

Electron impact excitation of the $n = 2$ level in He^+ and H at low energies

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Abstract. Two Coulomb-exchange distorted-wave (CEDW) approximations are developed and applied to the electron impact excitation of the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ transitions in He^+ and H at low energies. In the first approximation, CEDW1, partial waves are distorted by various direct multipole potentials. In the second approximation, CEDW2, particular partial waves are additionally distorted by an exchange monopole potential.

Results for cross sections presented here are compared with those of the three-state close-coupling and Coulomb–Born–Oppenheimer approximations, and with experiment. Despite the unfavourable degeneracy of the $2s$ and $2p$ states in hydrogenic atoms, the CEDW2 approximation gives satisfactory agreement with the three-state close-coupling approximation for the $1s \rightarrow 2s$ transition and fairly good agreement for the $1s \rightarrow 2p$ transition together with a significant reduction in computing time. Thus our distorted-wave approach can be useful at low energies for singly-ionised and neutral atoms and is sufficiently promising to justify further development for application to more complex systems, where we no longer have the degeneracy of states that we do with hydrogenic atoms.

1. Introduction

The excitation of positive ions by electron impact has been reviewed by Henry (1981) and, for the case of neutral atoms, by Bransden and McDowell (1977, 1978). Since then Chidichimo (1981) has shown that, by including the distortion of partial waves by multipole potentials, the distorted-wave approach to electron–ion collisions can give good results at low energies for a singly-ionised system, namely Ca^+ . Electron exchange between the incident and atomic electrons was neglected. In the distorted-wave approximation, the coupling between states is treated as a perturbation and the collision equations are uncoupled. This gives it a distinct advantage, in terms of computing resources, over the close-coupling approximation and provides the main motivation for this work. Thus at low energies it is important that the role of exchange be examined.

In § 2 we develop two Coulomb-exchange distorted-wave (CEDW) approximations for the electron impact excitation of hydrogenic atoms. In the first approximation, CEDW1, partial waves are distorted by various direct multipole potentials. In the second approximation, CEDW2, particular partial waves are additionally distorted by an exchange monopole potential. In both approximations, both the incident and scattered partial waves are distorted. In the CEDW2 approximation we also investigate the case of equivalent electrons in a bound-state problem. In § 3 we apply these approximations to the $1s \rightarrow 2s$ and $1s \rightarrow 2p$ transitions in He^+ and H. In § 4 we present

our results and compare them with other theoretical results, in particular the three-state close-coupling approximation, and with experiment.

There do of course exist more accurate and time-consuming theoretical results, especially between the $n = 2$ and $n = 3$ thresholds and these can predict the resonance structure that exists there. For He^+ see Ormonde *et al* (1967), Burke and Taylor (1969) and Morgan (1979). For H see e.g. Taylor and Burke (1967), Callaway *et al* (1975), Morgan *et al* (1977), Callaway (1982) and also the experiment of Williams (1976). Our model cannot predict resonances so the results can only be regarded as an averaged-out value for the cross sections there. Typically these elaborate calculations are only carried out for the first few angular momenta and are supplemented at higher L by results from simpler approximations. For positive ions more partial waves must be taken into account than for neutral atoms thus increasing further the computation time. We note also the polarised-orbital results of McDowell *et al* (1977).

All quantities are in atomic units except energies which are given in rydbergs. In the figures the cross sections are given in units of πa_0^2 .

2. Theory

The partial-wave theory of electron-hydrogen-atom collisions was developed by Percival and Seaton (1957). Following their approach we take the total wavefunction of the electron-hydrogenic-atom system to satisfy the collisional Hartree-Fock equations and solve to get radial equations of the form,

$$\left(\frac{d^2}{dr^2} - \frac{l'(l'+1)}{r^2} + \frac{2z}{r} + k_\nu^2\right) \mathcal{F}_{\nu'l\nu}^\pm(r) = \sum_{\nu'\lambda} (V_{\nu'l\nu'}^\lambda(r) \pm W_{\nu'l\nu'}^\lambda(r)) \mathcal{F}_{\nu'\lambda}^\pm(r) \quad (2.1)$$

where

$$V_{\nu'l\nu'}^\lambda(r) = 2f_\lambda(l'_a l', l''_a l''; L) (y_\lambda(P_{n'l'_a}, P_{n'l''_a} | r) - \delta_{\nu'l\nu'} \delta_{\lambda 0} / r) \quad (2.2)$$

$$\begin{aligned} W_{\nu'l\nu'}^\lambda \mathcal{F}_{\nu'l\nu'}^\pm(r) &= g_\lambda(l'_a l', l''_a l''; L) \left(\delta_{\lambda 0} (E_n - k_\nu^2) \right. \\ &\times \int_0^\infty P_{n'l'_a}(r') \mathcal{F}_{\nu'l\nu'}^\pm(r') dr' + 2y_\lambda(P_{n'l'_a}, \mathcal{F}_{\nu'l\nu'}^\pm | r) \left. \right) P_{n'l''_a}(r) \end{aligned} \quad (2.3)$$

$$y_\lambda(P, F | r) = \frac{1}{r^{\lambda+1}} \int_0^r P(r') F(r') r'^{\lambda} dr' + r^\lambda \int_r^\infty \frac{P(r') F(r')}{r'^{\lambda+1}} dr' \quad (2.4)$$

and $P_{nl_a}(r)$ satisfies

$$\left(\frac{d^2}{dr^2} - \frac{l_a(l_a+1)}{r^2} + \frac{2Z}{r} + E_n\right) P_{nl_a}(r) = 0. \quad (2.5)$$

$\mathcal{F}_{\nu'l\nu'}^\pm(r)$ is the radial function of the free electron, $-$ for the case of parallel electron spins and $+$ for the case of anti-parallel electron spins. $P_{nl_a}(r)$ is the radial function of the atomic electron described by quantum numbers nl_a and corresponds to a state with energy E_n .

$$E = E_n + k_\nu^2 \quad (2.6)$$

is the total energy of the system, $\nu = nl_a l$ are quantum numbers describing the system

in a coupled angular momentum representation and the angular coefficients, f_λ and g_λ , are defined by Percival and Seaton (1957). Z is the nuclear charge of the target and $z = Z - 1$.

2.1. The solution of the CEDW2 radial equation

We now consider the solution of the radial equation for the free electron in the CEDW approximations described in the introduction and defined later in § 2.5. The CEDW1 radial equation is no more complicated to solve numerically than the CBO radial equation in Burgess *et al* (1970) and is a special case of the CEDW2 radial equation. Thus we consider solutions of the CEDW2 radial equation,

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2z}{r} + k_\nu^2 - \sum_\lambda U_{\nu\nu}^{\lambda\pm} \right) F_\nu^\pm(r) = 0 \quad (2.7)$$

with

$$U_{\nu\nu}^{\lambda\pm} = V_{\nu\nu}^\lambda \pm \delta_{\lambda 0} W_{\nu\nu}^\lambda. \quad (2.8)$$

Using (2.2)–(2.4) and (2.8) we may rewrite (2.7) as

$$\begin{aligned} & \left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2z}{r} + k_\nu^2 \right) F_\nu^\pm(r) \\ &= 2 \sum_\lambda f_\lambda(l_a l, l_a l; L) \left(y_\lambda(P_{n l_a}, P_{n l_a} | r) - \frac{\delta_{\lambda 0}}{r} \right) F_\nu^\pm(r) \pm 2g_0(l_a l, l_a l; L) \\ & \quad \times \left(c + \frac{1}{r} \int_0^r P_{n l_a}(r') F_\nu^\pm(r') dr' - \int_0^r \frac{P_{n l_a}(r')}{r'} F_\nu^\pm(r') dr' \right) P_{n l_a}(r) \end{aligned} \quad (2.9)$$

where c is a constant given by

$$c = \frac{1}{2}(E_n - k_\nu^2) \int_0^\infty P_{n l_a}(r) F_\nu^\pm(r) dr + \int_0^\infty \frac{P_{n l_a}(r)}{r} F_\nu^\pm(r) dr. \quad (2.10)$$

On substituting the following expansions

$$F_\nu^\pm(r) = \sum_{n=0}^\infty a_n r^{n+l+1} \quad (2.11)$$

$$P_{n l_a}(r) = \sum_{i=0}^\infty p_i r^{i+l_a+1} \quad (2.12)$$

and

$$\sum_\lambda V_{\nu\nu}^\lambda(r) = \frac{2z}{r} + \sum_{j=0}^\infty v_{j-1} r^{j-1} \quad (2.13)$$

into (2.9) we obtain a recurrence relation of the form

$$\begin{aligned} & n(n+1+2l)a_n - \sum_{i,j=0}^\infty v_{i-1} a_j \delta(n, i+j+1) + a_{n-2} k_\nu^2 \\ & \mp g_0 \left(c p_{n-2} - \sum_{i,j,k=0}^\infty \frac{a_i p_j p_k \delta(n-2l_a-3, i+j+k+1)}{(n-k-1)(n-k-2)} \right) = 0 \end{aligned} \quad (2.14)$$

valid for $n > 1$ with a_1 given by

$$a_1 = -\frac{Za_0}{l+1}. \tag{2.15}$$

a_0 determines the normalisation and

$$g_s = 2g_0(la, la; L). \tag{2.16}$$

This gives us a power series solution for (2.9) with an infinite radius of convergence. However there is an effective radius of convergence, since we can only retain a finite number of terms in (2.11)–(2.13), so we seek a numerical extension of our analytic solution. Equation (2.9) is of the form

$$Y''(x) = G(x, Y) \tag{2.17}$$

for which a power series solution may be extended using the summed Cowell–Numerov formula (see Fröberg 1969),

$$Y_{n+1} = Y_n + \frac{h^2}{12} G_{n+1} - \frac{h^2}{12} G_n + h^2 \sum_{j=1}^n G_j + Y_1 - Y_0 - \frac{h^2}{12} G_1 + \frac{h^2}{12} G_0 \tag{2.18}$$

where $Y_n = Y(x_n)$ and $x_{n+1} = x_n + h$. By the application of (2.17)–(2.18) to (2.9) we obtain

$$\begin{aligned} & \left(1 - \frac{h^2}{12} \phi_{n+1}\right) F_{n+1}^\pm \\ &= \left(1 - \frac{h^2}{12} \phi_n\right) F_n^\pm \pm \frac{h^2}{12} g_s c (P_{n+1} - P_n) \\ & \pm \frac{h^2}{12} g_s \left[\left(\frac{1}{r_{n+1}} \int_0^{r_{n+1}} PF^\pm dr - \int_0^{r_{n+1}} \frac{PF^\pm}{r} dr\right) P_{n+1} \right. \\ & \left. - \left(\frac{1}{r_n} \int_0^{r_n} PF^\pm dr - \int_0^{r_n} \frac{PF^\pm}{r} dr\right) P_n \right] \\ & + h^2 \sum_{j=1}^n \left[\phi_j F_j^\pm \pm g_s P_j \left(\frac{1}{r_j} \int_0^{r_j} PF^\pm dr - \int_0^{r_j} \frac{PF^\pm}{r} dr + c\right) \right] \\ & + \sum_{i=0}^1 (-1)^{i+1} \left\{ F_i^\pm - \frac{h^2}{12} \left[\phi_i F_i^\pm \pm g_s P_i \left(\frac{1}{r_i} \int_0^{r_i} PF^\pm dr - \int_0^{r_i} \frac{PF^\pm}{r} dr + c\right) \right] \right\} \end{aligned} \tag{2.19}$$

where P_n now denotes $P(r_n)$ and

$$\phi(r) = \frac{l(l+1)}{r^2} - \frac{2z}{r} - k_v^2 + \sum_\lambda V_{\nu\nu}^\lambda(r). \tag{2.20}$$

We can approximate the term in F_{n+1}^\pm on the RHS of (2.19) in two ways (a) and (b) thus, (a)

$$\begin{aligned} & P_{n+1} \left(\frac{1}{r_{n+1}} \int_0^{r_{n+1}} PF^\pm dr - \int_0^{r_{n+1}} \frac{PF^\pm}{r} dr \right) \\ & \simeq P_{n+1} \left(\frac{1}{r_{n+1}} \int_0^{r_{n-1}} PF^\pm dr - \int_0^{r_{n-1}} \frac{PF^\pm}{r} dr \right) - \frac{2h^2}{3} \frac{P_{n+1}}{r_{n+1}} \left(\frac{P_{n-1} F_{n-1}^\pm}{r_{n-1}} + \frac{2P_n F_n^\pm}{r_n} \right) \end{aligned} \tag{2.21}$$

using a three-point Simpson rule on $\int_{r_{n-1}}^{r_{n+1}}$ or, (b)

$$P_{n+1} \left(\frac{1}{r_{n+1}} \int_0^{r_{n+1}} PF^\pm dr - \int_0^{r_{n+1}} \frac{PF^\pm}{r} dr \right) \\ \approx P_{n+1} \left(\frac{1}{r_{n+1}} \int_0^{r_n} PF^\pm dr - \int_0^{r_n} \frac{PF^\pm}{r} dr \right) - \frac{h^2}{6} \frac{P_{n+1}}{r_{n+1}} \left(\frac{4P_n F_n^\pm}{r_n} - \frac{P_{n-1} F_{n-1}^\pm}{r_{n-1}} \right) \quad (2.22)$$

using a three-point (r_{n-1}, r_n, r_{n+1}) Newton–Cotes integration formula (see Fröberg 1969) on $\int_{r_n}^{r_{n+1}}$.

In the cases of He^+ and H it was found that the difference between approximations (a) and (b) for the extension of the power series solution was less than the accuracy of the summed Cowell–Numerov method for a given step length. In (a), using a three-point Simpson rule at each step, $\int_0^{r_{n-1}}$ depends only on alternate previous integrals. During computation $\int_0^{r_m}$, m odd, drift apart from $\int_0^{r_m}$, m even. In (b) $\int_0^{r_n}$ depends on all the previous values and the above effect does not arise. For this reason approximation (b) was preferred.

Thus we have succeeded in, numerically, extending our power series solution.

2.2. The collision equation

We consider first, by setting $\nu = nssS$ in (2.9), s-wave scattering off He^+ or H in an s state. In this case $\lambda = 0$ is the only non-zero contribution to the sum over λ . Using Percival's method, see Marriott (1958), we evaluate F_ν^+ with two different arbitrary values of c and take a linear combination of the two solutions that satisfies (2.10). For the case of parallel electron spins whatever the value of c we choose we get a function F_ν^- that automatically satisfies (2.10) because if F_ν^- is a solution of (2.9) then $F_\nu^- + \beta P_{ns}$ is also a solution (β arbitrary). If we multiply (2.9) through by P_{ns} and integrate over all r we can reduce the resulting equation to (2.10), for F_ν^- . In this case we can impose F_ν^- orthogonal to P_{ns} .

For p-wave scattering off p states we do not include the $W_{\nu\nu}^2$ term of (2.3) in (2.7) and we can evaluate F_ν^\pm as we did previously for the case of F_ν^+ .

The appropriate asymptotic boundary conditions for a solution of (2.7) are

$$F_\nu^\pm(r) \sim 0 \quad (2.23) \\ r \rightarrow 0$$

and

$$F_\nu^\pm(r) = \zeta_\nu^{-1/2} \sin(\phi_\nu + \tau_\nu^\pm) \quad (2.24)$$

with ϕ_ν and ζ_ν given by (2.34)–(2.35) for $k > 0$ and by (2.36)–(2.37) for $k = 0, z > 0$ and evaluated according to Burgess (1963).

2.3. Equivalent electrons

To investigate further properties of the CEDW2 radial equation and as a check on the numerical methods and programs which solve it, we turn the $\text{He}^+ + e^-$ collision problem into one of evaluating the ground-state energy of He . The solution of this is already

well known in terms of the Hartree–Fock bound-state equation (see e.g. Froese Fischer 1977). Thus we set $\nu = nssS$ and $P_{nl_a} \equiv F_\nu^+$ in (2.9) and we impose the following asymptotic boundary conditions

$$F_\nu^+(r) \underset{r \rightarrow 0}{\sim} 0$$

and

$$F_\nu^+(r) \underset{r \rightarrow \infty}{\sim} 0 \quad (2.25)$$

with the normalisation

$$\int_0^\infty (F_\nu^+(r))^2 dr = 1. \quad (2.26)$$

Again $\lambda = 0$ is the only term contributing to the sum over λ . For equivalent electrons, with spins anti-parallel, the direct and exchange potentials reinforce. The resulting equation differs from the Hartree–Fock bound-state equation only by a numerical factor multiplying the integrals. Thus this problem provides a good test of the solution of the CEDW2 collision equation since it is the integral terms which are the most difficult to deal with, see (2.14) and (2.19).

The differences between the Hartree–Fock bound-state equation and that derived in the limit of the collision problem arise because the eigenvalue problem which leads to (2.1) and to (2.9) is equivalent to a variational problem in which one eigenfunction is set initially and the other determined when the variation of the expectation value of the Hamiltonian vanishes. However, for equivalent electrons both wavefunctions must be varied. This leads to (2.27) the radial equation for an eigenfunction of He $1s^2$, the Hartree–Fock bound-state equation, in agreement with Froese Fischer (1977).

$$\left(\frac{d^2}{dr^2} + \frac{4}{r}\right)F_\nu^+(r) = \left(\frac{2}{r} \int_0^r (F_\nu^+(r'))^2 dr' - 2 \int_0^r \frac{(F_\nu^+(r'))^2}{r'} dr' + \eta\right)F_\nu^+(r) \quad (2.27)$$

where

$$\eta = 2 \int_0^\infty \frac{(F_\nu^+(r))^2}{r} dr + \frac{\varepsilon}{2} \quad (2.28)$$

and

$$\varepsilon = -(E + F^0) \quad (2.29)$$

where E is still the total energy of the system and

$$F^0 = 4 \int_0^\infty \frac{(F_\nu^+(r))^2}{r} \int_0^r (F_\nu^+(r'))^2 dr' dr \quad (2.30)$$

is the interaction energy.

For comparison with Froese Fischer (1977) we note that we have simplified (2.30) using

$$\int_0^\infty (F_\nu^+(r_1))^2 \int_0^{r_1} \frac{(F_\nu^+(r_2))^2}{r_2} dr_2 dr_1 = \int_0^\infty \frac{(F_\nu^+(r))^2}{r} dr - \int_0^\infty \frac{(F_\nu^+(r_1))^2}{r_1} \int_0^{r_1} (F_\nu^+(r_2))^2 dr_2 dr_1 \quad (2.31)$$

which is easily verified by integrating the LHS by parts with respect to r_1 . The equations obtained in the limit of the collision problem have factors of four instead of two on the RHS of (2.27) and (2.28) and F^0 is replaced by $3F^0$ in (2.29).

Equation (2.27) is non-linear in F_ν^+ and to solve it we make a two-dimensional search varying a_0 , the normalisation coefficient, and η until we satisfy (2.26) and the boundary condition (2.25). For He and the H^- ion the appropriate values for a_0 and η are

$$\begin{aligned} a_0(\text{He}) &= 4.753\,296 & a_0(\text{H}^-) &= 1.393\,82 \\ \eta(\text{He}) &= 5.210\,477 & \eta(\text{H}^-) &= 1.463\,79. \end{aligned}$$

The integrals in (2.28) and (2.30) can now be evaluated numerically to give the following values for ε and F^0 ,

$$\begin{aligned} \varepsilon(\text{He}) &= 3.671\,818 & \varepsilon(\text{H}^-) &= 0.1848 \\ F^0(\text{He}) &= 2.051\,542 & F^0(\text{H}^-) &= 0.7910. \end{aligned}$$

E can then be evaluated from (2.29),

$$E(\text{He}) = -5.723\,360 \quad E(\text{H}^-) = -0.9758$$

in agreement with Froese Fischer (1977).

For collisional ionisation, di-electronic recombination or autoionisation similar changes need to be made to the collision equations in the case of equivalent electrons.

2.4. The ρ matrix and cross sections

Writing

$$\mathcal{F}_{\nu'\nu}^\pm(r) = \zeta_\nu^{-1/2} [\sin(\phi_{\nu'} + \tau_{\nu'}^\pm) \delta_{\nu'\nu} + \cos(\phi_{\nu'} + \tau_{\nu'}^\pm) \rho^\pm(\nu', \nu)] \quad (2.32)$$

we impose the following asymptotic boundary conditions on solutions of (2.1),

$$\mathcal{F}_{\nu'\nu}^\pm(r) \underset{r \rightarrow 0}{\sim} 0 \quad (2.33)$$

$$\phi_\nu \underset{r \rightarrow \infty}{\sim} k_\nu r - \frac{l\pi}{2} + \frac{z}{k_\nu} \ln(2k_\nu r) + \arg \Gamma\left(l + 1 - \frac{iz}{k_\nu}\right) \quad (2.34)$$

and

$$\zeta_\nu^{-1/2} \underset{r \rightarrow \infty}{\sim} k_\nu^{-1/2} \quad k_\nu > 0 \quad (2.35)$$

with

$$\phi_\nu \underset{r \rightarrow \infty}{\sim} (8zr)^{1/2} - (l + \frac{1}{4})\pi \quad (2.36)$$

and

$$\zeta_\nu^{-1/2} \underset{r \rightarrow \infty}{\sim} \left(\frac{r}{2z}\right)^{1/4} \quad k_\nu = 0, z > 0. \quad (2.37)$$

Then (see Seaton 1962),

$$\rho^\pm(\nu', \nu) = - \sum_{\nu''} \int_0^\infty F_{\nu''}^\lambda(r) (V_{\nu'\nu''}^\lambda(r) \pm W_{\nu'\nu''}^\lambda - U_{\nu'\nu''}^\pm) \mathcal{F}_{\nu''\nu}^\pm(r) dr \quad (2.38)$$

is related to the total cross section Q and total collision strength Ω as follows:

$$Q(nl_a \rightarrow n'l'_a) = \frac{1}{4}(Q^+ + 3Q^-) \quad (2.39)$$

where

$$Q^\pm(nl_a \rightarrow n'l'_a) = \frac{\pi \Omega^\pm(n'l'_a, nl_a)}{k_\nu^2(2l_a + 1)} \quad (2.40)$$

and

$$\Omega^\pm(n'l'_a, nl_a) = \sum_{l'l} (2L + 1) |T^\pm(n'l'_a l', nl_a l; L)|^2 \quad (2.41)$$

where we may derive the following relationships (see Eissner and Seaton 1972),

$$T^\pm(\nu, \nu) = 1 + \exp(2i\tau_\nu^\pm) (\mathcal{T}^\pm(\nu, \nu) - 1) \quad (2.42)$$

$$T^\pm(\nu', \nu) = \mathcal{T}^\pm(\nu', \nu) \exp(i\tau_\nu^\pm + i\tau_{\nu'}^\pm) \quad \nu \neq \nu' \quad (2.43)$$

and

$$\mathcal{T}^\pm = \frac{-2i\rho^\pm}{1 - i\rho^\pm} \quad (2.44)$$

2.5. Approximations for ρ

The second Coulomb-exchange distorted-wave (CEDW2) approximation for ρ is given by

$$\sum_\lambda V_{\nu'\nu''}^\lambda = 0 = \sum_\lambda W_{\nu'\nu''}^\lambda \quad \forall \nu'' \neq \nu \quad (2.45a)$$

$$\sum_\lambda U_{\nu'\nu''}^{\lambda\pm} = 0 \quad \forall \nu'' \neq \nu' \quad (2.45b)$$

$$\mathcal{F}_{\nu''\nu}^\pm(r) = F_\nu^\pm(r) \quad (2.45c)$$

where F_ν^\pm is given by (2.7), and

$$U_{\nu\nu}^{\lambda\pm} = V_{\nu\nu}^\lambda \pm \delta_{\lambda_0} W_{\nu\nu}^\lambda \quad \forall \nu, \lambda. \quad (2.45d)$$

The first Coulomb-exchange distorted-wave (CEDW1) approximation for ρ is given by (2.45a)–(2.45c) and by

$$U_{\nu\nu}^{\lambda\pm} = V_{\nu\nu}^\lambda \quad \forall \nu, \lambda. \quad (2.46)$$

The usual Coulomb–Born–Oppenheimer (CBO) approximation is given by (2.45a)–(2.45c) and by

$$U_{\nu\nu}^{\lambda\pm} = 0 \quad \forall \nu, \lambda. \quad (2.47)$$

In this case $\tau^\pm \equiv \mathbf{0}$ and the ρ matrix reduces to the usual \mathbf{R} matrix.

If the expression (2.44) is used, the \mathbf{S} matrix is unitary and (2.44) is denoted approximation II. When coupling is weak we may write

$$\mathcal{T}^\pm \approx -2i\rho^\pm \quad (2.48)$$

\mathbf{S} is not unitary and (2.48) is denoted approximation I. Unless otherwise stated we use approximation II for the CEDW approximations and thus drop the II. For neutral atoms we also drop the prefix Coulomb.

3. Applications to He^+ and H

We use three-state CEDW approximations (1s-2s-2p) which, when l_a couples to l , give rise to a 5×5 matrix for ρ . The matrix elements may be classified as in Burgess *et al* (1970).

3.1. Long-range integrals

The numerical evaluation of ρ -matrix elements (2.38) involving a 2p state are complicated by long-range, slowly convergent, integrals (see Burgess *et al* (1970)).

For $k_\nu \neq k_{\nu'}$ we can use the amplitude-phase method of Burgess and Sheorey (1974). For hydrogenic atoms we must also deal with the case $k_\nu = k_{\nu'}$. Considering the long-range part of the integral only, from (2.45), (2.24) and (2.38) and in the notation of Burgess and Sheorey (1974), we have to evaluate integrals of the form,

$$I = I^+ - I^- \quad (3.1)$$

where

$$I^\pm = \int \alpha_\pm \cos \phi_\pm d\phi_\pm \quad (3.2)$$

$$\phi_\pm = \phi_2 \pm \phi_1 \quad (3.3)$$

$$\alpha_\pm = \frac{1}{2} \frac{\zeta_1^{-1/2} \zeta_2^{-1/2} \zeta_\pm^{-1}}{r^{\lambda+1}} \quad (3.4)$$

and

$$\zeta_\pm = \zeta_2 \pm \zeta_1. \quad (3.5)$$

I^+ can still be evaluated using the amplitude-phase method. For

$$I^- = \frac{1}{2} \int_{\mathcal{R}} \zeta_1^{-1/2} \zeta_2^{-1/2} \frac{\cos \phi_-}{r^{\lambda+1}} dr \quad (3.6)$$

we make the substitution

$$I_{\lambda-1}(r) = c \int_r^\infty \frac{dr'}{r'^{\lambda+1} [k_\nu^2 + 2z/r' - l(l+1)/r'^2]^{1/2}} \quad (3.7)$$

where $l = \frac{1}{2}(l_1 + l_2)$, to leave the integrand slowly varying over a finite range of integration. For $l \neq 0$, writing

$$a^2 = k_\nu^2/l(l+1) \quad b^2 = 2z/l(l+1) \quad c^2 = l(l+1) \quad (3.8)$$

we have

$$I_\lambda(r) = a\delta_{\lambda 1} - \left(a^2 + \frac{b^2}{r} - \frac{1}{r^2}\right)^{1/2} \frac{1}{\lambda r^{\lambda-1}} \\ + \frac{(2\lambda-1)}{2\lambda} b^2 I_{\lambda-1} + \frac{(\lambda-1)}{\lambda} a^2 I_{\lambda-2} \quad \lambda > 0 \quad (3.9)$$

with

$$I_0(r) = \sin^{-1} \left(\frac{2r^{-1} - b^2}{(4a^2 + b^4)^{1/2}} \right) + \sin^{-1} \left(\frac{b^2}{(4a^2 + b^4)^{1/2}} \right). \quad (3.10)$$

For $l = 0$, $z \neq 0$, writing

$$c^2 = 2z \quad \text{and} \quad d^2 = \frac{2k_v^2}{z} \quad (3.11)$$

we have

$$I_\lambda(r) = \left(d^2 + \frac{4}{r}\right)^{1/2} \sum_{n=0}^{\lambda} \frac{(-1)^n d^{2n} (\lambda!)^2 (2\lambda - 2n)!}{(2\lambda + 1)! [(\lambda - n)!]^2 r^{\lambda - n}} - (-1)^\lambda \frac{d^{2\lambda + 1} (\lambda!)^2}{(2\lambda + 1)!}. \quad (3.12)$$

3.2. Contributions to the collision strength from large values of angular momentum

For the dipole transitions, partial collision strengths, $\Omega_{l' l}$, were evaluated up to $l = l_0$ in the particular approximation required and the sum from $l = l_0 + 1$ to ∞ was evaluated using the analytic formula of Burgess (1974). In the case of the CB and CBO approximations, using this more powerful approach to completing the sum as opposed to the geometric approach used by Burgess *et al* (1970) we were able to confirm their results for the $1s \rightarrow 2p$ total collision strength but not those of McDowell *et al* (1975, p 1059, table 1).

The CBI, CBII, CBOI, CBOII, \mathbf{R} matrix, partial and total collision strengths for $Z = 2$, ∞ in tables 1–10 of Burgess *et al* (1970) were confirmed.

4. Results

We are interested in comparing our CEDW results with the three-state close-coupling and CBOII calculations since they are the closest relations to the CEDW approximations and so provide the most insight into their behaviour. We also wish to compare our CEDW results with experiment.

Thus we present graphs of total excitation cross sections plotted against the incident electron energy in Rydbergs and tables of scaled CEDW collision strengths.

4.1. He^+

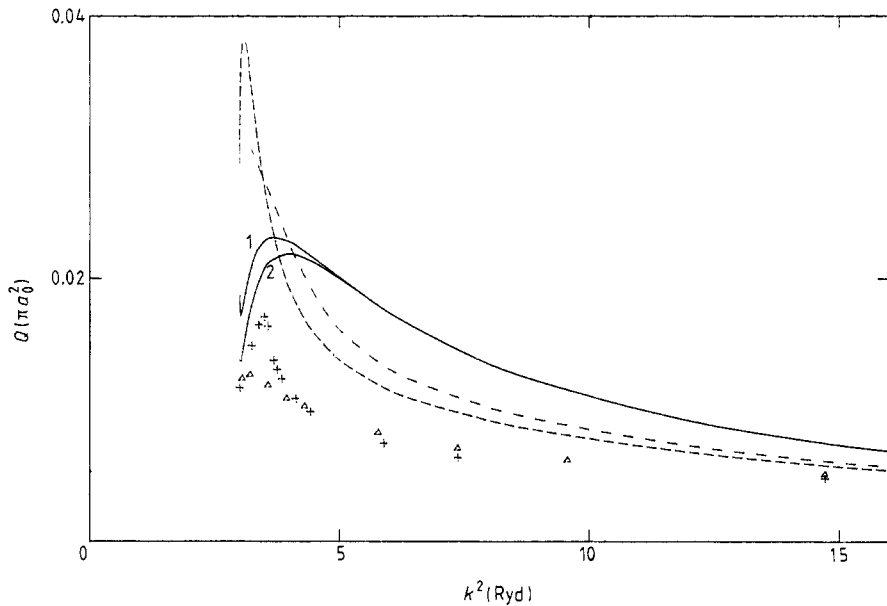
Total scaled collision strengths for electron impact excitation of the $1s \rightarrow 2s$ transition in He^+ , at selected energies, calculated in the CEDW1 and CEDW2 approximations discussed earlier are given in table 1. + and – refer to singlet and triplet contributions respectively ($Z = 2$).

In figure 1 we compare our CEDW cross sections for the $1s \rightarrow 2s$ transition with the three-state ($1s-2s-2p$) close-coupling (3CC) calculations including exchange of Burke *et al* (1964), the CBOII approximation and the experiments of Dance *et al* (1966) and Dolder and Peart (1973).

The CEDW2 cross section is more than 50% below the extrapolated 3CC value at threshold and in good agreement, presumably fortuitous, with both experiments. It is also nearly 50% below the results (not shown), at threshold, of Burke and Taylor (1969) and Morgan (1979). The CEDW curves merge at about 5 Ryd and tend to the Born approximation at high energies. Comparison of the CBOII and CEDW curves shows that treating the short-range direct potential term exactly results in a major reduction of the cross section at threshold while inclusion of the exchange potential in the same way produces a further, although smaller, reduction. Comparison of the

Table 1. Total collision strengths for $\text{He}^+ 1s \rightarrow 2s$. Approximation II.

k^2/Z^2	CEDW1			CEDW2		
	$\frac{1}{4}Z^2\Omega^+$	$\frac{3}{4}Z^2\Omega^-$	$Z^2\Omega$	$\frac{1}{4}Z^2\Omega^+$	$\frac{3}{4}Z^2\Omega^-$	$Z^2\Omega$
0.75	0.1645	0.0598	0.2242	0.1067	0.0588	0.1655
0.80	0.1494	0.1109	0.2603	0.1136	0.1078	0.2214
0.90	0.1891	0.1440	0.3330	0.1637	0.1421	0.3059
1.00	0.2034	0.1620	0.3654	0.1894	0.1615	0.3510
1.10	0.2084	0.1755	0.3839	0.2017	0.1756	0.3772
1.25	0.2092	0.1917	0.4008	0.2078	0.1919	0.3997
1.50	0.2043	0.2124	0.4167	0.2058	0.2125	0.4182
2.00	0.1904	0.2405	0.4309	0.1927	0.2401	0.4328
3.00	0.1692	0.2711	0.4403	0.1708	0.2705	0.4413
4.00	0.1563	0.2872	0.4436	0.1574	0.2867	0.4441

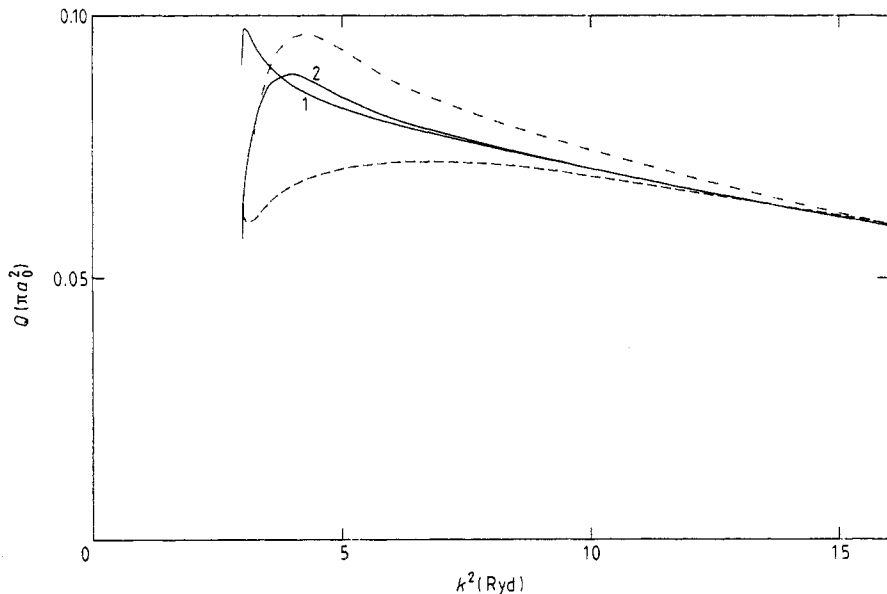
**Figure 1.** Excitation cross section for the $1s \rightarrow 2s$ transition in He^+ . —, CEDW1 and CEDW2; - - - -, CBOII; ·····, 3CC (Burke *et al* 1964). +, experimental points from Dance *et al* (1966); Δ , from Dolder and Peart (1973).

relative singlet and triplet contributions to the total cross section in the CEDW and 3CC approximations shows that they behave in the same manner in that the singlet dominates to about 1.5 Ryd and the triplet from there on. The CBOII behaviour is completely different in that the triplet dominates at all energies. Results for the $1s \rightarrow 2p$ transition are presented in table 2.

In figure 2 we compare our CEDW cross sections for the $1s \rightarrow 2p$ transition with the three-state close-coupling (3CC) calculations of Burke *et al* (1964) and the CBOII approximation.

Table 2. Total collision strengths for He⁺ 1s → 2p. Approximation II.

k^2/Z^2	CEDW1			CEDW2		
	$\frac{1}{4}Z^2\Omega^+$	$\frac{3}{4}Z^2\Omega^-$	$Z^2\Omega$	$\frac{1}{4}Z^2\Omega^+$	$\frac{3}{4}Z^2\Omega^-$	$Z^2\Omega$
0.75	0.9490	0.1391	1.088	0.5510	0.1405	0.6915
0.80	1.048	0.1704	1.219	0.8125	0.1738	0.9863
0.90	1.045	0.2473	1.293	1.007	0.2508	1.258
1.00	1.039	0.3492	1.388	1.071	0.3518	1.423
1.10	1.029	0.4607	1.489	1.076	0.4625	1.539
1.25	1.013	0.6318	1.645	1.054	0.6330	1.687
1.50	0.9972	0.9083	1.906	1.020	0.9093	1.930
2.00	1.001	1.396	2.397	1.008	1.397	2.405
3.00	1.073	2.136	3.209	1.073	2.138	3.211
4.00	1.161	2.674	3.835	1.161	2.675	3.836

**Figure 2.** Excitation cross section for the 1s → 2p transition in He⁺. —, CEDW1 and CEDW2; ----, CBOII; - · - ·, 3CC (Burke *et al* 1964).

All theoretical results are in broad agreement with the only reported experimental results to date (Dashchenko *et al* 1975), which are subject to large errors. The CEDW2 curve agrees with the projected 3CC value at threshold.

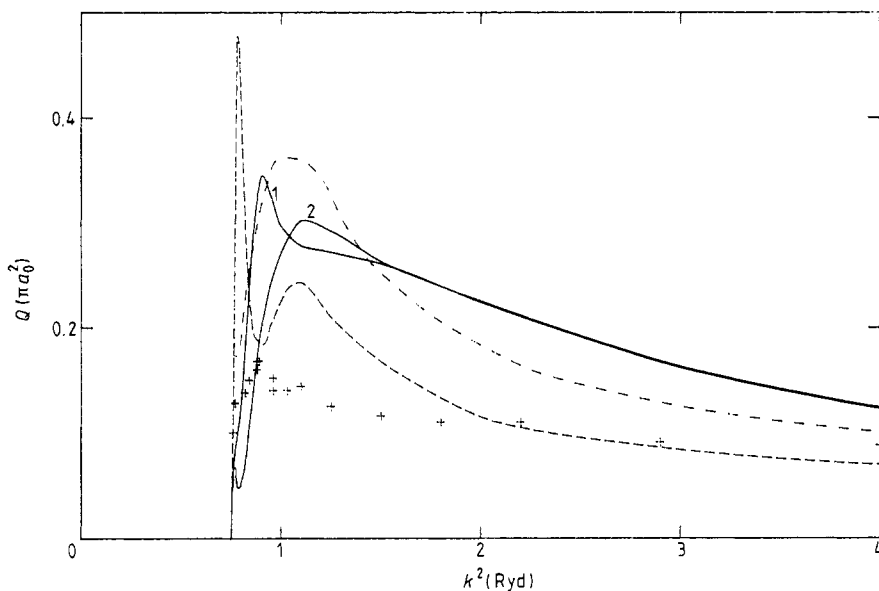
4.2. H

Total collision strengths for the 1s → 2s transition in H at selected energies are given in table 3.

In figure 3 we compare our EDW cross sections for the 1s → 2s transition with the three-state (1s–2s–2p) close-coupling (3CC) calculations of Burke *et al* (1963, 1967), the BOII approximation and the experiment of Kauppila *et al* (1970).

Table 3. Total collision strengths for $\text{H } 1s \rightarrow 2s$. Approximation II.

k^2	EDW1			EDW2		
	$\frac{1}{4}\Omega^+$	$\frac{3}{4}\Omega^-$	Ω	$\frac{1}{4}\Omega^+$	$\frac{3}{4}\Omega^-$	Ω
0.75001	0.0005	0.0006	0.0010	0.0003	0.0006	0.0008
0.80	0.0854	0.0153	0.1007	0.0274	0.0150	0.0424
0.90	0.1924	0.1175	0.3098	0.0637	0.1136	0.1774
1.00	0.1362	0.1607	0.2969	0.1172	0.1542	0.2713
1.10	0.1271	0.1783	0.3055	0.1574	0.1744	0.3318
1.25	0.1427	0.1977	0.3404	0.1665	0.1988	0.3653
1.50	0.1669	0.2250	0.3919	0.1660	0.2282	0.3943
2.00	0.1841	0.2649	0.4489	0.1829	0.2672	0.4500
3.00	0.1807	0.3052	0.4858	0.1826	0.3056	0.4882
4.00	0.1707	0.3231	0.4937	0.1725	0.3229	0.4954

**Figure 3.** Excitation cross section for the $1s \rightarrow 2s$ transition in H . —, EDW1 and EDW2; ---, BOII; - · - ·, 3CC (Burke *et al* 1963, 1967). +, experimental points from Kauppila *et al* (1970).

The EDW1 results are poor below 1 Ryd and illustrate the importance of treating the exchange distorting potential exactly. The EDW curves merge at about 1.5 Ryd and tend to the Born approximation at high energies. Comparison of the EDW curves with the BOII curve below 1.1 Ryd again shows the importance of including the direct distorting potential exactly. The behaviour of the relative singlet and triplet contributions to the cross sections in the EDW and 3CC approximations is the same and differs from that of the BOII approximation. The results of Callaway *et al* (1975), not shown, are in good agreement with the experiment of Kauppila *et al* (1970) over the energy range 0.75 to 2.25 Ryd.

Results for the $1s \rightarrow 2p$ transition are presented in table 4.

Table 4. Total collision strengths for H $1s \rightarrow 2p$. Approximation II.

k^2	EDW1			EDW2		
	$\frac{1}{4}\Omega^+$	$\frac{3}{4}\Omega^-$	Ω	$\frac{1}{4}\Omega^+$	$\frac{3}{4}\Omega^-$	Ω
0.75001	0.0028	0.0021	0.0048	0.0012	0.0020	0.0032
0.80	0.1566	0.0152	0.1718	0.1464	0.0153	0.1617
0.90	0.4286	0.1590	0.5876	0.2025	0.1608	0.3634
1.00	0.5884	0.2329	0.8213	0.3352	0.2369	0.5722
1.10	0.6755	0.2883	0.9638	0.5022	0.2922	0.7944
1.25	0.7467	0.4056	1.152	0.7175	0.4073	1.125
1.50	0.7940	0.6411	1.435	0.8407	0.6415	1.482
2.00	0.8473	1.105	1.953	0.8674	1.107	1.974
3.00	0.9517	1.857	2.809	0.9529	1.860	2.813
4.00	1.058	2.418	3.475	1.057	2.421	3.477

In figure 4 we compare our EDW cross sections for the $1s \rightarrow 2p$ transition with the three-state close-coupling (3CC) calculations of Burke *et al* (1963, 1967), the BOII approximation and the experiment of McGowan *et al* (1969).

Again the behaviour of the triplet and singlet contributions to the cross section is the same in the EDW and 3CC approximations and differs from the BOII approximation. The results of Callaway *et al* (1975), not shown, are in good agreement with the experiment of McGowan *et al* (1969) over 0.75 to 2.25 Ryd.

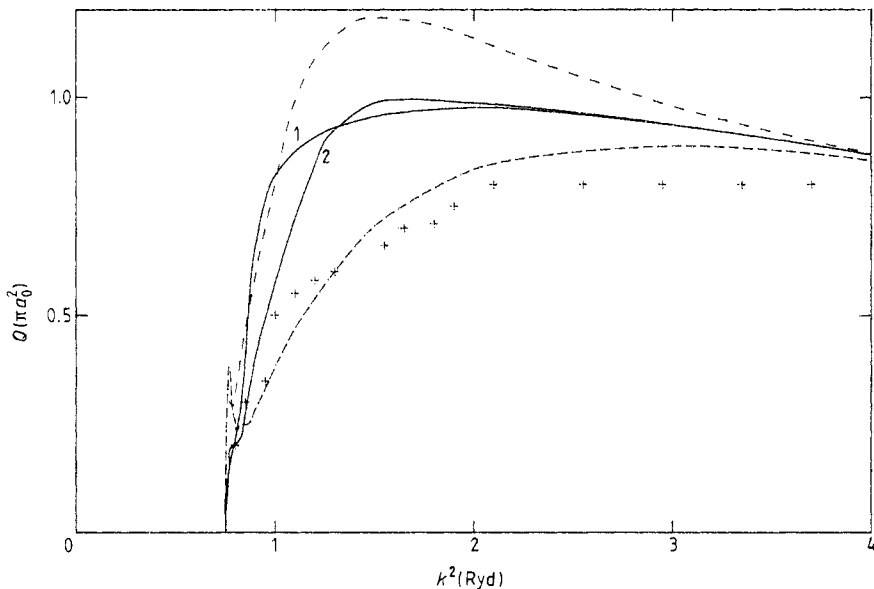


Figure 4. Excitation cross section for the $1s \rightarrow 2p$ transition in H. —, EDW1 and EDW2; ---, BOII; - · - ·, 3CC (Burke *et al* 1963, 1967). +, experimental points from McGowan *et al* (1969).

5. Conclusions

Bearing in mind that the degeneracy of the 2s and 2p states in hydrogenic atoms is unfavourable to the distorted-wave approach and that the convergence of the close-coupling expansion is poor for H, we can draw the following conclusions.

(i) Distortion of the free electron by direct and exchange potentials is important for all channels at low energies;

(ii) The CEDW2 approximation, for He^+ and H, gives satisfactory agreement with the three-state close-coupling approximation for the $1s \rightarrow 2s$ transition and fairly good agreement for the $1s \rightarrow 2p$ transition together with a significant reduction in computing time;

(iii) Future work on the inclusion into our trial wavefunctions of coupling to the 2p state, directly, and other p states, indirectly (polarisation), is desirable.

(iv) The simplicity of the CEDW2 approximation as it stands and the results it gives are sufficiently promising to justify further development to investigate the excitation of complex systems, where we no longer have degeneracy of the nl and nl' states, and ionisation.

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