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LETTER TO THE EDITOR

The multistate eikonal treatment of electron–atom collisions

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Abstract. The basic equation for the scattering amplitude as determined from a multistate eikonal description of electron–atom collisions is presented. The relationship with other semiclassical treatments is examined. Four-state eikonal calculations of the cross sections for elastic and the 2s and 2p excitations of H(1s) by electrons with incident energy E in the range $13{\cdot}6\,\mathrm{eV} \le E \le 200\,\mathrm{eV}$ are carried out, and are compared with other refined theoretical treatments and with experiment.

Recently, a variety of theoretical models have been proposed for elastic and inelastic electron–atom collisions at low and intermediate energies. These descriptions include the close-coupling expansion with its pseudo-state modifications (Burke and Webb 1970), a polarized orbital distorted-wave model of McDowell *et al* (1973), the Glauber approximation (Tai *et al* 1970), the impact-parameter approach (Bransden and Coleman 1972, Bransden *et al* 1972), the eikonal approximation of Byron (1971), and the distorted-wave eikonal theory of Chen *et al* (1972). The purpose of this letter is (*a*) to present a preliminary account of a new generalization of the eikonal method, (*b*) to illustrate its explicit relationship with other eikonal treatments and with the impact parameter approximation and (*c*) to present its comparison with experiment and various theories.

Flannery and McCann (1974, in preparation) have developed a multistate eikonal formulation of the stationary state description of a collision between an incident particle B with an atomic system (A + e). The treatment differs from previous approaches of Byron (1971) and of Bransden *et al* (1972) in that no additional assumptions, other than the eikonal approximation to the relative motion and a multistate expansion for the electronic motions, are made. Different speeds for various channels are acknowledged. The basic equation derived for the amplitude for scattering into $\hat{\boldsymbol{k}}_\mathrm{f}(\theta, \phi)$ about the incident Z-direction $\hat{\boldsymbol{k}}_\mathrm{i}$ is, in the centre-of-mass frame,

$$f_{\mathrm{if}}(\theta, \phi) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int \exp(\mathrm{i}\boldsymbol{K}\,.\,\boldsymbol{R})\,\mathrm{d}\boldsymbol{R}\sum_n B_n(\boldsymbol{\rho}, Z)V_{\mathrm{f}n}(\boldsymbol{R})\exp \mathrm{i}(k_n - k_\mathrm{i})Z \qquad (1)$$

where k_n is the wavenumber of relative motion in each channel n, $\boldsymbol{K} = \boldsymbol{k}_\mathrm{i} - \boldsymbol{k}_\mathrm{f}$ is the momentum change caused by the collision, and $V_{\mathrm{f}n}$ is the interaction matrix element $\langle\phi_\mathrm{f}(\boldsymbol{r})|\mathscr{V}(\boldsymbol{r}, \boldsymbol{R})|\phi_n(\boldsymbol{r})\rangle$ where $\phi_n(\boldsymbol{r})$ are the eigenstates describing the isolated systems with reduced mass μ. The electrostatic interaction between the B and (A + e) systems at separation $\boldsymbol{R} \equiv (R, \Theta, \Phi) \equiv (\rho, \Phi, Z)$, in spherical and cylindrical coordinate frames respectively, is $\mathscr{V}(\boldsymbol{R}, \boldsymbol{r})$. The coefficients B_n satisfy the set of coupled differential (phase Φ-dependent) equations,

$$\frac{\mathrm{i}\hbar^2 k_\mathrm{f}}{\mu}\frac{\partial B_\mathrm{f}}{\partial Z} = \sum_{n=1}^{N} B_n(\boldsymbol{\rho}, Z)V_{\mathrm{f}n}(\boldsymbol{R})\exp \mathrm{i}(k_n - k_\mathrm{f})Z \qquad \mathrm{f} = 1, 2, \ldots, N \qquad (2)$$

where N is the number of channels considered. It can be observed that (1), with $B_n = \delta_{ni}$ (where i is the initial state), reproduces the Born-wave amplitude. Also, after some algebraic manipulation, the distorted-wave Born formula of Chen *et al* (1972) is recovered from (1) and (2). Moreover, the expressions for the eikonal elastic scattering amplitude (cf Bransden 1970) follows by solving (2) with $B_n = B_i\delta_{ni}$ for B_i and by performing the Φ-integration in (1). The chief attributes of equations (1) and (2) above are that they account explicitly for different relative speeds in the various channels, and that they permit full inclusion of as many states (or pseudo-states) as desired. It is hoped that more complete details of the theory and its relationship with other theories will eventually be provided in a later paper.

The different exponents within the summation signs of (1) and (2) are significant. With the aid of (2), the scattering amplitude (1) reduces to

$$f_{\mathrm{if}}(\theta, \phi) = -\frac{\mathrm{i}k_{\mathrm{f}}}{2\pi}\int \exp \mathrm{i}[\boldsymbol{K}.\boldsymbol{R}-(k_{\mathrm{i}}-k_{\mathrm{f}})Z]\frac{\partial B_{\mathrm{f}}(\boldsymbol{\rho}, Z)}{\partial Z}\,\mathrm{d}\boldsymbol{R}. \tag{3}$$

Since $\mathscr{V}$ is composed of central potentials, $V_{nm}(\boldsymbol{R}) \equiv V_{nm}(R, \Theta)\exp(\mathrm{i}\Delta\Phi)$ where $\Delta = M_m - M_n$, the integral change in the azimuthal quantum number M, and hence the substitution $C_n(\rho, Z) = B_n(\boldsymbol{\rho}, Z)\exp(-\mathrm{i}\Delta\Phi)$ yields a set of phase-independent equations for C_n similar to (2). The amplitude reduces on Φ-integration, to

$$f_{\mathrm{if}}(\theta, \phi) = -\mathrm{i}k_{\mathrm{f}}\mathrm{i}^{\Delta}\int_0^{\infty} J_{\Delta}(K'\rho)I(\rho, \theta)\rho\,\mathrm{d}\rho \tag{4}$$

where K' is the XY-component $k_{\mathrm{f}}\sin\theta$ of K, where J_{Δ} are Bessel functions of integral order Δ, and where the function

$$I(\rho, \theta) = \int_{-\infty}^{\infty} \exp(\mathrm{i}\alpha Z)\frac{\partial C_{\mathrm{f}}(\rho, Z)}{\partial Z}\,\mathrm{d}Z \tag{5}$$

in which the difference between K_Z, the Z-component of the momentum change at angle θ, and the minimum momentum change $(k_{\mathrm{i}}-k_{\mathrm{f}})$ in the collision is

$$\alpha(\theta) = k_{\mathrm{f}}(1-\cos\theta). \tag{6}$$

We note, in the heavy-particle high-energy limit, when $\theta \approx 0$, that $\alpha \approx 0$ and hence

$$I(\rho, \theta) \approx I_{\mathrm{A}}(\rho) = (C_{\mathrm{f}}(\rho, \infty)-\delta_{\mathrm{if}}). \tag{7}$$

Thus the eikonal approximation of Byron (1971) is reproduced from (3) with (7) together with the further assumptions that the quantities k_{f}, and $(k_{\mathrm{i}}-k_{\mathrm{f}})$ appearing explicitly in (3) are taken as k_{i}, and $\epsilon_{\mathrm{fi}}/v_{\mathrm{i}}$ respectively. If, in addition $k_{\mathrm{f}}\sin\theta$ is approximated by $k_{\mathrm{i}}\sin\theta \approx 2k_{\mathrm{i}}\sin\frac{1}{2}\theta$ for small θ and large k_{f}, then the scattering amplitude based on the impact parameter description of Bransden and colleagues is recovered.

As a test of the present full eikonal model, calculations based on (1)–(6) have been performed for the processes

$$\mathrm{e}+\mathrm{H}(1\mathrm{s}) \rightarrow \mathrm{e}+\mathrm{H}(1\mathrm{s}, 2\mathrm{s}, 2\mathrm{p}_{0,\pm 1}) \tag{8}$$

in which the 1s, 2s, $2\mathrm{p}_0$, $2\mathrm{p}_{\pm 1}$ states of atomic hydrogen are closely coupled. The total elastic and inelastic cross sections $Q(nl)$ computed by direct integration of $(k_{\mathrm{f}}/k_{\mathrm{i}})|f_{\mathrm{if}}(\theta, \phi)|^2$ over all solid angles are displayed in the table and compared with other refined theoretical calculations (Burke and Webb 1970, Sullivan *et al* 1972, McDowell *et al* 1973), and with experimental data (Long *et al* 1968, Kauppila *et al* 1970) in figures

Table 1. Elastic and inelastic cross sections $Q(nl)\pi a_0^2$ for the processes $e+H(1s) \to e+H(nl)$; nl = 1s, 2s, $2p_{0,\pm 1}$, at electron energy E_i (eV)

E (eV)	Q(1s)	Q(2s)	$Q(2p_0)$	$Q(2p_{\pm 1})$	Q(2p)
13.6	0·988	0·143	0·140	0·077	0·217
20	0·703	0·131	0·319	0·297	0·616
30	0·522	0·113	0·362	0·441	0·803
50	0·332	0·085	0·347	0·514	0·861
100	0·202	0·050	0·191	0·439	0·630
200	0·125	0·028	0·118	0·335	0·453

1 and 2. Note that the $2\,^2S$ measurements include the cascade contribution 0·23 Q(3p) from the 3p level such that direct comparison is not possible until we perform similar multistate calculations for the 3p-excitation. Also, the experimental 2p-cross sections are normalized to our value of 0·453 πa_0^2 at 200 eV instead of the corresponding Born value of 0·485 πa_0^2, which is 7% higher.

The agreement for the 2p-excitation between the present treatment, the pseudo-state method and experiment is very good down to impact energies $E_i \sim 20$ eV, below which the effects of exchange and polarization distortion neglected in the present description, become important. Also shown are cross sections computed from the standard four-state impact parameter prescription. The comparison of these results with those labelled S of Sullivan *et al* (1972) is then a direct measure of the effect arising from their inclusion of second-order potentials.

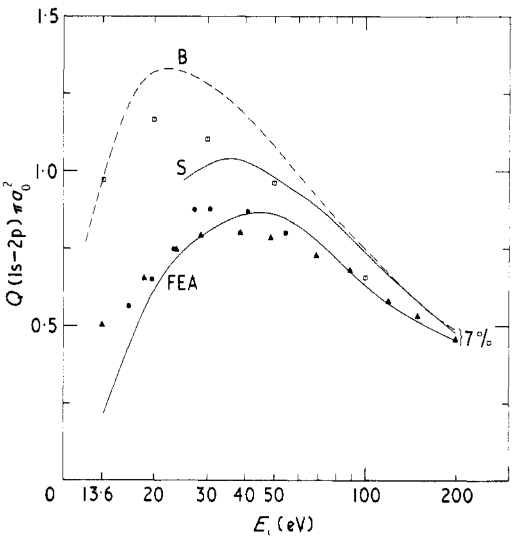

Figure 1. Total cross sections Q(1s–2p) for $e+H(1s) \to e+H(2p)$ at electron energy E_i (eV). FEA four-state eikonal approximation (present treatment), ▲ experiment (Long *et al* 1968), ● pseudo-state (Burke and Webb 1970), □ four-state impact-parameter treatment, S second-order potential method: four-channel approximation (Sullivan *et al* 1972), B Born approximation.

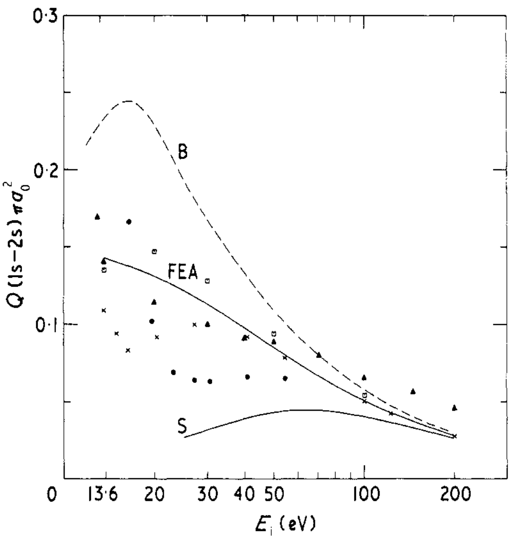

Figure 2. Total cross sections Q(1s–2s) for e + H(1s) → e + H(2s) at electron energy E_i (eV). FEA four-state eikonal approximation (present treatment), ● pseudo-state (Burke and Webb 1970), × polarized-orbital distorted wave model (McDowell *et al* 1973), ☐ four-state impact-parameter treatment, S second-order potential method: four-channel approximation (Sullivan *et al* 1972), B Born approximation, ▲ Q(1s–2s) + 0·23Q(1s–3p): experiment Kauppila *et al* 1970).

For the 2s-excitation, the agreement between the present results and the recent polarized-orbital distorted wave model of McDowell *et al* (1973) is encouraging. All the theoretical results show different variations with impact energy E_i below 40 eV. The experimental situation is somewhat obscured by the difficulty in obtaining direct account of the contributions arising from cascade, mainly from the 3p level. The large difference between the impact parameter cross sections indicates the sensitivity of the 2s-cross section to modification.

Finally, since the main object of this letter is to present the basic outline of the new treatment and to give some preliminary indication as to its success, it is our intention to eventually furnish a more complete theoretical description and a more detailed comparison (including differential cross sections, in particular) with other theoretical models.

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