational levels of the molecular anion as, e.g. for $N_2$ molecule. This displacement depends on the details of the dynamics, especially on the resonance width. There is, in general, no clear assignment of the cross-section peaks to vibrational levels of the negative ion, not even for the elastic cross-section.

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