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WAVE PACKET EVOLUTION SCHEME TO IONIZATION OF ATOMS AND MOLECULES BY FAST ELECTRONS

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1 Introduction

New experimental methods, particularly, based on the multiple coincidence detection technique [1, 2, 3] stimulate the interest to fundamental theoretical studies of the dissociative ionization of diatomic molecules by electron impact. In this context the molecular hydrogen ion can be considered as the basic system in which the removal of the unique electron causes dissociation. Substantial theoretical analysis of the dissociative ionization of H_2^+ by fast electrons was recently carried out in [4]. As mentioned in [4], the crucial point of calculating the cross-section of such processes is that no closed exact analytical wave functions of the continuum states exist. In [4] the final-state wave function of the ejected electron was found by taking a product of two approximate functions that take into account the two scattering centers. To improve the calculation it seems straightforward to obtain these functions with the exact numerical solutions of the two-center continuum problem. However, this approach involves a cumbersome procedure of calculating multi-dimensional integrals of the functions presented numerically that requires huge computer facilities and may cause additional computational problems. It seems reasonable to search for direct computational approaches, in which the basis of exact two-center continuum wave functions is not involved. Note that the potential advantage of such methods is that they could be generalized over a wider class of two-center systems starting from the molecular hydrogen ion as a test object. In the present paper we develop a direct approach to the ionization of hydrogen molecular ion by fast electrons that involves the reduction of the initial 6D Schrödinger equation to a 3D evolution problem followed by modeling of the wave packet dynamics.

Here we develop and apply a direct approach to the calculation of the angular distribution of scattered and ejected electrons that involves the reduction of the initial 6D Schrödinger equation to a 3D evolution problem followed by modeling of the wave packet dynamics. The approach does not make use of the basis of stationary Coulomb two-center functions of the continuous spectrum for the ejected

electron, whose proper choice is a crucial point of other model calculations. Our approach can be considered as the linearized version of the phase function method [5] for the multi-dimensional scattering problem. The evolution problem is solved using the method based on the split-step technique with complex scaling, recently proposed by us and tested in paraxial optics [7]. In the present paper the method as a whole is also tested using the well known problem of electron scattering by hydrogen atom [6].
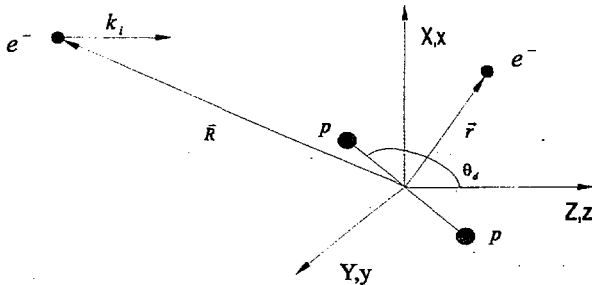

Figure 1: Coordinate frame

2   Basic equations

The 6D stationary Schrödinger equation for the scattering problem which describes two electrons in the field of two fixed protons

$$\left[H_0(\vec{r}) - \frac{1}{2}\nabla_{\vec{R}}^2 + V(\vec{r}, \vec{R}) \right] \Psi(\vec{r}, \vec{R}) = \left(\frac{k_i^2}{2} + E_0 \right) \Psi(\vec{r}, \vec{R}), \qquad (1)$$

where $\vec{r}$ is the radius-vector of the electron initially bound in H_2^+ and finally ejected, $\vec{R}$ is the radius-vector of the impact electron, k_i is the momentum of the incident electron, $-E_0$ is the ionization potential, $\hat{H}_0 = -\frac{1}{2}\nabla_{\vec{r}}^2 + U(\vec{r})$ is Hamiltonian of ejected electron in the field of two protons, $V(\vec{r}, \vec{R}) = U(\vec{R}) + U_{int}(\vec{r}, \vec{R})$ is the interaction between the impact electron and molecular ion, $U(\vec{r}) = -1/r_1 - 1/r_2$ is the attractive potential between the ejected electron and the protons, $U(\vec{R}) =$

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$-1/R_1 - 1/R_2$ is one for scattered electron, the distances from nuclei to ejected and scattered electrons are $r_1 = |\vec{r} - \vec{r}_{1p}|$, $r_2 = |\vec{r} - \vec{r}_{2p}|$ and $R_1 = |\vec{R} - \vec{r}_{1p}|$, $R_2 = |\vec{R} - \vec{r}_{2p}|$, where $\vec{r}_{ip}$ is the radius-vector of the i-th proton, $U_{int}(\vec{r}, \vec{R}) = 1/|\vec{r} - \vec{R}|$ is the repulsive potential of interaction between the electrons [4]. The origin of the coordinate frame is chosen in the center of symmetry of the molecular ion with the Z and z axis directed along the momentum of the incident electron.

Let us seek the solution of Eq.(1) in the form

$$\Psi(\vec{r}, X, Y, Z) = \psi(\vec{r}, \vec{R}_\perp, Z) \exp(ik_i Z).$$

Under the condition that $(k_e^2 + k_\perp^2 - 2E_0)/k_i^2 << 1$ one can neglect the second derivative of ψ with respect to Z. As a result we get the evolution-like equation for the envelope function $\psi(\vec{r}, \vec{R}_\perp, Z)$

$$ik_i \frac{\partial \psi(\vec{r}, \vec{R}_\perp, Z)}{\partial Z} = \left\{ \hat{H}_0(\vec{r}) - \frac{1}{2}\nabla^2_{\vec{R}_\perp} - E_0 + V(\vec{r}, \vec{R}) \right\} \psi(\vec{r}, \vec{R}_\perp, Z). \tag{2}$$

Neglecting the large-angle scattering one can write the initial condition for ψ as

$$\psi(\vec{r}, \vec{R}_\perp, -\infty) = \psi_0(\vec{r}). \tag{3}$$

To solve the 5D Schrödinger evolution equation(2) we use Fourier transformation with respect to the variable $\vec{R}_\perp$

$$\psi(\vec{r}, \vec{R}_\perp, Z) = \frac{1}{2\pi} \int \psi_{\vec{k}_\perp}(\vec{r}, Z) \exp(i\vec{k}_\perp \vec{R}_\perp) d\vec{R}_\perp. \tag{4}$$

Then Eq.(2) takes the form

$$ik_i \frac{\partial \psi_{\vec{k}_\perp}(\vec{r}, Z)}{\partial Z} = \left\{ \hat{H}_0(\vec{r}) + \left(\frac{k_\perp^2}{2} - E_0 \right) \right\} \psi_{\vec{k}_\perp}(\vec{r}, Z) + \frac{1}{(2\pi)^2} \int V_{\vec{k}_\perp \vec{k}'_\perp}(\vec{r}, Z) \psi_{\vec{k}'_\perp}(\vec{r}, Z) d\vec{k}'_\perp, \tag{5}$$

where

$$V_{\vec{k}_\perp \vec{k}'_\perp}(\vec{r}, Z) = \int \exp(-i(\vec{k}_\perp - \vec{k}'_\perp)\vec{R}_\perp) V(\vec{r}, \vec{R}_\perp, Z) d\vec{R}_\perp \tag{6}$$

is the Fourier transform of the interaction potential $V(\vec{r}, \vec{R}_\perp, Z)$.

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Further simplification of the problem is possible if the amplitude of the incident wave is much greater than that of the scattered wave. In this case one can put

$$\psi_{\vec{k}_\perp}(\vec{r}, Z) = \delta(\vec{k}_\perp)\psi_0(\vec{r}) \tag{7}$$

in the integral term of Eq.(5). As a result we get the inhomogeneous equation

$$ik_i\frac{\partial\psi_{\vec{k}_\perp}(\vec{r}, Z)}{\partial Z} = \left\{\hat{H}_0(\vec{r}) + \left(\frac{k_\perp^2}{2} - E_0\right)\right\}\psi_{\vec{k}_\perp}(\vec{r}, Z) + \frac{1}{(2\pi)^2}V_{\vec{k}_\perp}(\vec{r}, Z)\psi_0(\vec{r},) \tag{8}$$

where $V_{\vec{k}_\perp}(\vec{r}, Z) = V_{\vec{k}_\perp\vec{0}}(\vec{r}, Z)$, with the initial condition $\psi_{\vec{k}_\perp}(\vec{r}, -\infty) = 0$.

To calculate the integral with respect to transverse variables in the expression for $V_{\vec{k}_\perp}(\vec{r}, Z)$ it is easier to start from the known integral

$$\int \exp(-i\vec{k}\vec{R})\frac{1}{R}d\vec{R} = \frac{4\pi}{k^2} = \frac{4\pi}{k_Z^2 + k_\perp^2}. \tag{9}$$

Carrying out the inverse Fourier transformation

$$\int_{-\infty}^{\infty} \exp(ik_Z Z)\frac{dk_Z}{k_Z^2 + k_\perp^2} = \frac{\pi}{k_\perp}e^{-k_\perp|Z|}, \tag{10}$$

For molecular ion one gets

$$V_{\vec{k}_\perp}(\vec{r}, Z) = \frac{2\pi}{k_\perp}\left\{-\left[e^{-k_\perp|Z-d_Z|-i\vec{k}_\perp\vec{d}_\perp} + e^{-k_\perp|Z+d_Z|+i\vec{k}_\perp\vec{d}_\perp}\right] + e^{-k_\perp|Z-z|-i\vec{k}_\perp\vec{r}_\perp}\right\}. \tag{11}$$

Here $k_\perp = k_i\sin\theta_s$ is the transverse momentum component of the scattered electron, θ_s is the scattering angle, $\pm\vec{d}$ are the positions of the nuclei with respect to the center of symmetry, $\vec{d} = \frac{\vec{r}_{p2}-\vec{r}_{p1}}{2}$. Note that the first two terms in (11) determine the elastic scattering of the incident electron by the nuclei.

Due to the exponential decrease of the source term with $|Z|$ the integration may be actually carried out within a certain finite interval $(-Z_{max}, Z_{max})$. Hence the zero initial condition should be imposed at the point $-Z_{max}$.

Note that the approximation (7) is actually equivalent to the first Born approximation [6]. Multiply Eq.(8) by the complex conjugate function of the continuous spectrum of $\hat{H}_0$ and integrate over all $\vec{r}$. Then

$$ik_i\frac{dC_{\vec{k}_\perp}(\vec{k}_e, Z)}{dZ} = \left\{\frac{k_e^2}{2} + \frac{k_\perp^2}{2} - E_0\right\}C_{\vec{k}_\perp}(\vec{k}_e, Z) + \frac{1}{(2\pi)^2}\int \psi^*(\vec{k}_e, \vec{r})V_{\vec{k}_\perp}(\vec{r}, Z)\psi_0(\vec{r})d\vec{r}, \tag{12}$$

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where

$$C_{\vec{k}_\perp}(\vec{k}_e, Z) = \int \psi^*(\vec{k}_e, \vec{r})\psi_{\vec{k}_\perp}(\vec{r}, Z)d\vec{r}$$

is the probability density amplitude for the transition of the initially bound electron into the state with the momentum $\vec{k}_e$. Let us substitute

$$C_{\vec{k}_\perp}(\vec{k}_e, Z) = \tilde{C}_{\vec{k}_\perp}(\vec{k}_e, Z)\exp(ik_Z Z),$$

where k_Z is the increment of the longitudinal component of the momentum of the impact electron determined by the relation

$$k_Z = -\frac{1}{k_i}\left(\frac{k_e^2}{2} + \frac{k_\perp^2}{2} - E_0\right). \tag{13}$$

This relation is actually equivalent to the energy conservation law written neglecting the terms of the order of k_Z^2. The substitution yields

$$ik_i\frac{d\tilde{C}_{\vec{k}_\perp}(\vec{k}_e, Z)}{dZ} = \frac{1}{(2\pi)^2}\exp(-ik_Z Z)\int \psi^*(\vec{k}_e, \vec{r})V_{\vec{k}_\perp}(\vec{r}, Z)\psi_0(\vec{r})d\vec{r}, \tag{14}$$

and

$$\tilde{C}_{\vec{k}_\perp}(\vec{k}_e, \infty) = \frac{1}{ik_i(2\pi)^2}\int\int e^{-i(\vec{k}_s - \vec{k}_i)\vec{R}}\psi^*(\vec{k}_e, \vec{r})V(\vec{r}, \vec{R})\psi_0(\vec{r})d\vec{r}d\vec{R}, \tag{15}$$

where $\vec{k}_s = \vec{k}_i - \vec{K}$ is the momentum of the scattered electron, $\vec{K} = (-k_X, -k_Y, -k_Z)$ is the momentum transfer.

Provided that the ejected electron has the momentum $\vec{k}_e$, the asymptotic form of the solution of Eq. (1) for the wave function of the scattered electron when $R \to \infty$ is

$$\Psi^{as}_{\vec{k}_e}(\vec{R}) = \exp(ik_i Z) + \frac{\exp(ik_s R)}{R}f_{\vec{k}_e}(\theta_s, \phi_s). \tag{16}$$

The scattering differential cross-section(DCS) can be then expressed as

$$\sigma_{\vec{k}_e}(\theta_s, \phi_s) = \frac{k_e k_s}{k_i}\left|f_{\vec{k}_e}(\theta_s, \phi_s)\right|^2, \tag{17}$$

On the other hand, the asymptotic form of the wave function resulting from the solution of Eq.(8) under the condition $Z \to \infty$ can be presented as

$$\Psi^{as}_{\vec{k}_e}(\vec{R}) = \exp(ik_i Z) + \exp(ik_i Z)\int \tilde{C}_{\vec{k}_\perp}(\vec{k}_e, \infty)\exp(i\vec{k}_\perp\vec{R}_\perp + ik_Z Z)d\vec{k}_\perp. \tag{18}$$

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Making use of the fact that the integrand has a stationary point we finally get

$$\Psi_{\vec{k}_e}^{as}(\vec{R}) = \exp(ik_i Z) + \frac{1}{Z}\exp\left\{i\left(k_i - \frac{k_e^2/2 - E_0}{k_i}\right)Z + i\frac{k_i}{2Z}R_\perp^2\right\}(-2\pi i k_i)\tilde{C}_{\vec{k}_\perp^0}(\vec{k}_e,\infty),(19)$$

where $\vec{k}_\perp^0 = k_i\sin\theta_s(\cos\phi_s,\sin\phi_s)$, $R_\perp = R\sin\theta_s$, $Z = R\cos\theta_s$. The expression (18) agrees with (16) within the accuracy of the order of θ_s^2 if we set

$$f_{\vec{k}_e}(\theta_s,\phi_s) = -2\pi i k_i\tilde{C}_{\vec{k}_\perp^0}(\vec{k}_e,\infty) = -\frac{1}{2\pi}\int\int e^{-i(\vec{k}_s-\vec{k}_i)\vec{R}}\psi^*(\vec{k}_e,\vec{r})V(\vec{r},\vec{R})\psi_0(\vec{r})d\vec{r}d\vec{R}.$$
$$(20)$$

The latter expression is similar to the formula for $f_{\vec{k}_e}(\theta_s,\phi_s)$ derived in [6] using the first Born approximation.

3   Calculation of the angular distribution

The asymptotic expression of the radial part of the wave function corresponding to the continuous spectrum of $\hat{H}_0$ can be written as

$$\psi_E^{as}(r,t) = \frac{1}{\sqrt{v(r)\,r}}\exp\left(-iEt + i\int_{r_0}^r v(r')dr'\right) \tag{21}$$

where $t = Z/k_i$ is the evolution variable, $v(r) = \sqrt{2(E - U^{as}(r))}$, $E = \frac{k_e^2}{2} + \frac{k_i^2}{2} - E_0$, $U^{as}(r) = -Z'/r$, $Z' = 2$ is charge of two protons, $0 \ll r_0 < r_{max}$. In the asymptotic limit one can take only the radial component of the momentum of the ejected electron into account. Then, according to [8], the expression for calculating the amplitude $A(k,\theta,\phi)$ takes the form

$$A_{\vec{k}_\perp}(k_e,\theta_e,\phi_e) = \frac{1}{\sqrt{2\pi}}\int_{t_0}^{t_1} dt' j(\psi_{\vec{k}_\perp}(r,\theta,\phi,t'),\psi_E^{as}(r,t'))\Big|_{r=r_{max}}, \tag{22}$$

where

$$j(\Psi,\Phi) = \frac{i}{2}\left\{\Psi\,r^2\frac{\partial\Phi^*}{\partial r} - \Phi^*\,r^2\frac{\partial\Psi}{\partial r}\right\}, \tag{23}$$

is the flux introduced in [8], $t_0 = -Z_{max}/k_i$ and $t_1 >> Z_{max}/k_i$. The approximate relation (22) becomes exact when $t_1 \to +\infty$ and simultaneously $r_{max} \to +\infty$.

The amplitudes defined by (22) are related with the coefficients introduced in Eq.(15) by

$$\left| A_{\vec{k}_\perp}(k_e, \theta_e, \phi_e) \right|^2 = k_e \left| \tilde{C}_{\vec{k}_\perp}(\vec{k}_e, \infty) \right|^2 \tag{24}$$

Using (17),(20) and (24) we get the final expression for the differential cross-section

$$\sigma_{\vec{k}_e}(\theta_s, \phi_s) = (2\pi)^2 k_s k_i \left| A_{\vec{k}_\perp}(k_e, \theta_e, \phi_e) \right|^2. \tag{25}$$

In the region where $r > r_{max}$ we made use of the complex scaling technique [9] to suppress the non-physical reflection from the grid boundary.

4 Numerical scheme

The inhomogeneous Schrödinger equation in spherical coordinates (here axis of coordinate system $z' \parallel \vec{d}$) after the substitution $\Psi(r, \theta, \phi, t) = r\psi(r, \theta, \phi, t)$ and replace $\eta = \cos\theta$ can be written as

$$i\frac{\partial \Psi(r, \eta, \phi, t)}{\partial t} = \hat{H}_0 \Psi(r, \eta, \phi, t) + F(r, \eta, \phi, t), \tag{26}$$

where Hamiltonian reads as

$$\hat{H}_0 = -\frac{1}{2}\left[\frac{\partial^2}{\partial r^2} + \frac{1}{r^2}\left(\frac{\partial}{\partial \eta}(1-\eta^2)\frac{\partial}{\partial \eta} + \frac{1}{1-\eta^2}\frac{\partial^2}{\partial \phi^2}\right)\right] + U(r, \eta). \tag{27}$$

A solution within the second-order terms in Δt may be get by using of the numerical scheme

$$
\begin{aligned}
\hat{S}_{jj'}\Psi_1^{ij'k} &= \hat{S}_{jj'}\Psi_1^{ij'k}(t) - \frac{i\Delta t}{2}F^{ijk}(t); \\
\Psi_1^{ijk} &\overset{FFT}{\to} \Psi_2^{ijm} \\
(\hat{S}_{jj'}\delta_{ii'} + i\frac{\Delta t}{2}\hat{H}_{ii',jj'}^m)\Psi_3^{i'j'm} &= (\hat{S}_{jj'}\delta_{ii'} - i\frac{\Delta t}{2}\hat{H}_{ii',jj'}^m)\Psi_2^{i'j'm}; \\
\Psi_3^{ijm} &\overset{FFT}{\to} \Psi_4^{ijk} \\
\hat{S}_{jj'}\Psi^{ij'k}(t+\Delta t) &= \hat{S}_{jj'}\Psi_4^{ij'k} - \frac{i\Delta t}{2}F^{ijk}(t+\Delta t).
\end{aligned}
\tag{28}
$$

Here $i = 1, .., N$, $j = 1, .., L$, $k = 1, .., M$, $i' = 1, .., N$, $j' = 1, .., L$, $m = -M/2 + 1, .., 0, .., M/2$, where L is the number of splines, M and N are the numbers of grid

points in ϕ and r, respectively. For the η variable using expansion of function on B_2-splines, i.e.

$$\Psi(r_i, \eta, \phi_k, t) = \sum_j \Psi^{ijk} b_j(\eta) = \sum_{j,m} \Psi^{ijm} b_j(\eta) \exp(im\phi_k),$$

and

$$F(r_i, \eta, \phi_k, t) = \sum_j F^{ijk} b_j(\eta),$$

where b_j is j-th B_2-spline with nodes $\eta_{j-2}, .., \eta_{j+1}$. The $\hat{S}$ is the overlap or mass matrix

$$\hat{S}_{jj'} = \int\limits_{-1}^{1} b_j\, b_{j'}\, d\eta. \tag{29}$$

A finite-difference Hamiltonian is

$$\hat{H}_{ii',jj'}^m = -\frac{1}{2}\left\{ \hat{S}_{jj'}\hat{D}_{ii'} + \delta_{ii'}\frac{\hat{L}_{jj'} - m^2\hat{M}_{jj'}}{r_i^2} \right\} + \delta_{ii'}\hat{Q}_{i,jj'} \tag{30}$$

For r is used simple three-point finite-difference scheme

$$\hat{D}_{ii'}\Psi^{i'} = \frac{(\Psi^{i+1} - \Psi^i)/(r_{i+1} - r_i) + (\Psi^i - \Psi^{i-1})/(r_i - r_{i-1})}{(r_{i+1} - r_{i-1})/2}$$

Other matrixes in (30) are

$$\hat{L}_{jj'} = \int\limits_{-1}^{1} b_j'\, b_{j'}'\, d\eta; \tag{31}$$

$$\hat{M}_{jj'} = \int\limits_{-1}^{1} b_j\, (1 - \eta^2)^{-1}\, b_{j'}\, d\eta; \tag{32}$$

$$\hat{Q}_{i,jj'} = \int\limits_{-1}^{1} b_j\, U(r_i, \eta)\, b_{j'}\, d\eta. \tag{33}$$

Direct solution of the set of equations (28) requires NL^2M operations at each step in t. To reduce the number of operation we propose a double-cycle split-step scheme [7]. A double-cycle partial coordinate splitting scheme can be formulated as follows

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$$\Psi_{s1}^{ijm} = \Psi_2^{ijm};$$

$$\left\{ \hat{S}_{jj'} + i\frac{\Delta t}{4}(\hat{H}_A^{mi})_{jj'} \right\} \Psi_{s2}^{ij'm} = \left\{ \hat{S}_{jj'} - i\frac{\Delta t}{4}(\hat{H}_A^{mi})_{jj'} \right\} \Psi_{s1}^{ij'm};$$

$$\left\{ \delta_{ii'}\delta_{jj'} + i\frac{\Delta t}{4}(\hat{H}_{RA}^m)_{ii',jj'} \right\} \Psi_{s3}^{i'j'm} = \left\{ \delta_{ii'}\delta_{jj'} - i\frac{\Delta t}{4}(\hat{H}_{RA}^m)_{ii',jj'} \right\} \Psi_{s2}^{i'j'm};$$

$$\left\{ \delta_{ii'}\delta_{jj'} + i\frac{\Delta t}{4}(\hat{H}_{RA}^m)_{ii',jj'} \right\} \Psi_{s4}^{i'j'm} = \left\{ \delta_{ii'}\delta_{jj'} - i\frac{\Delta t}{4}(\hat{H}_{RA}^m)_{ii',jj'} \right\} \Psi_{s3}^{i'j'm};$$

$$\left\{ \hat{S}_{jj'} + i\frac{\Delta t}{4}(\hat{H}_A^{mi})_{jj'}) \right\} \Psi_{s5}^{ij'm} = \left\{ \hat{S}_{jj'} - i\frac{\Delta t}{4}(\hat{H}_A^{mi})_{jj'}) \right\} \Psi_{s4}^{ij'm};$$

$$\Psi_3^{ijm} = \Psi_{s5}^{ijm}.$$

Parts of initial Hamiltonian reads as

$$(\hat{H}_A^{mi})_{jj'} = (1 - p(r_i))\hat{A}_{i,jj'}^m, \tag{34}$$

$$(\hat{H}_{RA}^m)_{ii',jj'} = \hat{R}_{ii'} + p(r_i)\delta_{ii'}(\hat{S}^{-1}\hat{A}^m)_{i,jj'}, \tag{35}$$

where $\hat{H}_{ii',jj'}^m = (\hat{S}\hat{H}_{RA}^m)_{ii',jj'} + \delta^{ii'}(\hat{H}_A^{mi})_{jj'}$. The radial $\hat{R}$ and angular $\hat{A}$ operators have following forms

$$\hat{A}_{i,jj'}^m = -\frac{1}{2}\frac{\hat{L}_{jj'} - m^2\hat{M}_{jj'}}{r_i^2} + \hat{Q}_{i,jj'} - U_i\hat{S}_{jj'}, \tag{36}$$

$$\hat{R}_{ii'} = -\frac{1}{2}\hat{D}_{ii'} + \hat{U}_i\delta_{ii'}, \tag{37}$$

here $U_i = U^{as}(r_i)$. It is reasonable to choose the r-dependent weighting function $p(r)$ as a cubic polynomial

$$p(r) = \begin{cases} 2\left(\frac{r-r_a}{a_p}\right)^3 - 3\left(\frac{r-r_a}{a_p}\right)^2 + 1, & r_a < r < r_a + a_p; \\ 1, & r \le r_a; \\ 0, & r \ge r_a + a_p; \end{cases} \tag{38}$$

where r_a is the radius of the vicinity of $r = 0$ where the splitting is absent, a_p is the width of the area of partial splitting.

This scheme needs only $N(\alpha L + \beta L^2)M + \gamma NLM\log_2 M$ operations, where $\beta \ll \alpha$, conserves a norm

$$N = 2\pi \sum_{ijmj'} \frac{r_{i+1} - r_{i-1}}{2} \overset{*}{\Psi}{}^{ijm}\hat{S}_{jj'}\Psi^{ij'm}, \tag{39}$$

and approximately conserves the average energy

$$\langle E \rangle = 2\pi \sum_{ijmi'j'} \frac{r_{i+1} - r_{i-1}}{2} \stackrel{*}{\Psi}{}^{ijm} \hat{H}^m_{ii',jj'} \Psi^{i'j'm}, \tag{40}$$

when inhomogeneous term is absent.

Actually, the program works in two regimes: "integrating" regime, in which needs small step in time Δt_{int}, and "flowing out" regime with step Δt_{fl}. The angular distribution must be calculated in "flowing out' regime.

5   Numerical calculations and results

The method was tested using the well-studied example of the impact ionization of atomic hydrogen. We compared our results with those given by the well-known expression obtained in the first Born approximation [10]. Good agreement was demonstrated in the energy interval of interest E_e from 1 to 3 a.u., E_e being the energy of the ejected electron. The Figs.2 demonstrate convergence of the method with respect of the grid parameters.

Our numerical studies concerning the molecular hydrogen ion focused on the variation of the multi-fold differential cross section (MDCS) concerning a coincidence detection of the two emerging electrons and one of the protons with the ejection angle θ_e at different orientations of the molecular axis, provided that the scattering angle is small. The examples of our results illustrated by Figs.3 are obtained under the following conditions: the momentum of the impact electron k_i =12.13 a.u. ($E_i \simeq$ 2000 eV); the angle of scattering $\theta_s = 1^o$; the energy of the ejected electron $E_e = 1.85$ a.u.=50.3 eV. The impact and ejected electron trajectories and the molecular axis are supposed to lie in one plane. The latter restriction is not imposed by the method as such, it is just an example. Generally, one gets full information about the ejected electron after each run of the code at given values of the impact energy, scattering angle and molecular axis orientation.
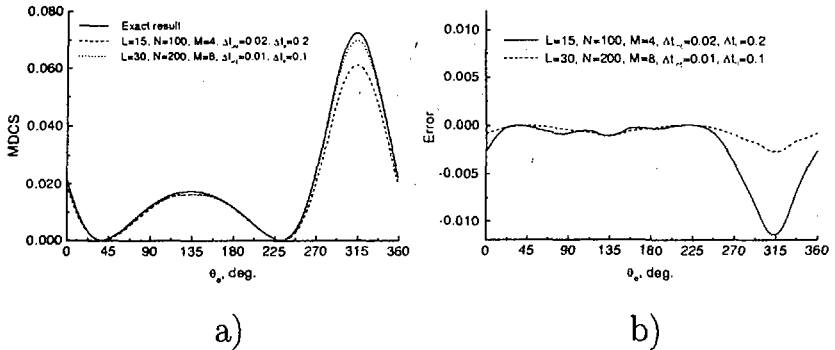
Figure 2: a)The multi-fold differential cross section (MDCS) of the ionization of atomic hydrogen versus the ejection angle θ_e: theoretical result(solid line), dashed line is the results given by proposed method for grid with parameters $N = 100$, $L = 15$, $M = 4$, $\Delta t_{int} = 0.02$, $\Delta t_{fl} = 0.2$; dotted line is one for $N = 200$, $L = 30$, $M = 8$, $\Delta t_{int} = 0.01$, $\Delta t_{fl} = 0.1$; b)discrepancy for rough(solid line) and more accurate(dashed line) grids. The momentum of the impact electron k_i =12.13 a.u. ($E_i \simeq 2000$ eV); the angle of scattering $\theta_s = 1^o$; the energy of the ejected electron $E_e = 2$ a.u.

6 Conclusion

We have developed a procedure which determines the multiply differential cross section of the (e,2e) ionization of hydrogen molecular ion by fast electron impact, using a direct approach which reduces the problem to a 3D evolution problem solved numerically. Our method avoids the cumbersome stationary perturbative calculations, and opens the way for near future applications to the (e,2e) ionisation of more complex atomic and molecular targets.
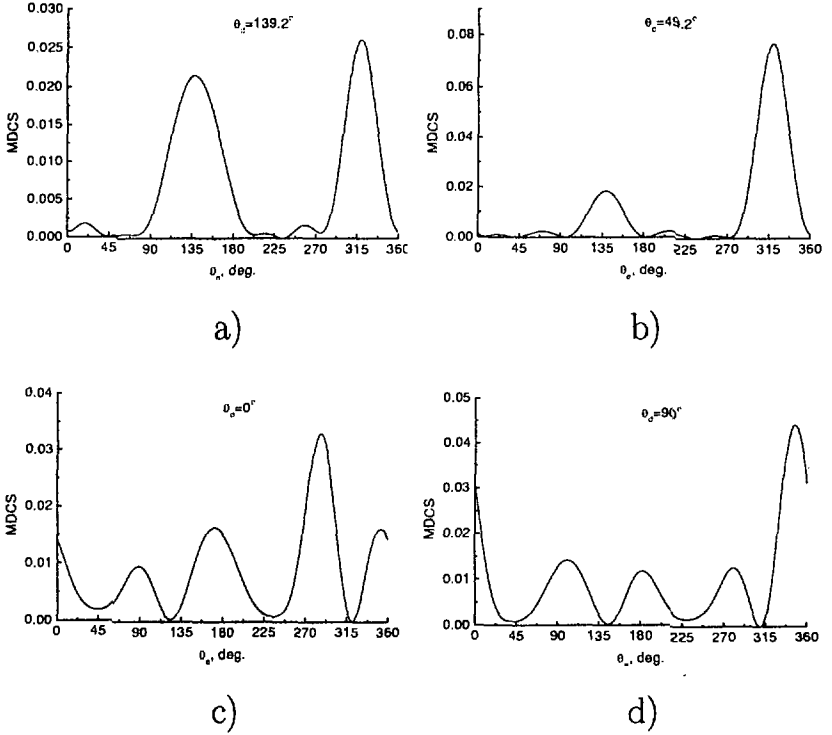
Figure 3: The multifold differential cross section (MDCS) of the ionization of H_2^+ versus the ejection angle θ_e for different angles θ_d: a)$\theta_d = 139.2^o$ that corresponds to $\vec{d} \parallel \vec{K}$; b)$\theta_d = 49.2^o$ that corresponds to $\vec{d} \perp \vec{K}$; c)$\theta_d = 0^o$; d) $\theta_d = 90^o$. The momentum of the impact electron $k_i =12.13$ a.u.; the angle of scattering $\theta_s = 1^o$; the energy of the ejected electron $E_e = 1.85$ a.u. Parameters of grid $N = 200$, $L = 30$, $M = 8$, $\Delta t_{int} \approx 0.01$, $\Delta t_{fl} = 0.1$

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References

[1] Y.D.Wang, J.H.McGuire, and R.D.Rivarola, Phys. Rev. A **40**, 3673 (1989).

[2] S.E.Corchs, R.D.Rivarola, J.H.McGuire, and Y.D.Wang, Phys. Rev. A **47**, 201 (1993).

[3] S.E.Corchs, R.D.Rivarola, J.H.McGuire, and Y.D.Wang, Phys. Scr. **50**, 469 (1994).

[4] B.Joulakian, J.Hassen, R.Rivarola, and A.Motassim, Phys. Rev. A, **54**, 1473 (1996)

[5] F.Calogero, Variable phase approach to potential scattering, Acad. Press, N.Y., London, 1967

[6] N.F.Mott and H.S.W.Massey, The theory of atomic function, Oxford, Clarendon Press, 1965

[7] V.V.Serov, A.I.Bychenkov, V.L.Derbov, and S.I.Vinitsky. Numerical scheme with external complex scaling for 2D Schrodinger equation in paraxial optics. Proc. SPIE, **4002** (2000) (to be published)

[8] A.M.Ermolaev, I.V.Puzynin, A.V.Selin, and S.I.Vinitsky, Phys. Rev. A, **60**, 4831 (1999)

[9] C.W.McCurdy and C.K.Stroud, Eliminating wavepacket reflection from grid boundaries using complex coordinate contours, Computer Phys. Commun., **63**, pp. 323-330, 1991.

[10] L.D.Landau and E.M.Lifshitz. Quantum Mechanics: Non-Relativistic Theory. London, Pergamon Press, 1958, p. 458.

[11] C.J.Joachain and B.Piraux. Comments At. Mol. Phys., **17**, 261 (1986).