Aust. J. Phys., 1994, **47**, 123–7

Calculation of Electron Impact Ionisation of Atomic Hydrogen with the Exact Final-state Boundary Conditions

Dmitry A. Konovalov and Ian E. McCarthy

Electronic Structure of Materials Centre, School of Physical Sciences,
Flinders University of South Australia, G.P.O. Box 2100,
Adelaide, S.A. 5001, Australia.
email: dima@esm.ph.flinders.edu.au and ian@esm.ph.flinders.edu.au

Abstract

We present a new and very powerful theoretical method—a distorted-wave Born approximation (DWBA) with an arbitrary final-state electron–electron correlation function. This method combines the flexibility of including any theoretically desired electron–electron correlation and the physical clarity of the DWBA method. Calculations explore the use of an auxiliary final-state wave function with the exact boundary condition, in attempting to describe the absolute cross sections for ionisation of helium in coplanar symmetric kinematics and to resolve discrepancies between theory and experiment.

1. Introduction and Theoretical Background

Some questions have been raised since Brauner, Briggs and Klar (BBK) (1989) first used a final state with the exact boundary condition (Rosenberg 1973) in a calculation of the (e, 2e) reaction on the hydrogen atom:

Question 1: Can the analogous state be incorporated in a calculation for a larger atom?

Question 2: Is the correct final-state boundary condition formally necessary for a correct calculation of ionisation?

Question 3: Is it relatively simple to find a universally valid method of calculating ionisation by incorporating the exact boundary condition?

Recently these or similar questions have generated extensive theoretical and experimental work (Brauner *et al.* 1991; Jones *et al.* 1993; Pochat *et al.* 1993; Klar *et al.* 1993).

In discussing these questions it is sufficient, at energies where resonances in two-body subsystems (McCarthy and Bo Shang 1993) are unimportant, to use a three-body model of ionisation, two bodies being the electrons, for which the relevant dynamical variables are distinguished by subscripts $i = 1, 2$, and the third being the residual ion, which plays the part of a massive, charged, inert core. The electron–core interactions are represented by static exchange potentials V_i. The subscript 0 is used for dynamical variables of the incident electron.

The analogue of the BBK final state is

$$\langle \Phi^{(-)}(\mathbf{k}_1, \mathbf{k}_2)| = \langle \chi^{(-)}(\mathbf{k}_1)\chi^{(-)}(\mathbf{k}_2)C(\mathbf{k}_1 - \mathbf{k}_2)|\,, \tag{1}$$

0004-9506/94/020123$05.00

where $|\chi^{(-)}(\mathbf{k}_i)\rangle$ are distorted waves, defined by

$$(E_i - K_i - V_i)|\chi^{(-)}(\mathbf{k}_i)\rangle = 0\,, \tag{2}$$

and the coordinate-space representation of the final-state correlation factor C is

$$C_{\mathrm{BBK}}(\eta, \mathbf{k}, \mathbf{r}) = \Gamma(1 - i\eta)\mathrm{e}^{-\pi\eta/2}\, F_{11}\big(\mathrm{i}\eta; 1; -\mathrm{i}(kr + \mathbf{k}\,.\,\mathbf{r})\big)\,. \tag{3}$$

Here

$$\eta = 1/2k\,, \qquad \mathbf{k} = \tfrac{1}{2}(\mathbf{k}_1 - \mathbf{k}_2), \qquad \mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2\,. \tag{4}$$

We use a formalism in which two-electron states are not explicitly antisymmetrised. Antisymmetrisation is achieved in ionisation amplitudes by means of an exchange term obtained by reversing the roles of $\mathbf{k}_1$ and $\mathbf{k}_2$. Antisymmetric states are used in calculations if necessary.

The first question above was affirmatively answered by Klar *et al.* (1993), who calculated coplanar symmetric cross sections for helium using the amplitude

$$\langle \mathbf{k}_1\mathbf{k}_2|T|\alpha\mathbf{k}_0\rangle = \langle \Phi^{(-)}(\mathbf{k}_1, \mathbf{k}_2)|V|\alpha\chi^{(+)}(\mathbf{k}_0)\rangle\,, \tag{5}$$

where V is the electron–target potential, $|\alpha\rangle$ is the orbital of the struck electron in the independent-particle model, and $|\chi^{(+)}(\mathbf{k}_0)\rangle$ is a distorted wave calculated in the potential $\langle\alpha|V|\alpha\rangle$. The numerical method uses Cartesian coordinates and six-dimensional Gaussian quadratures. Coplanar symmetric kinematics was chosen because of the existence of absolute experimental data and because the data provide a severe test of theory since they scan a wide range of recoil momentum $p = |\mathbf{k}_0 - \mathbf{k}_1 - \mathbf{k}_2|$ and momentum transfer $K = |\mathbf{k}_0 - \mathbf{k}_1|$, where $\mathbf{k}_1$ is the momentum of the faster electron.

The second question was answered negatively (Klar *et al.* 1993), where three forms of the formal T-matrix element for the three-body problem were considered:

$$\begin{aligned}
\langle \mathbf{k}_1\mathbf{k}_2|T|\alpha\mathbf{k}_0\rangle &= \langle \chi^{(-)}(\mathbf{k}_1)\chi^{(-)}(\mathbf{k}_2)|V - U_1|\Psi_\alpha^{(+)}(\mathbf{k}_0)\rangle \\
&= \langle \Psi^{(-)}(\mathbf{k}_1, \mathbf{k}_2)|V - U_1|\alpha\chi^{(+)}(\mathbf{k}_0)\rangle \qquad (6) \\
&= \langle \Phi^{(-)}(\mathbf{k}_1, \mathbf{k}_2)|V - U_1|\alpha\chi^{(+)}(\mathbf{k}_0)\rangle \qquad (7) \\
&\quad + \langle \Phi^{(-)}(\mathbf{k}_1, \mathbf{k}_2)|\overline{H} - E|\Psi_\alpha^{(+)}(\mathbf{k}_0) - \alpha\chi^{(+)}(\mathbf{k}_0)\rangle\,. \qquad (8)
\end{aligned}$$

Here $U_1 = \langle\alpha|V|\alpha\rangle$, $\Psi^{(\pm)}$ represent exact eigenstates of the three-body Hamiltonian H with initial/final-state boundary conditions, $\chi^{(-)}(\mathbf{k}_1)$ is calculated in the potential U_1 [not V_1 as in (1)] and $\Phi^{(-)}(\mathbf{k}_1, \mathbf{k}_2)$ is an auxiliary final-state function, whose choice is arbitrary. The notation $\overline{H}$ in (8) indicates that H operates on the bra state.

We calculate the first term of (8), considering the second term as a correction that is to be minimised. The choice $\Phi^{(-)} = \Psi^{(-)}$ reduces the second term to zero and makes (8) equivalent to (7). Equating the bra vectors of (6) and (8) reduces (8) to (6).

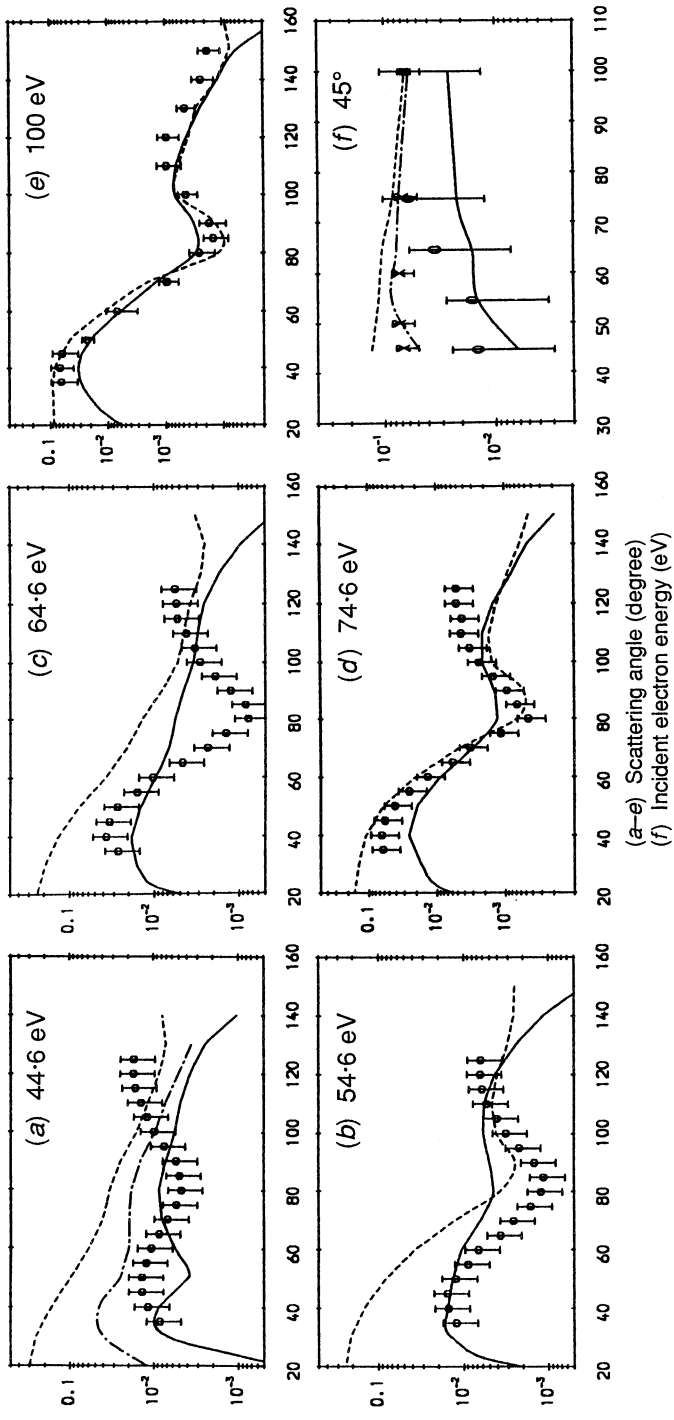

Fig. 1. Comparison of calculations with experimental data for the coplanar symmetric ionisation of helium. Experimental data are as follows: (*a*)–(*d*) Murray and Read (1993); (*e*) Gélébart and Tweed (1990); (*f*) absolute 45° differential cross sections measured by Pochat *et al.* (1993) (crosses); and Murray and Read (1993) (circles). Calculated curves are solid: BBK, short dashes: DWBA, dash–dot for (*a*) with $\beta = 2$ and for (*f*) with $\beta = 6$: see text. Experimental data of Murray and Read (1993) and Gélébart and Tweed (1990) are normalised at 45° and at 100 eV to the absolute measurements of Pochat *et al.* (1993).

The answer to the second question is obtained by considering the correction term of (8). The state $|\alpha\chi^{(+)}(\mathbf{k}_0)\rangle$ has the same asymptotic form as the exact state $|\Psi_\alpha^{(+)}(\mathbf{k}_0)\rangle$. Therefore the coordinate representation of the ket vector is zero in the asymptotic region so that the asymptotic form of $\Phi^{(-)}(\mathbf{k}_1, \mathbf{k}_2)$ is irrelevant. Nevertheless it is sensible to start with the correct asymptotic form in trying to choose $\Phi^{(-)}$ as close to $\Psi^{(-)}$ as possible in a given situation.

The object of the present work is to discuss the third question in terms of choices of the arbitrary auxiliary function $\langle \mathbf{r}_1, \mathbf{r}_2|\Phi^{(-)}(\mathbf{k}_1, \mathbf{k}_2)\rangle$. The ultimate objective of this approach to the ionisation problem is to choose a function that makes the second term of (8) negligibly small. Complete calculation of this term of course requires a solution of the problem, so other criteria must be found for judging whether it is small enough.

Here we use an experimental criterion, comparison of a calculation using the first term of (8) with coplanar symmetric cross sections. These data provide a severe test of theory since absolute experimental data exist and since they scan a wide range of recoil momentum $p = |\mathbf{k}_0 - \mathbf{k}_1 - \mathbf{k}_2|$ and momentum transfer $K = |\mathbf{k}_0 - \mathbf{k}_1|$.

2. Calculation and Results

The forms used for the auxiliary function $\langle \mathbf{r}_1, \mathbf{r}_2|\Phi^{(-)}(\mathbf{k}_1, \mathbf{k}_2)\rangle$ are all summarised by (1) with different expressions for the correlation factor C. The calculation denoted BBK uses the form (3), while DWBA uses $C = 1$. Figs 1*a*–*e* show coplanar symmetric cases at different incident energies for helium. At 74·6 and 100 eV there is little to choose between BBK and DWBA. At the lower energies absolute cross sections favour BBK, but details do not agree with experiment.

It is certain that the product form (1)–(3) is invalid in the interior region. Since DWBA is known to be successful [see for example Konovalov and McCarthy (1992) and McCarthy (1992)], in many cases where final-state correlations are unimportant we have chosen a form for C that is 1 in the interior region and given by (3) at large (asymptotic) distances. This is

$$C_\beta(\eta, \mathbf{k}, \mathbf{r}) = \mathrm{e}^{-(r_1^2+r_2^2)/\beta^2} + (1 - \mathrm{e}^{-(r_1^2+r_2^2)/\beta^2}) C_{\mathrm{BBK}}(\eta, \mathbf{k}, \mathbf{r}) . \tag{9}$$

The first amplitude of (9) is BBK for small β and DWBA for large β.

Fig. 1*f* shows the energy dependence of the coplanar symmetric cross section at 45° observed in two different experiments by Pochat *et al.* (1993) and by Murray and Read (1993) [normalised to the data of Pochat *et al.* (1993) at 100 eV].

DWBA does not include any final-state electron–electron correlation. The effect of this correlation becomes very important for coplanar symmetric (e, 2e) processes in forward or backward scattering at any energy. For example, the differential cross section (see Fig. 1) should vanish at 0 and 180° due to electron–electron repulsion. DWBA gives a nonzero answer at these angles. On the other hand BBK includes this correlation for any r_1 and r_2. These two cases represent two extremes which, we expect, should give very realistic bounds for the correct answer. This statement is well illustrated by Figs 1*d* and 1*e*. The two experiments are in good agreement with each other (Fig. 1*f*) which makes the experimental data used in Fig. 1*d* and 1*e* appear quite reliable. Also, the points lie within

the region bounded by the DWBA and BBK calculations, especially for the front scattering angles.

Unfortunately the experimental data are incompatible for incident energies below 74·6 eV. This makes it difficult to draw any conclusions from Figs 1*a*–*c* where the theoretical bounds, the DWBA and BBK calculations, do not contain experimental points as they do in Figs 1*d* and 1*e*. To further illustrate this point, we choose two intermediate cases (Figs 1*a* and 1*f*). Fig. 1*f* shows the $\beta = 6$ calculation, which agrees with the experiment of Pochat *et al.* (1993), while the BBK calculation agrees with the data of Murray and Read (1993). Also, Fig. 1*a* shows that the cross section for $\beta = 2$ is intermediate between BBK and DWBA, although it does not seem that a different choice of β would yield detailed agreement with experiment. A more sophisticated parametrisation of C may be needed in the interior region to get better agreement with experiment.

Using the above reasoning we conclude that a good understanding of the (e, 2e) process is achieved at energies above 74·6 eV. The theory also gives quite a close description of the experimental data at these energies. However, the energy region below 74·6 eV still has some major discrepancies and further experimental and theoretical work is required to resolve this problem. The further experimental work will have to resolve the major disagreement between two experiments (Fig. 1*f*). Further theoretical development would be able to check the assumption that the correct answer lies within the bounds of DWBA and BBK (Figs 1*d*–*f*). Such theoretical work is under way (Bray and Stelbovics 1992, 1993).

Acknowledgments

We acknowledge support from the Australian Research Council. We would like to thank Professor F. Read, Dr A. Murray and Dr R. Tweed for providing their experimental data in tabular form.

References

Brauner, M., Briggs, J. S., and Klar, H. (1989). *J. Phys.* B **22**, 2265.
Brauner, M., Briggs, J. S., Klar, H., Broad, J. T., Rösel, T., Jung, K., and Ehrhardt, H. (1991). *J. Phys.* B **24**, 657.
Bray, I., and Stelbovics, A. T. (1992). *Phys. Rev.* A **46**, 6995.
Bray, I., and Stelbovics, A. T. (1993). *Phys. Rev. Lett.* **70**, 746.
Gélébart, F., and Tweed, R. J. (1990). *J. Phys.* B **23**, L641.
Jones, S., Madison, D. H., Franz, A., and Altick, P. L. (1993). *Phys. Rev.* A **48**, R22.
Klar, H., Konovalov, D. A., and McCarthy, I. E. (1993). *J. Phys.* B **26**, L711.
Konovalov, D. A., and McCarthy, I. E. (1992). *J. Phys.* B **25**, L451.
McCarthy, I. E. (1992). *Z. Phys.* D **23**, 287.
McCarthy, I. E., and Bo Shang (1993). *Phys. Rev.* A **47**, 4807.
Murray, A. J., and Read, F. H. (1993). *Phys. Rev.* A **47**, 3724.
Pochat, A., Zhang, X., Whelan, C. T., Walters, H. R. J., Tweed, R. J., Gélébart, F., Cherid, M., and Allan, R. J. (1993). *Phys. Rev.* A **47**, R3483.
Rosenberg, L. (1973). *Phys. Rev.* D **8**, 1833.

Manuscript received 7 December 1993, accepted 28 January 1994