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On the extension of (e,2e) theory to coincidence studies of ion–atom collisions

A.L. Godunov [a], Marco Kampp [b], B. Sulik [c], H.R.J. Walters [d], Colm T. Whelan [a,*]

[a] Department of Physics, Old Dominion University, Norfolk Virginia 23529, United States
[b] Jesus College, Cambridge, CB5 8BL, UK
[c] Institute of Nuclear Research of the Hungarian Academy of Sciences (ATOMKI), Debrecen, Hungary
[d] Department of Applied Mathematics and Theoretical Physics, The Queen's University of Belfast, BT7 1 NN, UK

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Abstract

The extension of (e,2e) theory to the coincidence studies of ion–atom collisions is considered. The simultaneous ionization of projectile and target is discussed and results are presented for transfer ionization.

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The proposed new international facility for anti-proton and ion research (FAIR) at the Gesellschaft für Schwerionenforschung (GSI) will open up exciting and far reaching prospects for atomic physics research in the realm of ion–atom collisions. There is an urgent need to develop the theoretical basis for a number of new experiments. It has to be emphasised that the planned measurements are so difficult and the cross sections so small and the range of possible parameters so varied that it is only if theory and experiment are developed in a close consort will it be possible to focus the experiments towards kinematical arrangements where meaningful Physics may be extracted. As well as the new experiments being considered for the future FAIR facility there are some exciting new advances being made in ion–atom studies with present experimental capabilities. In this paper we will consider two cases of current interest (a) (e,2e) on multicharged ions at relativistic energies, where one would need the full power of the new facility and (b) the transfer ionization process which is already being actively studied.

* Corresponding author. Tel.: +1 757 683 3468; fax: +1 757 683 3038.
E-mail address: cwhelan@odu.edu (C.T. Whelan).

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1. (e,2e) on Multicharged ions

Zhang et al. [1] have completely explained the discrepancy between the inner-shell ionization experiments of the Würzburg group [2,3] and earlier calculations, achieving near perfect accord between their approximation and the measurements. The key feature of their description was that it allowed for multiple scattering of the incident and scattered electron in the field of the atom/ion. This work was extended to the relativistic impact energies, [4,5] in order to compare with the experiments of Nakel and his collaborators at Tübingen [4]. These measurements were entirely unique being at impact energies, which were far greater than performed anywhere else. In the approximation, of [5] the exact eigenstates of the Dirac equation were used with an effective atomic potential for all electron wavefunctions. In other words they calculated the two particle $\boldsymbol{S}$ matrix elements of quantum electrodynamics to lowest order in the electron–electron interaction coupling constant α but to all orders in the effective electron–nucleon interaction coupling $Z(r)/\alpha$. The method can also be regarded as a direct generalisation of the distorted wave Born approximation [6,7] used in non-relativistic (e,2e) where we use Dirac spinors instead of Schrödinger wave functions and the full QED photon propagator (in a generalised multipole expansion) as the relativistic generalisation of the Coulomb potential, the method is consequently known as the relativistic distorted wave Born approximation (rDWBA). The theoretical and computational difficulties in extending the DWBA, to relativistic situations were not inconsiderable. Much of the computational difficulties faced were concerned with the efficient evaluation of the partial wave integrals which occur [4,5]. These integrals present subtle mathematical and computational problems even for the non-relativistic case [8]. In the relativistic case many tens of thousands of highly oscillatory partial wave integrals and millions of vector coupling coefficients had to be evaluated and then combined together in a sum of negative and positive terms in such a way that avoided cancellation errors which would have rendered the calculations meaningless. Methods for the evaluation of these integrals can be found in [9] and details of the calculation in [4,5]. A whole series of effects were predicted and observed – in particular the role of Mott scattering, Pauli blocking, fine structure as well as q.e.d. (retardation and magnetic) and spin flip effects [4] were elucidated.

Very recently it has been suggested that one could use ions produced in accelerators to bombard simple neutral atoms where the target and projectile are simultaneously ionised [10]. In [11] rDWBA calculations, which were presented for such an experiment, it was argued that one could for all practical purposes treat this as (e,2e) processes with an ionic target. This would parallel to some extent the pioneering inner shell experiments of Nakel and his collaborators on the innermost shells of neutral atoms. It would however allow a much wider range of geometries. Further, the close agreement between the rDWBA calculations with neutral asymptotics with the fully relativistic Coulomb Born calculations [24] suggests that the rDWBA should work well for (e,2e) on a multicharged ion in equivalent kinematics to the Nakel experiments.

The Tübingen measurements were restricted to only two energies and quite simple experimental arrangements. The effect of Lorentz and frame transformations means that in the laboratory one will predominantly see the ejected electrons in a narrow cone in the forward direction making the identification of the physical effects difficult. However one should be able to see interesting results in the plane perpendicular to the beam direction. Spin asymmetry measurements that parallel those of the Nakel group would also be very interesting. Recently the theoretical structure of the relativistic (e,2e) problem has undergone a further intense analysis [12]. In particular the symmetry properties of the S-matrix in the fully relativistic distorted wave treatment of electron impact ionization has been investigated and it has been shown that the square modulus of the scattering matrix element in which the spin states of all four electrons is not invariant under the reversal of the direction of alignment of all spins. The larger of two contributions to this non-invariance originates from the relativistic modifications of the continuum wave functions induced by the distorting potential of the target atom. A second smaller contribution is manifested on reducing the eight-dimensional matrix element of the QED covariant propagator to two purely spatial two-electron integrals. What this means is that we are predicting that the triple differential cross section will exhibit a spin asymmetry unless the entire scattering process occurs in one plane, i.e. there will be a difference in the TDCS between an (e,2e) process with spins polarized parallel or anti-parallel to the beam direction even if the target is unpolarized and the spins of the exiting electrons are not detected. The TDCS will, however, remain unchanged, if in addition to reversal of the direction of the spin alignment one appropriate momentum component of one of the exiting electrons is reversed. The purely mathematical analysis in [12] is supported by rDWBA calculations on uranium targets [13]. There is a need for experimental confirmation of this effect and the physical interpretation given in [13]. In this latter paper it is argued that the predicted effects are a result of post-collisional 'spin–orbit' type interactions in the final channel and the rotation of the relative direction of polarization by the first elastic scattering. It is reasonable to ask how one can simulate a spin polarized (e,2e) experiment using the simultaneous ionization of projectile and target ion–atom experimental set up. One idea which we would suggest is to use metastable helium, rather than ground state helium as the target. He 2^3S has remarkably long lifetime, and if it were possible to separate out the components with both spin aligned, either (up, up) or (down, down), then one could attempt spin asymmetry measurements. Clearly the direction of the spin axis can be chosen at will.

2. Transfer ionization

One of the primary reasons for performing coincidence measurements is to try to learn something about the target. It has been an aspiration for some time to learn about highly correlated target states by studying double excitation processes [14]. Unfortunately the double excitation processes so far studied, ((γ,2e), (e,3e) excitation–ionization) though sensitive to target effects are hugely dependent on post-collisional interactions between the charged particles in the final state [15,16]. Transfer ionization is another such double ionization process, for proton impact the projectile captures one electron to become atomic hydrogen and one could therefore hope that post-collisional Coulombic interactions would be neutralized and the full sensitivity to target effects would be become apparent. The fully differential cross section for the transfer ionization process:

$$H^+ + He \rightarrow e + H + He^{2+}$$

has been measured using the COLTRIMS technique [17–19]. The experiments were performed with proton impact energies of the order of half an MeV and ejected electron energies of a few eVs. Results for coplanar and noncoplanar geometries have been presented. The measurements reveal that

1. The ejected electron is predominantly emitted into the backward direction.
2. The direction of maximum ejection is insensitive to the impact energy but shows some dependence on the momentum transfer.
3. The captured electron, recoil He^{2+} ion and ejected electron always have comparable momenta.

Until recently theory was unable to reproduce these general features. Godunov et al. [20] produced a simple theoretical model which explained the observed qualitative features in terms of target correlation and gave quantitative predictions for triple differential cross sections which explicitly demonstrated the sensitivity to terms beyond the (ns^2) in a multiconfiguration Hartree Fock description of the target, confirming a suggestion first made by Schmidt Böcking. The quantitative predictions given in [20] have been confirmed by new COLTRIMS experiment, see Fig. 1 and [21].

The model in [16] is a first order model and it is reasonable to ask if the dependence on target wave function will be lost in a second order model. In Godunov et al. [22], the model was extended to second order. In Fig. 2 we show a comparison between the experimental data and the first and second order models. The experimental data being relative is shown twice, normalized to both the first order and second order approximations. We conclude that for the case of proton impact that the second order results are in good agreement with experiment is maintained provided the model contains a high degree of correlation in the target wave function.

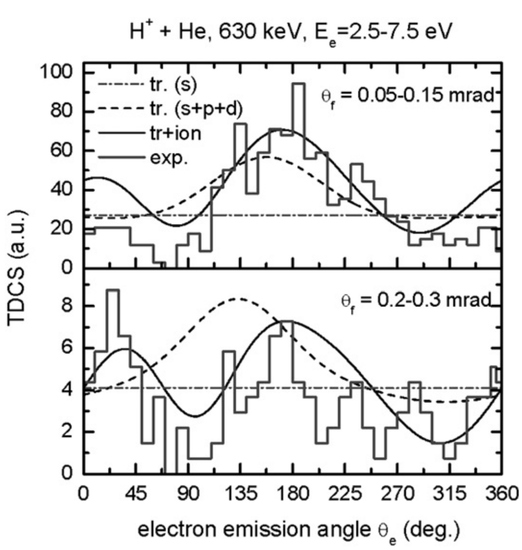

Fig. 1. Triple differential cross section comparison between theory and experiments, theory of Godunov et al. [20], experiment, histogram [21,22] t_1 – the transfer first cross section, t_2 – ionization first, $t_1 + t_2$ the full cross section allowing for both mechanisms and their interference, the set marked (s) corresponds to using a ground state helium model within the multiconfiguration Hartree Fock method using only $(ns)^2$ terms, the other set models the helium target using $(ns)^2$, $(ps)^2$ and $(nd)^2$ terms, with n less than or equal 5. Note: the calculations were performed in advance of the experiment.

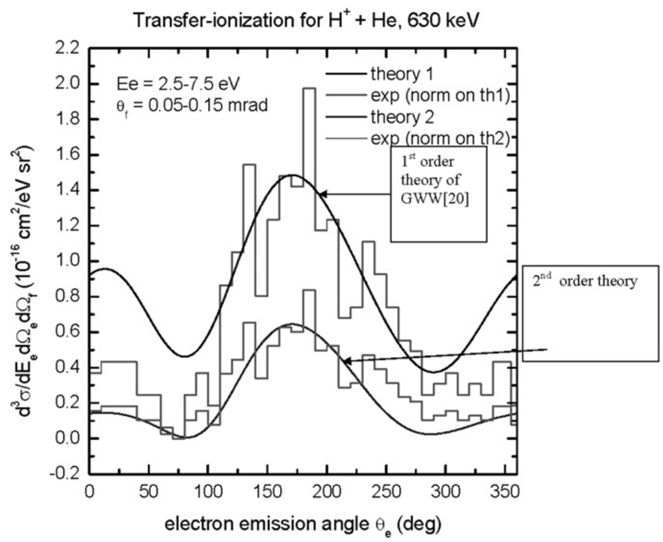

Fig. 2. Triple differential cross section showing both the first order model of [20], upper solid curve and second order calculation using the model of [23], lower solid curve. The experimental data is relative and is shown twice normalized to the different approximations. Note the target wave function is calculated in both case within the multiconfiguration Hartree Fock method using $(ns)^2$, $(ps)^2$ and $(nd)^2$ terms, with n less than or equal 5.

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