

# Theory of atomic ionization and the coulomb three-body breakup

A. S. Kadyrov\*, A. M. Mukhamedzhanov†, A. T. Stelbovics\* and I. Bray\*

\*Centre for Atomic, Molecular and Surface Physics, Division of Science and Engineering,  
Murdoch University, Perth 6150, Australia

†Cyclotron Institute, Texas A&M University, College Station, TX 77843, USA

**Abstract.** An alternative surface-integral formulation of the theory of electron-impact ionization of atoms and the Coulomb three-body breakup is presented.

The Peterkop-Rudge [1, 2] formalism for electron-impact ionization of atoms and the Faddeev-Merkuriev [3] formalism for the three-body problem in general were given almost four decades ago. Despite the knowledge that these formulations suffer from a number of serious formal problems little progress has been made in their resolution. An integral representation for the ionization amplitude that is free of ambiguity and divergence problems has been given recently [4]. Subsequently, we have presented a new formulation of the theory of electron-impact ionization of atoms [5] that addressed these issues. In particular, we showed that the ionization amplitude has four alternative, but equivalent, surface-integral forms ideally suited for practical calculations. The formulation was extended to amplitudes of all possible scattering processes taking place in an arbitrary three-body system. A well-defined *post* form of the breakup amplitude valid for arbitrary potentials including the long-range Coulomb interaction has also been presented. Here we recapitulate some of these results.

The ionization amplitude in the *prior* form is given as

$$T^{(prior)}(\vec{k}_1, \vec{k}_2) = \langle \Psi_f^- | \bar{V}_i | \Phi^{(i)} \rangle. \quad (1)$$

Here  $\Psi_f^-$  is the total scattering wave function developing from an initial state of three particles in the continuum with incoming scattered-wave boundary condition. It satisfies

$$(E - H)\Psi_f^-(\vec{r}_1, \vec{r}_2) = 0, \quad (2)$$

where  $H = H_0 + V$  is the total three-body Hamiltonian,  $H_0$  is the free three-body Hamiltonian,  $V$  is the full interaction and  $E$  is the total energy of the system,  $\bar{V}_i = V - V_i$  is the interaction of the incident electron with the target particles,  $\vec{r}_1$  and  $\vec{r}_2$  are the coordinates of the electrons relative to the proton and  $\vec{k}_1$  and  $\vec{k}_2$  are their momenta. The wave function representing the initial two-fragment channel satisfies

$$(E - H_0)\Phi^{(i)}(\vec{r}_1, \vec{r}_2) = V_i\Phi^{(i)}(\vec{r}_1, \vec{r}_2), \quad (3)$$

where  $V_i$  is the potential responsible for the bound state in the initial channel.

The ionization amplitude given by the form (1) is not convenient for practical calculations because it requires the total wave function  $\Psi_f^-$  which evolves from a free three-particle initial state  $\Psi^{(f)-}$ . Generally  $\Psi^{(f)-}$  is very complex. In addition, for the ionization amplitude to be calculated from this definition, a knowledge of  $\Psi_f^-$  in the entire space is necessary. It is more convenient to work with the total wave function  $\Phi_i^+$  evolving from the two-fragment state  $\Phi^{(i)}$  with outgoing scattered-wave boundary condition. It is a solution of the Schrödinger equation

$$(E - H)\Phi_i^+(\vec{r}_1, \vec{r}_2) = 0. \quad (4)$$

In the stationary theory the *post* form of the breakup amplitude is defined by

$$T^{(post)}(\vec{k}_1, \vec{k}_2) = \langle \vec{k}_1, \vec{k}_2 | V | \Phi_i^+ \rangle, \quad (5)$$

where  $\langle \vec{r}_1, \vec{r}_2 | \vec{k}_1, \vec{k}_2 \rangle = e^{i\vec{k}_1 \cdot \vec{r}_1 + i\vec{k}_2 \cdot \vec{r}_2}$  is the undistorted three-body plane wave. However, this form is valid only when  $V$  is short-ranged. The stationary scattering theory fails to define the same for long-range interactions unless it refers to some screening technique. This only leads to additional problems since convergence of the screening procedure when the screening radius is extended to infinity still remains to be proven.

To overcome this problem we first note that Eq. (4) can be written as

$$(E - H)\Phi_i^{(sc)+}(\vec{r}_1, \vec{r}_2) = \bar{V}_i \Phi^{(i)}(\vec{r}_1, \vec{r}_2), \quad (6)$$

where we separated the scattered-wave part of  $\Phi_i^+$  according to  $\Phi_i^{(sc)+} = \Phi_i^+ - \Phi^{(i)}$ . Combining this with Eq. (2) it follows that

$$\begin{aligned} T^{(prior)}(\vec{k}_1, \vec{k}_2) &\equiv \langle \Psi_f^- | \bar{V}_i | \Phi^{(i)} \rangle \\ &= \langle \Psi_f^- | E - \vec{H} | \Phi_i^{(sc)+} \rangle \\ &= \langle \Psi_f^- | \overleftarrow{H} - E | \Phi_i^{(sc)+} \rangle + \langle \Psi_f^- | E - \vec{H} | \Phi_i^{(sc)+} \rangle \\ &= \langle \Psi_f^- | \overleftarrow{H}_0 - \vec{H}_0 | \Phi_i^{(sc)+} \rangle \equiv T^{(a)}(\vec{k}_1, \vec{k}_2), \end{aligned} \quad (7)$$

where a left (right) arrow on the differential Hamiltonian operator indicates that it acts on the *bra* (*ket*) state. This form readily leads to a surface-integral representation for the ionization amplitude [4]. In addition, taking into account Eqs. (2) and (3) we get

$$\begin{aligned} T^{(prior)}(\vec{k}_1, \vec{k}_2) &\equiv \langle \Psi_f^- | V - V_i | \Phi^{(i)} \rangle \\ &= \langle \Psi_f^- | E - \overleftarrow{H}_0 - (E - \vec{H}_0) | \Phi^{(i)} \rangle \\ &= -\langle \Psi_f^- | \overleftarrow{H}_0 - \vec{H}_0 | \Phi^{(i)} \rangle \equiv T^{(b)}(\vec{k}_1, \vec{k}_2). \end{aligned} \quad (8)$$

Separating the unscattered (i.e., incident) and scattered parts of  $\Psi_f^-$  according to  $\Psi_f^- = \Psi^{(f)-} + \Psi_f^{(sc)-}$  we can also get

$$T^{(c)}(\vec{k}_1, \vec{k}_2) = \langle \Psi^{(f)-} | \overleftarrow{H}_0 - \vec{H}_0 | \Phi_i^+ \rangle, \quad (9)$$

$$T^{(d)}(\vec{k}_1, \vec{k}_2) = -\langle \Psi_f^{(sc)-} | \overleftarrow{H}_0 - \vec{H}_0 | \Phi_i^+ \rangle. \quad (10)$$

The new forms obtained for ionization amplitudes can be extended to amplitudes of all other processes taking place in the collisional system. If in the final channel we had a two-fragment state instead of a three-body state then the total wave function  $\Phi_f^-$  developed from the final state will be similar to  $\Phi_i^+$ . However, all the scattered parts of this wave function would have to satisfy the incoming-wave boundary condition. Thus in a similar way we introduce surface-integral forms for the scattering amplitude:

$$F^{(a)}(\vec{k}_f, \vec{k}_i) = \langle \Phi_f^- | \overleftarrow{H}_0 - \vec{H}_0 | \Phi_i^{(sc)+} \rangle, \quad (11)$$

$$F^{(b)}(\vec{k}_f, \vec{k}_i) = -\langle \Phi_f^- | \overleftarrow{H}_0 - \vec{H}_0 | \Phi^{(i)} \rangle, \quad (12)$$

$$F^{(c)}(\vec{k}_f, \vec{k}_i) = \langle \Phi^{(f)} | \overleftarrow{H}_0 - \vec{H}_0 | \Phi_i^+ \rangle, \quad (13)$$

$$F^{(d)}(\vec{k}_f, \vec{k}_i) = -\langle \Phi_f^{(sc)-} | \overleftarrow{H}_0 - \vec{H}_0 | \Phi_i^+ \rangle. \quad (14)$$

Eq. (9) leads to a well-defined conventional volume-integral form of the ionization amplitude in terms of the total three-body scattering wave function  $\Phi_i^+$ . From the *c*-form of the ionization amplitude we get

$$\begin{aligned} T^{(c)}(\vec{k}_1, \vec{k}_2) &= \langle \Psi^{(f)-} | \overleftarrow{H}_0 + V - E - \vec{H}_0 - V + E | \Phi_i^+ \rangle \\ &= \langle \Psi^{(f)-} | \overleftarrow{H}_0 + V - E | \Phi_i^+ \rangle \equiv T^{(post)}(\vec{k}_1, \vec{k}_2). \end{aligned} \quad (15)$$

Eq. (15) takes the form of Eq. (5) when the full interaction  $V$  is short-ranged. Thus, Eq. (15) extends the definition of the *post*-form of the breakup amplitude to arbitrary potentials including the long-range Coulomb interaction. This resolves a long-standing formal problem of the scattering theory.

In our formalism we have not been required to reference the masses of the particles or the explicit forms of the interactions between them. Therefore the amplitudes of all processes in an arbitrary three-body system can be written in this surface-integral form. The surface-integral forms for the breakup and scattering amplitudes are ideal for numerical calculations as the result depends only on the asymptotic behaviour of the wave functions. The formalism is readily applicable to extraction of the amplitudes in calculations of atomic and molecular breakup processes including the double photoionization of helium or breakup and photodisintegration calculations in nuclear physics. For the rigorous proof of the presented forms and their partial-wave analysis see Ref. [5].

The work was supported by the Australian Research Council, U.S. DOE Grant DE-FG03-93ER40773 and NSF Grant PHY-0140343.

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