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The multichannel eikonal treatment of atomic collisions: e–H(1s) elastic and inelastic scattering

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Abstract. A multichannel eikonal description of atomic collisions is presented. The basic formula for the scattering amplitude reduces upon successive approximation to expressions previously derived. In particular, the equations, in the heavy-particle or high-energy limit reduce to the standard impact parameter formulae. A four-state treatment of e–H(1s) elastic and 2s and 2p inelastic scattering is carried out. The calculated cross sections, which illustrate the effects of various approximations, compare very favourably with other refined theoretical methods and with experiment.

1. Introduction

A variety of methods have been proposed for the theoretical description of e–atom collisions at low and intermediate energies. The close coupling expansion with its pseudo-state modifications (Burke and Webb 1970), and the polarized orbital distorted wave model of McDowell *et al* (1973) are among those that follow from the full wave treatment of the collision. Other methods, termed as semiclassical—the eikonal approximations of Byron (1971) and of Chen *et al* (1972), the impact parameter approach (Bransden and Coleman 1972) and the Glauber approximation (cf Tai *et al* 1970)—all essentially separate the relative motion of the incident electron (described by an eikonal-type or Born wavefunction for the electron in a static field) from the internal electronic motions of the atomic system which is described by a multistate expansion.

These semiclassical methods are all amenable to systematic improvement at little extra cost eg additional atomic states, electron-exchange, and polarization effects can be suitably incorporated into the treatment. Moreover, their application to collisions with complex atoms is without the almost insurmountable hurdles associated with the application of the full wave treatment to non-hydrogenic systems. In particular, e-excited atom collisions—important to analysis of gaseous discharges, laser development and astrophysical problems—can be treated with relative ease by these semiclassical methods. It is therefore highly desirable to investigate these methods in greater detail and to propose possible improvements.

In this paper, a new generalization of the eikonal approach to atomic collisions is presented. It accounts explicitly for the changes in speed associated with the various channels and for other effects not acknowledged by the previous semiclassical descriptions. Its relationship with the former treatments is discussed and its overall reliability is assessed by comparing the calculated differential and total cross sections for

e–H(1s) elastic and inelastic collisions with other refined treatments and with experiment. A preliminary account of this generalization has already been presented (Flannery and McCann 1974a).

2. Theory

Consider the collision of a particle B of mass M_B and incident velocity v_i along the Z-axis with a one-electron atomic system (A+e) of mass (M_A+m). The subsequent analysis can be immediately generalized so as to cover multi-electron systems. Let $\boldsymbol{R}, \boldsymbol{R}_B, \boldsymbol{r}$ and $\boldsymbol{r}_a$ denote the A–B, B–(Ae) centre of mass, e–(AB) centre of mass and e–A separations, respectively. In the (ABe) centre-of-mass reference frame, the scattering amplitude for direct transition between an initial state i and a final state f of the collision system, of reduced mass μ, is

$$f_{if}(\theta, \phi) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\langle \Psi_f(\boldsymbol{k}_f; \boldsymbol{r}, \boldsymbol{R})|V(\boldsymbol{r}, \boldsymbol{R})|\Psi_i^+(\boldsymbol{k}_i; \boldsymbol{r}, \boldsymbol{R})\rangle_{\boldsymbol{r},\boldsymbol{R}} \tag{1}$$

in which $V(\boldsymbol{r}, \boldsymbol{R})$ is the instantaneous electrostatic interaction between the collision species, and where the scattering is directed along the final relative momentum $\hbar\boldsymbol{k}_f(l, \theta, \phi)$. The final stationary state of the isolated atoms in channel f is Ψ_f, and Ψ_i^+ is the solution of the time independent Schrödinger equation,

$$\left[-\frac{\hbar^2}{2\mu}\nabla_R^2 + H_e(\boldsymbol{r}) + V(\boldsymbol{r}, \boldsymbol{R})\right]\Psi_i^+(\boldsymbol{r}, \boldsymbol{R}) = E_i\Psi_i^+(\boldsymbol{r}, \boldsymbol{R}) \tag{2}$$

solved subject to the asymptotic boundary condition,

$$\Psi_i^+(\boldsymbol{r}, \boldsymbol{R}) \xrightarrow{\text{large } R} \sum_n \left[e^{i\boldsymbol{k}_n\cdot\boldsymbol{R}_B}\,\delta_{ni} + f_{in}(\theta, \phi)\frac{e^{ik_nR_B}}{R_B}\right]\phi_n(\boldsymbol{r}_a) \tag{3}$$

in which $\phi_n(\boldsymbol{r}_a)$ are eigenfunctions of the Hamiltonian $H_e(\boldsymbol{r}) \approx H_e(\boldsymbol{r}_a)$ for the isolated atomic system (A+e) with internal electronic energy ϵ_n such that the total energy E_i in channel i is $\epsilon_i + \hbar^2k_i^2/2\mu$ which is conserved throughout the collision.

2.1. The multichannel eikonal approximation

The eikonal approximation to (2) sets

$$\Psi_i^+(\boldsymbol{r}, \boldsymbol{R}) = \sum_n A_n(\boldsymbol{\rho}, Z)\exp iS_n(\boldsymbol{\rho}, Z)\chi_n(\boldsymbol{r}, \boldsymbol{R}) \tag{4}$$

where the nuclear separation $\boldsymbol{R} \equiv (R, \Theta, \Phi) \equiv (\rho, \Phi, Z)$ in spherical and cylindrical coordinate frames respectively. The eikonal S_n in (4) is the characteristic-function solution of the classical Hamilton–Jacobi equation (ie the Schrödinger equation in the $\hbar \to 0$ limit) for the A–B relative motion under the static interaction $V_{nn}(\boldsymbol{R})$, and is therefore given by

$$S_n(\boldsymbol{\rho}, Z) = k_nZ + \int_{-\infty}^{Z}[\kappa_n(\boldsymbol{R}) - k_n]\,dZ \tag{5}$$

in which the local wavenumber of relative motion at $\boldsymbol{R}$ is

$$\kappa_n(\boldsymbol{R}) = \left[k_n^2 - \frac{2\mu}{\hbar^2}V_{nn}(\boldsymbol{R})\right]^{1/2} \tag{6}$$

and where dZ is an element of path length along the trajectory which, at present, is taken as a straight line. For electron–atom collisions, κ_n in (6) is always real. The use of the actual classical trajectory with its 'built-in' turning point is therefore not as essential as in, for example, positron–atom collisions when κ_n becomes imaginary for sufficiently close rectilinear encounters. The general problems associated with the choice of classical trajectory within a multichannel framework are at present unresolved, although the forced-common turning-point, two-state procedure of Bates and Crothers (1970) is attractive.

The interaction matrix elements

$$V_{nm}(\boldsymbol{R}) = \langle \chi_n(\boldsymbol{r}, \boldsymbol{R}) | V(\boldsymbol{r}, \boldsymbol{R}) | \chi_m(\boldsymbol{r}, \boldsymbol{R}) \rangle \tag{7}$$

connect the various electronic states

$$\chi_n(\boldsymbol{r}, \boldsymbol{R}) = \phi_n(\boldsymbol{r}_a) \exp(il\boldsymbol{k}_n \cdot \boldsymbol{r}) \qquad l = \frac{mM_{AB}}{M_A} \tag{8}$$

in which the phase factor which ensures satisfaction of the boundary condition (3) describes the translational motion of the electron relative to the (A–B) centre of mass, and is unimportant to the present development only when rearrangement channels are neglected. Moreover the eikonal (5) ensures that Ψ_i^+ contains, in addition to the incident wave, outgoing scattered waves which differ from the undistorted Born wave, $\exp(ik_nZ)$ by the following amount of phase-distortion,

$$\Phi_n(\boldsymbol{\rho}, Z) \equiv \int_{-\infty}^{Z} (\kappa_n - k_n)\, dZ$$

which vanishes outside a cylinder, with axis along the Z direction, with infinite length and with diameter corresponding to the range $\boldsymbol{R}_n$ of the static interaction $V_{nn}(\boldsymbol{R})$. Thus, at impacts less than the interaction-range, distortion to the incident plane-wave relative motion does occur, thereby causing actual scattering. Applicability of (5) is therefore not confined to small angle scattering alone, although a straight-line element dZ is normally taken in (5). On assuming that the main variation of Ψ_i^+ on $\boldsymbol{\rho}$ is contained in S_n, ie provided $V_{nn}(\boldsymbol{R})$ varies slowly over many wavelengths $2\pi/\kappa(\boldsymbol{R})$ of relative motion, and the coefficients $A_n(\boldsymbol{\rho}, Z)$ therefore vary primarily along Z, then substitution of (4) in (2) yields the set of coupled differential equations,

$$\frac{i\hbar^2}{\mu}\kappa_f \frac{\partial A_f(\boldsymbol{\rho}, Z)}{\partial Z} = \sum_{\substack{n=1 \\ \neq f}}^{N}{}' A_n(\boldsymbol{\rho}, Z) V_{fn}(\boldsymbol{R}) \exp i(S_n - S_f) \qquad f = 1, 2, \ldots, N \tag{9}$$

where N is the number of channels adopted in the expansion (4). The phase substitution

$$B_f(\boldsymbol{\rho}, Z) = A_f(\boldsymbol{\rho}, Z) \exp i \int_{-\infty}^{Z} (\kappa_f - k_f)\, dZ \equiv A_f(\boldsymbol{\rho}, Z) \exp i\Phi_f(\boldsymbol{\rho}, Z) \tag{10}$$

with the aid of (6), reduces (9) to

$$\frac{i\hbar^2}{\mu}\kappa_f \frac{\partial B_f(\boldsymbol{\rho}, Z)}{\partial Z} + \left[\frac{\hbar^2}{\mu}\kappa_f(\kappa_f - k_f) + V_{ff}(\boldsymbol{R})\right] B_f(\boldsymbol{\rho}, Z)$$
$$= \sum_{n=1}^{N} B_n(\boldsymbol{\rho}, Z) V_{fn}(\boldsymbol{R}) \exp i(k_n - k_f)Z \qquad f = 1, 2, \ldots, N \tag{11}$$

a set of N coupled equations to be solved subject to the asymptotic condition

$B_f(\boldsymbol{\rho}, -\infty) = \delta_{fi}$ which ensures that $\Psi_i \sim \phi_i(\boldsymbol{r}_a)\exp(ik_iZ)$ as $Z \to -\infty$. The scattering amplitude (1) with the undistorted final wave $\Psi_f = \phi_f(\boldsymbol{r}_a)\exp(i\boldsymbol{k}_f \cdot \boldsymbol{R})$ inserted, is therefore,

$$f_{if}(\theta, \phi) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int \exp(i\boldsymbol{K}\cdot\boldsymbol{R})\,d\boldsymbol{R}\sum_{n=1}^{N} B_n(\boldsymbol{\rho}, Z)V_{fn}(\boldsymbol{R})\exp i(k_n - k_i)Z \tag{12}$$

where $\boldsymbol{K}$ is the momentum change $\boldsymbol{k}_i - \boldsymbol{k}_f$ caused by the collision. Since the electrostatic interaction $V(\boldsymbol{r}, \boldsymbol{R})$ is composed of central potentials, $V_{fi}(\boldsymbol{R}) = V_{fi}(R, \Theta)\exp i\Delta\Phi$, where $\Delta = M_i - M_f$ is the change in the azimuthal quantum number of the atom. Hence the substitution

$$C_f(\boldsymbol{\rho}, Z) = B_f(\boldsymbol{\rho}, Z)\exp(-i\Delta\Phi) \tag{13}$$

yields the set of phase Φ-independent equations

$$\frac{i\hbar^2}{\mu}\kappa_f(\rho, Z)\frac{\partial C_f(\rho, Z)}{\partial Z} + \left[\frac{\hbar^2}{\mu}\kappa_f(\kappa_f - k_f) + V_{ff}(\rho, Z)\right]C_f(\rho, Z)$$
$$= \sum_{n=1}^{N} C_n(\rho, Z)V_{fn}(\rho, Z)\exp i(k_n - k_f)Z \tag{14}$$

solved subject to the boundary condition $C_f(\rho, -\infty) = \delta_{if}$. On completion of the Φ-integration in (12), the scattering amplitude reduces to

$$f_{if}(\theta, \phi) = -i^{\Delta+1}\int_0^{\infty} J_\Delta(K'\rho)[I_1(\rho, \theta) - iI_2(\rho, \theta)]\rho\,d\rho \tag{15}$$

where K' is the XY-component $k_f \sin\theta$ of $\boldsymbol{K}$ and where J_Δ are Bessel functions of integral order. Both the functions

$$I_1(\rho, \theta; \alpha) = \int_{-\infty}^{\infty} \kappa_f(\rho, Z)\left[\frac{\partial C_f(\rho, Z)}{\partial Z}\right]\exp(i\alpha Z)\,dZ \tag{16}$$

and

$$I_2(\rho, \theta; \alpha) = \int_{-\infty}^{\infty}\left[\kappa_f(\kappa_f - k_f) + \frac{\mu}{\hbar^2}V_{ff}\right]C_f(\rho, Z)\exp(i\alpha Z)\,dZ \tag{17}$$

contain a dependence on the scattering angle θ via

$$\alpha = k_f(1 - \cos\theta) = 2k_f\sin^2\frac{\theta}{2} \tag{18}$$

the difference between the Z-component of the momentum change $\boldsymbol{K}$ and the minimum momentum change $k_i - k_f$ in the collision. Equations (14–18) are the basic formulae given by the present treatment representing the full multistate eikonal description for the scattering amplitude, and can be easily generalized so as to cover collisions involving multielectron systems. It is apparent that a variety of approximations readily follow. Note that in the absence of all couplings except that connecting the initial and final channels ie $C_n = \delta_{ni}$, then either (12) or (15) directly yields,

$$f_{if}(\theta, \phi) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int V_{fi}(\boldsymbol{R})\exp(i\boldsymbol{K}\cdot\boldsymbol{R})\,d\boldsymbol{R} \tag{19}$$

which is the Born-wave scattering amplitude.

2.2. Approximations to the full multistate eikonal equations

(i) The first multistate approximation A to the above treatment follows by expanding κ_f in (17) as

$$\kappa_f(\boldsymbol{R}) \approx k_f - \frac{\mu}{\hbar^2 k_f} V_{ff}(\boldsymbol{R}) \tag{20}$$

valid for kinetic energies $\hbar^2 k_f^2/2\mu \gg V_{ff}$. Thus, with (6) for κ_f^2 and (20) for κ_f, both I_2 and the term within square brackets on the LHS of (14) vanish identically so that the scattering amplitude given by approximation A is

$$f_{if}^{\mathrm{A}}(\theta, \Phi) = -\frac{1}{4\pi}\frac{2\mu}{\hbar^2}\int \exp[\mathrm{i}(\boldsymbol{K}\cdot\boldsymbol{R} + \Delta\Phi)]\,\mathrm{d}\boldsymbol{R} \sum_{n=1}^{N} C_n^{\mathrm{A}}(\rho, Z) V_{fn}(R, \Theta) \exp \mathrm{i}(k_n - k_i)Z \tag{21a}$$

$$= -\mathrm{i}^{\Delta+1}\int_0^\infty J_\Delta(K'\rho)\rho\,\mathrm{d}\rho \int_{-\infty}^{\infty} \kappa_f \left(\frac{\partial C_f^{\mathrm{A}}}{\partial Z}\right) \exp(\mathrm{i}\alpha Z)\,\mathrm{d}Z \tag{21b}$$

where

$$\frac{\mathrm{i}\hbar^2}{\mu}\kappa_f \frac{\partial C_f^{\mathrm{A}}}{\partial Z} = \sum_{n=1}^{N} C_n^{\mathrm{A}}(\rho, Z) V_{fn}(\rho, Z) \exp \mathrm{i}(k_n - k_f)Z. \tag{22}$$

(ii) A related multistate approximation B involves setting all the local wavenumbers κ_n in A, ie in (21*b*) and (22), equal to their asymptotic values k_n. Both approximations A and B yield the Born-wave elastic and inelastic scattering amplitudes when $C_n^{\mathrm{A}} = \delta_{in}$ is substituted in (21*a*). When the effect of all inelastic channels is neglected, ie when $C_n^{\mathrm{B}} = C_i^{\mathrm{B}}\,\delta_{in}$ in (22) with $\kappa_f = k_f$, then

$$C_i^{\mathrm{B}}(\rho, Z) = \exp\left[-\frac{\mathrm{i}}{\hbar v_i}\int_{-\infty}^{Z} V_{ii}(\rho, Z')\,\mathrm{d}Z'\right]. \tag{23}$$

On performing the integrations in (21*a*) with (23), we find that the corresponding elastic scattering amplitude reduces to

$$f_{ii}^{\mathrm{E}}(\theta, \phi) = -\mathrm{i}k_i \int_0^\infty J_0\left(2k_i\rho \sin\frac{\theta}{2}\right)[\exp 2\mathrm{i}\chi(\rho) - 1]\rho\,\mathrm{d}\rho \tag{24}$$

where the eikonal

$$\chi(\rho) = -\frac{1}{\hbar v_i}\int_0^\infty V_{ii}[(\rho^2 + Z^2)^{1/2}]\,\mathrm{d}Z. \tag{25}$$

This is just the customary eikonal expression for elastic scattering (cf Glauber 1959, Bransden 1970) by a fixed potential.

In particular when the full wavefunction (4) is projected onto the distorted wave

$$\Psi_f(\boldsymbol{r}, \boldsymbol{R}) = \phi_f(\boldsymbol{r}_{\mathrm{a}}) \exp \mathrm{i}\left(\boldsymbol{k}_f \cdot \boldsymbol{R} - \frac{1}{\hbar v_f}\int_{+\infty}^{Z} V_{ff}\,\mathrm{d}Z\right) \tag{26}$$

for the final state, rather than onto the undistorted wave $\phi_f(\boldsymbol{r}_{\mathrm{a}})\exp(\mathrm{i}\boldsymbol{k}_f \cdot \boldsymbol{R})$, as previously used in equation (12), then the preceding analysis follows through with the result,

$$f_{if}^{\mathrm{DW}}(\theta, \phi) = -\mathrm{i}^{\Delta+1}\int_0^\infty J_\Delta(K'\rho)\rho\,\mathrm{d}\rho \int_{-\infty}^{\infty} k_k \left(\frac{\partial C_f^{\mathrm{B}}}{\partial Z}\right) \exp \mathrm{i}\left(\alpha Z + \frac{1}{\hbar v_f}\int_{\infty}^{Z} V_{ff}\,\mathrm{d}Z'\right)\mathrm{d}Z \tag{27}$$

where, in approximation B, C_f^B satisfies (22) with $\kappa_f = k_f$. Setting $C_n^B = C_i^B \delta_{in}$ in (22) then, with the aid of (23), the scattering amplitude (27) reduces to

$$f_{if}^{DWB}(\theta, \phi) = -\frac{i^{\Delta}\mu}{\hbar^2} \int_0^{\infty} J_{\Delta}(k_f \rho \sin\theta) \rho \, d\rho \int_{-\infty}^{\infty} V_{fi}(\rho, Z) \times \exp i[\{(k_i - k_f) + \alpha\}Z + \delta\Phi(Z)] \, dZ \tag{28}$$

where

$$\delta\Phi(Z) = -\frac{1}{\hbar v_i} \int_{-\infty}^{Z} V_{ii} \, dZ - \frac{1}{\hbar v_f} \int_{Z}^{\infty} V_{ff} \, dZ. \tag{29}$$

Equation (28) is the distorted-wave Born approximation which is identical to that derived by Chen *et al* (1972) from a different approach.

(iii) In the heavy-particle or high-energy limit, the asymptotic wavenumbers in approximation B tend to

$$k_f = k_i - \frac{\epsilon_{fi}}{\hbar v_i}\left(1 + \frac{\epsilon_{fi}}{2\mu v_i^2} + \ldots\right) \qquad \epsilon_{fi} = \epsilon_f - \epsilon_i \tag{30}$$

and a third approximation C(α) follows by setting all the individual k_n in approximation B equal to k_i, and any difference $k_n - k_f = \epsilon_{fn}/\hbar v_i$. Hence

$$f_{if}^{C}(\theta, \phi) = -i^{\Delta+1} k_i \int_0^{\infty} J_{\Delta}(K'\rho) \left[\int_{-\infty}^{\infty} \frac{\partial C_f^C(\rho, Z)}{dZ} \exp(i\alpha Z) \, dZ\right] \rho \, d\rho$$

$$\alpha = K_Z - \frac{\epsilon_{fi}}{\hbar v_i}. \tag{31a}$$

In addition, for small angle scattering, $\alpha \approx 0$ from (18) and the Z-integration above can therefore be performed so that a further approximation C($\alpha = 0$) is characterized by

$$f_{if}^{C(0)}(\theta, \phi) = -i^{\Delta+1} k_i \int_0^{\infty} J_{\Delta}(K'\rho)[C_f^C(\rho, \infty) - \delta_{if}] \rho \, d\rho \tag{31b}$$

where $K'^2 = K^2 - \epsilon_{fi}^2/\hbar^2 v_i^2$ and the amplitudes C_f^C satisfy

$$i\hbar v_i \frac{\partial C_f^C}{\partial Z} = \sum_{n=1}^{N} C_n^C(\rho, Z) V_{fn}(\rho, Z) \exp\left(\frac{i\epsilon_{fn} Z}{\hbar v_i}\right) \tag{32}$$

in which $v_i = \hbar k_n/\mu$ for $n = 1, 2, \ldots, N$, is the incident speed. These equations (31) and (32) are simply the familiar impact-parameter equations which have received widespread application to atom–atom and ion–atom scattering (Flannery and McCann 1973, 1974b–e). Also, (32) with (31*b*), in which $K' = 2k_i \sin\frac{1}{2}\theta$, have been modified by Bransden and Coleman (1972) so as to acknowledge implicitly the polarization effect on the incident channel due to couplings ignored explicitly by the truncated expansion (4). Byron (1971) has also obtained (31*a*) although he actually used (31*b*) and (32) for e–He collisions. The preceding analysis shows, however, that (31–32) are strictly valid only in the heavy-particle or high-energy limit.

In the limit of very high impact-speeds, the phase $\epsilon_{fn} Z/\hbar v_i$ in (32) can be neglected and Byron (1971) solved the infinite set ($N \to \infty$) of coupled equations exactly to give

$$C_f^G(\boldsymbol{\rho}, Z) = \langle \phi_f(\boldsymbol{r}_a) \left| \exp -\frac{i}{\hbar v_i} \int_{-\infty}^{Z} V(\boldsymbol{r}_a, \boldsymbol{R}) \, dZ \right| \phi_i(\boldsymbol{r}_a) \rangle \tag{33}$$

a solution easily verified and which includes the effects arising from all discrete and continuum atomic states. Substitution in either equation (31*a*) with $\alpha = K_Z$ since $\epsilon_{fi}/v_i = 0$, and with the Φ-integration re-introduced or in equation (31*b*) with $K' = K$, yields

$$f_{if}^{G}(\theta, \phi) = -\frac{ik_i}{2\pi} \int e^{i\mathbf{K}\cdot\boldsymbol{\rho}} \phi_f^*(\boldsymbol{r}_a)[e^{i\chi(\boldsymbol{\rho}, \boldsymbol{r}_a)} - 1]\phi_i(\boldsymbol{r}_a)\, d\boldsymbol{r}_a\, d\boldsymbol{\rho} \tag{34}$$

where the phase shift

$$\chi(\boldsymbol{\rho}, \boldsymbol{r}_a) = -\frac{1}{\hbar v_i} \int_{-\infty}^{\infty} V(\boldsymbol{r}_a, \boldsymbol{\rho}, Z)\, dZ \tag{35}$$

thereby providing an alternative derivation of the expression of Glauber (1959). Thus, the Glauber approximation is a high-energy approximation which acknowledges all couplings between all discrete and continuum atomic eigenstates. The approximation has been applied by Tai *et al* (1970) to e–H(1s) excitation.

In general, for all the above approximations, the total cross section is given by

$$\sigma_{if}(k_i) = 2\pi \frac{k_f}{k_i} \int_0^{\pi} |f_{if}(\theta, \phi)|^2 \sin\theta\, d\theta \tag{36}$$

which, for the special case of approximation $C(\alpha = 0)$ alone, reduces to the customary impact-parameter expression

$$\sigma_{if}(k_i) = 2\pi \frac{k_f}{k_i} \int_0^{\infty} |C_f^C(\rho, \infty) - \delta_{if}|^2 \rho\, d\rho \tag{37}$$

for the total cross section. This expression is valid provided the energy is sufficiently high ($k_i \approx k_f$) and the scattering is into small angles such that the quantity $K'^2 \approx K^2 \approx 2k_i^2(1 - \cos\theta)$ can be used in the integrand of (31*b*) and (36) and that the integral

$$\int_{(k_i - k_f) \approx 0}^{(k_i + k_f) \approx \infty} J_\Delta(K\rho) J_\Delta(K\rho') K\, dK \approx \frac{1}{\rho}\, \delta(\rho - \rho') \tag{38}$$

can be used to reduce (36) to (37). The JWKB approach of Bates and Holt (1966) involves the use of (37) with C_f^C replaced by the solution A_f of (9). In the next section, the effect of all the various approximate schemes A, B, C(α) and C(0) above to the full multistate eikonal treatments equations (14–15) will be fully examined by direct calculation.

3. Results and discussion

The theory derived in the previous section is now applied to the examination of the elastic and inelastic collisions,

$$e + H(1s) \rightarrow e + H(1s, 2s, 2p_{0, \pm 1}) \tag{39}$$

in which the lowest five states 1s, 2s, $2p_0$ and $2p_{\pm 1}$ of atomic hydrogen are closely coupled. It is worth pointing out that the resulting set of coupled equations are *not* approximations to the five actual coupled differential equations obtained from the full quantal close-coupling method. One advantage of the present procedure is that an infinite number of distorted partial waves of relative motion are automatically acknowledged via the eikonal in (4) and all these waves in turn are further correlated with the target wavefunctions via A_n in (4). This is done at the expense of the full correlation between the incident and atomic electrons included in a quantal close-coupling description of a *given* partial wave.

Differential and total cross sections for (39) are calculated for incident energies E_i in the range 13·6 eV $\leqslant E_i \leqslant$ 200 eV. In table 1 are displayed the total cross sections obtained from the full eikonal treatment equations (14–18, 36) at three representative impact energies together with comparison values obtained from the approximate schemes A, B, C(α), C(0) and IP previously discussed, and summarized in figure 1.

Table 1. Total cross sections (πa_0^2) at impact energy E_i(eV) for the processes e + H(1s) → e + H(nl); nl = 1s, 2s, $2p_{0,\pm1}$, obtained from various approximate schemes.

E_i(eV)	nl	Full eikonal treatment equations (14–18)	Approximate eikonal treatments A	B	C(α)	Impact parameter treatment C(0)	IP
20	1s	0·841	0·923	0·703	0·651	0·714	1·056
	2s	0·145	0·174	0·131	0·070	0·122	0·147
	$2p_0$	0·398	0·524	0·319	0·347	0·373	0·447
	$2p_{\pm1}$	0·322	0·355	0·297	0·307	0·931	0·720
	2p	0·720	0·879	0·616	0·654	1·304	1·167
50	1s	0·365	0·378	0·332	0·373	0·371	0·519
	2s	0·090	0·095	0·085	0·076	0·089	0·083
	$2p_0$	0·350	0·360	0·347	0·352	0·303	0·279
	$2p_{\pm1}$	0·515	0·522	0·514	0·515	0·717	0·569
	2p	0·865	0·882	0·861	0·867	1·020	0·848
100	1s	0·224	0·229	0·202	0·202	0·213	0·271
	2s	0·052	0·053	0·050	0·049	0·053	0·054
	$2p_0$	0·190	0·192	0·191	0·196	0·176	0·173
	$2p_{\pm1}$	0·439	0·441	0·439	0·443	0·506	0·484
	2p	0·629	0·633	0·630	0·639	0·682	0·657

A: equations (20–22, 36); B: equations (21, 22, 36) with $\kappa_n = k_n$; C(α): equations (31*a*, 32, 36); C(0): equations (31*b*, 32, 36); IP: equations (31*b*, 32, 37).

3.1. Total cross sections

The comparison between the last two columns C(0) and IP in table 1 is a direct measure of the error introduced by the use of (37) rather than (36) for the total cross section. In general, IP exceeds C(0) except for the $2p_{\pm1}$ and 2p excitations. The overestimates for $\Delta = 1(2p_{\pm1})$ transitions and the underestimate for $\Delta = 0(2p_0)$ transitions are direct consequences of the different behaviour of the Bessel functions J_0 and J_1 in (38) at the non-physical small momentum changes $K < k_i - k_f$ and at the non-physical large momentum changes $K > k_i + k_f$ which are automatically included in equation (37) via assumption (38).

Inclusion of the phase α by approximation C(α), equation (31*a*), causes a further reduction in the total cross sections at all energies. The difference between the asymptotic speeds v_n is acknowledged via approximation B, equations (21–22) with $\kappa_n = k_n$. This inclusion yields cross sections, column B, in general larger than those given by C(α), particularly at the lower incident speeds, as expected from examination of the LHS of (22). The effect of adopting in (21) the approximate local wavenumber κ_f given by (20), rather than the asymptotic value k_n as in B, is examined in columns A and B. The cross sections become greater at all energies with the result that the impact parameter cross sections

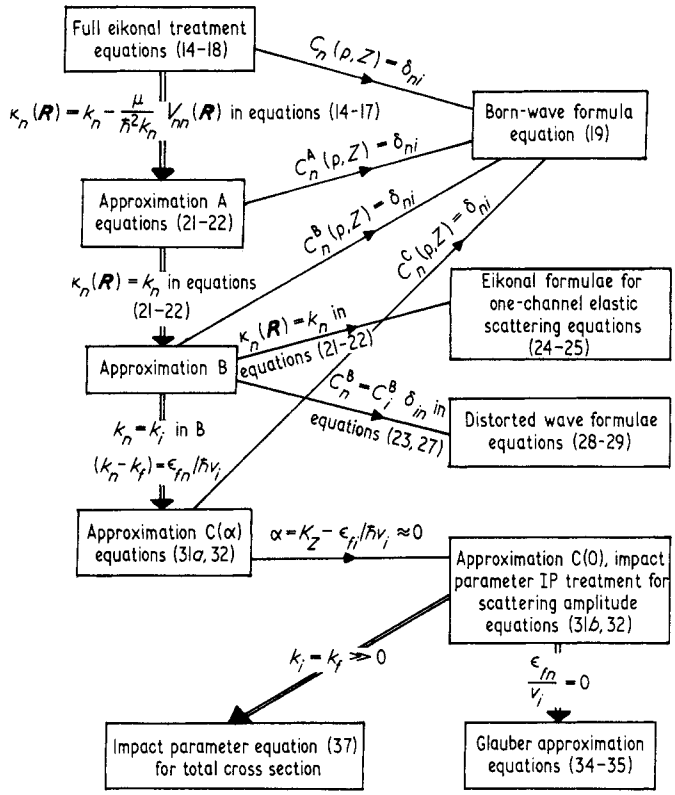

Figure 1. Schematic diagram illustrating approximations to full eikonal multistate treatment.

(column IP) are effectively better than the actual approximation merits; the effect of the various refinements introduced via C(0) and C(α) is largely offset by those acknowledged via B and A.

Finally, the cross sections given by the full multistate description equations (14–18) with the additional integral (17), are somewhat less than those given by A. In conclusion, the changes introduced by the various modifications to the full eikonal treatment are, as exhibited by table 1, significant at the lower incident energies and become vanishingly small at the high impact energies, as they should, since the basic framework of the model is essentially preserved.

3.2. Comparison of various theories and experiment

In table 2 are presented the final elastic and inelastic cross sections $\sigma_{1s-nl}(E_i)$ obtained from the present full multistate eikonal treatment of processes (39) for various impact energies E_i (eV). The present 2s and 2p excitation cross sections are compared in figures 2 and 3, curve FE, with those given by other refined treatments—the pseudo-state method of Burke and Webb (1970), the second-order potential approach of Sullivan *et al* (1972) and the polarized orbital distorted-wave model of McDowell *et al* (1973). Also displayed in figures 2 and 3 are results of approximation B, of the impact parameter IP treatment and of the Born approximation. The 2p experimental data of Long *et al*

Table 2. Elastic and inelastic cross sections (πa_0^2) from the full eikonal approximation to the processes e + H(1s) → e + H(nl), nl = 1s, 2s, $2p_0$, $2p_{\pm 1}$ at electron energy E_i(eV).

E_i(eV) \ nl	1s	2s	$2p_0$	$2p_{\pm 1}$	2p
13·6	1·290	0·120	0·345	0·115	0·460
20	0·841	0·145	0·398	0·322	0·720
30	0·615	0·124	0·387	0·449	0·836
50	0·365	0·090	0·350	0·515	0·865
100	0·224	0·052	0·190	0·439	0·629
200	0·129	0·028	0·118	0·335	0·453

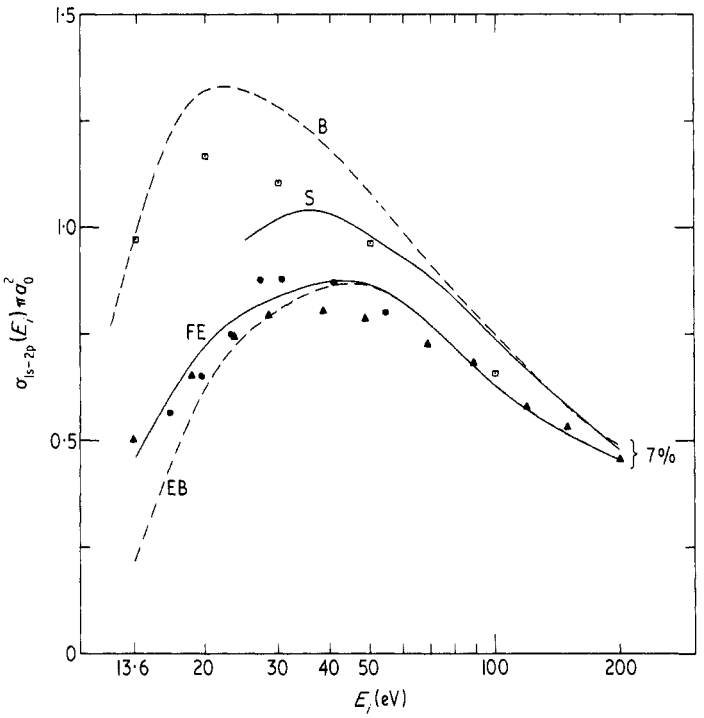

Figure 2. Total cross sections $\sigma_{1s-2p}(E_i)$ for e + H(1s) → e + H(2p) at impact energy E_i(eV). FE: full eikonal approximation, equations (14–18), four-state treatment; EB: eikonal approximation B, equations (21–22) with $\kappa_n = k_n$, four-state treatment; ▲: experiment (Long *et al* 1968); ●: pseudo-state (Burke and Webb 1970); ⊡: four-state impact parameter treatment, equations (32, 37); S: second-order potential method, four-channel approximation (Sullivan *et al* 1972); B: Born approximation.

(1968), normalized to the present value of $0{\cdot}453\pi a_0^2$ at 200 eV (rather than to the corresponding Born results of $0{\cdot}485\pi a_0^2$ which is 7% higher), and values of $\sigma_{1s-2s} + 0{\cdot}23\sigma_{1s-3p}$ measured by Kauppila *et al* (1970) are also shown in figures 2 and 3, respectively. Although the Glauber treatment involved a heavy-particle high-energy limit, the Glauber results of Tai *et al* (1970) which are not shown, agree very well with experiment.

The agreement between FE, pseudo-state values and experiment is very good for the 2p excitation. The EB results which were reported earlier (Flannery and McCann 1974a) are indistinguishable from the full treatment FE for $E_i \gtrsim 50$ eV. The difference

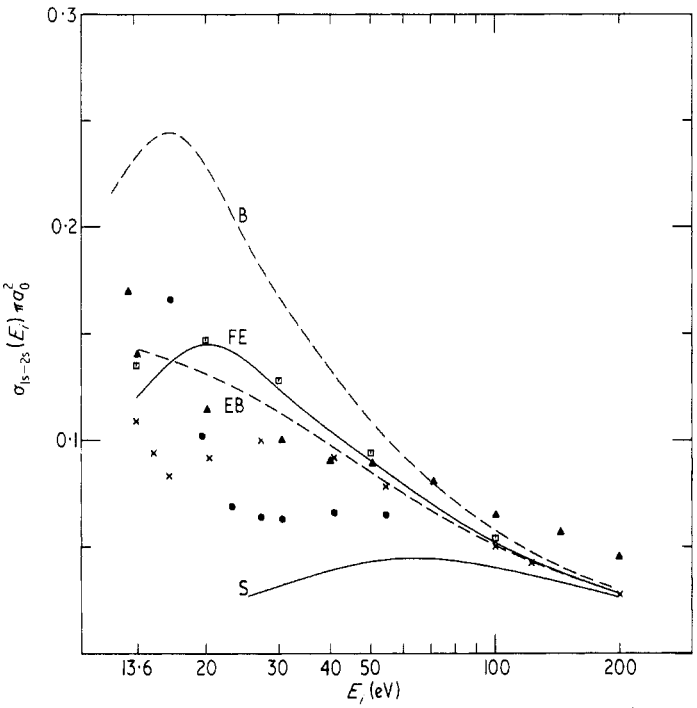

Figure 3. Total cross sections $\sigma_{1s-2s}(E_i)$ for e + H(1s) → e + H(2s) at impact energy E_i (eV). FE: full eikonal approximation, equations (14–18), four-state treatment; EB: eikonal approximation B, equations (21–22) with $\kappa_n = k_n$, four-state treatment; ●: pseudo-state (Burke and Webb 1970); ×: polarized-orbital distorted wave model (McDowell *et al* 1973); ⊡: four-state impact parameter treatment, equations (32, 37); S: second-order potential method, four-channel approximation (Sullivan *et al* 1972); B: Born approximation; ▲: $\sigma_{1s-2s}(E_i) + 0{\cdot}23\sigma_{1s-3p}(E_i)$, experiment (Kauppila *et al* 1970).

between S and ⊡ is a direct measure of the effect of the second-order potential introduced by Bransden and Coleman so as to reproduce exactly the long-range interaction in the incident channel. The present treatment represents a considerable improvement over both the Born and impact-parameter approximations.

For the 2s excitation, there is a much greater scatter between the refined theoretical cross sections for impact energies $E_i < 50$ eV. The measured values of Kauppila *et al* (1970) do not offer any definition since the 3p cascade contribution $0.23\sigma_{1s-3p}$ which, of course, varies with E_i, was included. Direct comparison between FE and experiment will only be possible when the higher $n = 3$ channels are included in the multistate expansion (9). Inclusion of κ_f as in FE rather than the use of k_f as in EB introduces a maximum to the 2s excitation.

The close agreement, for energies $E_i > 40$ eV, of the present treatment with that of McDowell *et al* (1973) who included exchange and polarization effects is either fortuitous or else demonstrates that exchange and polarization effects make little contribution at these energies.

3.3. Differential cross sections

Examination of the differential cross sections,

$$\frac{d\sigma}{d\Omega} = \frac{k_f}{k_i}|f_{if}(\theta, \phi)|^2 \tag{40}$$

permits additional insight into the accuracy and possible limitations of the present treatment. Although the treatment can be suitably modified so as to theoretically acknowledge electron-exchange and that portion of the polarization distortion not included by virtue of the four-state expansion, the present analysis has neglected such effects.

3.3.1. Elastic scattering. Results (MEA) for elastic scattering at 50 eV and 100 eV are shown in figure 4 together with the measured values of Teubner *et al* (1973) and the theoretical predictions of Winters *et al* (1973) and the Glauber results of Franco (1968) and

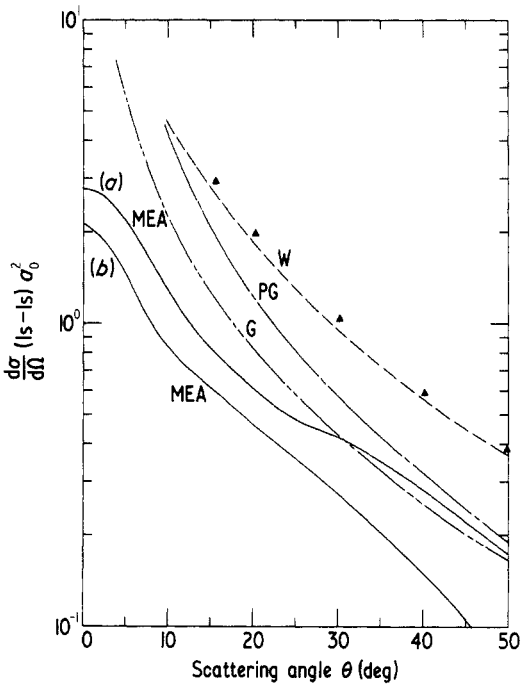

Figure 4. Differential cross sections for elastic scattering at 50 eV. MEA: present four-state (1s, 2s, $2p_0$, $2p_{\pm 1}$) eikonal treatment at (*a*) 50 eV, (*b*) 100 eV; G: Glauber approximation (Franco 1968); PG: polarized Glauber approximation (Mathur 1974); W: second-order potential theory with exchange (Winters *et al* 1973); ▲ Teubner *et al* (1973).

of Mathur (1974). Although the experimental data are subject to $\pm 35\%$ error, comparison between MEA and W clearly demonstrates the necessity of including the full polarization distortion (for distant encounters) electron-exchange and a wave treatment modification (for the closer encounters), all of which were acknowledged by the one-channel approximation of Winters *et al* (1973). The present differential cross sections were rather insensitive to the approximations in § 2.2 (cf table 1).

Further accord with experiment is introduced by inclusion of electron-exchange and a wave treatment of the close collisions (with angular momentum $l \leqslant 7$) as carried out by Winters *et al* (1973). In conclusion, figure 4 displays the inadequacy of the present treatment to properly describe elastic scattering at all angles; polarization distortion mainly affects small-angle scattering while electron-exchange becomes dominant for larger angle scattering.

3.3.2. Inelastic scattering. In figures 5(*a*), (*b*) are displayed the $2p_{0,\pm 1}$ and 2p differential cross sections at 50 eV and 100 eV, together with the distorted-wave calculations of Chen *et al* (1972). Comparison shows that the effect of coupling with the 2s channel is to decrease the 2p scattering only at small angles $\lesssim 10°$. The Glauber results of Tai *et al* (1970) are also shown at 100 eV.

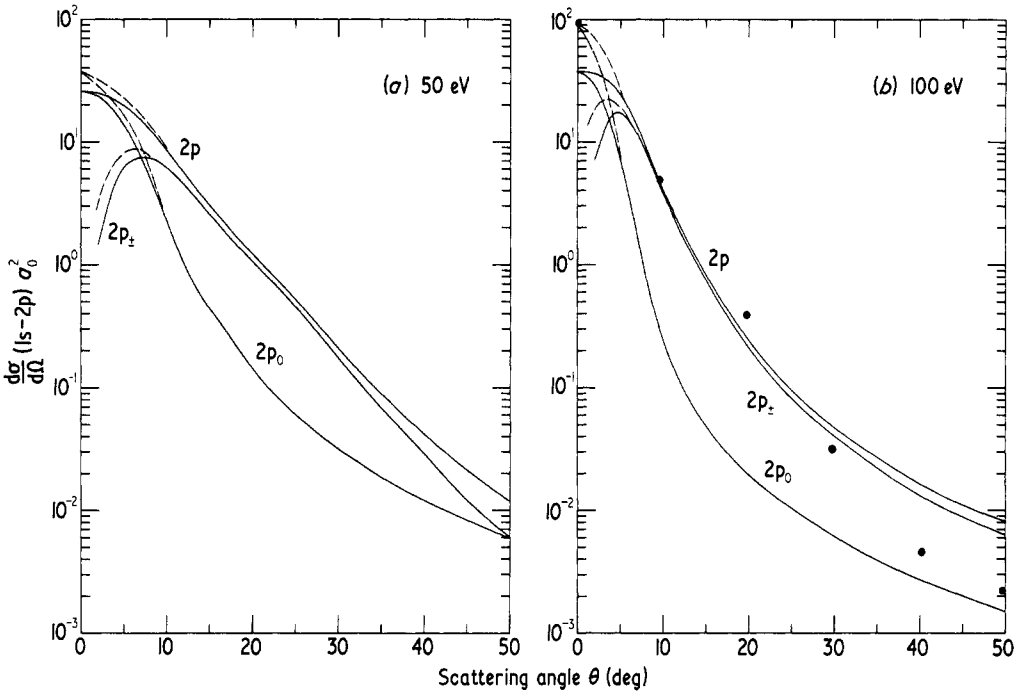

Figure 5. Differential cross sections for the $2p_0$, $2p_{\pm 1}$ and 2p excitations of atomic hydrogen by electron impact at (*a*) 50 eV and (*b*) 100 eV incident energy; —— present four-state (1s, 2s, $2p_0$, $2p_{\pm 1}$) eikonal treatment; – – – distorted-wave treatment (Chen *et al* 1972); ● Glauber approximation (Tai *et al* 1970).

Figures 6(*a*), (*b*) display the corresponding 2s scattering. A two-state treatment has also been carried out and the results agree closely with Chen *et al*, who found that electron-exchange, the importance of which increases with θ, is very small. Figures 6(*a*) and (*b*) show that the more important effect arises via coupling with the 2p channel, particularly for small momentum transfers. The Glauber approximation is in general agreement with the four-channel calculations except at high-momentum changes.

In summary, a multichannel generalization of the eikonal approach to atomic collisions has been presented. Various approximate schemes have been proposed, and examined in detail for e–H(1s) collisions. In the heavy-particle or high-energy limit, the basic formulae reduce to the standard impact parameter method. For e–H(1s) collisions at low and intermediate energies E, the additional refinements introduced are necessary for an adequate description of excitation. Very good agreement with experiment and with other refined treatments is obtained for the 2p excitation while the 2s excitation (the cross section for which being less definitive for $E < 40$ eV) is in satisfactory accord. However polarization distortion and electron-exchange which are neglected in the present description are very important for elastic scattering at all angles.

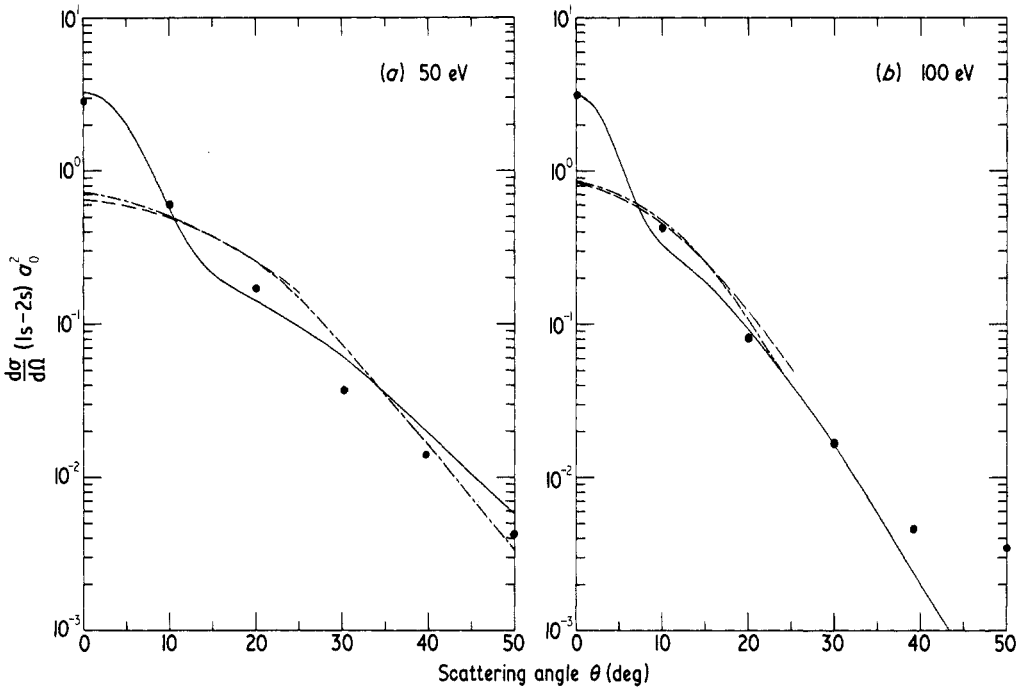

Figure 6. Differential cross sections for the 2s-excitation of atomic hydrogen by electron-impact at (*a*) 50 eV and (*b*) 100 eV incident energy: —— present four-state (1s, 2s, $2p_0$, $2p_{\pm 1}$) eikonal treatment; — — — present two-state (1s, 2s) eikonal treatment; – – – distorted-wave treatment (Chen *et al* 1972); ● Glauber approximation (Tai *et al* 1970).

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