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Incorporation of Threshold Phenomena in Three-body Coulomb Continuum Wavefunctions

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Abstract

In this work a three-body Coulomb wavefunction for the description of two continuum electrons moving in the field of a nucleus is constructed such that the Wannier threshold law for double escape is reproduced and the asymptotic Coulomb boundary conditions as well as the Kato cusp conditions are satisfied. It is shown that the absolute value of the total cross section, as well as the spin asymmetry, are well described by the present approach. Further, the excess-energy sharing between the two escaping electrons is calculated and analysed in light of the Wannier theory predictions. This is the first time an analytical three-body wavefunction is presented which is asymptotically exact and capable of describing threshold phenomena.

1. Introduction

An understanding of the fragmentation dynamics of few-body Coulomb systems is the ultimate goal of many experimental and theoretical investigations. Our present knowledge of the analytical properties of the motion of three particles above the complete dissociation threshold is limited to some specific region of the phase space. Close to the three-body break-up threshold the total cross section for two continuum electrons receding from a charged ion has been investigated by Wannier (1953) using a classical analysis. Wannier (1953) pointed out that the excess-energy functional dependence of the total ionisation cross section at the three-particle fragmentation threshold can be deduced from the volume of the phase space available for double escape of the two electrons. Since then a large amount of theoretical and experimental studies (e.g. Peterkop 1971; Cvejanović and Read 1974; Read 1984; Rau 1971, 1984; Klar 1981; Feagin 1984; Kossmann *et al.* 1988; Lablanquie *et al.* 1990; Rost 1995; Macek and Ovchinnikov 1995) using quite different approaches has been carried out which basically confirm the Wannier-threshold law.

On the other hand, the analytical properties of three-body Coulomb continuum wavefunctions are known in some limited region in six dimensional Hilbert space. When two particles approach each other (in configuration space), while the size of the triangle formed by the three particles is large, the three-body wavefunction satisfies the Kato (1957) cusp conditions. When the size of this

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triangle diminishes, i.e. at the three-body coalescence point, the wavefunction possesses a Fock (1958) expansion which contains power and logarithmic terms in the size of the triangle. For large interparticle separations the eigenfunction of the non-relativistic three-body Schrödinger equation has been given by Redmond (see Rosenberg 1973). Recently, Alt and Mukhamedzhanov (1993) showed that a correct description of the whole asymptotic region requires the introduction of local relative momenta. The latter asymptotic behaviour can also be accounted for by the introduction of local Sommerfeld parameters depending on the internal degrees of freedom (Berakdar 1996*a*).

The aim of the present theoretical study is to incorporate all this fragmentary knowledge and some further properties of the total potential surface in one analytic (holomorph) wavefunction. This is vital for calculating reaction cross sections at arbitrary energies of the system, since evaluation of ionisation amplitudes involves integration over the whole configuration space. To this end the three-body system has been broken down into three (in configuration space) non-interacting two-body subsystems that are subsequently coupled to each other by a coupling matrix, which is determined such that the resulting wavefunction solves for the three-body Schrödinger equation in the whole asymptotic region and satisfies the Kato cusp conditions (Berakdar 1996*a*, hereafter this work is referred to as Paper I). In addition, the motion on the Wannier saddle, i.e. when the two electrons travel outward on opposite sides of, and equal distances from, the residual ion, has been accounted for. Here we show how the Wannier threshold law can be incorporated in this model to give, for the first time, an analytic wavefunction which is valid at threshold and possesses the correct asymptotic behaviour. It should be mentioned that the wavefunction derived in this work has already been successfully applied to evaluate fully differential cross sections (Berakdar and Briggs 1994*a*, 1994*b*, 1996). Atomic units are used throughout.

2. Theoretical Considerations

We consider the motion of two electrons receding from a nucleus of charge Z at the total energy E. Following Paper I the three-body time-independent Schrödinger equation with outgoing-wave boundary conditions is reformulated in the coordinate system

$$\{\xi_k = r_{ij} + \hat{\mathbf{k}}_{ij} \cdot \mathbf{r}_{ij};\ \xi_m = r_{ij}\}, \quad \epsilon_{ijk} \neq 0;\ j > i, k \in [1,3];\ m \in [4,6]\,. \quad (1)$$

In (1) the $\hat{\mathbf{k}}_{ij}$ denote the directions of the momenta $\mathbf{k}_{ij}$ which are conjugate to the interparticle distances r_{ij}. As has been shown in Paper I the three-body Hamiltonian H, expressed in the coordinate system (1), splits into two *parametrically* coupled differential operators; an operator $H_{\xi_{1\ldots3}}$ which is differential in the coordinates $\xi_{1\ldots3}$ only and an operator differential in internal degrees of freedom r_{ij}; $j > i \in [1,3]$. An additional mixing term arises from the off-diagonal elements of the metric tensor. The decisive point is that the Hamiltonian $H_{\xi_{1\ldots3}}$ is the sum of three commuting, two-body Coulomb Hamiltonians, i.e., it is exactly separable in the coordinates $\xi_{1\ldots3}$. Thus, within the approximation $H \approx H_{\xi_{1\ldots3}}$ the three-body system is considered as the sum of three spatially decoupled

two-body Coulomb systems. The exact regular eigenfunction of $H_{\xi_{1\ldots3}}$ at a given total energy E has the explicit form (compare Paper I)

$$\Psi_{\mathrm{DS3C}}(\xi_1,\xi_2,\xi_3)|_{(\xi_4,\xi_5,\xi_6)} = (2\pi)^{-3}\exp(i\ \mathbf{r}_{ij}\cdot\mathbf{k}_{ij} + i\ \mathbf{R}_k\cdot\mathbf{K}_k)$$
$$\times N\prod_{n=1}^{3}\ {}_1F_1(i\beta_{lm}(\xi_4,\xi_5,\xi_6),1,\ -ik_{lm}\ \xi_n);$$
$$\epsilon_{lmn}\neq 0;\ \ m>l\in[1,3];\ \ \epsilon_{ijk}\neq 0;\ \ j>i\in[1,3]. \quad (2)$$

In (2) the coordinate $\mathbf{R}_k$ refers to the particle 'k' with respect to the centre of mass of the pair 'ij', while $\mathbf{K}_k$ designates the momentum conjugate to this coordinate and N is a normalisation factor. The Sommerfeld parameters β_{ij} are given by

$$\beta_{ij} = \frac{Z_{ij}(\xi_{4\ldots6})\mu_{ij}}{k_{ij}}, \quad (3)$$

where the reduced mass of the pair 'ij' is denoted by μ_{ij}. The parametric dependence of $H_{\xi_{1\ldots3}}$ on the internal coordinates is reflected by the product charges $Z_{ij}(\xi_{4\ldots6})$ being allowed to be functions of the internal coordinates $\xi_{4\ldots6}$ under the constraint that these functions do not alter the Schrödinger equation. This additional freedom allows the introduction of three-body coupling, i.e. coupling of each two-body Coulomb subsystem to the third charged continuum particle. Thus, we assume that the interaction between two continuum particles depends not only on their mutual Coulomb interaction but on the strength of coupling to the third particle, i.e.

$$V^i = \sum_{j=1}^{3} a_{ij}V^j,\ \ i=1,2,3, \quad (4)$$

where $V^k \equiv V_{ij};\ \epsilon_{ijk}\neq 0$ is the Coulomb potential between particles 'i' and 'j' and the 3×3 matrix $\mathcal{A}$ with elements $a_{ij}(\xi_{4\ldots6})$ describes the amount of three-body coupling. The matrix elements a_{ij} are subject to the constraint $\sum_{j=1}^{3} a_{ij}=1$ which ensures the invariance of $H_{\xi_{1\ldots3}}$, and thus the total Hamiltonian H under the transformation given by (4). The identity transformation $\mathcal{A}=I$ fulfils all the requirements on $\mathcal{A}$, but it means that coupling (in configuration space) between two-body subsystems is neglected. In this case the Sommerfeld parameters (3) reduce to $\beta_{ij} = (Z_iZ_j\mu_{ij}/k_{ij})$, where Z_j is the charge of particle 'j'. The wavefunction, given by (2), simplifies in the case of $\mathcal{A}=I$ to the well known expression (Garibotti and Miraglia 1980; Brauner *et al.* 1989)

$$\lim_{\mathcal{A}\to I}\Psi_{\mathrm{DS3C}}(\xi_1,\xi_2,\xi_3)|_{(\xi_4,\xi_5,\xi_6)} \to \Psi_{3\mathrm{C}}(\xi_1,\xi_2,\xi_3)$$
$$= (2\pi)^{-3}\exp(i\ \mathbf{r}_{ij}\cdot\mathbf{k}_{ij} + i\ \mathbf{R}_k\cdot\mathbf{K}_k)$$
$$\times N\prod_{n=1}^{3}\ {}_1F_1\left(i\frac{Z_lZ_m\mu_{lm}}{k_{lm}},1,\ -ik_{lm}\ \xi_n\right);$$
$$\epsilon_{lmn}\neq 0;\ \ l>m\in[1,3];\ \ \epsilon_{ijk}\neq 0;\ \ j>i\in[1,3]. \quad (5)$$

The actual task in deriving the expression (2) lies in determining the matrix elements a_{ij} which are different depending on the specific type of three-particle systems under consideration. For two electrons moving in the field of a nucleus these expansion coefficients a_{ij} have been determined on the grounds that the wavefunction, given by (2), has to be an exact asymptotic solution of the Schrödinger equation and the Kato cusp conditions have to be satisfied. In addition, the Wannier threshold-ionisation mode should be correctly described (see Paper I). If we take r_{12} to be the interelectronic coordinate, the form of the local product charges $Z_{ij}(\xi_4, \xi_5, \xi_6) = V_{ij} r_{ij}$ are then

$$Z_{12}(r_{13}, r_{23}, r_{12}) = 1 - \eta\,, \tag{6}$$

where Z_{12} is the interelectronic dynamical product charge. The function η is given by

$$\eta = \left(\frac{3 + \cos^2 4\alpha}{4} \frac{r_{12}}{r_{13} + r_{23}} \right)^2 , \tag{7}$$

where $\tan\alpha = r_{23}/r_{13}$. The dynamical electron–nucleus product charges are

$$Z_{13}(r_{13}, r_{23}, r_{12}) = -Z + (1 - Z_{12}) \frac{r_{13}^{1+s}}{(r_{13}^s + r_{23}^s) r_{12}} , \tag{8}$$

$$Z_{23}(r_{13}, r_{23}, r_{12}) = -Z + (1 - Z_{12}) \frac{r_{23}^{1+s}}{(r_{13}^s + r_{23}^s) r_{12}} , \tag{9}$$

where s is a non-vanishing positive real number which can be chosen as $s = 1$. The physical and mathematical justification for equations (6), (8) and (9) have been given in Paper I. For the following the limiting cases of (6), (8) and (9) are important. When one electron is close to the nucleus and the other electron is far away the first electron 'sees' the full nuclear charge Z, whereas the latter electron experiences a screened nuclear field $Z - 1$. The interelectronic interaction is totally screened ($Z_{12} = 0$), i.e.

$$\lim_{\substack{r_{23}\to\infty \\ (r_{13}/r_{23})\to 0}} Z_{23} \to -Z + 1,\ Z_{13} \to -Z,\ Z_{12} \to 0\ , \tag{10}$$

$$\lim_{\substack{r_{13}\to\infty \\ (r_{23}/r_{13})\to 0}} Z_{13} \to -Z + 1,\ Z_{23} \to -Z,\ Z_{12} \to 0\ . \tag{11}$$

As the distance between the two electrons diminishes they experience the full repulsive electronic interaction

$$\lim_{\substack{r_{12}\to 0 \\ (r_{13}/r_{12})\to\infty, (r_{13}/r_{12})\to\infty}} Z_{23} \to -Z,\ Z_{13} \to -Z,\ Z_{12} \to 1\ . \tag{12}$$

When the motion of the two electrons proceeds along the Wannier ridge the force exerted on the two-electron subsystem vanishes. The interelectronic correlation is minimised and completely subsumed into an effective nuclear charge

$$\lim_{\mathbf{r}_{13}\to-\mathbf{r}_{23}} Z_{23} \to -Z+1/4,\ Z_{13} \to -Z+1/4,\ Z_{12} \to 0,. \tag{13}$$

Furthermore, the dynamical product charges Z_{ij} conserve the total potential, i.e.

$$\sum_{j>i=1}^{3} \frac{Z_{ij}}{r_{ij}} = \sum_{j>i=1}^{3} \frac{Z_i Z_j}{r_{ij}}\,. \tag{14}$$

In addition, the dynamical product charges (6), (8) and (9) are bound in the whole Hilbert space, more specifically

$$Z_{12} \in [0,1],\ Z_{13} \in [-Z,0],\ Z_{23} \in [-Z,0]\,. \tag{15}$$

Equations (15) mean that an interaction between two Coulomb particles can be screened by the presence of a third charged particle, however, it does not change its sign.

Although the Wannier threshold ionisation mode is correctly accounted for by the dynamical product charges (6), (8) and (9) it is still not clear whether the Wannier threshold law is reproduced by the cross section when employing the wavefunction (2) as final state. This is due to the fact that, in the Wannier theory and its modifications (Peterkop 1971; Rau 1971, 1984; Klar 1981; Feagin 1984), the total potential is linearised around the Wannier configuration while the kinetic energy operator is exactly treated. In contrast, in the present treatment the total potential is exactly diagonalised because the Hamiltonian H is invariant under the transformation (4), whereas parts of the kinetic energy are neglected as demonstrated in Paper I. Thus, it is desirable to explicitly incorporate the Wannier threshold law in the present model. According to the Wannier stability analysis, the excess-energy functional dependence of the total cross section for double escape is described by

$$\sigma(E) \propto E^{\mu/2\ -\ 1/4}\,, \tag{16}$$

where the Wannier index μ is given by

$$\mu = \tfrac{1}{2}\sqrt{\frac{100Z-9}{4Z-1}}\,. \tag{17}$$

On the other hand, the total cross section can be directly calculated from the transition amplitude using the formula

$$\sigma(E) = \frac{(2\pi)^4}{v_i}\int |T|^2 \delta(E-E_i) d^3k_{13} d^3k_{23}\,, \tag{18}$$

where E_i, v_i are the energy in the initial channel and the velocity of the incoming projectile with respect to the nucleus. The transition-matrix element occurring in (18) has the form

$$T = \langle\ \Psi_{\mathrm{DS3C}} | W_i | \Phi\ \rangle\,, \tag{19}$$

where the perturbation operator in the initial channel is denoted by W_i and the initial state of the three-body system is described by $|\Phi\ \rangle$. To evaluate the transition amplitude (19) a six-dimensional integral has to be performed which is not feasible at present. However, if we follow the treatment of Peterkop (1977) and Rudge and Seaton (1965; see also Jetzke and Faisal 1992), which are based on a consideration of the classical motion of three Coulomb particles in the total three-body Coulomb potential at asymptotically large distances, the radial dependence of the dynamical charges (6), (8) and (9) can be converted into a velocity dependence using the formula $r_{ij} = k_{ij}/\mu_{ij} t$ where t is the time. The validity of this relation has been reinforced by Redmond (see Rosenberg 1973) who showed that for large t, i.e. in the asymptotic region, the wavepackets of n charged particles are centred around the classical trajectories:

$$\mathbf{r}_j = \mathbf{v}_j\ t - \sum_{k \neq j}^{n} \frac{Z_{jk}}{m_j\ v_{jk}^2}\ \hat{\mathbf{r}}_{jk}\ \ln|t|\,. \tag{20}$$

Here $\mathbf{r}_i$, $\mathbf{v}_i$ refer to the position and velocities of the particles with respect to an arbitrary origin and $\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j$; $\mathbf{v}_{ij} = \mathbf{v}_i - \mathbf{v}_j$. From (20) it is clear that for $|t| \to \infty$ the wavepackets are well separated and their motion is uniform, i.e. $\lim_{|t|\to\infty} \mathbf{r}_i = \mathbf{v}_i\ t$. The same conclusions have also been drawn by Peterkop and Rabik (1977) and Gailitis (1990). Using the momentum dependent dynamical charges (6), (8) and (9) $[Z_{ij}(r_{13}, r_{23}, r_{12}) = Z_{ij}(r_{13} = k_{13}/\mu_{13}t, r_{23}k_{23}/\mu_{23}t, r_{12}k_{12}/\mu_{12}t)]$ the six-dimensional integral (19) can be analytically reduced to two-dimensional integrals on the real axis which are performed numerically. In addition, the normalisation of the wavefunction, given by (2), is readily deduced

$$N = N_{13} N_{23} N_{12}\,, \tag{21}$$

where

$$N_{ij} = \exp(-\beta_{ij}\pi/2)\Gamma(1 - i\beta_{ij})\,. \tag{22}$$

3. Incorporation of the Wannier Threshold Law

As discussed in Paper I the wavefunction Ψ_{DS3C}, given by (2), aims at diagonalising the total potential in an exact manner whilst disregarding some parts of the kinetic energy operator. In addition, Ψ_{DS3C} is constructed to possess the correct asymptotic behaviour. The latter property is ensured by requiring the dynamical product charges (6), (8) and (9) to have the limiting cases given by equation (10)–(15). As these conditions are limits, there will naturally be other functional forms of Z_{ij} extrapolating between these limits. Different choices for Z_{ij} correspond to different parts of the kinetic energy operator being neglected. Here we will

use this additional freedom to construct product charges Z_{ij} which lead to the Wannier threshold law when calculating the cross section (18). To this end we remark that at threshold the functional dependence $\sigma(E)$ is determined by properties of the final state wavefunction, irrespective of the initial state from which or the transition operator via which this final state is achieved. This is due to the fact that the initial binding energy of the system, i.e. the minimal energy needed to bring about the transition of the two electrons to the double continuum, is usually much larger than the excess energy E at which the system is to be considered. This fact is also one of the ingredients of the Wannier theory which, for this reason, treats the reaction as a 'half collision'. Thus the threshold behaviour of the function Ψ_{DS3C} is decisive for $\sigma(E)$. For inspection of this behaviour we introduce hyperspherical momenta

$$K := (k_{13}^2 + k_{23}^2)/2 = E, \quad \tan\beta = \frac{k_{23}}{k_{13}}, \quad \text{and} \quad \cos\theta_k = \hat{\mathbf{k}}_{13} \cdot \hat{\mathbf{k}}_{23}\,. \tag{23}$$

Taking (15) into account the wavefunctions Ψ_{DS3C} and Ψ_{3C}, given by (2) and (5), can be expanded in terms of Bessel functions (Luke 1975; Abramowitz and Stegun 1984) and, for small excess energies $E \to 0$, taking leading order terms in excess energy we obtain

$$\lim_{E\to 0} \Psi_{\mathrm{DS3C}}(\xi_{1\cdots 6}) = (2\pi)^{-3} N J_0(2\sqrt{-Z_{23}\xi_1})\, J_0(2\sqrt{-Z_{13}\xi_2})\, I_0(\sqrt{2Z_{12}\xi_3})\,, \tag{24}$$

where $J_0(x), I_0(x)$ are Bessel and modified Bessel functions respectively. A similar equation applies to Ψ_{3C} with the replacement $Z_{23} = -Z = Z_{13}, Z_{12} = 1$. Reformulating (18) in the coordinates given by (23), the integration over the coordinate K is readily performed. In addition, due to the overall rotational invariance of the system (18) reduces to

$$\sigma(E) = \frac{(2\pi)^{-2}}{v_i}\; 2E^2 \int \sin^2 2\beta\; |N|^2 |T_r|^2\; d\beta\; d\cos\theta_k\; d\varphi_{12}\; d\varphi_{23}\,. \tag{25}$$

In (25) φ_{12} and φ_{23} denote the azimuthal angles of $\mathbf{k}_{12}$ and $\mathbf{k}_{13}$ with respect to an appropriate axis, whereas T_r is the transition matrix element T (19) with the normalisation factor of the final-state wavefunction being factored out. As evident from (25) the excess-energy dependence of $\sigma(E)$ is directly related to the excess-energy behaviour of $|N|^2$ since, for $E \ll 1$, T_r is an insignificantly slow varying function of E and thus irrelevant regarding the functional form of $\sigma(E)$. This is in accordance with the Wannier theory in that $\sigma(E)$ is a property of the phase space occupied by the two continuum electrons. On the other hand the function N, being a normalisation constant (with regard to radial dependence), is determined by the radial part of the wavefunction, in particular, by its asymptotic behaviour. This is clearly seen when inspecting the threshold behaviour (24) and its implication for $\sigma(E)$. The Bessel function $J_0(x)$ has an oscillatory bound asymptotic behaviour whereas the modified Bessel function $I_0(x)$, corresponding to the electron–electron interaction, is unbound for large arguments x. Hence, to account for this behaviour, the normalisation $|N_{12}|^2$ of

the electron–electron Coulomb wave must decrease exponentially with vanishing excess energy. In fact we have

$$|N_{ij}|^2 = 2\pi\beta_{ij}\left(e^{2\pi\beta_{ij}} - 1\right)^{-1} \tag{26}$$

and thus for $E \ll 1$ the factors N_{ij} take on the forms

$$|N_{13}|^2 = -2\pi\beta_{13} = \frac{-2\pi Z_{13}}{\sqrt{2E}\cos\beta}, \quad \forall Z_{13} < 0 \tag{27}$$

$$|N_{23}|^2 = -2\pi\beta_{23} = \frac{-2\pi Z_{13}}{\sqrt{2E}\sin\beta}, \quad \forall Z_{23} < 0 \tag{28}$$

$$|N_{12}|^2 = \frac{2\pi Z_{12}}{\sqrt{2E}f(\theta_k,\beta)} \exp\left(-2\pi\frac{Z_{12}}{\sqrt{2E}f(\theta_k,\beta)}\right), \quad \forall Z_{12} > 0\,, \tag{29}$$

where

$$f(\theta_k,\beta) = \sqrt{1 - \sin 2\beta\cos\theta_k}.$$

For $Z_{12} > 0$ (Ψ_{3C} employs $Z_{12} = 1$) the behaviour (29) is directly reflected into $\sigma(E)$ which declines exponentially at lower excess energy. Cross sections calculated with Ψ_{DS3C} do not exhibit this spurious behaviour as the argument of $I_0(\sqrt{2Z_{12}\xi_3})$ remains bound in the whole Hilbert space (because $Z_{12} \to 0$ for $\xi_3 \to \infty$); however, the analytic dependence (16) of the cross section is not explicitly reproduced. It is worth noting at this stage that the analytic dependence $\sigma(E)$ in certain approximations is readily deduced from (25), (27) and (28). In an independent neutral particle model, i.e. when the motion of the two electrons is described by plane waves, we deduce from (22) that $N = 1$ and (25) shows then the behaviour $\sigma(E) \propto E^2$. In contrast in an independent Coulomb particle model, i.e. $Z_{12} \equiv 0$, $Z_{13} = -Z = Z_{23}$, we end up with $N_{12} = 1$ and thus $\sigma(E) \propto E$ as it is evident upon substitution of (27) and (28) into (25). In the first Born approximation, i.e. $Z_{13} \equiv 0 \equiv Z_{12}$, $Z_{23} = -Z$, (25) and (28) yield $\sigma(E) \propto E^{1\cdot 5}$. Now the question arises whether it is possible to find product charges Z_{ij} which fulfil the conditions given by (10)–(15) and lead to the threshold law (16). To answer this question we insert (27)–(29) in (25) to arrive at

$$\sigma(E) = \frac{2\pi}{v_i}\, E \int \frac{Z_{13}Z_{23}Z_{12}}{\sqrt{2E}}\, \exp\left(-2\pi\frac{Z_{12}}{\sqrt{2E}}\, f^{-1}(\theta_k,\beta)\right)$$

$$\times\, [\sin 2\beta\; f^{-1}(\theta_k,\beta)\; |T_r(\theta_k,\beta,\varphi_{13},\varphi_{23})|^2] d\beta d\varphi_{13} d\varphi_{23}\; d\cos\theta_k\,. \tag{30}$$

Equation (30) is valid for $Z_{ij} \neq 0$. From (30) it is clear that the energy dependence of the integrand can be considerably smoothed by an appropriate choice of Z_{12}. Suppose Z_{12} has the form

$$Z_{12} = (1 - \eta\; a^g)a^h\,, \tag{31}$$

where the dimensionless quantity $a = E/E_i$ has been introduced and where E_i is the initial total energy of the system before fragmentation. The functions g and h are determined such that the conditions (10)–(15) are satisfied. Upon substitution of (31) in (30) and requiring $\sigma(E)$ to behave as given by (16), the excess-energy dependence of the function h is concluded to be

$$h \propto n \qquad \text{where} \qquad n = 0{\cdot}5 + \frac{\mu}{2} - \tfrac{1}{4} - 1\,. \tag{32}$$

It is readily established that with this functional dependence of Z_{12} the Wannier threshold law is reproduced and the integrand in (30) is a slowly varying function of E. Now to establish the condition $\lim_{r_{12}\to 0} Z_{12} \to 1$ the function h must vanish in this case. Thus, we assume $h = (\mathbf{k}_{13} - \mathbf{k}_{23})^2/(k_{13} + k_{23})^2\ n$. The class of functions for g is limited by the conditions (10)–(11). A simple choice for g which fulfils these relations is

$$g = \frac{2k_{13}\ k_{23}\ \cos\theta_k/2}{k_{13}^2 + k_{23}^2}\ . \tag{33}$$

As f and g are now determined we can, in principle, substitute for Z_{12} in (9) and (18) to arrive at the final forms of the product charges. One has to bear in mind, however, that (30) is only valid in the case where Z_{13} or Z_{23} do not vanish. The latter product charges do indeed vanish in certain cases and if $Z = 1$ [compare (10) and (11)]. However, the choice $s = a$ considerably minimises the region in which Z_{13} or Z_{23} are zero. In fact this region does not contribute to the integrand in (30). Now upon inspection of the integral (30) at small excess energy one can deduce

$$\sigma(E) = E^{\mu/2-1/4} \int \mathcal{T}_{abs}(\mathbf{k}_{13}, \mathbf{k}_{23})\ d\varphi_{13}\ d\varphi_{23}\ d\cos\theta_k\ d\beta\,, \tag{34}$$

where $\mathcal{T}_{abs}(\mathbf{k}_{13}, \mathbf{k}_{23})$ is an insignificantly slow varying function of E. The accuracy and range of validity of (34) is explicitly shown in the next section where (30) is evaluated numerically. It is straightforward to show that the above constructed product charges satisfy the conditions (10)–(15). In particular the total potential is conserved along the trajectories of free particles, i.e. $\sum_{j>i=1}^{3} Z_{ij}\mu_{ij}/k_{ij} = \sum_{j>i=1}^{3} Z_i Z_j \mu_{ij}/k_{ij}$. Further, as the limits (10)–(13) are fulfilled a procedure similar to that applied in Paper I can be used to show that the wavefunction Ψ_{DS3C} satisfies the Kato cusp conditions. Finally, it should be mentioned that all the modifications made to the product charges Z_{ij} at threshold depend on the factor a which goes to unity for higher energies. In this case it is a simple matter to deduce that the original product charges (6), (8) and (9) are obtained.

4. Numerical Results

In the last section we designed the product charges Z_{ij} so as to reproduce the analytical dependence (16) of the cross section $\sigma(E)$. The absolute value of $\sigma(E)$ will depend on the detailed reaction dynamic which is contained in $\mathcal{T}_{abs}(\mathbf{k}_{13}, \mathbf{k}_{23})$,

as seen from (34). The Wannier treatment does not provide any information about the magnitude of $\sigma(E)$. That the magnitude is a very sensitive quantity is illustrated by the behaviour of the cross section in the independent Coulomb particle model which, as shown above, yields a linear dependence of the cross section on the excess energy, $\sigma(E) \propto E$. Although the latter dependence of $\sigma(E)$ does not deviate much from the Wannier threshold law (16) the absolute value of $\sigma(E)$ within the independent Coulomb particle model is largely overestimated (compare Fig. 1). If we employ the wavefunction Ψ_{DS3C}, with the dynamical product charges described in the preceding section, for the description of two

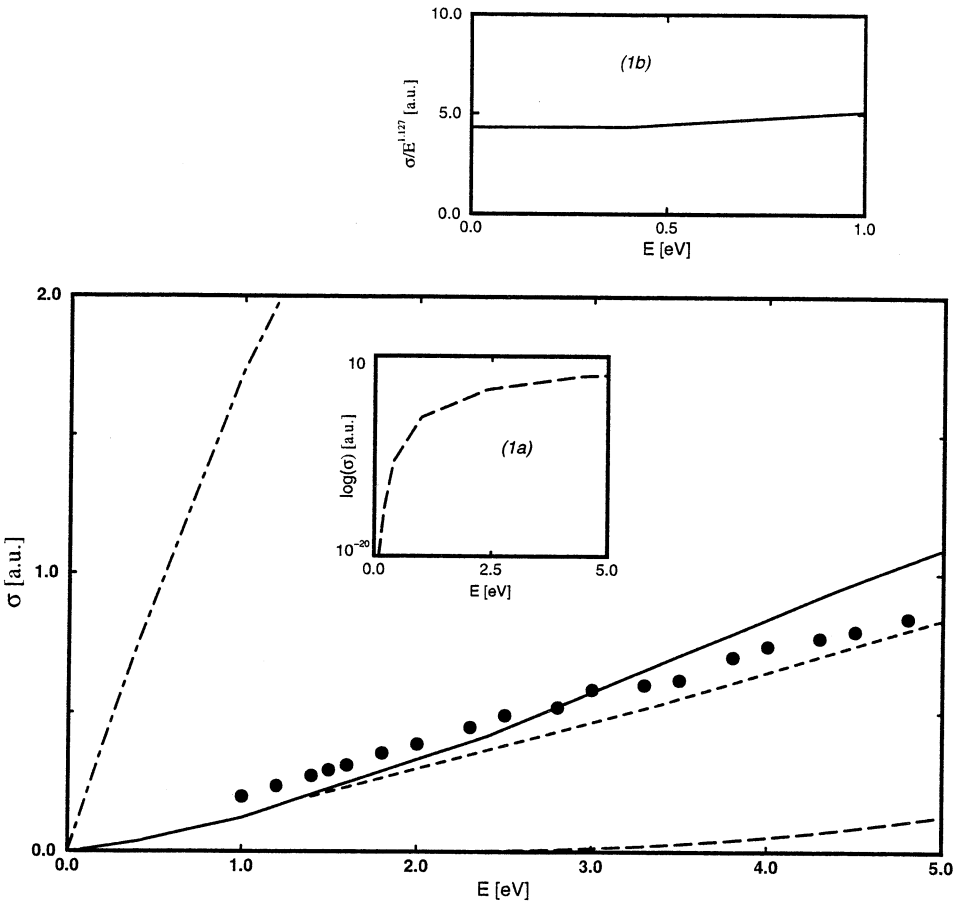

Fig. 1. Total cross section for the electron-impact ionisation of atomic hydrogen as a function of the excess energy E. The solid (long dashed) curve shows the results for $\sigma(E)$ when representing the two continuum electrons by Ψ_{DS3C} (Ψ_{3C}), whereas the dot–dash curve denotes the results of the independent Coulomb particles model (see text). Results of the CCC method are also included (short dashed curve). Experimental data are due to Shah *et al.* (1987). Inset (1a) shows the results of the Ψ_{3C} wavefunction on a logarithmic scale, whereas in inset (1b) the quantity $\sigma(E)/E^{1\cdot 127}$ as function of E is evaluated using Ψ_{DS3C} for the description of the continuum electrons.

continuum electrons resulting from electron-impact ionisation of atomic hydrogen and numerically evaluate the integral given by (30) we end up with the behaviour depicted in Fig. 1. First we remark that the absolute magnitude of the total cross section is satisfactorily reproduced. It should be stressed that this feature is not enforced by any choice of Z_{ij}. To examine the analytical behaviour of $\sigma(E)$ calculated using Ψ_{DS3C} we plot in inset (1b) the quantity $\sigma(E)/E^{1\cdot 127}$. According to the Wannier-threshold law the latter quantity should be a constant function of E and gives the absolute value of the cross section. As seen in inset (1b) the Wannier threshold law is in fact reproduced by Ψ_{DS3C} within a range of $E \in [0, 0\cdot 5\ \mathrm{eV}]$. For $E > 0\cdot 5$ eV the analytical dependence of $\sigma(E)$ evaluated with Ψ_{DS3C} slowly deviates from the Wannier threshold law. When using the Ψ_{3C} wavefunction for the description of the two escaping electrons we end up, as expected, with the wrong analytical behaviour for $\sigma(E)$, as well as with the wrong absolute value for the total cross section (inset 1a) which indicates that, at lower excess energies, the fragmentation dynamics are poorly described by Ψ_{3C}. This is in accordance with the analysis of Paper I which shows that Ψ_{3C} reveals a threshold behaviour which is incompatible with properties of the total potential. Also included in Fig. 1 are the results of the convergent-close coupling (CCC) method, (Bray and Stelbovics 1993). The results of the CCC method are in very good agreement with the experimental $\sigma(E)$ for higher energies (Bray and Stelbovics 1993); however, close to threshold the evaluation of $\sigma(E)$ is limited by the computational resources as an ever increasing number of pseudo states is needed to achieve convergence.

In addition to the magnitude of the cross section, the spin asymmetry A offers a further way of probing the dynamical properties of the electron-impact ionisation of atomic systems. The spin asymmetry A is defined as

$$A(E) := \frac{\sigma^s(E) - \sigma^t(E)}{\sigma^s(E) + 3\sigma^t(E)}, \tag{35}$$

where σ^s and σ^t are the total ionisation cross sections for singlet and triplet scattering respectively. In the case where the two continuum electrons are treated on an equal footing, the normalisation N (22) of approximate wavefunctions is invariant under exchange of the electron momenta, i.e. $N(\mathbf{k}_{13}, \mathbf{k}_{23}) = N(\mathbf{k}_{23}, \mathbf{k}_{13})$ (this is not the case in the first Born approximation). Hence, A depends strongly on the behaviour the radial part of the wavefunction and therefore it is a dynamical property of the ionisation mechanism. The Wannier theory for threshold ionisation predicts a constant value of A with increasing excess energy but provides no information on the numerical value (Greene and Rau 1982). Measurements of A at threshold reveal a slightly positive slope of the spin asymmetry with increasing excess energies (Guo *et al.* 1990).

In Fig. 2 the results for A are shown in the case where the two-electron continuum final state is represented by Ψ_{3C} and Ψ_{DS3C}. Also depicted in Fig. 2 are the results of the CCC approach (Bray and Stelbovics 1993) and the method using hidden-crossing theory (Macek and Ovchinnikov 1995). Although all theories, except for that using Ψ_{3C}, are in reasonable agreement with experiment the positive slope of A at threshold is not reproduced. Again the spurious radial

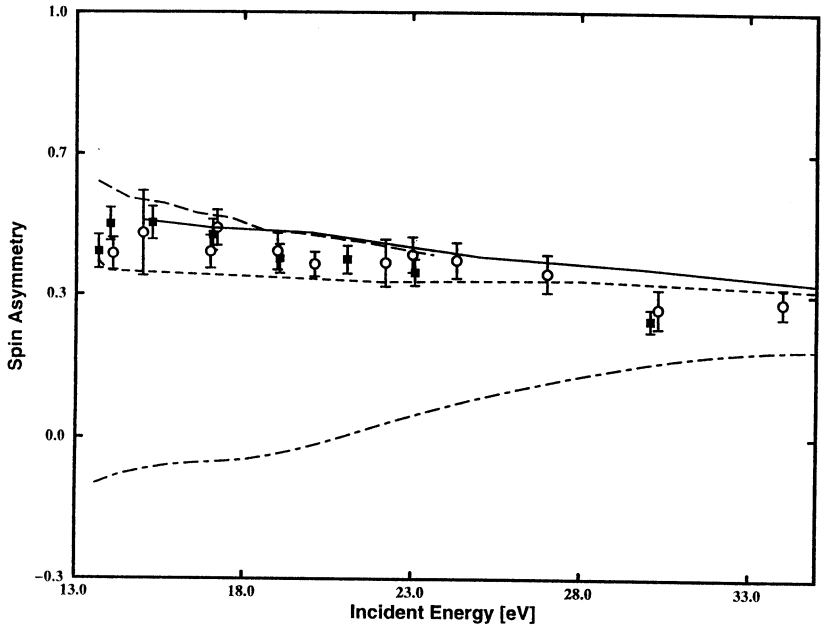

Fig. 2. Spin asymmetry (35) in the total cross section for the electron-impact ionisation of atomic hydrogen. Results of the hidden crossing theory (Macek and Ovchinnikov 1995) (long dashed curve) and the CCC method (Bray and Stelbovics 1993) (solid curve) are depicted. Representing the final state by Ψ_{DS3C} (Ψ_{3C}) yields for the spin asymmetry the results shown by the short-dashed (dot–dash) curve. The experimental data are due to Fletcher *et al.* (1985) (full squares) and Crowe *et al.* (1990) (open circles).

behaviour of Ψ_{3C} at the fragmentation threshold, as has been discussed in the preceding section, results in completely wrong behaviour of the calculated spin asymmetry. With increasing excess energy Ψ_{3C} becomes more and more an adequate description. It should be emphasised that the design of the dynamical product charges Z_{ij}, as done in the preceding section, aims at controlling the threshold excess energy behaviour of the normalisation $|N|^2$ so as to reproduce the threshold law (16) of the total cross section. The results (Fig. 2) for the spin asymmetry using Ψ_{DS3C} are, however, determined by the behaviour of radial part of Ψ_{DS3C} which is independent of N and thus not *a priori* imposed.

We can further assess the behaviour of the integrand in (34) by investigating the excess-energy sharing between the two electrons regardless of their emission directions, i.e. $d\sigma(E,\beta)/d\beta$. The Wannier treatment, supported by experiment (Cvejanović and Read 1974; Lablanquie *et al.* 1990; Cvejanović *et al.* 1995), predicts a basically flat energy distribution at threshold. In Fig. 3 results for the energy-sharing calculated with Ψ_{3C} and Ψ_{DS3C} are depicted. In contrast to the Wannier theory prediction Ψ_{3C} yields an energy distribution sharply peaked around equal energy–sharing whereas Ψ_{DS3C} indicates a much flatter energy–sharing, dependence. A possible explanation for this behaviour is given by Berakdar (1996*b*).

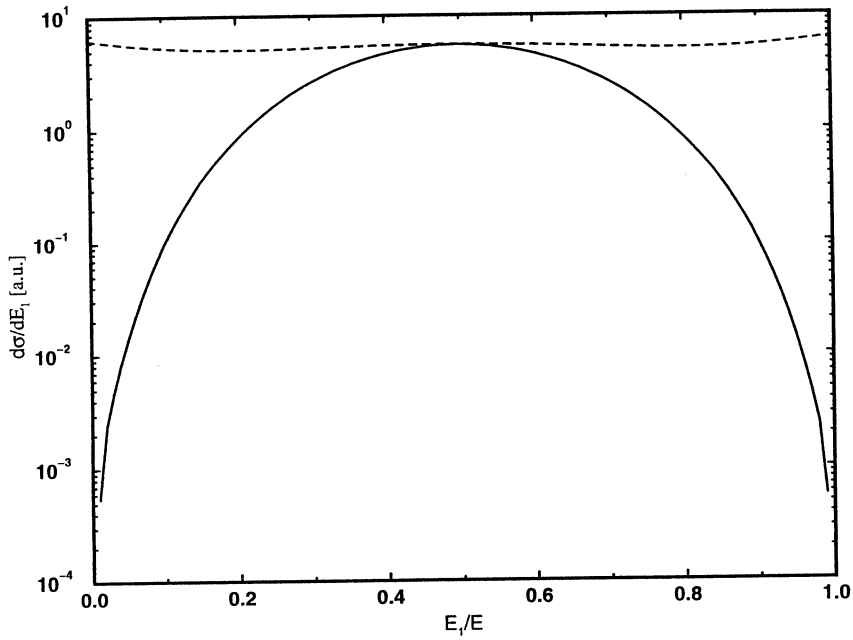

Fig. 3. Single differential cross section for the electron-impact ionisation of atomic hydrogen as function of the ratio E_1/E where E_1, is the energy of one of the final-state electrons and E is the total excess energy which is chosen as $E = 200$ meV. Using the Ψ_{DS3C} approximation yields the dashed curve, whereas the solid curve represents the results when employing Ψ_{3C} for the final state. The results of Ψ_{3C} have been multiplied by a factor of 10^{13}.

5. Conclusions

For the description of the motion of two electrons receding from an ion a three-body Coulomb wavefunction has been constructed which reproduces the Wannier threshold law for the total cross section. In addition, this wavefunction is analytical in the whole Hilbert space and constitutes an exact solution of the non-relativistic three-body Schrödinger equation in the asymptotic region. Furthermore, the Kato cusp conditions are satisfied. Using this wavefunction the total cross section for the electron-impact ionisation of atomic hydrogen has been calculated and analysed, as well as the spin asymmetry in this cross section. In addition, the excess-energy sharing between the two escaping electrons has been shown to be consistent with the Wannier theory predictions when employing the designed wavefunction.

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