INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS B: ATOMIC, MOLECULAR AND OPTICAL PHYSICS

J. Phys. B: At. Mol. Opt. Phys. **37** (2004) 2607–2616 PII: S0953-4075(04)76825-X

Modified two-centre continuum wavefunction: application to the dissociative ionization of H_2^+ by fast electrons

Ochbadrakh Chuluunbaatar[1], Boghos B Joulakian[2], Khinyat Tsookhuu[3] and Sergue I Vinitsky[4]

[1] Laboratory of Information Technologies, Joint Institute for Nuclear Research, Dubna, Moscow Region 141980, Russia
[2] Institut de Physique, Laboratoire de Physique Moléculaire et des Collisions, Université de Metz, Technopôle 2000, 1 Bd Arargo, 57078 Metz Cedex 3, France
[3] National University of Mongolia, School of Physics and Electronics, Ulaanbaatar, Mongolia
[4] Bogoliubov Laboratory of Theoretical Physics, Joint Institute for Nuclear Research, Dubna, Moscow Region 141980, Russia

E-mail: chuka@cv.jinr.ru, joulak@sciences.univ-metz.fr, tsookhuu@yahoo.com and vinitsky@thsun1.jinr.ru

Received 25 February 2004
Published 7 June 2004
Online at stacks.iop.org/JPhysB/37/2607
doi:10.1088/0953-4075/37/12/015

Abstract

A 3C-type two-centre wavefunction with four parameters that we will call a modified two-centre continuum wavefunction (MTCC) is proposed. This function is constructed in a closed analytical form by solving the Schrödinger equation of an electron (with wave vector $\vec{k}$ and position vector $\vec{r}$) in the Coulomb field of two fixed charged nuclei. The obtained solution fulfils the correct boundary conditions asymptotically up to the order $O((kr)^{-2})$. The MTCC function is applied to calculations of the seven-fold differential cross section of the dissociative ionization of the simplest homo-nuclear diatomic system H_2^+ by fast electrons. The good agreement of the obtained results with exact ones shows that the MTCC function could be a very elegant and useful compromise in the description of slow electrons emerging from diatomic targets.

1. Introduction

The coincidence detection techniques measuring the momenta of fragments emerging from atomic collision processes and particularly from dissociative ionization experiments of diatomic species by electron impact are now undergoing a very rapid development [1–5]. Studying the differential cross sections of these processes can deliver information, which is

necessary in larger domains, such as plasma sciences (in Tokamaks), biological sciences (in the study of cellular death) and the study of interstellar reactions. In the case of ionization, the coincidence detection of the scattered and ejected electrons and one of the protons, can deliver information about the electronic structure, the mechanism of simultaneous ionization and dissociation, and permits one to study the dependence of the differential cross section on the orientation of the inter-nuclear axis. This type of coincidence detection has already been performed in collision experiments involving multiply charged ionic projectiles and hydrogen molecules [6–8].

One of the basic difficulties to tackle the problem of the theoretical modelling of these types of experiments is to find a correct description of continuum states of the ejected electron moving in the field of two charged nuclei. For many years, investigations of the continuum states of the Coulomb three-body problem have been the object of great interest. In the case of large inter-particle distances, a simple wavefunction was first proposed by Redmond [9] and presented in the literature by Rosenberg [10] and Peterkop [11]. A more general type of asymptotic wavefunction, referred to as the 3C functions, is used by Brauner *et al* [12], and Merkuriev [13] in their study of the electronic continuum of a helium atom constructed by three Coulomb wavefunctions. Later Alt and Mukhamedzanov [14] have shown that, if the distance between any two particles is small compared to their respective distance from the third particle, the correct description requires introducing a local relative momentum. Other additional terms in these types of functions were introduced by Kim and Zubarev [15]. It is worth mentioning that Berakdar and Briggs [16] corrected the 3C wavefunction by introducing momentum-dependent Sommerfeld parameters. They used the invariance properties of a total potential under overall rotations in the parabolic–hyperspherical coordinates.

The electronic two-centre problem we face when studying ionization and/or scattering of electrons from diatomic targets is a particular case of the Coulomb three-body problem. In the last few years, many elegant models have been proposed to describe the dynamics of the ejected electron in an (e, 2e) experiment, which presents a unique physical situation together with that of (γ, e), where an electron (in this case the ejected electron) can be found in the field of two fixed nuclei. Joulakian *et al* [17] used an approximate 3C-type one parameter wavefunction inspired from the Pluvinage model [18] constructed by the product of two Coulomb functions. However, the calculated cross sections in this model are in some disagreement with those obtained lately, both by a wave packet evolution approach (Serov *et al* [19]) and by a partial wave approach constructed by the exact solutions in prolate spheroidal coordinates of the two-centre Coulomb problem (Serov *et al* [20]). The latter should be considered as the most reliable approach because it uses the exact solutions, while its application to more complex diatomic systems demands some very cumbersome calculations.

In this paper we propose, for the same physical situation of the electronic continuum, a general 3C-type two-centre wavefunction with four parameters that we will call the modified two-centre continuum wavefunction (MTCC). This function is obtained in a closed analytical form by solving the Schrödinger equation of an electron (with wave vector $\vec{k}$ and position vector $\vec{r}$) in the field of two fixed charged nuclei. The obtained solution fulfils the correct boundary conditions asymptotically up to the order $O((kr)^{-2})$. In what follows, it will be evident that the application of this model to diatomic systems is far less cumbersome due to its closed elegant form than that of the exact partial wave expansion in the prolate spheroidal coordinates. In what follows, we will give the details of the determination of this function and its application in the calculation of the seven-fold differential cross section of the simple (e, 2e) ionization of H_2^+ where one of the protons is detected in coincidence with the scattered and ejected electrons. We compare our results with those given by the application of the partial

wave approach constructed by the exact solutions in prolate spheroidal coordinates of the two centre Schrödinger equation (Serov *et al* [20]).

The paper is organized as follows. In section 2, we give briefly the basic expressions to calculate the seven-fold ionization cross section of the ground state hydrogen molecule ion by a fast electron. In subsection 2.1.1, a reduction of the Coulomb two-centre problem into a set of two separable ones is proposed. In subsection 2.1.2, a solution of this problem is given with an accuracy of the order $O((kr)^{-2})$ and the MTCC function is determined. In section 3, the MTCC function is examined in the calculation of the ionization cross section of H_2^+.

2. Theory

The differential cross section of general out-of-plane detection of two electrons and one of the nuclei of a H_2^+ target is sevenfold and is given by

$$\sigma^{(7)} = \frac{d^7\sigma}{d\Omega_\rho\, d\Omega_e\, d\Omega_s\, d\left(k_s^2/2\right)} = \frac{k_e k_s}{k_i}|T_{fi}|^2, \tag{1}$$

where Ω_s, Ω_e and k_s, k_e are respectively the solid angles and moduli of the wave vectors of the scattered and ejected electrons, Ω_ρ is the solid angle of the inter-nuclear axis $\vec{\rho}$ and k_i is the modulus of the wave vector of the incident electron. The T matrix element, T_{fi}, is given in the case of an unpolarized fast electron beam by

$$T_{fi} = \frac{1}{2\pi}\int d\vec{R}\, d\vec{r}\frac{\exp(i\vec{K}\vec{R})}{|\vec{R}-\vec{r}|}\chi^*(\vec{r}_1,\vec{r}_2)\phi_{1\sigma_g}(\vec{r}_1,\vec{r}_2), \tag{2}$$

where $\vec{R}$ represents the position of the fast (2 keV) incident (and scattered) electron described here by a plane wave; $\vec{r}$ refers to the position of the bound (ejected) electron. The position of this electron with respect to the two centres is given by $\vec{r}_1 = \vec{r} + \vec{\rho}/2$ and $\vec{r}_2 = \vec{r} - \vec{\rho}/2$; $\vec{K} = \vec{k}_i - \vec{k}_s$ gives the momentum transferred to the target. The wavefunction $\phi_{1\sigma_g}$ describes the initial electronic $1\sigma_g$ fundamental state of the target and was obtained by a variational two-parameter calculation borrowed from [17]

$$\phi_{1\sigma_g}(\vec{r},\vec{\rho}) = N(\rho)(\exp(-ar_1 - br_2) + \exp(-br_1 - ar_2)), \tag{3}$$

where $a = 0.224\,086$ and $b = 1.136\,03$ are variational parameters that we have determined for the equilibrium inter-nuclear distance $\rho = 2$ au with the normalization constant $N(\rho) = 0.6217$. The wavefunction $\chi(\vec{r}_1,\vec{r}_2)$ represents a state of continuous spectra of the slow ejected electron. Its determination will be one of the main objects of this work as mentioned in the introduction.

2.1. The final state wavefunction

2.1.1. 3C-type solution of the two-centre electronic continuum. Let us consider the Hamiltonian of an electron moving in the field of two fixed nuclei of charges Z_1 and Z_2

$$H = -\frac{1}{2}\Delta_r - \frac{Z_1}{r_1} - \frac{Z_2}{r_2}. \tag{4}$$

We seek for a solution to the Schrödinger equation

$$(H - E)\Psi(\vec{k},\vec{r}) = 0, \tag{5}$$

in the form of a product of two functions

$$\Psi(\vec{k},\vec{r}) = \Psi_1(\vec{k},\vec{r}_1)\Psi_2(\vec{k},\vec{r}_2), \tag{6}$$

where $\vec{k}$ represents a wave vector. We will take each function in the form

$$\Psi_l(\vec{k},\vec{r}_l) = \exp(\mathrm{i}\vec{k}\vec{r}_l/2)\,Q_l(\vec{k},\vec{r}_l). \tag{7}$$

Substituting this function in equation (5), we get the following equation:

$$\left[\frac{1}{2}\Delta_1 Q_1 + \mathrm{i}\vec{k}\vec{\nabla}_1 Q_1 + \frac{Z_1}{r_1}Q_1 + \frac{\vec{\nabla}_1 Q_1 \vec{\nabla}_2}{2}\right] Q_2 + \left[\frac{1}{2}\Delta_2 Q_2 + \mathrm{i}\vec{k}\vec{\nabla}_2 Q_2 + \frac{Z_2}{r_2}Q_2 + \frac{\vec{\nabla}_2 Q_2 \vec{\nabla}_1}{2}\right] Q_1 = 0, \tag{8}$$

where the notation $\Delta_l = \Delta_{r_l}$ and $\vec{\nabla}_l = \vec{\nabla}_{r_l}$ are used. Now we suppose that the expression in each bracket equals identically zero. This gives

$$\left[\frac{1}{2}\Delta_l Q_l + \mathrm{i}\vec{k}\vec{\nabla}_l Q_l + \frac{Z_l}{r_l}Q_l + \frac{\vec{\nabla}_l Q_l \vec{\nabla}_n}{2}\right] Q_n = 0, \qquad l,n = 1,2. \tag{9}$$

In the last equation let us first neglect the last term with the scalar product. The resulting equation has a conventional solution

$$Q_l(\vec{k},\vec{r}_l) \equiv {}_1F_1(\mathrm{i}\alpha_l, 1, -\mathrm{i}[kr_l + \vec{k}\vec{r}_l]), \tag{10}$$

where ${}_1F_1$ is the Kummer confluent hyper geometric function and $\alpha_l = -Z_l/k$ is the Sommerfeld parameter. In this approximation the solution to equation (5) is of the form

$$\Psi(\vec{k},\vec{r}) = (2\pi)^{-3/2}\exp(\mathrm{i}\vec{k}\vec{r})\prod_{l=1}^{2} N_l Q_l(\vec{k},\vec{r}_l), \tag{11}$$

which fulfils the orthonormalization condition

$$\langle\Psi(\vec{k}',\vec{r})|\Psi(\vec{k},\vec{r})\rangle = \delta(\vec{k}-\vec{k}'), \tag{12}$$

with a normalization factor

$$N_l = \exp(-\pi\alpha_l/2)\Gamma(1-\mathrm{i}\alpha_l). \tag{13}$$

The expression on the right-hand side of equation (11) is just a 3C-type solution [17] (more precisely, a 2C-type, because the two Coulomb centres are supposed to be fixed). It satisfies the exact asymptotic Redmond condition

$$\lim_{r\to\infty}\Psi(\vec{k},\vec{r}) \longrightarrow (2\pi)^{-3/2}\exp(\mathrm{i}\vec{k}\vec{r})\exp(-\mathrm{i}(\alpha_1+\alpha_2)\ln(kr+\vec{k}\vec{r})). \tag{14}$$

As mentioned above, this solution fulfils equation (9) within an accuracy of the order $\mathrm{O}((kr)^{-2})$, since

$$\vec{\nabla}Q(\vec{k},\vec{r}) = \alpha(k\hat{r}+\vec{k})\,{}_1F_1(\mathrm{i}\alpha+1, 2, -\mathrm{i}[kr+\vec{k}\vec{r}]), \tag{15}$$

becomes at $kr\to\infty$

$$\vec{\nabla}Q(\vec{k},\vec{r}) = \frac{\alpha(k\hat{r}+\vec{k})\exp(\pi\alpha/2)}{\mathrm{i}(kr+\vec{k}\vec{r})}(f(\vec{k},\vec{r}) - \exp(-\mathrm{i}(kr+\vec{k}\vec{r}))\,f^*(\vec{k},\vec{r})) + \mathrm{O}((kr)^{-2}), \tag{16}$$

where

$$f(\vec{k},\vec{r}) = \frac{\exp(-\mathrm{i}\alpha\ln(kr+\vec{k}\vec{r}))}{\Gamma(1-\mathrm{i}\alpha)}. \tag{17}$$

This fact permits us to estimate finally the order of magnitude of the neglected term

$$\vec{\nabla}_1 Q_1 \vec{\nabla}_2 Q_2 \approx \mathrm{O}((kr)^{-2}). \tag{18}$$

2.1.2. The modified 3C-type solution. Now let us introduce an asymptotic expression of the term $\vec{\nabla}_1 Q_1 \vec{\nabla}_2 Q_2$ in equation (9). Using equation (16), we can rewrite each factor in the form

$$\vec{\nabla} Q(\vec{k},\vec{r}) \approx \frac{\alpha(k\hat{r}+\vec{k})\exp(\pi\alpha/2)}{\mathrm{i}(kr+\vec{k}\vec{r})} f(\vec{k},\vec{r}) q(\vec{k},\vec{r}) \approx \frac{\alpha(k\hat{r}+\vec{k})}{\mathrm{i}(kr+\vec{k}\vec{r})} Q(\vec{k},\vec{r}) q(\vec{k},\vec{r}), \tag{19}$$

where

$$q(\vec{k},\vec{r}) = 1 - \exp(-\mathrm{i}(kr+\vec{k}\vec{r}))\frac{f^*(\vec{k},\vec{r})}{f(\vec{k},\vec{r})}, \tag{20}$$

which gives

$$|1 - q(\vec{k},\vec{r})| = 1. \tag{21}$$

This shows that $q(\vec{k},\vec{r})$ is finite. Now to uncouple equation (9) we will admit that $\alpha q(\vec{k},\vec{r})$ in the asymptotic expression (19) can be replaced by a free parameter ϵ. This permits us to transform equation (9) into

$$\frac{1}{2}\Delta_l Q_l + \mathrm{i}\vec{k}\vec{\nabla}_l Q_l + \frac{Z_l}{r_l} Q_l - \frac{\mathrm{i}\epsilon_n}{2}\frac{\hat{r}_l + \hat{k}}{1+\hat{r}_l\hat{k}}\frac{\vec{\nabla} Q_l}{r_l} = 0, \tag{22}$$

where we have replaced $\vec{r}_n$ by $\vec{r}_l$ using the approximation $r_n^{-1} = r_l^{-1} + \mathrm{O}(r_l^{-2})$.

To solve equation (22), we introduce a new variable $x_l = -\mathrm{i}(kr_l + \vec{k}\vec{r}_l)$ and consider the relations

$$\begin{aligned} \nabla_l Q_l &= -\mathrm{i}k(\hat{r}_l + \hat{k}) Q_l', \\ \Delta_l Q_l &= -2k^2(1+\hat{k}\hat{r}_l) Q_l'' - \frac{2k^2}{x_l}(1+\hat{k}\hat{r}_l) Q_l'. \end{aligned} \tag{23}$$

Then finally we get a differential equation

$$x_l Q_l'' + (1 - \mathrm{i}\epsilon_l - x_l) Q_l' - \mathrm{i}\alpha_l Q_l = 0, \tag{24}$$

which also has a conventional analytical solution

$$Q_l(\alpha_l, \epsilon_l, \vec{k}, \vec{r}_l) \equiv {}_1F_1(\mathrm{i}\alpha_l, 1 - \mathrm{i}\epsilon_l, -\mathrm{i}[kr_l + \vec{k}\vec{r}_l]), \tag{25}$$

depending on the supplementary parameter ϵ_l which reduces to equation (10) for $\epsilon_l = 0$. Using this solution instead of the previous one in equation (11), we get a new expression of the approximate wavefunction

$$\Psi(\vec{k},\vec{r}) = (2\pi)^{-3/2}\exp(\mathrm{i}\vec{k}\vec{r})\prod_{l=1}^{2} N(\alpha_l,\epsilon_l) Q_l(\alpha_l,\epsilon_l,\vec{k},\vec{r}_l), \tag{26}$$

that fulfils the orthonormalization condition with a new normalization factor

$$N(\alpha_l,\epsilon_l) = \exp(-\pi\alpha_l/2)\frac{\Gamma(1-\mathrm{i}\alpha_l - \mathrm{i}\epsilon_l)}{\Gamma(1-\mathrm{i}\epsilon_l)}. \tag{27}$$

The basic difference between the function given in equation (11) and the MTCC function given in equation (26) is that in the latter the electronic motion relative to one of the Coulomb centres depends on the Sommerfeld parameter of the other centre. Finally, we express the wavefunction of the slow ejected electron in a symmetric form for the homo-nuclear case of $Z_1 = Z_2$

$$\begin{aligned} \chi(\vec{r}_1,\vec{r}_2) = \frac{\exp(\mathrm{i}\vec{k}_\mathrm{e}\vec{r})}{2(2\pi)^{3/2}} N(\alpha,\beta)N(\nu,\gamma)[&Q_1(\alpha,\beta,\vec{k}_\mathrm{e},\vec{r}_1) Q_2(\nu,\gamma,\vec{k}_\mathrm{e},\vec{r}_2) \\ &+ Q_1(\alpha,\beta,\vec{k}_\mathrm{e},\vec{r}_2) Q_2(\nu,\gamma,\vec{k}_\mathrm{e},\vec{r}_1)], \end{aligned} \tag{28}$$

where $\alpha = -Z_1/k_e$, $\nu = -Z_2/k_e$ are the Sommerfeld parameters and $\beta = -z_3/k_e$, $\gamma = -z_4/k_e$ are the supplementary ones. Note that z_3 and z_4 will be considered as free variational parameters related to the small parameter ϵ in equation (22). Integrating over the coordinates $\vec{R}$ of the fast incident electron with the help of the relation

$$\int \frac{d\vec{R}}{|\vec{R}-\vec{r}|}\exp(i\vec{K}\vec{R}) = \frac{4\pi\exp(i\vec{K}\vec{r})}{K^2}, \tag{29}$$

and substituting the functions defined in equations (3) and (28) into equation (2), we get

$$T_{fi} = \frac{-N(\rho)}{(2\pi)^{3/2}K^2}\frac{\Gamma(1+i\alpha+i\beta)}{\Gamma(1+i\beta)}\frac{\Gamma(1+i\nu+i\gamma)}{\Gamma(1+i\gamma)}\exp(-\pi(\alpha+\nu)/2)(I(a,b)+I(b,a)), \tag{30}$$

where

$$I(a,b) = J(a,b,\alpha,\beta,\nu,\gamma) + J(a,b,\nu,\gamma,\alpha,\beta), \tag{31}$$

with

$$J(a,b,\alpha,\beta,\nu,\gamma) = \int d\vec{r}\exp(i(\vec{K}-\vec{k}_e)\vec{r} - ar_1 - br_2) \times {}_1F_1(-i\alpha, 1+i\beta, i[k_e r_1 + \vec{k}_e\vec{r}_1])\,{}_1F_1(-i\nu, 1+i\gamma, i[k_e r_2 + \vec{k}_e\vec{r}_2]). \tag{32}$$

Using the Fourier transform for one of the centres, we reduce this integral to a three-dimensional integral having the form

$$J(a,b,\alpha,\beta,\nu,\gamma) = \frac{\exp(i(\vec{K}-\vec{k}_e)\vec{\rho}/2)}{(2\pi)^3} \times \int d\vec{\tau}\exp(i\vec{\tau}\vec{\rho})W_{(\alpha,\beta)}(\vec{k}_e,\vec{\tau},a)W_{(\nu,\gamma)}(\vec{k}_e,-\vec{K}-\vec{\tau}+\vec{k}_e,b). \tag{33}$$

The integrand function $W_{(\alpha,\beta)}(\vec{k}_e,\vec{q},\lambda)$ reads as

$$W_{(\alpha,\beta)}(\vec{k}_e,\vec{q},\lambda) = \int d\vec{r}\exp(-i\vec{q}\vec{r}-\lambda r)\,{}_1F_1(-i\alpha, 1+i\beta, i(k_e r + \vec{k}_e\vec{r})) = \frac{8\pi}{(q^2+\lambda^2)^2}\left(\lambda\,{}_2F_1(-i\alpha,2,1+i\beta,x) - \frac{\alpha k_e}{1+i\beta}\,{}_2F_1(1-i\alpha,2,2+i\beta,x)\right), \tag{34}$$

where $x = 2(\vec{q}\vec{k}_e + i\lambda k_e)/(q^2+\lambda^2)$ and ${}_2F_1$ is the hypergeometric function. Note that these integrals are calculated much more easily than the hypergeometric functions in equation (32). Moreover, at zero value of supplementary parameter $\beta = 0$, the integral in equation (34) is evaluated analytically

$$W_{(\alpha,0)}(\vec{k}_e,\vec{q},\lambda) = \frac{8\pi}{(q^2+\lambda^2)^2}(1-x)^{i\alpha}\left(\lambda(1+i\alpha) - i\alpha\frac{\lambda - ik_e}{1-x}\right). \tag{35}$$

Note that the three-dimensional integral in equation (33) is calculated only by the numerical quadratures. The proposed reduction reveals the diatomic nature of the problem by the appearance of the interference terms represented by the factor $\exp(i(\vec{K}-\vec{k}_e)\vec{\rho}/2)$.

3. Results

The basic aim of this work is to test the validity of our approach presented in subsection 2.1.2 which as mentioned above seems to be an elegant alternative for the cumbersome exact description of the two-centre electronic continuum. We restrict our presentation to a case of the homo-nuclear diatomic situation taking $Z_1 = Z_2 = 1$ and considering situations studied in

Table 1. The 7DCS for different values of $z_3 = z_4 = z$, for the case $\vec{k}_e \| \vec{K}$ at $\theta_s = 9^\circ$ and $\theta_\rho = 0^\circ$. The last column shows the difference between 7DCS obtained by the exact solution and the preceding column.

$Z_1 = Z_2$	z	$\sigma^{(7)}$ by MTCC	$\Delta\sigma^{(7)}$
1.00	0.00	0.137 41	0.008 13
	0.10	0.142 52	0.003 03
	0.16	0.145 46	0.000 09
	0.17	0.145 94	−0.000 39
	0.20	0.147 37	−0.001 82
	0.50	0.160 43	−0.014 88
	1.00	0.177 77	−0.032 22
$\sigma^{(7)}$ exact solution [20]		0.145 55	

Table 2. The same as in table 1 for $\theta_s = 9.5^\circ$ and $\theta_\rho = 90^\circ$.

$Z_1 = Z_2$	z	$\sigma^{(7)}$ by MTCC	$\Delta\sigma^{(7)}$
1.00	0.00	0.120 31	0.005 59
	0.10	0.123 95	0.001 95
	0.15	0.125 88	0.000 02
	0.16	0.126 27	−0.000 37
	0.20	0.127 86	−0.001 96
	0.50	0.139 97	−0.014 06
	1.00	0.157 73	−0.031 83
$\sigma^{(7)}$ exact solution [20]		0.125 90	

some recent papers [17, 19, 20]. We will fix the energy value of the incident electron to 2 keV such that its state can be represented by a plane wave in the transition matrix. Following the preceding calculations, we consider that the ejected electron emerges with an energy value of 50 eV, which seems to be a judicious choice for different reasons. It gives an optimal magnitude to the multiply differential cross section of this process, justifies neglecting the exchange terms [17] between the scattered and ejected electrons in the transition matrix element as $k_s \gg k_e$ and permits us to admit that the ionization process is much faster than the motion of the nuclei. Now we consider a coincidence detection of the scattered and ejected electrons with one of the protons whose momentum gives the orientation of the molecular target. We will give the seven-fold differential cross section for two particular directions, $\varphi_\rho = 0^\circ$, $\theta_\rho = 0^\circ$ and 90°, of the inter-nuclear axis defined by the polar angles around the direction of incidence chosen as that of the Z axis. In the homo-nuclear case we consider equal Sommerfeld parameters and put $\beta = \gamma = -z/k_e = \epsilon$, which should take small values, as shown in equation (22). To determine the most appropriate value for z, we compare our results shown in tables 1 and 2 for different values of z with those obtained by the application of the exact solution [20] in an optimal situation, when the momentum of the ejected electron is equal and parallel to the momentum transferred to the target by the incident electron $\vec{K} = \vec{k}_e$. The results show that z should not exceed 0.2. A required value of z is identified by a sign changing that corresponds to a coincidence of the neighbourhood maxima of the 7DCS. This circumstance can be used as a key point to realize an effective algorithm of fitting both theoretical and experimental data of any conventional multi-fold differential cross sections of the problem under consideration and its further application to more complex diatomic systems.

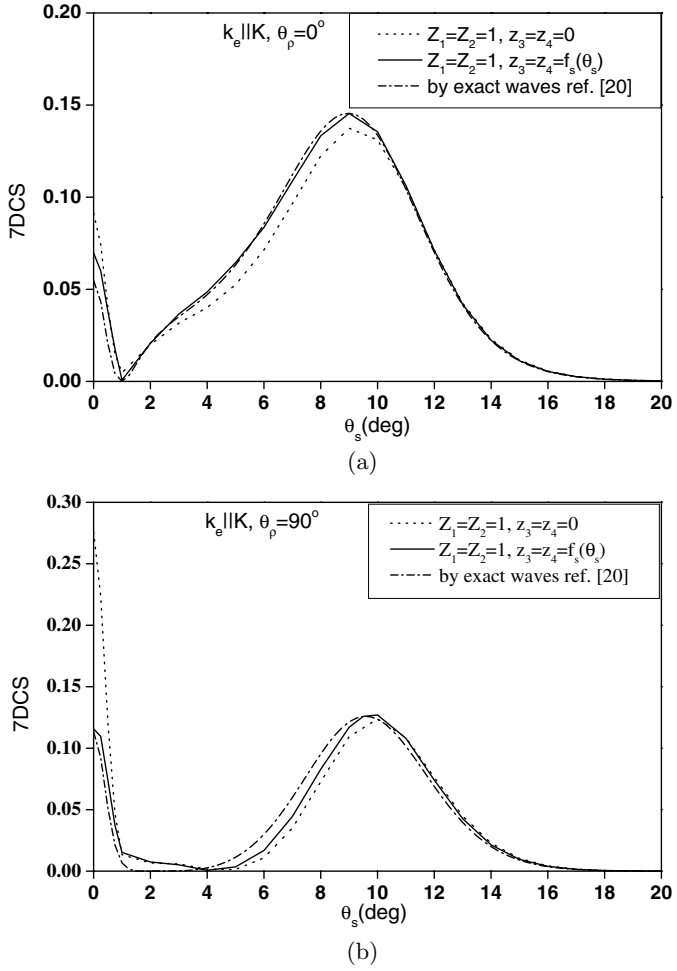

Figure 1. The variation of the 7DCS of the (e, 2e) ionization of H_2^+ with the scattering angle θ_s for the case $\vec{k}_e \| \vec{K}$, with optimal $z_3 = z_4 = f_s(\theta_s)$.

Then we consider in figures 1(a) and (b) the variation of the seven-fold differential cross section with the scattering angle for two directions of the nuclear axis $\varphi_\rho = 0^\circ$, $\theta_\rho = 0^\circ$ and 90°, respectively. The dynamical situations are such that for each value of θ_s, the ejected electron comes out in a direction parallel to the momentum transfer which, as mentioned above, is a favourable direction, as in this situation the recoil momentum has its lowest value, and the energy is mostly transferred to the ejected electron, thus creating an optimal condition for ejection for each value of θ_s. Now as seen on the two curves, the introduction of the supplementary parameter, ϵ_l, improves the agreement with that obtained by the application of the exact wavefunction especially in the region of small scattering angles, where the two-centre model proposed by [17] fails completely.

Now, to see the effect of the introduction of β and γ (or z_3 and z_4) in more detail, we consider the variation of the seven-fold differential cross section with the ejection angle for two particular values of the scattering direction $\theta_s = 3^\circ$ in figure 2 and $\theta_s = 9^\circ$ in figure 3 for the particular orientation of the inter-nuclear axis $\varphi_\rho = 0^\circ$, $\theta_\rho = 0^\circ$. Both cases show that

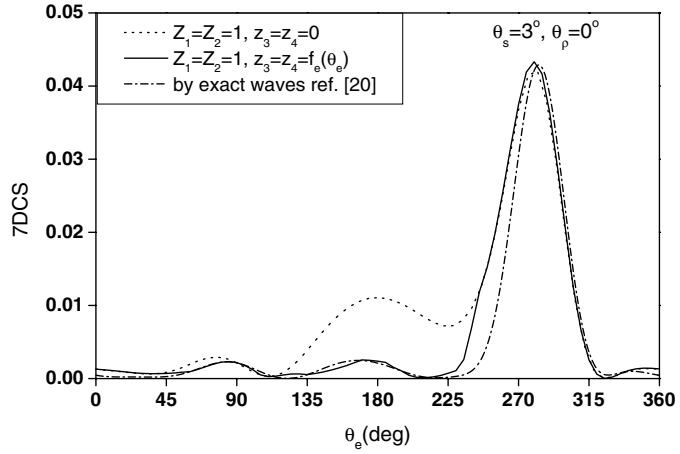

Figure 2. Variation of the 7DCS of (e, 2e) of H_2^+ with the ejection angle θ_e, with optimal $z_3 = z_4 = f_e(\theta_e)$. Here $\theta_s = 3^\circ$ and $\theta_\rho = 0^\circ$.

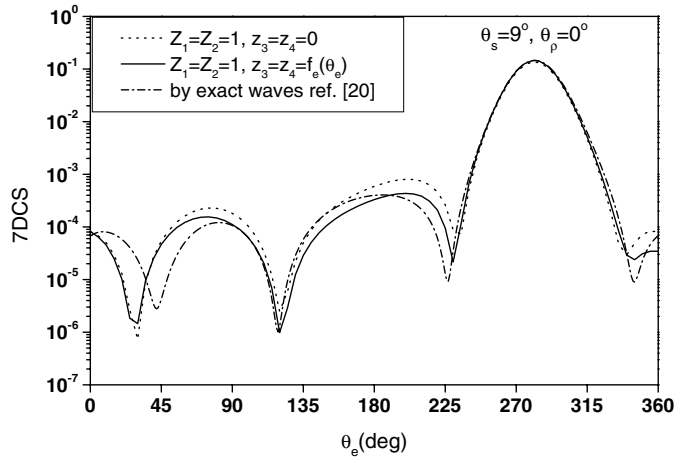

Figure 3. Same as figure 2, but for $\theta_s = 9^\circ$.

the interference patterns due to the diatomic nature of the target identified in our approach via the term $\exp(-i(\vec{K} - \vec{k}_e)\vec{\rho}/2)$ in equation (33) persist and are very similar to those obtained by the exact solutions. The improvement brought about by the introduction of ϵ_l is evident in the two figures, especially in the region $100^\circ < \theta_e < 240^\circ$ in figure 2. Many disagreements persist, especially in the region $0 < \theta_e < 100^\circ$ in figure 3, which are very difficult to interpret as the order of magnitude of the multiply differential cross section is relatively very small in this region and could be explained by the approximate nature (up to order $O((kr)^{-2})$) of our wavefunction.

4. Conclusion

We have proposed a new four-parameter continuum wavefunction describing the slow electron in the Coulomb field of two positively charged nuclei and applied it to the determination of

the seven-fold differential cross section of the dissociative ionization of the simplest homonuclear diatomic system H_2^+. Our results show that the introduction of a supplementary parameter permits us to obtain elegantly a good agreement with the results obtained by rather cumbersome calculations using the exact solution of the two-centre Schrödinger equation in prolate spheroidal coordinates for the same physical situation. We believe that this approach will be particularly useful for the description of the ejected electrons from more complex diatomic targets for which the exact solution is inapplicable.

Acknowledgments

We would like to thank Drs T Zhanlav, V V Serov and N Tsogbadrakh for valuable discussions. We also thank the CINES (Centre Informatique National de l'Enseignement Superieur) for providing computing facilities. This work was partially supported by the grant no 03-02-16263 of the Russian Foundation for Basic Research and no 40.018.1.1.1314 of the Russian Ministry of Industry, Science and Technologies.

References

[1] Corche S E, Busnengo H F and Rivarola R D 1999 *Nucl. Instrum. Methods* B **149** 247
[2] Dörner R *et al* 1996 *Phys. Rev. Lett.* **77** 1024
[3] Lafosse A, Houver J C and Dowek D 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** 819
[4] Edwards A K and Zheng Q 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** 1539
[5] Weber Th *et al* 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** 3669
[6] Wang Y D, McGuire J H and Rivarola R D 1989 *Phys. Rev.* A **40** 3673
[7] Corchs S E, Rivarola R D, McGuire J H and Wang Y D 1993 *Phys. Rev.* A **47** 201
[8] Corchs S E, Rivarola R D, McGuire J H and Wang Y D 1994 *Phys. Scr.* **50** 469
[9] Redmond P J 1972 unpublished
[10] Rosenberg L 1973 *Phys. Rev.* D **8** 1833
[11] Peterkop R J 1977 *Theory of Ionization of Atoms by Electron Impact* (Boulder, CO: University of Colorado Press)
[12] Brauner M, Briggs J S and Klar H 1989 *J. Rev.* B **22** 2265
[13] Merkuriev S P 1977 *Theor. Math. Phys.* **32** 680
[14] Alt E O and Mukhamedzhanov A M 1993 *Phys. Rev.* A **47** 2004
[15] Kim Y E and Zubarev A L 1997 *Phys. Rev.* A **56** 521
[16] Berakdar J and Briggs J S 1994 *Phys. Rev. Lett.* **72** 3799
[17] Joulakian B, Hanssen J, Rivarola R and Motassim A 1996 *Phys. Rev.* A **54** 1473
[18] Pluvinage P 1951 *Phys. Radium* **12** 789
[19] Serov V V, Derbov V L, Joulakian B B and Vinitsky S I 2001 *Phys. Rev.* A **63** 062711
[20] Serov V V, Joulakian B B, Pavlov D V, Puzynin I V and Vinitsky S I 2002 *Phys. Rev.* A **65** 062708