Dissociative attachment of low-energy electrons to vibrationally excited hydrogen molecules [*]

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Dissociative electron attachment to hot hydrogen molecules is studied in the framework of nonlocal resonance model. The method based on the use of the Bateman approximation, well known in nuclear physics, is adapted for solving the Lippmann–Schwinger integral equation of the nonlocal resonance model and applied to the calculation of cross sections of inelastic resonant electron-molecule collisions. The proposed method is compared with the Schwinger–Lanczos algorithm used extensively for the treatment of these processes. It is shown that the Bateman approximation is very useful and efficient for treating the non-separable nonlocal potentials appearing in the integral kernels of the nonlocal resonance models. The calculated cross sections for the dissociative attachment of electrons to vibrationally excited hydrogen molecules are of importance for astrophysics.

1   Introduction

The process of dissociative attachment (DA) of electrons to hydrogen molecules

$$e^- + H_2(\nu_i) \to H + H^-, \tag{1}$$

and its inverse, the process of associative detachment (AD),

$$H + H^- \to H_2 + e^-, \tag{2}$$

play an essential role in many areas of physics and chemistry. In astrophysics, for example, it is assumed that the process of AD is responsible for the creation of the hydrogen molecule at early stages of the development of the Universe after the Big Bang. The occurence of H_2 molecules turns on a very efficient cooling mechanism of the hot materia which eventually lead to the creation of stars and galaxies. These processes are of importance also in fusion plasma, gas lasers, molecular switches, etc.

In this paper these processes are described by the nonlocal resonance model (NRM) [1] which represents the most advanced theory of the resonance inelastic processes in the electron–molecule system.

The nonlocal resonance model makes use of the Feshbach projector formalism [2] to separate the full Hilbert space (electronic and nuclear degrees of freedom) to

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[*] This paper is dedicated to Prof. J. Bičák on the occasion of his 60th birthday.

a resonant part corresponding to the state $(AB)^-$, and a background part corresponding to the continuum states $e^- + AB$. Projecting out the electronic degrees of freedom we get the basic equation of the nonlocal resonance model for radial motion of the nuclei in the resonance state [1].

There are two possible descriptions of these processes: time-independent and time-dependent picture. In the time-independent picture we get the Lippmann–Schwinger equation

$$\psi(R) = \phi(R) + \int\limits_0^\infty \int\limits_0^\infty \mathrm{d}fR' \, \mathrm{d}fR'' G_\mathrm{d}(E, R, R') F(E, R', R'')\psi(R''), \qquad (3)$$

where $\phi(R)$ is a scattering solution describing incoming particles and $G_\mathrm{d}(E, R, R')$ is the Green function for the potential $V_\mathrm{d}(R)$ of the discrete state $(AB)^-$. $F(E, R, R')$ is a nonlocal, complex and energy-dependent potential of the general form

$$F(E, R, R') = \sum_n \!\!\!\!\!\!\!\!\!\int \chi_n(R)[\Delta(E - E_n, R, R') - \tfrac{1}{2}\mathrm{i}\Gamma(E - E_n, R, R')]\chi_n(R') \qquad (4)$$

with

$$\Gamma(\epsilon, R, R') = 2\pi V_{\mathrm{d}\epsilon}(R)V_{\mathrm{d}\epsilon}^*(R'), \qquad (5)$$

$$\Delta(\epsilon, R, R') = \frac{1}{2\pi}\int \mathrm{d}f\epsilon' \frac{\Gamma(\epsilon', R, R')}{\epsilon - \epsilon'}, \qquad (6)$$

describing the interaction between the discrete state of $(AB)^-$ and the continuum through the matrix element $V_{\mathrm{d}\epsilon}(R)$. The functions $\chi_n(R)$ are vibrational states of the neutral molecule AB (including the continuum).

In the time-dependent picture one has to solve the Schrödinger equation

$$\mathrm{i}\frac{\partial}{\partial t}\psi(R, t) = \left(-\frac{1}{2\mu}\frac{\mathrm{d}f^2}{\mathrm{d}fR^2} + V_\mathrm{d}(R)\right)\psi(R, t) + \frac{1}{\mathrm{i}}\int_0^t \mathrm{d}ft' \int_0^\infty \mathrm{d}fR' F(R, R', t-t')\psi(R', t'), \qquad (7)$$

with the initial condition $\psi(R, 0) = V_{\mathrm{d}\epsilon_i}(R)\chi_{\nu_i}(R)$, which indicates that the molecule AB in the initial state $\chi_{\nu_i}(R)$ captures an electron of energy ϵ_i with the probability governed by $V_{\mathrm{d}\epsilon_i}$. The kernel

$$F(R, R', \tau) = \sum_n \!\!\!\!\!\!\!\!\!\int \chi_n(R) \int \mathrm{d}f\epsilon \, V_{\mathrm{d}\epsilon}(R)\mathrm{e}^{-\mathrm{i}(\epsilon + E_n)\tau} V_{\mathrm{d}\epsilon}^*(R')\chi_n(R'), \qquad (8)$$

which is nonlocal, complex and time-dependent, represents the memory of the system and the dynamics is therefore non-Markovian. The two quantities $F(E, R, R')$ and $F(R, R', \tau)$ are related by the Laplace transform.

In both time-dependent and time-independent formalisms the essential technical difficulty for numerical solution is the nonseparability (in coordinates R and R') of the quantity F which is furthermore rapidly oscillating, nonhermitian and strongly

energy dependent. Separable expression for F is easily found if the coupling $V_{d\epsilon}(R)$ is separable in ϵ and R. Numerical treatment of Eq.(3) and Eq.(7) in this case is described in [3] (time-independent picture) and in [4] (time-dependent picture). First goal of this paper is to treat the general case. We discuss the Bateman approximation [5], which was used successfully in nuclear physics, to produce separable approximations (finite rank operators) to generally non-separable integral kernels. It is shown that the Bateman approximation is useful also in the case of electron-molecule scattering. A very precise and robust algorithm for the calculation of the Bateman approximation is proposed. We will focus here on the time-independent description.

In the present work this technique is applied to the calculation of the cross sections for DA process in the case of highly vibrationally excited hydrogen molecules. To our knowledge this problem, which is very important for example for cooling fusion plasma, has never been studied in the full nonlocal treatment.

This paper is organized as follows: The Bateman approximation is introduced and techniques for solution of scattering integral equations are briefly discussed in Section 2. A model problem is solved by both the Schwinger–Lanczos [6] and the Bateman technique [5]. Section 3 is devoted to the application of the proposed numerical technique to a realistic problem, namely to the calculation of DA cross section for HCl molecule (Subsection 3.1). This represents a severe test of the proposed algorithm. Finally in Subsection 3.2 we present DA cross sections for highly vibrationally excited H_2 molecules. The paper is summarized in Section 4.

2 Numerical solution of the basic NRM equation

The equation (3) is a Fredholm-type integral equation of the second kind which has a general form

$$\psi(x) = \phi(x) + \int_a^b V(x,y)\psi(y)\,\mathrm{d}y\,. \tag{9}$$

There exists a plethora of methods for solving scattering integral equations (see e.g. [7, 8]). A very general method how to solve integral equations is to approximate the integrals by a quadrature rule, say of the Gauss-type, and to convert the integral equation into an algebraic one. This method is widely used in solving nuclear scattering problems in momentum representation [9] because the number of mesh points needed to obtain reliable cross sections is relatively low. In the present case, however, this method seems not to be practical because the number of mesh-points required to yield even a very rough estimate of the results is generally large. This is caused by the nature of the integral kernel of the NRM approach which is nonhermitian, rapidly oscillating and strongly energy-dependent. In this paper we shall consider two approaches which are based on a different way of solving integral equations, namely on the use of separable approximation of the integral kernel and which are expected to work efficiently even if the number of meshpoints is large.

If the kernel $V(x, y)$ is separable,

$$V(x, y) = \sum_{i=1}^{M} \lambda_i f_i(x) g_i(y), \qquad (10)$$

(this is the case of Eq.(3) provided the coupling $V_{d\epsilon}(R)$ is separable in energy and space) then the equation (9) can be transformed to a set of M linear equations. This set can be then solved by standard methods (e.g. LU-decomposition). Coefficients of these linear equations are known integrals, the number of which is $M(M + 1)$. $M^2 N + O(MN) + O(M^3)$ operations are thus needed to obtain the approximate solution in N grid points. The problem, however, arises if the integral kernel is nonseparable. In what follows we shall discuss two methods which in some sense generate an optimized separable approximations to the kernels of the NRM theory.

2.1 Schwinger–Lanczos algorithm

A method, which requires $M_{\mathrm{SL}} N^2 + O(M_{\mathrm{SL}} N)$ multiplications and additions (M_{SL} will be specified later) and N^2 evaluations of kernel, is the Schwinger–Lanczos algorithm [6]. Since this algorithm has been described in detail in the literature [6], we give here only a brief description. This algorithm generates an appropriate basis (Krylov basis) using the leading term $\phi(x)$ and the kernel $V(x, y)$. In this basis the operator V is tridiagonal and it is possible to determine its inverse operator exactly.

In the process of construction of the basis it is necessary to apply the kernel $V(x, y)$ to basis vectors; this operation is an $O(N^2)$ process. The whole algorithm is of the order $M_{\mathrm{SL}} N^2$, where M_{SL} is the number of the basis vectors used. If the kernel is separable, then the application of $V(x, y)$ on one basis vector is an $O(MN)$ process and the whole calculation is of the order $M_{\mathrm{SL}} MN$. Provided $M_{\mathrm{SL}} \ll M$, i.e., $M_{\mathrm{SL}} MN \ll M^2 N$ (in NRM calculations typically $M \simeq (50\text{--}100)$ and a good precision is achieved for $M_{\mathrm{SL}} \simeq 10$), then it makes sense to use the Schwinger–Lanczos algorithm even for separable kernels.

2.2 Bateman approximation

The Bateman approximation was originally designed for generating separable approximations of integral kernels of infinite rank [5], but it might also be useful in treatment of integral kernels of high rank, i.e., kernels which are separable, but in which the number of separable terms is large. An advantage of this method is that it requires generally $5 M_{\mathrm{B}}^2 N + O(M_{\mathrm{B}} N) + O(M_{\mathrm{B}}^3)$ operations, where M_{B} is a number of terms in the separable approximation (the rank of the operator), Eq. (10), that is independent on N. This method is clearly very fast if $N \gg M_{\mathrm{B}}$.

The first Bateman approximation is given by [5]

$$V_1(x, y) = \frac{V(x, y_1) V(x_1, y)}{V(x_1, y_1)}, \qquad (11)$$

where (x_1, y_1) is a point in the integration range. A good choice of this point is essential for a good performance of the Bateman approximation. We will discuss this later. It is easy to see that

$$V_1(x, y_1) = V(x, y_1) \quad \text{and} \quad V_1(x_1, y) = V(x_1, y). \tag{12}$$

The M-th approximation is then given by

$$V_M(x, y) = V_{M-1}(x, y) + \frac{W_{M-1}(x, y_M)W_{M-1}(x_M, y)}{W_{M-1}(x_M, y_M)}, \tag{13}$$

where

$$W_{M-1}(x, y) = V(x, y) - V_{M-1}(x, y) \tag{14}$$

is the "error" of the $(M-1)$-th approximation. From the construction it is clear that

$$\begin{aligned} W_{M-1}(x, y) = 0 \quad & \text{for } x = x_1, \ldots, x_{M-1} \text{ or for } y = y_1, \ldots, y_{M-1}, \\ V_M(x, y) = V(x, y) \quad & \text{for } x = x_1, \ldots, x_M \text{ or for } y = y_1, \ldots, y_M, \end{aligned} \tag{15}$$

i.e., the Bateman approximation is exact on lines which are parallel to the y-axis for $x = x_1, \ldots, x_{M-1}$ and on lines which are parallel to the x-axis for $y = y_1, \ldots, y_{M-1}$. If the kernel is of the form (10), then it is easy to show that the Bateman approximation is exact for $M_{\mathrm{B}} = M$.

The numerical realisation of the M-th Bateman approximation of the original kernel requires $2M_{\mathrm{B}}^2 N$ multiplications, $M_{\mathrm{B}}^2 N$ additions and evaluating of $2M_{\mathrm{B}} N$ values of the kernel (compare with N^2 evaluations of the Schwinger-Lanczos algorithm). To solve the integral equation, Eq. (9), $M_{\mathrm{B}}(M_{\mathrm{B}} + 1)$ integrals have to be calculated; this requires $M_{\mathrm{B}}^2 N$ multiplications and additions. Finally a set of M_{B} linear equations is solved which is of the order M_{B}^3. The whole algorithm is thus of the order $O(M_{\mathrm{B}}^2 N) + O(M_{\mathrm{B}}^3)$.

The main problem connected with the Bateman approximation is to find a good choice of the points (x_i, y_i). It is possible to construct methods based on minimization of some functionals but these methods are usually nonlinear and not easy to use numerically. Here we suggest a simple way of choosing the points (x_i, y_i), which reduces numerical problems connected with the occurrence of zeros in the denominators of the expressions (11) and (13). The idea is to take the first point, (x_1, y_1) so that $|V(x, y)|$ is maximal at (x_1, y_1) and the subsequent points (x_i, y_i) so that $|W_{i-1}(x, y)|$ attain maxima at (x_i, y_i).

Searching for maxima of $W_i(x, y)$ at all points is not practical because evaluation of a large number (N^2) of functional values is needed. Since all nonlocal potentials appearing in NRM calculations are always symmetrical $(V(x, y_i) = V(y_i, x))$ we suggest to choose the points (x_i, y_i) only on the diagonal, $x = y$. This restriction accelerates the calculation significantly and as will be shown below leads to a very reliable and stable algorithm. Generally, it is difficult to make an estimate of the error of the Bateman approximation. Practical calculations, however, showed that this method is convergent for relatively small M_{B} and gives good results for a broad class of problems.

2.3   Model example

To see how the Bateman approximation works for simplified cases, let us first consider the equation

$$\psi(x) = \sin 10x + 10 \int_0^{10} e^{-(x-5)^2-(y-5)^2} \sin xy \, \psi(x) \, dy \,, \tag{16}$$

the kernel of which models a real part of the nonlocal potential GF. The integral kernel of this equation is non-separable and because of the term $\sin xy$, which is rapidly oscillating, one has to take into account a large number of meshpoints to describe correctly all the oscillations (e.g., $N \approx 1000$ if a relative precision of the solution 10^{-12} is required when Newton–Cotes formulas of the order $O(1/N^6)$ are used for the integration).

Table 1 shows convergence rate of the L^2-norm of the solution of Eq. (16) at increasing order M_B of the Bateman approximation and also at increasing order M_{SL} of the Schwinger–Lanczos algorithm.

The convergence of the latter method is faster and smoother than that of the former one, but the computational cost, as shown in the 4th and 7th column, is significantly lower for the Bateman approximation.

Table 2 shows how many iteration steps are needed to get the wave function of the prescribed accuracy. In this table δ represents the maximal relative error of the solution ψ on the whole integration range. Again M_B denotes the number of terms in the Bateman approximation and M_{SL} the number of Schwinger–Lanczos iterations. The entries in the third and fifth column show the time needed for

Table 1. Convergence of the L^2-norm of the solution for the Bateman and the Schwinger–Lanczos method. M_B and M_{SL} denote the number of terms (iterations) of the Bateman and Schwinger–Lanczos method, respectively. The entries in the second and fifth columns show the L^2-norm of the solution $\psi(x)$, the third and sixth the error of the L^2-norm and fourth and seventh the time needed for the calculation.

M_B, M_{SL}	$\|\psi\|_B$	$\Delta\|\psi\|_B$	τ_B (s)	$\|\psi\|_{SL}$	$\Delta\|\psi\|_{SL}$	τ_{SL} (s)
1	5.02183083	−0.00233591	0.0001	5.02119854	−0.00296820	0.04
3	5.02190118	−0.00226555	0.002	5.02046574	−0.00370100	0.13
5	5.02333382	−0.00083291	0.006	5.02545659	0.00128986	0.22
7	5.02342891	−0.00073782	0.010	5.02414255	−0.00002418	0.30
9	5.02181191	−0.00235483	0.017	5.02416673	0.00000000	0.39
11	5.02303986	−0.00112688	0.024			
13	5.02467722	0.00051049	0.032			
15	5.02416752	0.00000079	0.041			
17	5.02416752	0.00000079	0.053			
19	5.02416717	0.00000044	0.066			
21	5.02416657	−0.00000016	0.079			
23	5.02416673	0.00000000	0.092			

Table 2. Number of steps and computational cost for a given maximal relative error (δ) of the solution using the Bateman approximation and the Schwinger–Lanczos algorithm.

δ	M_{B}	τ_{B} (s)	M_{SL}	τ_{SL} (s)
10^{-2}	16	0.046	8	0.933
10^{-4}	19	0.066	10	1.158
10^{-6}	23	0.091	11	1.280
10^{-8}	28	0.140	12	1.395
10^{-10}	32	0.160	14	1.626
10^{-12}	38	0.225	15	1.747

the calculation. It is observed that the computational time for the Schwinger–Lanczos method is almost independent on the required accuracy of the solution. The Bateman method, on the contrary, is very fast if high accuracy is not required and the CPU time increases more rapidly at increasing accuracy.

3   Dissociative attachment to diatomic molecules

In this section we briefly describe applications of the nonlocal resonance model [1] to the collisions of electrons with HCl and H_2 molecules. To calculate cross sections for vibrational excitation, dissociative attachment or associative detachment for a particular molecule, we have to specify the potential $V_0(R)$ of the neutral molecule, the so-called discrete-state potential $V_{\mathrm{d}}(R)$ of the resonance $(AB)^-$ and the discrete-state-continuum coupling $V_{\mathrm{d}\epsilon}(R)$. Before we come over to the goal of this paper, i.e. the calculation of DA cross sections for molecular hydrogen in its highly vibrationally excited states, we first discuss the process of DA to HCl molecule. The DA process for HCl molecule has been studied by several authors (e.g. [10–12]), and represents a test case for all methods designed for the treatment of electron-molecule resonance scattering. HCl molecule has a nonzero permanent dipole moment. This long-range force makes the calculation difficult.

3.1   HCl

We adopt the form of the functions $V_0(R)$, $V_{\mathrm{d}}(R)$ and $V_{\mathrm{d}\epsilon}(R)$ from [12]. For the purpose of the further discussion we specify here only the form of the discrete-state-continuum coupling

$$V_{\mathrm{d}\epsilon}(E,R) = f(E,R)g(R), \tag{17}$$

where

$$f(E,R) = \sqrt{\frac{A}{2\pi}} \left(\frac{E}{B}\right)^{\alpha(R)/2} \mathrm{e}^{-E/2B}. \tag{18}$$

The behavior of $f(E,R)$ for $E \to 0$, Eq.(18), corresponds to the so-called Wigner threshold law [1]. For polar molecules with a non-zero dipole moment the threshold exponent α depends on the internuclear distance R.

The NRM was generalized to the case of the variable threshold exponent by Horáček et al. [13]. The R-dependence of the threshold exponent is a reason why the nonlocal potential $F(E, R, R')$ is non-separable. Actually the resonance width $\Gamma(E, R, R')$ is separable in the NRM theory, but the resonance shift $\Delta(E, R, R')$ is not, due to a Hilbert integral transform (6). Explicitly,

$$\Delta(E, R, R') = g(R)\delta(E, R, R')g(R'), \qquad (19)$$

where

$$\delta(E, R, R') = \int \mathrm{d}\epsilon' \frac{f(E, R)f(E, R')}{E - \epsilon'} = \int \mathrm{d}\epsilon' \frac{\dfrac{A}{2\pi}\left(\dfrac{E}{B}\right)^{(\alpha(R)+\alpha(R'))/2} \mathrm{e}^{E/B}}{E - \epsilon'}. \qquad (20)$$

In application of the above numerical procedure to Eq.(3) it is sufficient (and simpler) to apply the Bateman approximation only to the potential F and not to the full kernel GF. Figure 1 shows the real part of $F(E, R, R')$ at the energy $E = 1\,\mathrm{eV}$ and the absolute error of the 20-th Bateman approximation of this real part for the HCl molecule. The magnitude of the error is less than 5×10^{-6} on the full range of the internuclear distances R and R' and therefore the 20-th Bateman approximation represents an excellent approximation to $F(E, R, R')$. There exist, however, another way how to apply the Bateman approximation which may combine the speed of the Bateman approximation with the excellent convergence properties of the Schwinger–Lanczos method. The idea is to apply the Batemann approximation not to the full potential operator $F(E, R, R')$ but only to the term $\delta(E, R, R')$, Eq.(20), and then to solve the resulting equation by the Schwinger–Lanczos method. This approach combines good properties of both methods. Contrary to the full potential operator $F(E, R, R')$ the term $\delta(E, R, R')$ is a smooth and nonoscillatory
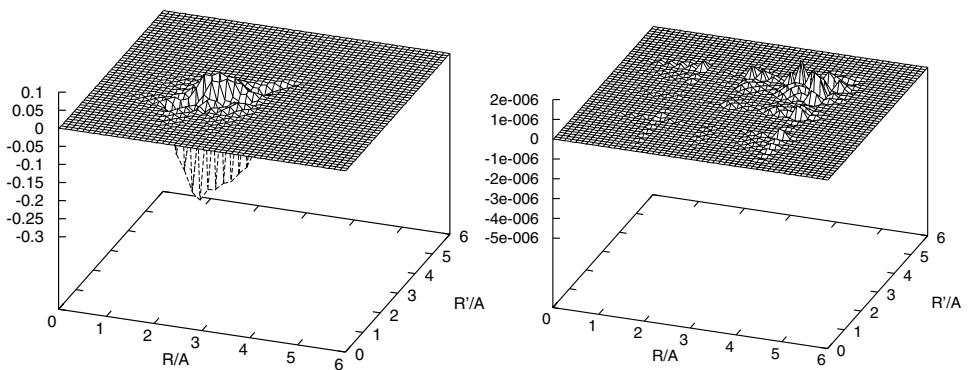

Fig. 1. The real part of the non-local potential $F(E, R, R')$ at $E = 1\,\mathrm{eV}$, left, and the absolute error of the Bateman approximation for $M_B = 20$, right. The plot corresponds to the model of Čížek, Horáček, and Domcke [12].

function of the coordinates R and R' and, hence, is much more easily approximated by the Bateman method. For example, at the energy $E = 1.0\,\text{eV}$ the relative error of the third Bateman approximation to $\delta(E, R, R')$ is less than 10^{-7}. This precision highly exceeds the accuracy of any available ab initio calculation providing Γ.

We may conclude this section by saying that the Bateman approximation is well suited for the treatment of the process of DA to HCl molecule and we apply this approach to molecular hydrogen with confidence.

3.2 Dissociative electron attachment to hot hydrogen molecules

It was suggested [14, 15] that the dissociative electron attachment to vibrationally excited molecular hydrogen plays an important role in molecular activated recombination in fusion divertor plasmas. This process is also believed to be the primary source of negative-ion production in low-density hydrogen plasmas [4,22,23]. A vast literature is devoted to the study of DA process in molecular hydrogen, see e.g. [16–22,24,25]. For most recent works see [26] and [27].

In this paper we employ the recent NRM of Čížek et al. [26] for the calculation of the DA cross sections. The calculated DA cross sections for rotationless ($J = 0$) vibrational states of H_2 for initial vibrational states of the target molecule, $v = 4$–15, are plotted in Fig. 2.
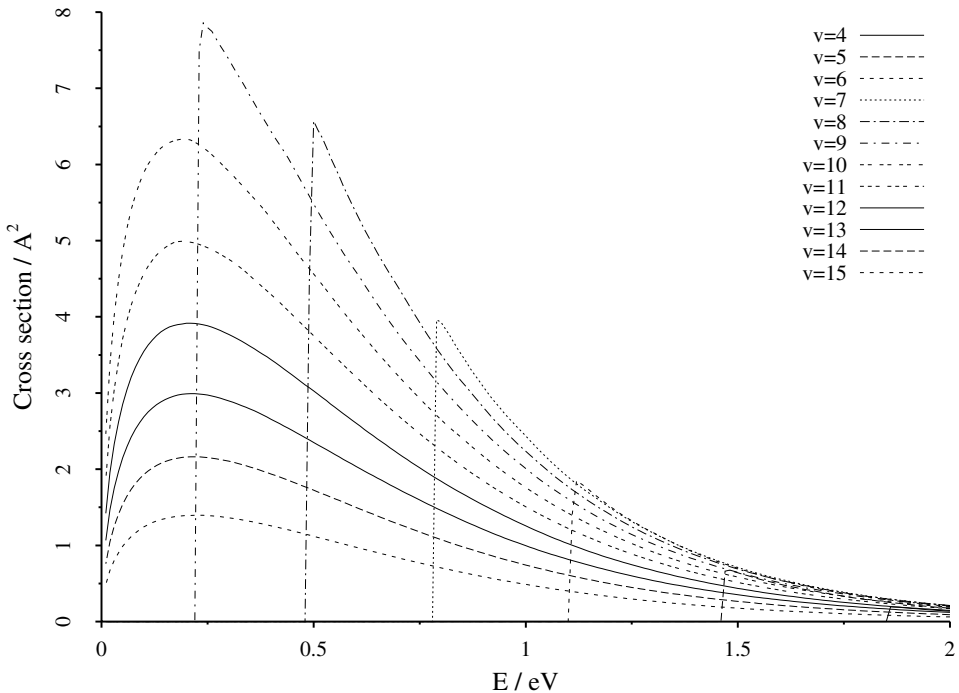

Fig. 2. Cross sections for DA to H_2 for $J = 0$ and $v = 4$–15.

It is seen that the peak value of the DA cross section increases with increasing vibrational quantum number v up to $v = 9$ attaining the highest value of about 8 Å^2; for higher values of v it decreases with increasing v. The cross sections are very smooth functions of energy without pronounced structures. Since H$_2$ molecule has no dipole moment, the DA cross sections show no noticeable Wigner cusps at openings of new vibrational channels.

The calculated DA cross sections are in good agreement with the calculation of Hickman [24], Bardsley and Wadehra, [17] and Launay et al. [21].

The most recent calculation of DA cross sections to highly vibrationally excited molecules H$_2$ ($v = 10$–15) was published by Xu and Fabrikant [27]. Their peak values are by 20-30% higher than the present results. This difference might be attributed partly to the different way of solution of the nuclear dynamics in the resonance state. Our calculation is fully quantum mechanical, whereas the calculation of Xu and Fabrikant [27] is based on the quasiclassical theory of Kalin and Kazansky [28]. The accuracy of the quasiclassical approach is difficult to assess mainly in the threshold region. The difference might be also due to different long-range behavior of their $V_d(R)$ potential.

For astrophysical applications rate constants for the DA process depending on the temperature of the electrons are required. For this the rotational heating of the target molecules must be taken into account. This problem will be deferred to a separate paper.

4   Conclusions

This paper is devoted to the study of the process of dissociative attachment of electrons to diatomic molecules using the nonlocal resonance model. The basic equation of the nonlocal resonance model, which is the most advanced present theory of resonance electron-molecule scattering, leads to the problem of solving Lippmann–Schwinger integral equations with very complicated nonlocal interactions. In this paper the Bateman approximation for treating equations of this type was used and tested. A very stable and robust numerical algorithm based on the use of the Bateman approximation is proposed. It was found that a combination of the Bateman approximation, which is used to approximate the non-separable part of the nonlocal potential, and of the Schwinger–Lanczos algorithm for the remaining part of the interaction, represent a very efficient and precise method for calculation of the DA cross sections. The use of the Bateman approximation as an alternative to the Schwinger–Lanczos algorithm is found to be useful in cases of slow convergence of the Schwinger–Lanczos method.

The Bateman approximation can also be used in the framework of the time-dependent picture (see equations (7) and (8)). Since the threshold exponent α in the coupling $V_{d\epsilon}$ (see (17) and (18)) generally depends on the internuclear distance R, the memory kernel (8) is nonseparable due to integration over energy. The approximation of this kernel by a separable one using the Bateman approximation may significantly accelerate the calculation. The time-dependent approach which is

essential for understanding of the dynamics of the process of DA will be considered in a separate paper.

Summarizing, we can conclude that the Bateman approximation may represent a very efficient numerical technique for solving scattering integral equations of the NRM theory. In this paper the newly developed numerical technique was applied to the calculation of DA cross section for HCl and H_2 molecules in highly vibrationally excited states of the target molecules in good agreement with the available calculations.

References

[1] W. Domcke: Phys. Rep. **208** (1991) 97.

[2] H. Feshbach: Annals of Phys. **19** (1962) 287.

[3] M. Čížek: *Resonant processes in atomic collisions*, PhD thesis, Charles University Prague, 1999.

[4] P.L. Gertitschke and W. Domcke: Phys. Rev. A **47** (1993) 1031.

[5] H. Bateman: Proc. Roy. Soc. London, Ser. A **100** (1922) 441.

[6] H.-D. Meyer, J. Horáček and L.S. Cederbaum: Phys. Rev. A **43** (1991) 3587.

[7] C. Baker: *The Numerical Treatment of Integral Equations*, Clarendon Press, Oxford, 1977.

[8] L.M. Delves and J.L. Mohamed: *Computational Methods for Integral Equations*, Cambridge University Press, Cambridge, 1985.

[9] S.K. Adhikari and K.L. Kowalski: *Dynamical Collision Theory and Its Applications*, Academic Press, Boston, 1991.

[10] W. Domcke and C. Mündel: J. Phys. B **18** (1985) 4491.

[11] L.A. Morgan, P.G. Burke, and C.J. Gillan: J. Phys. B **23** (1990) 99.

[12] M. Čížek, J. Horáček, and W. Domcke: Phys. Rev. A **60** (1999) 2873.

[13] J. Horáček, M. Čížek, and W. Domcke: Theor. Chem. Acc. **100** (1998) 31.

[14] D.E. Post: Nucl. Mater. **143** (1995) 220.
S.I. Krasheninnikov, A.Yu. Pigarov, and D.J. Sigmar: Phys. Lett. A **214** (1996) 285.

[15] N. Ohno, N. Ezumi, S. Takamura, S.I. Krasheninnikov, and A.Yu. Pigarov: Phys. Rev. Lett. **81** (1998) 818.

[16] J.P. Gauyacq: J. Phys. B **18** (1985) 1859.

[17] J.N. Bardsley and J.M. Wadehra: Phys. Rev. A **20** (1979) 1398.

[18] D.E. Atems and J.M. Wadehra: Phys. Rev. A **42** (1990) 5201.

[19] J.M. Wadehra: Phys. Rev. A **29** (1984) 106.

[20] C. Mündel, M. Berman, and W. Domcke: Phys. Rev. A **32** (1985) 181.

[21] J.M. Launay, M. Le Dourneuf, and C.J. Zeippen: Astron. Astrophys. **252** (1991) 842.

[22] J.R. Hiskes: Comments At. Mol. Phys. **19** (1987) 75.

[23] J.R. Hiskes and A.M. Karo: Appl. Phys. Lett. **54** (1989) 508.

[24] A.P. Hickman: Phys. Rev. A **43** (1991) 3495.

[25] D.E. Atems and J.M. Wadehra: J. Phys. B **26** (1993) L759.

[26] M. Čížek, J. Horáček, and W. Domcke: J. Phys. B **31** (1998) 2571.

[27] Y. Xu and I.I. Fabrikant: Appl. Phys. Lett. **78** (2001) 2598.

[28] S.A. Kalin and A.K. Kazansky: J. Phys. B **23** (1990) 4377.