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The hyperbolic matrix method for wave packet treatment of atomic and molecular dynamics

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Abstract. The hyperbolic matrix method for the treatment of atomic and molecular nuclear dynamics is derived by means of the wave packet technique within the Born–Oppenheimer approach formalism. This method allows one to calculate the evolution of a wave packet by means of the product of usual matrices instead of the time propagation of matrix exponentials. We provide a detailed description of this method, considering Tully's model as an example. We also show good agreement with the Landau–Zener model application.

Keywords: wave packet, atomic and molecular collisions, non-adiabatic transitions, nuclear dynamics, matrix exponential

Introduction

The wave packet method is an efficient method of inelastic process investigation. In this method, a wave function evolution is calculated based on a time-dependent Schrodinger equation with initial conditions for a free particle written in the form of a superposition of de Broglie waves, the so-called wave packet. It has been proven that wave packet propagation is an efficient technique for investigating nuclear dynamics in atomic and molecular collisions. There are many investigations of wave packet application for nuclear and molecular collisions: see, for example, (Akpinar, Surucu 2011; Mao et al. 2022; Tully 1990; Vaeck, et al. 1998) and references therein. Time propagation of a wave packet can be calculated by different means: see, e. g., (Balakrishnan et al. 1997). One of them is propagation by an evolution operator and the split-operator method. This approach leads to matrix exponentials, which are a challenge for numerical calculations. Thus, we describe a new method for accomplishing time–evolution calculations without matrix exponentials.

Method

The main equations

The most widely used approach for treating inelastic atomic and molecular collisions, the Born–Oppenheimer approach, splits the total Hamiltonian of a molecule, as well as a collision into two parts: the kinetic energy operator of nucleus motion $\hat{T}_N$ and the electronic Hamiltonian $\hat{H}_e$:

$$\hat{H} = \hat{H}_e + \hat{T}_N \ . \tag{1}$$

In this case, the total wave function $\psi(\vec{R},\vec{r},t)$ of a quasi-molecule can be derived from the time-dependent Schrodinger equation:

$$i\hbar\frac{\partial}{\partial t}\psi(\vec{R},\vec{r},t) = (\hat{H}_e + \hat{T}_N)\psi(\vec{R},\vec{r},t) \ , \tag{2}$$

$\vec{R}$ being the internuclear vector and $\vec{r}$, the electronic coordinates. The wave function $\psi(\vec{R},\vec{r},t)$ can be written as a sum of partial wave functions:

$$\psi(\vec{R},\vec{r},t) = \sum_{J,M_J}\psi_{J,M_J}(\vec{R},\vec{r},t) \ , \tag{3}$$

where J is the quantum number of the total angular momentum of a molecule, and M_J is the quantum number of the projection of the total angular momentum onto the internuclear axis. Each partial wave function satisfies the Schrodinger equation (2). By expanding a partial wave function on the basis of diabatic electronic wave functions $\varphi_j^{di}(\vec{r};R)$, one gets:

$$\psi_{J,M_J}(\vec{R},\vec{r},t) = \sum_j \chi_j(\vec{R},t)\varphi_j^{di}(\vec{r};R) \ , \tag{4}$$

where $\chi_j(\vec{R},t)$ is the nuclear wave function.

The nuclear wave function in Eq. (4) depends on molecule symmetry properties. Let us consider a case of the Σ symmetry. A nuclear wave function can be written as

$$\chi_j(\vec{R},t) = \frac{F_j(R,t)}{R}Y_{J,M_J}(\theta,\varphi) \ , \tag{5}$$

where $F_j(R,t)$ is the radial nuclear wave function and $Y_{J,M_j}(\theta,\varphi)$, the spherical nuclear wave function. Then the partial wave function reads:

$$\psi_{J,M_J}(\vec{R},\vec{r},t) = \sum_j \frac{F_j(R,t)}{R}Y_{J,M_J}(\theta,\varphi)\varphi_j^{di}(\vec{r};R) \ . \tag{6}$$

By substituting the partial wave function into Eq. (2), multiplying by a complex conjugate wave function $\left(\varphi_k^{di}(\vec{r};R)\right)^*$ and integrating over the electronic coordinates, one obtains a system of differential equations:

$$i\hbar\frac{\partial F_k(R,t)}{\partial t} = \left(-\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial R^2} + \frac{\hbar^2}{2\mu}\frac{J(J+1)}{R^2} + H_{kk}\right)F_k(R,t) + \sum_{j\neq k}F_j(R,t)H_{kj} \ , \tag{7}$$

where $H_{kj} = \langle\varphi_k^{di}(\vec{r};R)|\hat{H}_e|\varphi_j^{di}(\vec{r};R)\rangle$ is an element of the Hamiltonian matrix and μ is a reduced mass.

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Let us write the system of differential equations (7) in the matrix form:

$$\dot{\boldsymbol{F}} = (\boldsymbol{T} + \boldsymbol{H})\boldsymbol{F} \tag{8}$$

where $\dot{\boldsymbol{F}} = (\partial F_1(R,t)/\partial t, \dots, \partial F_n(R,t)/\partial t)^T$, $\boldsymbol{F} = \left(F_1(R,t), \dots, F_n(R,t)\right)^T$,

$$[\boldsymbol{T}]_{kj} = \left(-\frac{i}{\hbar}\frac{\hbar^2\hat{k}^2}{2\mu}\right)\delta_{kj}, \qquad [\boldsymbol{H}]_{kj} = -\frac{i}{\hbar}\left(\frac{\hbar^2}{2\mu}\frac{J(J+1)}{R^2}\right)\delta_{kj} - \frac{i}{\hbar}H_{kj}\,. \tag{9}$$

The solution can be written as a matrix exponential:

$$\boldsymbol{F} = e^{(\boldsymbol{T}+\boldsymbol{H})t}\boldsymbol{F_0}\,, \tag{10}$$

$\boldsymbol{F_0} = \left(F_1(R,0), \dots, F_n(R,0)\right)^T$ being the vector of initial functions.

The main problem is in the calculation of a derivative of $\hat{k}$ in the matrix exponent. The point is that the matrix exponential of a sum of two matrices is not equal to a product of two matrix exponentials because the matrices do not commute. The split-operator method (Balakrishnan et al. 1997) solves this by splitting the matrix exponential into three terms:

$$e^{(\boldsymbol{T}+\boldsymbol{H})t} = e^{\frac{\boldsymbol{H}}{2}t}e^{\boldsymbol{T}t}e^{\frac{\boldsymbol{H}}{2}t} + O(t^3) \approx e^{\frac{\boldsymbol{H}}{2}t}e^{\boldsymbol{T}t}e^{\frac{\boldsymbol{H}}{2}t}\,. \tag{11}$$

Thus, one can multiply the function on each matrix exponential one by one in the coordinate and momentum spaces. It allows one to treat $\hat{k}$ as a number, not as a derivative. Finally, the algorithm is the following:

1. $\boldsymbol{G}^{st.1} = e^{\frac{\boldsymbol{H}}{2}t}\boldsymbol{F_0}$;
2. $\boldsymbol{D}^{st.2} = FT[\boldsymbol{G}^{st.1}]$;
3. $\boldsymbol{D}^{st.3} = e^{\boldsymbol{T}t}\boldsymbol{D}^{st.2}$;
4. $\boldsymbol{G}^{st.4} = IFT[\boldsymbol{D}^{st.3}]$;
5. $\boldsymbol{F} = e^{\frac{\boldsymbol{H}}{2}t}\boldsymbol{G}^{st.4}$,

where $\boldsymbol{G}^{st.N}$ is the vector of the N-step wave function in the coordinate space, $\boldsymbol{D}^{st.N}$ is the vector of the N-step wave function in the momentum space; FT is the Fourier transform and IFT is the inverse Fourier transform. For numerical calculations, the Fast Fourier transform algorithm can be used.

The initial condition is set up as follows. The wave function of the initial state can be chosen in the form of a wave packet:

$$W(R,0) = \left(\frac{1}{a\sqrt{\pi}}\right)^{1/2} e^{-\frac{1}{2}\left(\frac{R-R_0}{a}\right)^2 + ik_0R}\,, \tag{12}$$

where a is the coefficient of the wave packet width, R_0, the center of the wave packet and k_0, the average momentum of the wave packet.

The hyperbolic matrix method

In practice, there is a problem of getting a matrix exponential. There are different methods and algorithms for this: The Taylor approximation, the Pade approximation, the scaling and squaring method (Al-Mohy, Higham 2010; 2011), etc. It is also possible to use the hyperbolic matrix method.

The method is based on the expansion of a matrix exponential by Taylor series and is valid for symmetric matrices. Off-diagonal Hamiltonian diabatic matrix elements should be equal for this method.

Let us consider the case of the matrix (2 × 2) :

$$\boldsymbol{A} = \begin{pmatrix} a & c \\ c & b \end{pmatrix}, \tag{13}$$

the matrix exponential $e^{\boldsymbol{A}}$ is defined as:

$$e^{\boldsymbol{A}} = \sum_{k=0}^{\infty} \frac{1}{k!} \boldsymbol{A}^k . \tag{14}$$

The matrix exponential $e^{\boldsymbol{A}}$ can be accepted as a multiplication of three matrix exponentials using a method similar to the split-operator method and with the same precision:

$$e^{\boldsymbol{A}} \approx e^{\frac{\boldsymbol{C}}{2}} e^{\boldsymbol{B}} e^{\frac{\boldsymbol{C}}{2}}, \tag{15}$$

where

$$\frac{\boldsymbol{C}}{2} = \begin{pmatrix} 0 & \frac{c}{2} \\ \frac{c}{2} & 0 \end{pmatrix}, \tag{16}$$

$$\boldsymbol{B} = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}. \tag{17}$$

Then the matrix exponentials $e^{\boldsymbol{B}}$ and $e^{\frac{\boldsymbol{C}}{2}}$ read:

$$e^{\boldsymbol{B}} = \sum_{k=0}^{\infty} \frac{1}{k!} \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}^k, \tag{18}$$

$$e^{\frac{\boldsymbol{C}}{2}} = \sum_{k=0}^{\infty} \frac{1}{k!} \begin{pmatrix} 0 & \frac{c}{2} \\ \frac{c}{2} & 0 \end{pmatrix}^k . \tag{19}$$

There is the following rule for raising matrices to powers:

$$\begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}^k = \begin{pmatrix} a^k & 0 \\ 0 & b^k \end{pmatrix} \tag{20}$$

and

$$\begin{pmatrix} 0 & \frac{c}{2} \\ \frac{c}{2} & 0 \end{pmatrix}^k = \begin{cases} \begin{pmatrix} \left(\frac{c}{2}\right)^k & 0 \\ 0 & \left(\frac{c}{2}\right)^k \end{pmatrix}, & k = 2n, \ \ n \in \mathbb{N}; \\ \begin{pmatrix} 0 & \left(\frac{c}{2}\right)^k \\ \left(\frac{c}{2}\right)^k & 0 \end{pmatrix}, & k = 2n+1, \ \ n \in \mathbb{N}. \end{cases} \tag{21}$$

Thus, for $e^{\boldsymbol{B}}$ we have the following:

$$e^{\boldsymbol{B}} = \begin{pmatrix} \sum_{k=0}^{\infty} \frac{1}{k!} a^k & 0 \\ 0 & \sum_{k=0}^{\infty} \frac{1}{k!} b^k \end{pmatrix} = \begin{pmatrix} e^a & 0 \\ 0 & e^b \end{pmatrix}, \tag{22}$$

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and for $e^{\frac{C}{2}}$ the matrix reads:

$$e^{\frac{C}{2}} = \begin{pmatrix} \sum_{k=0}^{\infty} \frac{1}{2k!}\left(\frac{C}{2}\right)^{2k} & \sum_{k=0}^{\infty} \frac{1}{(2k+1)!}\left(\frac{C}{2}\right)^{2k+1} \\ \sum_{k=0}^{\infty} \frac{1}{(2k+1)!}\left(\frac{C}{2}\right)^{2k+1} & \sum_{k=0}^{\infty} \frac{1}{2k!}\left(\frac{C}{2}\right)^{2k} \end{pmatrix}, \tag{23}$$

$$e^{\frac{C}{2}} = \begin{pmatrix} cosh\left(\frac{C}{2}\right) & sinh\left(\frac{C}{2}\right) \\ sinh\left(\frac{C}{2}\right) & cosh\left(\frac{C}{2}\right) \end{pmatrix}. \tag{24}$$

This method allows one to move from the matrix exponential to a usual matrix. This finding is strict because the Taylor series are exact.

Thus, returning to the solution (10), one can see that the matrix exponential should be split into the following three matrix exponentials:

$$e^{(\boldsymbol{T}+\boldsymbol{H})t} = e^{\frac{\boldsymbol{H_{od}}}{2}t} e^{(\boldsymbol{T}+\boldsymbol{U})t} e^{\frac{\boldsymbol{H_{od}}}{2}t} + O(t^3) \approx e^{\frac{\boldsymbol{H_{od}}}{2}t} e^{(\boldsymbol{T}+\boldsymbol{U})t} e^{\frac{\boldsymbol{H_{od}}}{2}t} \tag{25}$$

where

$$[\boldsymbol{H_{od}}]_{kj} = -\frac{i}{\hbar} H_{kj}(1-\delta_{kj}), \tag{26}$$

$$[\boldsymbol{U}]_{kj} = -\frac{i}{\hbar}\left(\frac{\hbar^2}{2\mu}\frac{J(J+1)}{R^2} + H_{kj}\right)\delta_{kj}, \qquad [\boldsymbol{T}]_{kj} = \left(-\frac{i}{\hbar}\frac{\hbar^2\hat{k}^2}{2\mu}\right)\delta_{kj}. \tag{27}$$

Then the split-operator method can be applied to the central matrix exponential of Eq. (25):

$$e^{(\boldsymbol{T}+\boldsymbol{H})t} \approx e^{\frac{\boldsymbol{H_{od}}}{2}t} e^{\frac{\boldsymbol{U}}{2}t} e^{\boldsymbol{T}t} e^{\frac{\boldsymbol{U}}{2}t} e^{\frac{\boldsymbol{H_{od}}}{2}t}. \tag{28}$$

Using the hyperbolic matrix method for external matrix exponentials and taking into account that $H_{12} = H_{21}$, we get:

$$e^{(\boldsymbol{T}+\boldsymbol{H})t} = \boldsymbol{H_y U_e T_e U_e H_y}, \tag{29}$$

where

$$[\boldsymbol{U_e}]_{kj} = \exp\left(-\frac{1}{2}\frac{i}{\hbar}t\left(\frac{\hbar^2}{2\mu}\frac{J(J+1)}{R^2} + H_{kj}\right)\right)\delta_{kj}, \tag{30}$$

$$[\boldsymbol{T_e}]_{kj} = \exp\left(\left(-\frac{i}{\hbar}t\frac{\hbar^2\hat{k}^2}{2\mu}\right)\right)\delta_{kj}, \tag{31}$$

$$[\boldsymbol{H_y}]_{kj} = \begin{cases} cosh\left(-\frac{i}{\hbar}t\frac{H_{12}}{2}\right), & k = j; \\ sinh\left(-\frac{i}{\hbar}t\frac{H_{12}}{2}\right), & k \neq j. \end{cases} \tag{32}$$

Finally, the solution (10) can be written as:

$$\boldsymbol{F} = \boldsymbol{H_y U_e T_e U_e H_y F_0}. \tag{33}$$

Thus, we found that the final solution, which was initially expressed via the matrix exponential, see Eq. (10), can be calculated as a product of the number of usual matrices without any matrix exponential, see Eq. (33).

Extension and generalization of the hyperbolic matrix method

Simplicity of the hyperbolic matrix method is marred by the heavy calculations it requires. The key point of the matrix exponential method is to express $e^{\boldsymbol{A}}$, $\boldsymbol{A}$ being a symmetric $(N \times N)$ matrix, via a multiplication of $2C_N^2 + 1$ matrices, where C_n^k is the combination number.

Assume $\boldsymbol{A}$ contains $a_{jk} = a_{kj}$, then

$$e^{\boldsymbol{A}} = \left(\prod_{m=1}^{N-1}\prod_{n>m}^{N}(\boldsymbol{I} + \boldsymbol{C^{mn}})\right)\boldsymbol{B}\left(\prod_{m=N-1}^{1}\prod_{n>m}^{N}(\boldsymbol{I} + \boldsymbol{C^{mn}})\right), \tag{34}$$

where $\boldsymbol{I}$ is the identity matrix, and

$$[\boldsymbol{C^{mn}}]_{jk} = \left(\delta_{jm}\delta_{kn} + \delta_{km}\delta_{jn}\right)\sinh\left(\frac{a_{mn}}{2}\right) + \delta_{jk}\left(\delta_{jn} + \delta_{jm}\right)\left(\cosh\left(\frac{a_{mn}}{2}\right) - 1\right), \tag{35}$$

$$[\boldsymbol{B}]_{jk} = \delta_{jk}e^{a_{jk}}. \tag{36}$$

The formula (34) is obtained by repeating the split-operator method C_N^2 times.

Application example

Tully's model (Tully 1990) is an analytic two diabatic-state model with a non-adiabatic region. The model can be used to demonstrate a possible application of the wave packet method for investigating an inelastic collision process. Tully's article contains three different models: with a single non-adiabatic region; with a pair of adiabatic regions; and with an extended coupling with reflection. We performed a test calculation for the first model with a single adiabatic region (fig. 1).

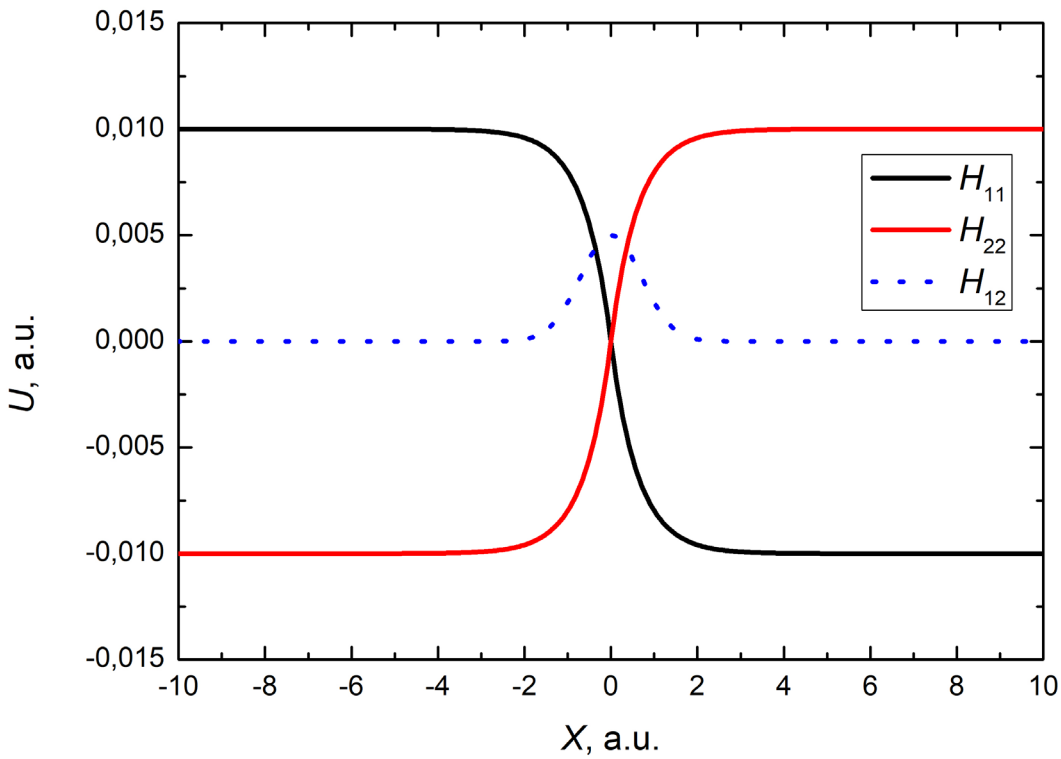

Fig. 1. Diabatic potentials and off-diagonal Hamiltonian matrix element as a function of the scattering coordinate. The solid black line is the first potential, the solid red line is the second potential, and the dotted blue line is the off-diagonal Hamiltonian matrix element

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The potentials and off-diagonal Hamiltonian matrix element are determined as

$$H_{11} = \begin{cases} A(1 - e^{-Bx}), & x > 0; \\ -A(1 - e^{Bx}), & x < 0, \end{cases} \tag{37}$$

$$H_{22} = -H_{11}, \tag{38}$$

$$H_{12} = H_{21} = Ce^{-Dx^2}, \tag{39}$$

where A, B, C and D are some parameters and x is the coordinate used in the model. The diabatic higher asymptotic state was chosen as the initial channel. We used the following values for the above parameters: A = 0.01, B = 1.6, C = 0.005 and D = 1.

The initial wave function was taken as a wave packet (12) with the following parameters: $a = 20/k_0$ and m = 2000. The case was investigated for a range of 3.0 a.u. ≤ k ≤ 50 a.u. that corresponds to a collision energy of 0.00225 a.u. ≤ E_{col} ≤ 0.625 a.u or 0.0612 eV ≤ E_{col} ≤ 17 eV.

The hyperbolic matrix method was used for wave packet propagation. Probability was calculated by the reactive flux method (Balakrishnan et al. 1997; Neuhauser et al. 1991), which allows one to analyze the outgoing flux of the wave packet towards the asymptotic channel, where the flux is equal to

$$j(\tilde{x}, t) = \frac{\hbar}{m} \mathrm{Im} \left(F^*(x, t) \frac{\partial F(x, t)}{\partial x} \right)_{x=\tilde{x}}, \tag{40}$$

then

$$P = \int_0^\infty j(\tilde{x}, t) dt \ . \tag{41}$$

The main advantage of flux methods is that in order to calculate the outgoing flux, the wave function should be known only at one point $\tilde{x}$. The method provides nonadiabatic transition probability as a function of the average wave packet momentum k_0.

The results of the wave packet calculations of the nonadiabatic transition probabilities have been compared with the probabilities calculated by the Landau–Zener model:

$$P_{12} \approx e^{-\frac{2\pi H_{12}^2}{\left(\frac{dH_{11}}{dx} - \frac{dH_{22}}{dx}\right)v}}, \tag{42}$$

where $v = \frac{\hbar k_0}{m}$. The Landau–Zener probability is calculated at the point $\tilde{x} = 0$, which gives the following expression according to Eqs. (37)–(39):

$$P_{12} = e^{-\frac{\pi C^2}{ABv}}. \tag{43}$$

Note that probability does not depend on the parameter D, see Eq. (39). The comparison of the calculated probabilities is presented in Fig. 2.

As follows from this figure, the results for Tully's model agree well with each other, which proves the reliability and efficiency of the hyperbolic matrix method for wave packet propagation.

Conclusions

In conclusion, an inelastic collision can be treated by the time-dependent Schrodinger equation, which can be resolved by means of a matrix exponential. The hyperbolic matrix method is a way to solve the Schrodinger equation by transforming the matrix exponential into a usual matrix. This allows one to avoid calculating matrix exponentials. The simplicity of computing a usual matrix instead of a matrix exponential is one of the advantages of the method. Its disadvantage is a rapid increase in the number of matrix multiplications with an increase in the matrix dimension leading to heavy calculations. Thus, the hyperbolic matrix method works well for low-dimensional systems. An application example for

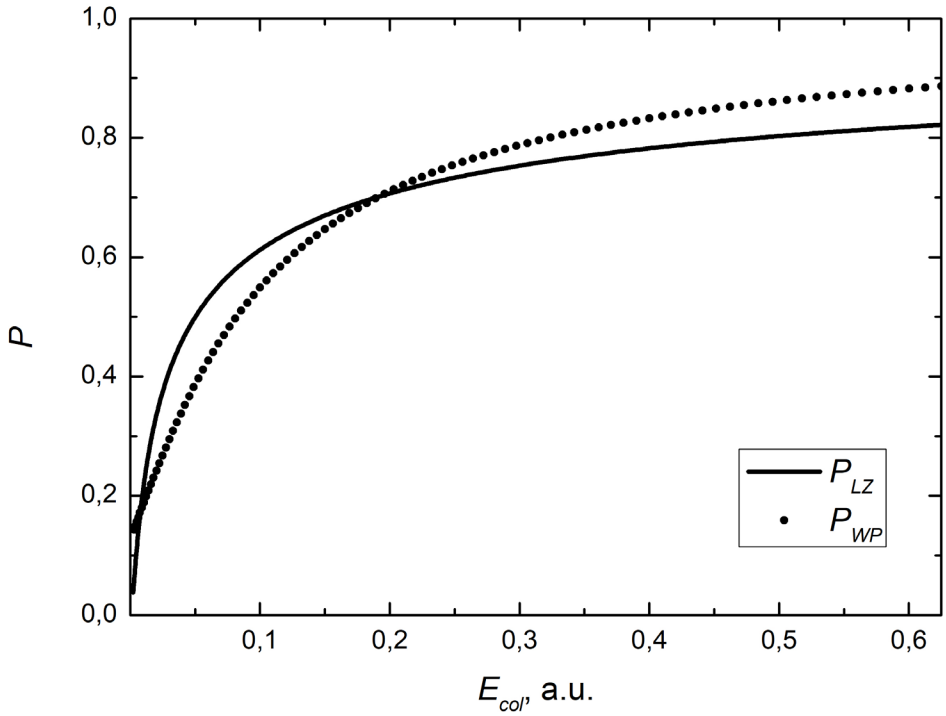

Fig. 2. Probabilities for transitions from higher to low diabatic states. The solid line represents the Landau–Zener probability while the circle symbols stand the wave-packet probabilities

Tully's model shows the method provides a good agreement with results of Landau-Zener model applications, and finally, applicability of the hyperbolic matrix method to other collision systems. In addition, it is worth emphasizing that the hyperbolic matrix method can be employed in other problems where matrix exponentials are used.

Conflict of Interest

The authors declare that there is no conflict of interest, either existing or potential.

Author Contributions

The authors have made an equal contribution to the paper.

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