Electron impact excitation of He

N R Badnell

Department of Applied Mathematics and Theoretical Physics, Silver Street, Cambridge
CB3 9EW, England

Abstract. A new approximation is developed for electron collisions with two-electron atoms and is applied to the excitation of He. The core orbital is taken to be that given by equivalent frozen $1s^2$ orbitals and the valence wavefunction is taken to be that given by a Hartree or Hartree–Fock frozen-core approximation. The resulting orthogonality of the core and valance wavefunctions enables the exact three-electron collision equations to be simplified to a form similar to that for a two-electron problem. The explicit dependence on the core wavefunction being removed, the effect of choosing a non-equivalent core is investigated within the Hartree frozen-core approximation. The collision equations are solved using a number of five-state exchange distoited-wave (EDW) approximations which include various multipole exchange distorting potentials exactly.

We calculate total collision strengths for all transitions between the 1^1S, 2^3S, 2^1S, 2^3P and 2^1P states of He for incident electron energies from just above threshold up to 15.0 Ryd. Using a screened hydrogenic Hartree frozen core, adjusted to lead to the exact $1^1S \to 2^1P$ line strength, and the EDW2 approximation, which includes the dominant monopole exchange distorting potential exactly, this rather simple, but physically motivated, approach gives good results in general and is much faster to apply than the more elaborate R-matrix approximation. It should prove useful for the calculation of reaction rates for He-like ions in the future.

1. Introduction

The knowledge of reaction rates for electron collisions with He and He-like ions is of particular importance in the study of laboratory and astrophysical plasmas. The close-coupling approximation including the first five atomic states (1^1S, 2^3S, 2^1S, 2^3P, 2^1P) could in theory provide much information; however, in practice it has proved difficult to apply widely. The first calculations for He, carried out over a narrow energy range (see Burke *et al* 1969, Oberoi and Nesbet 1973, Berrington *et al* 1975), were somewhat unreliable (see Fon *et al* (1981) for a detailed discussion). Fon *et al* (1979, 1980, 1981) have carried out a five-state close-coupling calculation for He using the R-matrix method, but the bound–bound terms in their eigenfunction expansion gave rise to pseudo-resonances and they were unable to give results over a wide range of energies. Bhadra *et al* (1979) carried out a standard five-state close-coupling (5CC) calculation, i.e. without bound–bound terms, and gave results for transitions from the ground state, those for the spin-allowed transitions being poor. Willis and McDowell (1981) have investigated a number of close-coupling approximations for the $1^1S \to 2^1S$ and $1^1S \to 2^1P$ transitions using both physical states and pseudo-states. The large amount of computing resources required by the close-coupling approximation for the three-electron system makes it unsuitable for the widespread calculation of reaction rates.

The application to He of the distorted-wave approximation, and variants thereof, has mainly been confined to spin-allowed transitions (see e.g. Scott and McDowell 1975, 1976, Flannery and McCann 1975) since the treatment of exchange as a perturbation gives poor results for spin-forbidden transitions (see however Tully (1978) and Baluja and McDowell (1979) for the $1^1S \rightarrow 2^3S$ transition) since these can only take place through electron exchange, on neglecting spin–orbit interaction. For a comprehensive review of the excitation of He at intermediate energies, both theoretical and experimental, see Bransden and McDowell (1978).

In this paper we develop an approximation for electron collisions with two-electron atoms and compare our results for the excitation of He with other theoretical results and with experiment, for transitions from the ground state. We also provide results for transitions between the $n = 2$ states, there being few others in the literature. Our approach is based on two approximations, both of which are made on physical grounds. The first is that the use of equivalent electron orbitals provides a good description of the ground state and that the excited valence wavefunctions are relatively insensitive to the core used. This enables us to reduce the exact three-electron collision equations to a form similar to those for a two-electron problem. The second is that spin-forbidden transitions can be calculated using the distorted-wave approximation if we include the exchange distorting potentials exactly. This reduces the collision equations to a set of uncoupled integro-differential equations.

This work is part of a programme to calculate excitation rates and di-electronic recombination rates for a wide range of ions of astrophysical interest. To do this we first require a fast approximation for the collision problem which is reliable at low energies. In an earlier paper (see Badnell 1983a, hereafter referred to as I) we developed two forms of exchange distorted-wave (EDW) approximation and tested them on the excitation of He$^+$ and H. A third variant was also investigated (see Badnell 1983b, hereafter referred to as II). For non-hydrogenic atoms we must also approximate the atomic structure—which can lead to appreciable errors. This paper provides a simple approach for He-like ions.

In § 2 we develop the required mathematical theory for our approach and in § 3 we discuss possible choices for the bound-state wavefunctions. In § 4 we deal with an arbitrariness that arises in some of our free wavefunctions within this formulation. In § 5 we present our results and compare them with those of other theoretical models, in particular the close-coupling approximation, and with experiment where possible. We use atomic units throughout except for energies which are in Rydbergs.

2. Theory

We take the Hamiltonian H for the electron–He atom system to be of the form

$$H = -\tfrac{1}{2}\left(\nabla_1^2 + \nabla_2^2 + \nabla_3^2 + \frac{2Z}{r_1} + \frac{2Z}{r_2} + \frac{2Z}{r_3} - \frac{2}{r_{12}} - \frac{2}{r_{13}} - \frac{2}{r_{23}} \right) \tag{2.1}$$

where z is the nuclear charge. We take the wavefunction $\Psi_{\nu''}^{LS}$ for this system to be of the form

$$\Psi_{\nu''}^{LS}(1, 2, 3) = \frac{1}{\sqrt{3}} \sum_\nu [\Psi_{\nu\nu''}^{LS}(\overline{12}, 3) + \Psi_{\nu\nu''}^{LS}(\overline{23}, 1) + \Psi_{\nu\nu''}^{LS}(\overline{31}, 2)] \tag{2.2}$$

(see e.g. Burke *et al* 1969) which is an expansion in terms of unperturbed atomic wavefunctions and also of partial waves for the free electron. ν'' denotes the initial state of the system and LS are the total orbital and spin angular momenta both separately conserved. $\nu = nl_a s_a l$ where $nl_a s_a$ are quantum numbers describing the atom and l is the orbital angular momentum of the free electron with spin $\frac{1}{2}$. 1, 2, 3 represent the space and/or spin coordinates of the three electrons (r_i, σ_i), $i = 1, 2, 3$.

We may write $\Psi^{LS}_{\nu\nu''}$ in terms of its space and spin components thus,

$$\Psi^{LS}_{\nu\nu''}(\overline{12}, 3) = \phi^{LS}_{\nu\nu''}(\overline{12}, 3)\chi^{SM_S}_{s_a 1/2}(\overline{12}, 3) \tag{2.3}$$

where $\phi^{LS}_{\nu\nu''}$ is given by

$$\phi^{LS}_{\nu\nu''}(\overline{12}, 3) = \sum_{m_{l_a} m_l} C^{l_a\, l\, L}_{m_{l_a} m_l M_L}\psi^{s_a}_{nl_a m_{l_a}}(r_1, r_2)\mathscr{F}^{LS}_{\nu\nu''}(r_3)\, Y_{lm_l}(\hat{r}_3)/r_3 \tag{2.4}$$

where $\psi^{s_a}_{nl_a m_{l_a}}$ is the spatial part of the atomic wavefunction and

$$\psi^{s_a}_q(r_1, r_2) = (-1)^{s_a}\psi^{s_a}_q(r_2, r_1) \tag{2.5}$$

where $q = nl_a m_{l_a}$. $\mathscr{F}^{LS}_{\nu''\nu}$ is the radial function of the free electron and $C^{l_a\, l\, L}_{m_{l_a} m_l M_L}$ is a vector-coupling coefficient. The spin component $\chi^{SM_S}_{s_a 1/2}$ is given by

$$\chi^{SM_S}_{s_a 1/2}(\overline{12}, 3) = \sum_{m_{s_a} m_{1/2}} C^{s_a\, 1/2\, S}_{m_{s_a} m_{1/2} M_S}\chi^{s_a}_{m_{s_a}}(1, 2)\chi^{1/2}_{m_{1/2}}(3) \tag{2.6}$$

where

$$\chi^{s_a}_{m_{s_a}}(1, 2) = \sum_{\mu_1 \mu_2} C^{1/2\, 1/2\, S}_{\mu_1 \mu_2 M_S}\,\delta_{\mu_1 \sigma_1}\,\delta_{\mu_2 \sigma_2} \tag{2.7}$$

and

$$\chi^{1/2}_{m_{1/2}}(3) = \delta_{m_{1/2} \sigma_3}, \qquad m_{1/2} = \pm 1/2. \tag{2.8}$$

For each final state of the system described by ν' we impose

$$\sum_{\sigma_i} \int {}^{F}\phi^{LS\dagger}_{\nu'\nu''}(\overline{12}, 3)\chi^{SM_S\dagger}_{s_a 1/2}(\overline{12}, 3)(H - \tfrac{1}{2}E)\Psi^{LS}_{\nu''}(1, 2, 3)\, dr_1\, dr_2\, d\hat{r}_3 = 0 \tag{2.9}$$

where ${}^{F}\phi$ may be written in terms of ϕ thus,

$$\phi^{LS}_{\nu'\nu''}(\overline{12}, 3) = {}^{F}\phi^{LS}_{\nu'\nu''}(\overline{12}, 3)\mathscr{F}^{LS}_{\nu'\nu''}(r_3)/r_3 \tag{2.10}$$

and E is the total energy of the system. On substituting (2.2)–(2.8) into (2.9) we may perform the sum over the spin coordinates to get

$$\sum_{\nu} \int {}^{F}\phi^{LS\dagger}_{\nu'\nu''}(\overline{12}, 3)(H - \tfrac{1}{2}E)(\phi^{LS}_{\nu\nu''}(\overline{12}, 3)\,\delta_{s'_a s_a} + \phi^{LS}_{\nu\nu''}(\overline{32}, 1)d^S_{s'_a s_a})\, dr_1\, dr_2\, d\hat{r}_3 = 0 \tag{2.11}$$

where

$$d^S_{s'_a s_a} = 2[(2s_a + 1)(2s'_a + 1)]^{1/2}\begin{Bmatrix} \frac{1}{2} & \frac{1}{2} & s_a \\ \frac{1}{2} & S & s'_a \end{Bmatrix} \tag{2.12}$$

and { } is the Wigner 6-*j* symbol which is obtained on summing the vector-coupling coefficients using equation (6.1.5) of Edmonds (1957). Explicitly

$$d^{1/2}_{00} = -1 \qquad d^{1/2}_{01} = \sqrt{3} = d^{1/2}_{10} \qquad d^{1/2}_{11} = 1 \qquad d^{3/2}_{11} = -2.$$

We may approximate $\psi_q^{s_a}$ in terms of one-electron wavefunctions thus,

$$\psi_q^{s_a}(\mathbf{r}_1, \mathbf{r}_2) = \frac{1}{\sqrt{2N}}\left(\frac{P_{nl_a}(r_1)P_C(r_2)}{\sqrt{4\pi r_1 r_2}}Y_{l_a m_{l_a}}(\hat{\mathbf{r}}_1) + 1 \leftrightarrow 2\right) \tag{2.13}$$

and we assume that P_C is frozen, i.e. independent of P_{nl_a}, thus $\psi_q^{s_a}$ satisfies the usual orthogonality condition. We take P_C, the radial function for the core electron, to satisfy

$$(\mathrm{d}^2/\mathrm{d}r^2 + 2Z/r - {}^CU(r) - \varepsilon_C)P_C(r) = 0 \tag{2.14}$$

where ε_C is the diagonal (or orbital) energy parameter of the core electron and ${}^CU(r)$ is to be defined below. We take P_{nl_a}, the radial function for the valence electron, to satisfy

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l_a(l_a+1)}{r^2} + \frac{2Z}{r} - {}^{FC}V(r) - \varepsilon_{nl_a}\right)P_{nl_a}(r) = 0 \tag{2.15}$$

where ${}^{FC}V$ is given by

$$^{FC}V(r) = \frac{2}{r}\int_0^r P_C^2(r')\,\mathrm{d}r' + 2\int_r^\infty \frac{P_C^2(r')}{r'}\,\mathrm{d}r'. \tag{2.16}$$

We now assume P_C to be equivalent to P_{1s}, i.e. ${}^CU \equiv {}^{FC}V$, thus P_C is orthogonal to P_{2s}, and $N = 1 + \delta_{n1}$. It is not necessary that the excited valence radial function (2.15) be given by a non-exchange approximation, however it is the form we consider in detail later.

Using (2.13)–(2.16) the collision equations (2.11) now reduce straightforwardly to

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{l'(l'+1)}{r^2} + \frac{2z}{r} - {}^{FC}V(r) + k_\nu^2\right)\mathscr{F}_{\nu'\nu''}^{LS}(r) = \sum_{\nu\lambda}(b_{\nu'\nu}V_{\nu'\nu}^{\lambda L}(r) + h_{\nu'\nu}^S\,W_{\nu'\nu}^{\lambda L})\mathscr{F}_{\nu\nu''}^{LS}(r) \tag{2.17}$$

where $z = Z - 1$,

$$h_{\nu'\nu}^S = \tfrac{1}{2}(1 + |\delta_{n'1} - \delta_{n1}|)^{1/2}(1 + \delta_{n1}\,\delta_{n1})d_{s_a's_a}^S \tag{2.18a}$$

and

$$b_{\nu'\nu} = (1 + |\delta_{n'1} - \delta_{n1}|)^{1/2}\,\delta_{s_a s_a'}. \tag{2.18b}$$

V^λ and W^λ are as in paper I except that $E_{n'}$ of (I2.3) is replaced by $-\varepsilon_{n'l_a'}$. Also the energy of the free electron k_ν^2 is now related to E by

$$E = k_\nu^2 - \varepsilon_C - \varepsilon_{nl_a} - F^0 \tag{2.19}$$

where F^0 is given by

$$F^0 = \int_0^\infty {}^CU(r)P_C^2(r)\,\mathrm{d}r \tag{2.20}$$

and $\varepsilon_C + F^0$ is the sum of the kinetic and potential energies of the core electron. No further approximations are required to reduce the direct term in (2.11) to the form given in (2.17), the same being true for the exchange term when q and q' both describe the ground state. However, when q and/or q' describe an excited state we approximate the exchange term

$$\sum_\nu \int {}^F\phi_{\nu'\nu''}^{LS\dagger}(\overline{12}, 3)(H - \tfrac{1}{2}E)\phi_{\nu\nu''}^{LS}(\overline{32}, 1)d_{s_a's_a}^S\,\mathrm{d}\mathbf{r}_1\,\mathrm{d}\mathbf{r}_2\,\mathrm{d}\hat{\mathbf{r}}_3 \tag{2.21}$$

in (2.11) by

$$\sum_\nu \int {}^F\phi_{\nu'\nu''}^{LS\dagger}(\overline{12}, 3)\left(\tfrac{1}{2}\nabla_2^2 + \frac{Z}{r_2} + \frac{1}{r_{13}} - \tfrac{1}{2}(k_\nu^2 + \varepsilon_{n'l'_n} + \varepsilon_C + F^0)\right)\phi_{\nu\nu''}^{LS}(\overline{32}, 1)d_{s_a's_a}^S \, d\boldsymbol{r}_1 \, d\boldsymbol{r}_2 \, d\hat{\boldsymbol{r}}_3. \tag{2.22}$$

The two forms are identical (generally) only when ψ_q is a solution of the two-electron Schrödinger equation and this approximation is similar to the approximation for the exchange term made by Burke *et al* (1969), and the main effect can be expected to be on the ^{2}S partial wave; we discuss this further in § 4. For transitions between excited states, we have also neglected terms which represent exchange between the core and free electrons. We note that, due to the orthogonality of the one-electron atomic radial functions, this only affects the $2^3L \rightarrow 2^3L, 2^1L$ transitions. These assumptions enable us to retain the important properties of the three-electron problem while reducing the collision equations to the same form as those for a two-electron problem, which were dealt with in paper I. Such a simplification has considerable advantages in terms of computing resources. The equations (2.17) may be solved in the EDW1,2 approximations, as defined in I, using the methods described in that paper. The solution in the EDW3 approximation of II is similar and details are given in an appendix to the present paper.

In the EDW1 approximation the free electron is subject to all the direct distorting potentials, see (I2.46) with

$$U_{\nu\nu}^{\lambda LS} = V_{\nu\nu}^{\lambda L} + {}^{FC}V\delta_{\lambda 0}. \tag{2.23}$$

In the EDW2 approximation the free electron is additionally distorted by a non-local monopole exchange potential, see (I2.45d) where

$$U_{\nu\nu}^{\lambda LS} = {}^{FC}V\delta_{\lambda 0} + V_{\nu\nu}^{\lambda L} + \delta_{\lambda 0}h_{\nu\nu}^S W_{\nu\nu}^{\lambda L}. \tag{2.24}$$

In the EDW3 approximation the free electron is distorted by the lowest multipole exchange potential, as well as by all the direct terms, see (I2.45d) and the appendix of the present paper with

$$U_{\nu\nu}^{\lambda LS} = {}^{FC}V\delta_{\lambda 0} + V_{\nu\nu}^{\lambda L} + \delta_{\lambda\lambda_m}h_{\nu\nu}^S W_{\nu\nu}^{\lambda L} \tag{2.25}$$

where $\lambda_m = |l_a - l|$ and we restrict λ_m to $\lambda_m \lesssim 3$.

The T matrix, which may be obtained in these approximations as discussed in paper I, is related to the total collision strength Ω by

$$\Omega(n'l'_a s'_a, nl_a s_a) = \tfrac{1}{2}\sum_{l'lLS}(2L+1)(2S+1)|T(\nu', \nu)_{LS}|^2. \tag{2.26}$$

The total cross section Q is given by

$$Q(nl_a s_a \rightarrow n'l'_a s'_a) = (\pi/k_\nu^2)\Omega(n'l'_a s'_a, nl_a s_a)/(2l_a + 1)(2s_a + 1). \tag{2.27}$$

We note that the definition (2.26) differs slightly from that used in I which, as is common practice for one-electron atoms, included the initial spin degeneracy of the atom in the denominator on the RHS.

3. Bound-state wavefunctions

Elaborate configuration-interaction atomic wavefunctions have been developed for use in the collision problem (see Berrington *et al* 1975). However, as discussed in § 1, we are interested in a fast approximation and thus look for simple wavefunctions that have direct physical interpretation.

3.1. The Hartree frozen-core approximation

Since equations (2.14) and (2.15) describe a frozen form of the Hartree self-consistent field approximation, as first solved by Wilson and Lindsay (1935), we denote their use as the Hartree frozen-core (HFC) approximation. As noted previously we may use a non-exchange (Hartree) or exchange (Hartree–Fock) frozen-core approximation for the valence electron. However, the Hartree frozen core is faster to use since the free wavefunctions corresponding to singlet and triplet atomic states are, in this case, the same for most partial waves. Also it is easier to use with different cores compared with the Hartree–Fock frozen-core approximation. So, in this paper, we investigate the results of our method with the Hartree frozen-core approximation.

The explicit dependence on the core radial function being removed, it is no longer necessary to take $P_C \equiv P_{1s}$. Our choice of core and thus valence wavefunctions is determined by our choice of ^CU in (2.14). We consider two cases (a) and (b).

(a) We take $^CU \equiv {}^{FC}V$; then $P_C \equiv P_{1s}$ is the (restricted) Hartree–Fock radial function for He $1s^2$ and, using (2.20), F^0 is given by

$$F^0 = 4 \int_0^\infty \frac{P_C^2(r)}{r} \int_0^r P_C^2(r')\, \mathrm{d}r'\, \mathrm{d}r \tag{3.1}$$

which is the interaction energy between the two ground-state electrons, in agreement with (I2.30). This is the form that we assumed for P_C and P_{nl_a} in our reduction of the collision equations.

(b) We take

$$^CU(r) = 2(Z - \zeta)/r \tag{3.2}$$

then

$$P_C(r) = 2\zeta^{3/2} r\, \mathrm{e}^{-\zeta r} \tag{3.3}$$

is a screened hydrogenic (SH) radial function and F^0 is given by

$$F^0 = 2(Z - \zeta)\zeta \tag{3.4}$$

which is an approximation for the ground-state interaction energy. We may treat ζ as a variable parameter and adjust it, for example, to give the exact value for the quantity $\sigma^2(1^1S \to 2^1P)$, which is related to the oscillator strength (see § 3.2), the appropriate value being $\zeta = 1.4289$.

The Hartree–Fock frozen-core approximation for He is often used in the collision problem (see e.g. Flannery and McCann 1975, Tully 1978); the ground-state electrons are not restricted to be equivalent and the core is taken to be that of He$^+$ 1s. This means that the resulting radial equations are the same as those obtained by considering the He$^+$ + e$^-$ collision problem, in the EDW3 approximation, as a bound-state problem; compare those of Cohen and Kelly (1966) and the appendix of this paper. On comparing radial functions for He in the approximations described above we find that

the diagonal energy parameter is a good guide to their quality. In table 1 we compare the diagonal energy parameters for the valence radial functions in the approximations described above, as well as those from the multiconfiguration Hartree–Fock (MCHF) approximation of Froese Fischer (1977) which can be regarded as 'exact' for our purposes.

Table 1. Diagonal energy parameters for the valence radial functions of He.

| | | MCHF (Froese Fischer 1977) | HFFC (He$^+$ 1s) | HF He 1s^2 (case (a)) | HFC SH (case (b)) | |
					$\zeta = 1.4289$	$\zeta = 2.0$
1s1s'	^{1}S	1.9181	1.7450	1.835 91	1.985 35	1.6414
	^{3}S	0.3504	0.3485			
1s2s				0.316 67	0.324 14	0.3061
	^{1}S	0.2919	0.2871			
	^{3}P	0.2665	0.2626			
1s2p				0.254 86	0.260 51	0.2523
	^{1}P	0.2476	0.2449			

In the frozen-core approximations the excitation energies are given by the difference between the diagonal energy parameters for the relevant states. From table 1 we see that, in the Hartree frozen-core approximation, the use of a non-hydrogenic core has little effect on the excited states compared with the He$^+$ core but greatly improves the ground-state wavefunction. We note that for the screened hydrogenic core ($\zeta = 1.4289$) $\varepsilon_C = \zeta^2 = 2.0417$ is close to $\varepsilon_{1s} = 1.985\,35$ and the two radial functions are approximately 'equivalent'. The use of a non-hydrogenic core for the excited states means that the core radial function itself is poor but the point of our approximation for the collision problem is that the only dependence of the collision equations on the core orbital is via ^{FC}V which is precisely where there is little difference between the use of a He$^+$ or non-hydrogenic core for P_{nl_a}; and we expect the same to be true for the free wavefunctions.

3.2. Oscillator strengths and optically allowed transitions

For optically allowed transitions, $nl_a s_a \to n'l'_a s'_a$ where $l' = l \pm 1$,

$$\Omega/\ln k_i^2 \underset{k_i^2 \to \infty}{\sim} 4\omega_i f/\Delta k_{if}^2 \tag{3.5}$$

where ω_i is the statistical weight of the initial atomic state $\Delta k_{if}^2 = k_i^2 - k_f^2$ and f is the oscillator strength (see Burgess and Tully 1978). We may write f as

$$4\omega_i f/\Delta k_{if}^2 = \tfrac{4}{3}S \tag{3.6}$$

where S is the line strength given by

$$S = \sum_\mu \left| \sum_{\sigma_i} \int \psi_{q'}^{s'_a}(r_1, r_2)\chi_{m'_{s_a}}^{s'_a}(1, 2)(r_1 + r_2)\psi_q^{s_a}(r_1, r_2)\chi_{m_{s_a}}^{s_a}(1,2)\,\mathrm{d}r_1\,\mathrm{d}r_2 \right|^2$$

$$\mu = m_{l_a}m_{l'_a}m_{s_a}m_{s'_a} \tag{3.7}$$

which can be written in terms of an algebraic coefficient $\mathscr{A}$ and a radial part σ^2 thus,

$$S = \omega_i \mathscr{A} \sigma^2 \tag{3.8}$$

where

$$\mathscr{A} = l_>(2l_a' + 1) \qquad l_> = \max(l_a, l_a') \tag{3.9}$$

(see e.g. Goldberg 1936). To obtain the σ relevant to our treatment of the collision problem we must assume equivalent ground-state electrons and use the resulting orthogonality of the one-electron orbitals, as in the reduction of the collision equations, σ can then be written as

$$\sigma = -\left(\frac{1 + |\delta_{n1} - \delta_{n'1}|}{4l_>^2 + 1}\right)^{1/2} \delta_{s_a s_a'} \int_0^\infty P_{nl_a} r P_{n'l_a'} \, dr. \tag{3.10}$$

We use

$$\sigma^2 = 3f / \mathscr{A} \Delta k_{if}^2 \tag{3.11}$$

to convert other author's oscillator strengths to σ^2, using their excitation energies. By (3.5) this is the quantity that we wish to compare in different approximations to measure differences in the collision strengths for optically allowed transitions.

In table 2 we compare the values for σ^2, in the Hartree frozen-core approximations, with the 'exact' results of Schiff and Pekeris (1964) as well as those of other authors with which we shall compare our collision results in § 5. The values given for the Hartree–Fock frozen core were evaluated from (3.7) assuming a non-equivalent (He$^+$ 1s) core, that being the form used by Flannery and McCann (1975).

Table 2. σ^2.

| | Schiff and Pekeris (1964) | Berrington et al (1975) | HFFC He$^+$ 1s | HFC | | Willis and McDowell (1981) | Bhadra et al (1979) |
				HF He 1s^2	SH $\zeta = 1.4289$		
1^{1}S–2^{1}P	0.1771	0.183 68	0.186	0.2097	0.1771	0.1894	0.216
2^{1}S–2^{1}P	8.504	8.008	8.820				
				7.547	7.302		
2^{3}S–2^{3}P	6.408	7.295	6.597				

4. Free wavefunctions

For the two-electron problem, we recall in paper I the arbitrariness of the solution of the free wavefunction in the EDW2 approximation for s-wave scattering off an s-state with parallel electron spins (see also Seaton 1953). A similar arbitrariness can arise for the three-electron problem but now the resulting ρ matrix is not automatically unique.

To illustrate, consider without loss of generality (2.11) and (2.12) with $\nu, \nu' = 1s0s$, 2s1s and denote them by $0 \equiv 1s0s$ and $1 \equiv 2s1s$. Since we have assumed the same angular dependence we suppress the spherical harmonics. We write

$$\psi_0(r_1, r_2) = P_{1s}(r_1) P_{1s}(r_2) \tag{4.1}$$

and

$$\psi_1(r_1, r_2) = (1/\sqrt{2})(P_{1s}(r_1)P_{2s}(r_2) - P_{1s}(r_2)P_{2s}(r_1)) \qquad (4.2)$$

and we are still considering the exact exchange problem. Then for $\{F_0, F_1\}$ a solution of the resulting pair of coupled integro-differential equations, $\{F_0 + \beta P_{1s}, F_1\}$ is also a solution. This follows on inspecting the two equations thus. For $\nu' = 0$, the term involving F_0 is (using (2.11) and (2.12))

$$\int \psi_0(r_1, r_2)(H - \tfrac{1}{2}E)(\psi_0(r_1, r_2)F_0(r_3) - \psi_0(r_3, r_2)F_0(r_1)) \, dr_1 \, dr_2. \qquad (4.3)$$

This vanishes identically when $F_0 \equiv P_{1s}$ (use 4.2). For $\nu' = 1$, the term involving F_0 is

$$\int \psi_1(r_1, r_2)(H - \tfrac{1}{2}E)\psi_0(r_3, r_2)F_0(r_1) \, dr_1 \, dr_2. \qquad (4.4)$$

Setting $F_0 \equiv P_{1s}$ we obtain

$$\int (P_{1s}(r_1)P_{2s}(r_2) - P_{1s}(r_2)P_{2s}(r_1))(H - \tfrac{1}{2}E)P_{1s}(r_1)P_{1s}(r_2)P_{1s}(r_3) \, dr_1 \, dr_2 \qquad (4.5)$$

which vanishes identically due to the symmetry in r_1 and r_2. This is true in general for P_{1s} and P_{2s}, in ψ_1, replaced by P_{nl_a} and $P_{n'l'_a}$ respectively, so long as the ground-state electrons are taken to be equivalent, i.e. of the form given by (4.1); the core need not be frozen. It follows that, in the exact exchange problem, the distorted-wave approximation for the ρ matrix is unique. However, our approximation (2.22) for the exchange term in the collision equations means that, when using the EDW2,3 approximations, the ^2S ρ-matrix elements are not unique in general. For example, the $1^1S\ ^2S$ free wavefunction F_0 may be written as

$$F_0^\beta = F_0^\perp + \beta P_{1s} \qquad (4.6)$$

where β is arbitrary, and the $^2S\ 1^1S \to 2^3S$ ρ-matrix element is just given by

$$\rho(1, 0) = -\sqrt{\tfrac{3}{2}} \int_0^\infty F_1(r) W_{10}^{0S} F_0(r) \, dr. \qquad (4.7)$$

Since in the exact exchange problem using the distorted-wave approximation, the only non-zero contribution to the ρ matrix comes from $F_0^\perp$, we argue that $\beta = 0$ is a consistent choice for the collision problem where we have approximated the exchange term. This should minimise the error introduced. We note that for ^4S scattering off the 2^3S state there is no arbitrariness in the free wavefunction in the exact exchange problem but that the approximation for the exchange term introduces it, cf the two-electron problem, and also that it cancels out, as in the two-electron problem, between the direct and exchange contributions to ρ. Thus again we expect the error introduced, by the approximation for the exchange term, to be minimised.

5. Results

We have calculated total collision strengths for all transitions between the 1^1S, 2^3S, 2^1S, 2^3P and 2^1P states of He, for incident electron energies from just above threshold up to 15.0 Ryd, using a number of five-state unitarised EDW approximations for the

free wavefunctions with screened hydrogenic ($\zeta = 1.4289$) and Hartree–Fock He $1s^2$ cores in the approximation for the valence electron. We present our results in the form of collision strengths in tables 3 and 4 and compare them with other theoretical results and with experiment, where possible, in figures 1–10. In these figures we plot the scaled collision strength Y against the (dimensionless) scaled energy X where $X = 1/\ln (k_f^2/c_1 + e)$ and $Y = \Omega/\ln (k_f^2/c_2 + c_3)$ for optically allowed transitions, $X = 1/(k_f^2/c_1 + 1)$ and $Y = \Omega$ for spin-allowed transitions, and $X = 1/(k_f^2/c_1 + 1)$ and $Y = \Omega(k_f^2/c_2 + c_3)^2$ for spin-forbidden transitions. k_f^2 is the energy of the free electron scattered off the final state. The values used for the constants c_i are given in the captions.

5.1. Transitions from the ground state

We set $c_1 = \Delta E_0 = c_2$, where ΔE_0 is the observed excitation energy taken from Moore (1949) and take $c_3 = e$ for the optically allowed transition and $c_3 = 1$ otherwise.

In table 3 we present our results for the total collision strengths obtained using the EDW2 approximation for the free wavefunctions and a screened hydrogenic ($\zeta = 1.4289$) Hartree frozen-core approximation for the valence electron.

Table 3. Total collision strengths for transitions from the ground state of He in the EDW2 approximation with the SH ($\zeta = 1.4289$) HFC.

k_f^2	$1^1S \to 2^3S$	$1^1S \to 2^1S$	k_f^2	$1^1S \to 2^3P$	$1^1S \to 2^1P$
$8.879 - 2\dagger$	$3.29 - 2$	$3.32 - 2$	$2.129 - 2$	$1.39 - 2$	$6.44 - 3$
$1.388 - 2$	$4.42 - 2$	$2.59 - 2$	$7.129 - 2$	$1.97 - 2$	$1.93 - 2$
$1.888 - 1$	$6.50 - 2$	$6.08 - 2$	$1.213 - 1$	$2.36 - 2$	$4.67 - 2$
$2.388 - 1$	$8.29 - 2$	$8.56 - 2$	$1.713 - 1$	$3.55 - 2$	$7.96 - 2$
$2.888 - 1$	$7.66 - 2$	$1.05 - 1$	$2.213 - 1$	$5.32 - 2$	$1.00 - 1$
$3.388 - 1$	$6.76 - 2$	$1.17 - 1$	$2.713 - 1$	$7.05 - 2$	$1.14 - 1$
$4.388 - 1$	$6.96 - 2$	$1.24 - 1$	$3.713 - 1$	$1.06 - 1$	$1.36 - 1$
$5.388 - 1$	$5.93 - 2$	$1.31 - 1$	$5.713 - 1$	$1.40 - 1$	$1.50 - 1$
$6.888 - 1$	$4.39 - 2$	$1.38 - 1$	$6.213 - 1$	$1.71 - 1$	$1.73 - 1$
$8.388 - 1$	$3.48 - 2$	$1.45 - 1$	$7.713 - 1$	$1.76 - 1$	$2.00 - 1$
1.339	$2.36 - 2$	$1.68 - 1$	1.271	$1.38 - 1$	$3.02 - 1$
1.839	$2.00 - 2$	$1.84 - 1$	1.771	$1.01 - 1$	$3.99 - 1$
2.339	$1.80 - 2$	$1.95 - 1$	2.271	$7.57 - 2$	$4.87 - 1$
3.339	$1.49 - 2$	$2.09 - 1$	3.271	$4.55 - 2$	$6.40 - 1$
4.339	$1.24 - 2$	$2.17 - 1$	4.271	$2.97 - 2$	$7.67 - 1$
6.339	$8.59 - 3$	$2.25 - 1$	6.271	$1.50 - 2$	$9.72 - 1$
8.339	$6.19 - 3$	$2.29 - 1$	8.271	$8.89 - 3$	1.13
$1.334 + 1$	$3.18 - 3$	$2.32 - 1$	$1.327 + 1$	$3.49 - 3$	1.43

† $8.879 - 2$ means 8.879×10^{-2}.

In figure 1 we compare the EDW scaled collision strengths, for the $1^1S \to 2^1P$ transition in He, with those of the five-state R-matrix calculation of Fon *et al* (1981), the five-state close-coupling (5CC) calculation of Bhadra *et al* (1979) and a $\overline{7CCLE}$ calculation by Willis and McDowell (1981) as well as with the experimental points from Westerveld *et al* (1979). We also include the 'exact' value for Y at $X = 0$, obtained using the f value from Schiff and Pekeris (1964) as described in § 3.2. $\overline{7CCLE}$ denotes a seven-state close-coupling calculation, with local exchange operator approximation, using the five lowest states of He as well as two pseudo-states. We see a great improvement in the
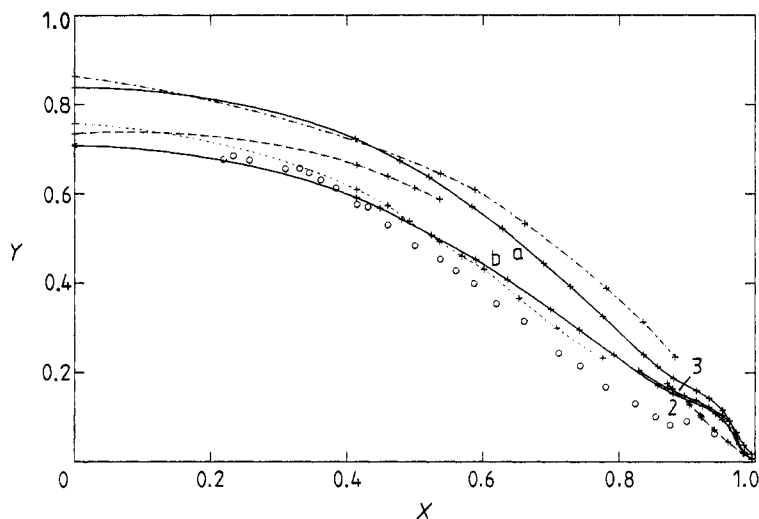
Figure 1. Scaled collision strengths for the $1^1S \to 2^1P$ transition in He. ——, EDW2,3, curve a, HF He $1s^2$ HFC, curve b, SH($\zeta = 1.4289$) HFC; — $\cdot$ —, SCC (Bhadra *et al* 1979); – – –, R matrix (Fon *et al* 1981); $\cdots\cdots$, $\overline{7CC}$LE (Willis and McDowell 1981); *, 'exact' limit point (Schiff and Pekeris 1964); $\bigcirc$, experimental points from Westerveld *et al* (1979). $c_1 = 1.5603$ Ryd $= c_2$, $c_3 =$ e.

EDW2 results on using the SH ($\zeta = 1.4289$) core as opposed to the HF He $1s^2$ core. The SH core chosen so as to reproduce the 'exact' value for Y in the infinite energy limit ($X = 0$) gives good results when compared with experiment down to quite low energies. The effect of including higher exchange multipoles ($\lambda > 0$) exactly (EDW3) is small. This illustrates that for an optically allowed transition the accuracy of the collision strengths is dominated at all energies by the accuracy of the line strength. What is essentially a five-state close-coupling calculation by Fon *et al* (1981) differs from the SCC calculation of Bhadra *et al* (1979) due to the inclusion of bound–bound terms in the eigenfunction expansion of the former to allow for three-electron correlation effects (see Fon *et al* 1979) as well as the use of more accurate atomic wavefunctions. Their inclusion of the bound–bound terms also gives rise to pseudo-resonances over the energy range $k_{1s}^2 \approx 2.2$–7.4 Ryd for all transitions.

From figure 2 we see that the main source of error for the $1^1S \to 2^1S$ transition is due to the neglect of an infinity of states on using a truncated eigenfunction expansion. Willis and McDowell (1981) allow for this approximately by including two pseudo-states, one chosen so as to give the experimental value for the static dipole polarisability of the ground state, and obtained good agreement with the experimental points from de Heer and Jansen (1977). The bound–bound terms in the eigenfunction expansion used by the R-matrix method (Fon *et al* 1979) also make some allowance for the neglected states. For this transition the use of the SH core does not give particularly good results compared with experiment, although there is some improvement over those obtained using the HF core. But we note that the SH results do exhibit good agreement with the SCC results of Bhadra *et al* (1979) at high energies. As with the $1^1S \to 2^1P$ transition, our results are sensitive to the core used but not to the collision approximation.

In figures 3 and 4 we compare our scaled EDW collision strengths for the $1^1S \to 2^3S$ and $1^1S \to 2^3P$ transitions in He with those of the R-matrix calculation of Fon *et al*
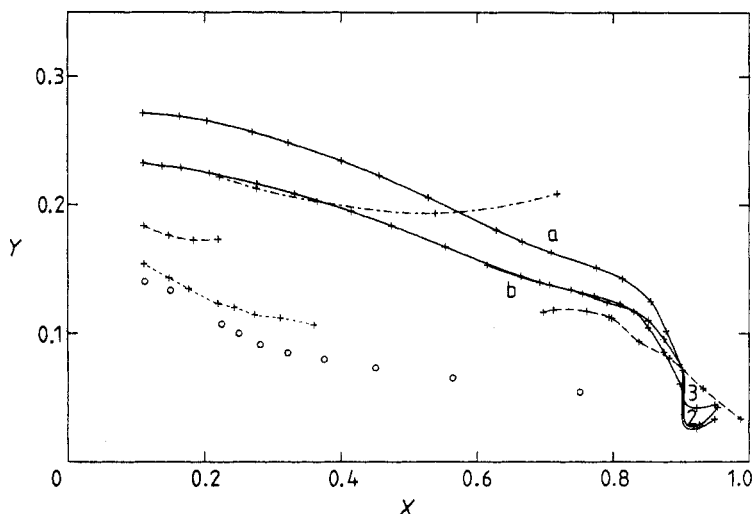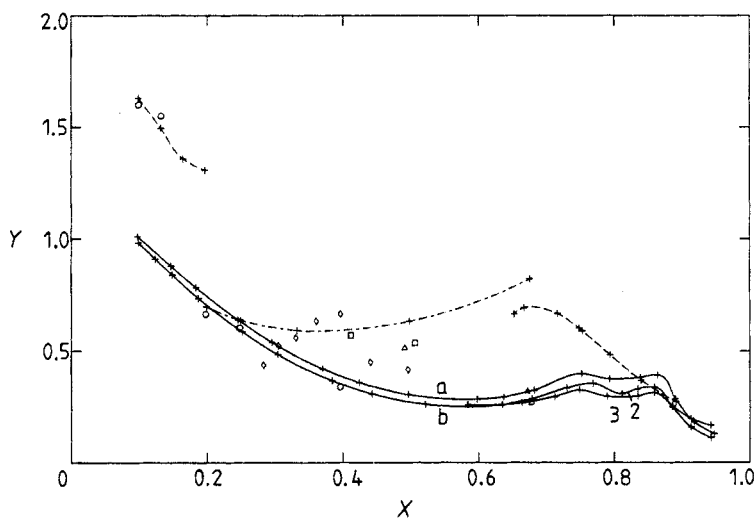
Figure 2. Scaled collision strengths for the $1^1S \rightarrow 2^1S$ transition in He. ———, EDW2,3, curve a, HF He $1s^2$ HFC, curve b, SH($\zeta = 1.4289$) HFC; — · —, 5CC (Bhadra *et al* 1979); – – –, *R* matrix (Fon *et al* 1981), · · · · · ·, $\overline{7CC}$LE (Willis and McDowell 1981); ○, experimental points from de Heer and Jansen (1977). $c_1 = 1.6584$ Ryd $= c_2$, $c_3 = 1$.

Figure 3. Scaled collision strengths for the $1^1S \rightarrow 2^3S$ transition in He. ———, EDW2,3, curve a, HF He $1s^2$ HFC, curve b, SH($\zeta = 1.4289$) HFC; — · —, 5CC (Bhadra *et al* 1979); – – –, *R* matrix (Fon *et al* 1981); □, experimental points from Hall *et al* (1973); △, from Trajmar (1973); ○, from Yagishita (1978, unpublished); ◇, from Crooks *et al* (1972). $c_1 = 1.4574$ Ryd $= c_2$, $c_3 = 1$.

(1981) and the 5CC calculation of Bhadra *et al* (1979) as well as with the experiments of Hall *et al* (1973), Trajmar (1973), Yagishita (1978) and Crooks *et al* (1972) for $1^1S \rightarrow 2^3S$ and Jobe and St John (1967, with cascade correction due to de Heer and Jansen 1977) for $1^1S \rightarrow 2^3P$. For these two spin-forbidden transitions there is little
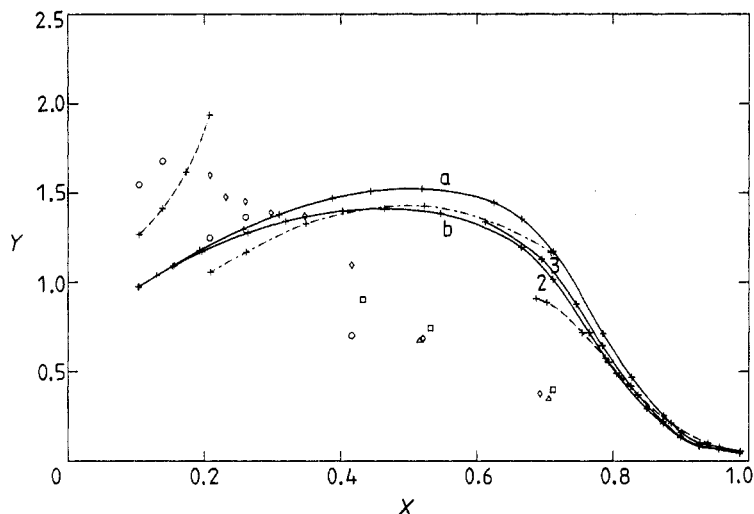
Figure 4. Scaled collision strengths for the $1^1S \to 2^3P$ transition in He. ———, EDW2,3, curve a, HF He $1s^2$ HFC, curve b, SH($\zeta = 1.4289$) HFC; — $\cdot$ —, SCC (Bhadra *et al* 1979); – – –, R matrix (Fon *et al* 1981); $\square$, experimental points from Hall *et al* (1973); $\triangle$, from Trajmar (1973); $\bigcirc$, from Yagishita (1978, unpublished); $\diamond$, from Jobe and St John (1967, with cascade correction due to de Heer and Jansen 1977). $c_1 = 1.5316$ Ryd $= c_2$, $c_3 = 1$.

difference in the EDW2 collision strengths for the two different cores used. Although results for the EDW3 approximation only differ slightly from those of the EDW2 approximation the EDW1 results (not shown) are poor as expected since exchange is treated as a perturbation (see also paper I). The monopole exchange potential is thus the dominant term, which is the basis of the EDW2 approximation.

For the $1^1S \to 2^3S$ transition, the EDW results are in quite good agreement with experiment. However, there is some disagreement at high energies between the EDW results and those of the R-matrix approximation of Fon *et al* (1981) and the unpublished experimental results of Yagishita (1978). From figure 3 we see that the trend from intermediate energies of the experimental results (including those of Yagishita (1978)) and of the SCC results (Bhadra *et al* 1979), is towards the high energy EDW results rather than those of the R matrix (Fon *et al* 1981). Vriens *et al* (1968) obtained experimental results (not shown) that are a factor of four smaller than those of Yagishita (1978) at high energies. But Baluja and McDowell (1979) have pointed out that the form assumed by Vriens *et al* (1968) for the dependence of their differential cross sections on the momentum transfer was incorrect and hence that their total (integrated) cross sections are invalid. However, Baluja and McDowell (1979) suggested that the corrected results should be a factor of two larger at 200 eV ($X \simeq 0.1$), i.e. a factor of two smaller than those of Yagishita (1978) and more in line with the EDW results. More experimental evidence is required at high energies to help resolve this discrepancy for the $1^1S \to 2^3S$ transition. We note that figure 1 of Fon *et al* (1979, p 1864) is misleading in its comparison of the original results of Vriens *et al* (1968) with those of Yagishita (1978). Fon *et al* (1979) plot the $1^1S \to 2^3S$ cross section in units of a_0^2 but the results of Vriens *et al* (1968, p 13 table VII) are in units of $\pi a_0^2 10^{-4}$ and Fon *et al* (1979) appear to have plotted the results of Vriens *et al* (1968) without first multiplying by π.

From figure 4 we see that there is little agreement in general between theory and experiment for the $1S \to 2^3P$ transition, although the EDW results are in good agreement with those of the R-matrix method (Fon *et al* 1981) at low energies and with those of the 5CC calculation (Bhadra *et al* 1979) at intermediate energies. Again the high energy behaviour of the results of the R-matrix approximation of Fon *et al* (1981) is at variance with that of the EDW and 5CC (Bhadra *et al* 1979) approximations.

5.2. Transitions between the n = 2 states

For transitions between the $n = 2$ states, the initial and final states are more strongly coupled than for transitions from the ground state and so we do not expect the EDW results to be particularly good at low energies. Consequently we hope to match up with the R-matrix results of Fon *et al* (1981) at energies just below those at which they encountered pseudo-resonances and to provide reliable results from there on. In the figures the c_i are chosen so as to emphasise this energy region and the particular values used are given in each caption. For spin-forbidden transitions we only compare EDW results obtained using the SH core since those obtained using the HF core differ by no more than a few per cent.

In table 4 we present our results for the total collision strengths at selected energies for transitions between the $n = 2$ states of He in the EDW2 approximation using the SH ($\zeta = 1.4289$) Hartree frozen-core approximation for the valence electron.

Table 4. Total collision strengths for transitions between the $n = 2$ states of He in the EDW2 approximation with the SH ($\zeta = 1.4289$) HFC.

k_i^2	$2^1S \to 2^1P$	$2^3S \to 2^3P$	$2^3S \to 2^1P$	$2^1S \to 2^3P$	$2^3P \to 2^1P$	k_i^2	$2^3S \to 2^1S$
$1.713-1$	$3.46+1$	$1.07+2$	2.53	1.67	6.34	$2.388-1$	2.31
$2.213-1$	$4.22+1$	$1.31+2$	2.73	1.79	6.17	$2.888-1$	1.68
$2.713-1$	$4.89+1$	$1.53+2$	2.43	1.69	6.20	$3.388-1$	1.49
$3.713-1$	$6.10+1$	$1.88+2$	1.98	1.71	5.96	$4.388-1$	1.23
$4.713-1$	$7.11+1$	$2.18+2$	1.56	1.46	5.10	$5.388-1$	$9.41-1$
$6.213-1$	$8.34+1$	$2.53+2$	1.04	1.03	3.70	$6.888-1$	$6.37-1$
$7.713-1$	$9.31+1$	$2.81+2$	$7.31-1$	$7.27-1$	2.66	$8.388-1$	$4.42-1$
1.271	$1.15+2$	$3.45+2$	$2.98-1$	$2.96-1$	1.08	1.339	$1.73-1$
1.771	$1.28+2$	$3.84+2$	$1.57-1$	$1.56-1$	$5.72-1$	1.839	$9.32-2$
2.271	$1.37+2$	$4.13+2$	$9.61-2$	$9.58-2$	$3.51-1$	2.339	$5.88-2$
3.271	$1.51+2$	$4.53+2$	$4.65-2$	$4.64-2$	$1.70-1$	3.339	$2.99-2$
4.271	$1.60+2$	$4.82+2$	$2.73-2$	$2.73-2$	$9.99-2$	4.339	$1.81-2$
6.271	$1.73+2$	$5.20+2$	$1.28-2$	$1.28-2$	$4.62-2$	6.339	$8.71-3$
8.271	$1.82+2$	$5.47+2$	$7.38-3$	$7.37-3$	$2.64-2$	8.339	$5.10-3$
$1.327+1$	$1.97+2$	$5.93+2$	$2.89-3$	$2.89-3$	$1.02-2$	$1.334+1$	$2.02-3$

In figures 5 and 6 we compare our scaled EDW2, SH and HF He $1s^2$ Hartree frozen-core collision strengths for the $2^3S \to 2^3P$ and $2^1S \to 2^1P$ transitions with those of the R-matrix calculation of Fon *et al* (1981) and a multichannel eikonal calculation by Flannery and McCann (1975). Again we have included the 'exact' value for Y at $X = 0$, using the results of Schiff and Pekeris (1964) as described in § 3.2. Apart from the spin
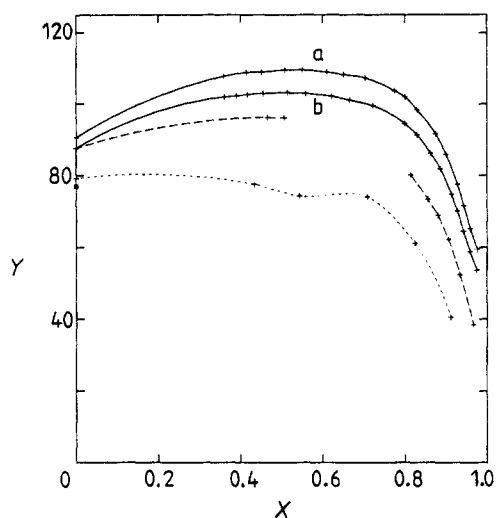
Figure 5. Scaled collision strengths for the $2^3S \to 2^3P$ transition in He. ———, EDW2, curve a, HF He $1s^2$ HFC, curve b, SH($\zeta = 1.4289$) HFC; ·······, eikonal (Flannery and McCann 1975); ———, R matrix (Fon *et al* 1981); *, 'exact' limit point (Schiff and Pekeris 1964). $c_1 = 1.0$ Ryd, $c_2 = 0.04$ Ryd, $c_3 = 1$.
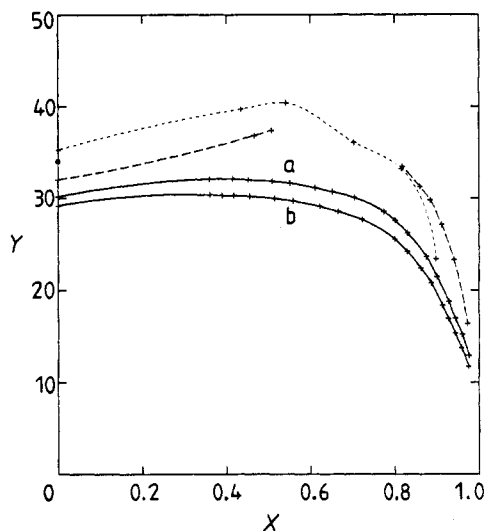
Figure 6. Scaled collision strengths for the $2^1S \to 2^1P$ transition in He. ———, EDW2, curve a, HF He $1s^2$ HFC, curve b, SH($\zeta = 1.4289$) HFC; ·······, eikonal (Flannery and McCann 1975); ———, R matrix (Fon *et al* 1981); *, 'exact' limit point (Schiff and Pekeris 1964). $c_1 = 1.0$ Ryd, $c_2 = 0.02$ Ryd, $c_3 = 1$.

weights, results in the EDW approximation for these two transitions are virtually identical except at low energies since, using the Hartree frozen-core approximation for the valence electron, only the first few partial waves are distinct and exchange scattering makes little contribution to the total collision strength. The differences between the results shown in figures 5 and 6 are probably solely due to the approximation used for the atomic wavefunctions rather than subsequent approximation to the solution of the collision equations.

In figures 7 and 8 we compare our scaled EDW2 and EDW3 collision strengths for the $2^3S \to 2^1P$ and $2^1S \to 2^3P$ transitions with those of the R-matrix calculation of Fon *et al* (1981). Their results, which they only give at energies below those at which pseudo-resonances occurred, appear to be the only ones available in the literature. Again, apart from the spin weights, there is little difference between results for these transitions in the EDW approximation using the Hartree frozen-core approximation for the valence electron.

In figures 9 and 10 we compare our scaled EDW2 and EDW3 collision strengths for the $2^3S \to 2^1S$ and $2^3P \to 2^1P$ transitions with those of the R-matrix calculation of Fon *et al* (1981). Although the excitation energy for these two transitions is zero, using the Hartree frozen-core approximation for the valence electron, the EDW collision strengths fall off correctly like $(k_f^2)^{-2}$. The same is not true for the R-matrix results of Fon *et al* (1981); as stated in their paper, their best fit was for $(k_f^2)^{-1}$.

We suggest that the R-matrix results of Fon *et al* (1981) are generally unreliable for spin-forbidden transitions at energies above those at which pseudo-resonances occurred and, hence, so is the interpolation formula that is based on them (see Fon *et al* 1981, p 2932 equation (2) and p 2933 table 5).
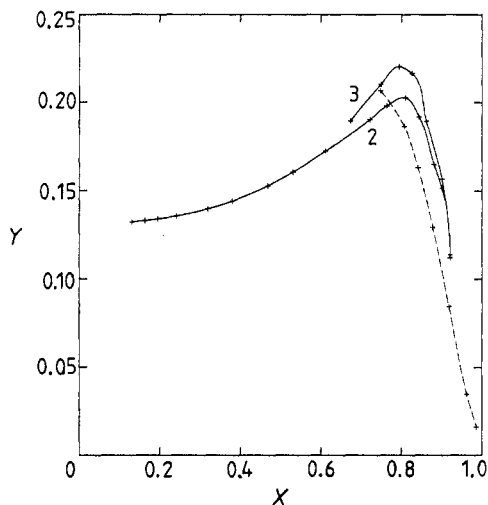
Figure 7. Scaled collision strengths for the $2^3S \to 2^1P$ transition in He. ——, EDW2,3 SH($\zeta = 1.4289$) HFC; – – –, R matrix (Fon *et al* 1981). $c_1 = 2.0$ Ryd $= c_2$, $c_3 = 0.125$.
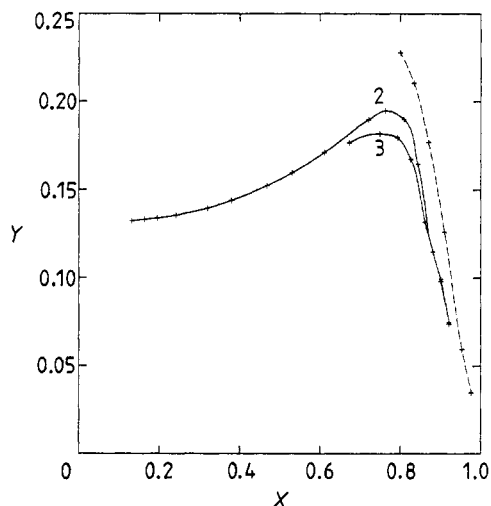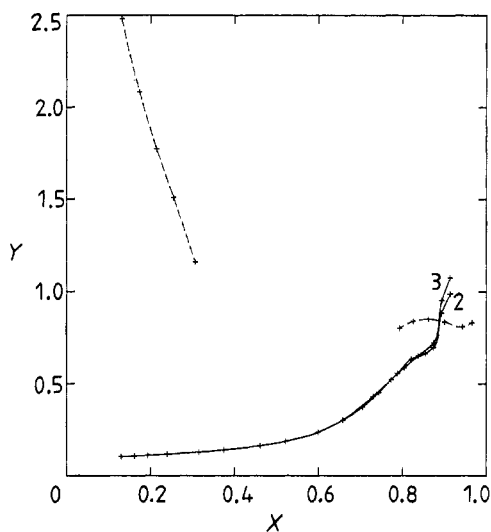
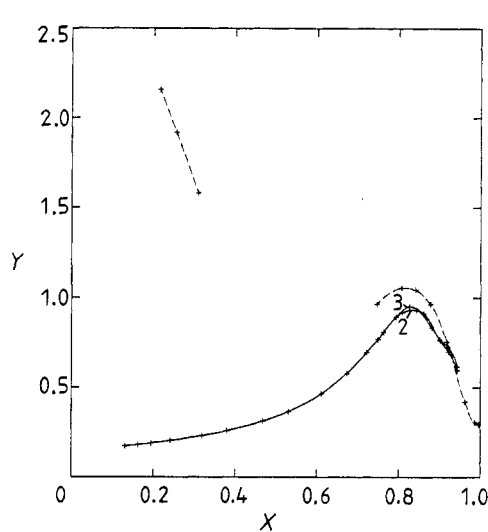**Figure 8.** Scaled collision strengths for the $2^1S \to 2^3P$ transition in He. ——, EDW2,3 SH($\zeta = 1.4289$) HFC; – – –, R matrix (Fon *et al* 1981). $c_1 = 2.0$ Ryd $= c_2$, $c_3 = 0.125$.

Figure 9. Scaled collision strengths for the $2^3S \to 2^1S$ transition in He. ——, EDW2,3 SH($\zeta = 1.4289$) HFC; – – –, R matrix (Fon *et al* 1981). $c_1 = 2.0$ Ryd $= c_2$, $c_3 = 0.5$.

Figure 10. Scaled collision strengths for the $2^3P \to 2^1P$ transition in He. ——, EDW2,3 SH($\zeta = 1.4289$) HFC; – – –, R matrix Fon *et al* (1981). $c_1 = 2.0$ Ryd $= c_2$, $c_3 = 0.5$.

6. Conclusions

We have developed a new approximation for electron collisions with two-electron atoms, based on the orthogonality of one-electron bound-state wavefunctions, and have applied it to the excitation of He. We have presented results for total collision

strengths for all inelastic transitions between the 1^1S, 2^3S, 2^1S, 2^3P and 2^1P states over a wide range of energies.

We have seen that, for spin-forbidden transitions, our results are good and that they are relatively insensitive to the valence wavefunctions used. Thus for spin-forbidden transitions, also bearing in mind table 1, we estimate that the effect on our results if we were to use a form of the Hartree–Fock frozen-core approximation (not necessarily with a He^+ 1s core) within our formulation of the collision problem, would be less than about 10%. For the $1^1S \rightarrow 2^1S$ transition the main source of error is due to the infinity of states neglected in the truncated eigenfunction expansion, so although our results are sensitive to the form of the valence wavefunctions used we would not necessarily gain any improvement on using a Hartree–Fock frozen-core approximation. For the $1^1S \rightarrow 2^1P$ transition we have seen that good results can be obtained by choosing a core that leads to valence wavefunctions that give the exact value for the quantity σ^2. The $2^3S \rightarrow 2^3P$ and $2^1S \rightarrow 2^1P$ transitions are the two transitions for which including exchange explicitly, in the approximation for the valence wavefunction, could be expected to give improved results, simply because the singlet and triplet $2l$ orbitals would then be non-degenerate (see also table 2).

Thus using a screened hydrogenic core, adjusted to lead to the exact value of $\sigma^2(1^1S \rightarrow 2^1P)$, and the EDW2 approximation, which includes the dominant monopole exchange distorting potential exactly, this rather simple, but physically motivated, approach gives good results in general and is much faster to apply than the more elaborate R-matrix approximation. It should prove useful for calculating excitation rates and di-electronic recombination rates for He-like ions in the future.

Acknowledgments

Appendix

In paper I we discussed the solution of the EDW2 radial equation; we now consider the solution of

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2z}{r} + k_\nu^2 - \sum_\lambda U_{\nu\nu}^{\lambda LS}\right) F_\nu^{LS}(r) = 0 \tag{A.1}$$

where

$$U_{\nu\nu}^{\lambda LS} = \delta_{\lambda 0}\,{}^{FC}V + V_{\nu\nu}^{\lambda L} + h_{\nu\nu}^S W_{\nu\nu}^{\lambda L}. \tag{A.2}$$

This contains the EDW2,3 radial equations as a special case, see (2.24) and (2.25). We write (A.1) and (A.2), in the notation of paper I, as

$$\left(\frac{d^2}{dr^2} - \frac{l(l+1)}{r^2} + \frac{2z}{r} - {}^{FC}V(r) + k_\nu^2\right) F_\nu^{LS}(r)$$

$$= \sum_\lambda \left[2f_\lambda(l_a l, l_a l; L)\left(y_\lambda(P_{n l_a}, P_{n l_a}|r) - \frac{\delta_{\lambda 0}}{r}\right) F_\nu^{LS}(r)\right.$$

$$+g_\nu^{\lambda S}\left(\frac{1}{r^{\lambda+1}}\int_0^r P_{nl_a}(r')F_\nu^{LS}(r')r'^\lambda\,\mathrm{d}r'\right.$$

$$\left.-r^\lambda\int_0^r \frac{P_{nl_a}(r')F_\nu^{LS}(r')}{r'^{\lambda+1}}\,\mathrm{d}r'+c_\lambda r^\lambda\right)P_{nl_a}(r)\Bigg] \tag{A.3}$$

where

$$g_\nu^{\lambda S}=2h_{\nu\nu}^S g_\lambda(l_a l, l_a l; L) \tag{A.4}$$

and

$$c_\lambda=-\frac{\delta_{\lambda 0}}{2}(\varepsilon_{nl_a}+k_\nu^2)\int_0^\infty P_{nl_a}(r)F_\nu^{LS}(r)\,\mathrm{d}r+\int_0^\infty \frac{P_{nl_a}(r)F_\nu^{LS}(r)}{r^{\lambda+1}}\,\mathrm{d}r. \tag{A.5}$$

For the three-electron problem, throughout paper I we replace $V_{\nu'\nu}^\lambda$ by $\delta_{\lambda 0}\,\delta_{\nu'\nu}\,{}^{FC}V+b_{\nu'\nu}V_{\nu'\nu}^{\lambda L}$ and $\pm W_{\nu'\nu}^\lambda$ by $h_{\nu'\nu}^S W_{\nu'\nu}^{\lambda L}$. We determine a power series solution as in I, the recurrence relation being of the form

$$n(n+1+2l)a_n-\sum_{i,j=0}^\infty v_{i-1}a_j\,\delta(n,i+j+1)+a_{n-2}k_\nu^2$$

$$-\sum_\lambda g_\nu^{\lambda S}\left(c_\lambda P_{n-d-2}-\sum_{\substack{i,j,k\\=0}}^\infty \frac{(2\lambda+1)a_i P_j P_k\,\delta(n-2l_a-3,i+j+k+1)}{(n-k-1-e)(n-k-2-d)}\right)$$

$$=0 \tag{A.6}$$

where

$$d=\lambda+l_a-l \qquad\text{and}\qquad e=l_a-l-\lambda$$

which is valid $\forall n\geq 0$ if we define

$$a_i\equiv 0 \qquad P_i\equiv 0 \qquad v_{i-1}\equiv 0 \qquad \forall i<0.$$

The numerical extension of the power series solution of (A.3), using the summed Cowell–Numerov method as in paper I, is

$$\left(1-\frac{h^2}{12}\phi_{n+1}\right)F_{n+1}^{LS}$$

$$=\left(1-\frac{h^2}{12}\phi_n\right)F_n^{LS}+\frac{h^2}{12}\sum_\lambda g^{\lambda S}\Bigg[c_\lambda(r_{n+1}^\lambda P_{n+1}-r_n^\lambda P_n)$$

$$+\left(\frac{1}{r_{n+1}^{\lambda+1}}\int_0^{r_{n+1}}PF^{LS}r^\lambda\,\mathrm{d}r-r_{n+1}^\lambda\int_0^{r_{n+1}}\frac{PF^{LS}}{r^{\lambda+1}}\,\mathrm{d}r\right)P_{n+1}$$

$$-\left(\frac{1}{r_n^{\lambda+1}}\int_0^{r_n}PF^{LS}r^\lambda\,\mathrm{d}r-r_n^\lambda\int_0^{r_n}\frac{PF^{LS}}{r^{\lambda+1}}\,\mathrm{d}r\right)P_n\Bigg]$$

$$+h^2\sum_{j=1}^n\left[\phi_j F_j^{LS}+\sum_\lambda g^{\lambda S}P_j\left(\frac{1}{r_j^{\lambda+1}}\int_0^{r_j}PF^{LS}r^\lambda\,\mathrm{d}r-r_j^\lambda\int_0^{r_j}\frac{PF^{LS}}{r^{\lambda+1}}\,\mathrm{d}r+c_\lambda r_j^\lambda\right)\right]$$

$$+\sum_{i=0}^1(-1)^{i+1}\left\{F_i^{LS}-\frac{h^2}{12}\Bigg[\phi_i F_i^{LS}+\sum_\lambda g^{\lambda S}P_i\right.$$

$$\left.\times\left(\frac{1}{r_i^{\lambda+1}}\int_0^{r_i}PF^{LS}r^\lambda\,\mathrm{d}r-r_i^\lambda\int_0^{r_i}\frac{PF^{LS}}{r^{\lambda+1}}\,\mathrm{d}r+c_\lambda r_i^\lambda\right)\Bigg]\right\} \tag{A.7}$$

where

$$\phi(r) = \frac{l(l+1)}{r^2} - \frac{2z}{r} - k_\nu^2 + {}^{FC}V(r) + \sum_\lambda V_{\nu\nu}^{\lambda L}(r). \tag{A.8}$$

Let

$$I = P_{n+1}\left(\frac{1}{r_{n+1}^{\lambda+1}} \int_0^{r_{n+1}} PF^{LS}r^\lambda \, dr - r_{n+1}^\lambda \int_0^{r_{n+1}} \frac{PF^{LS}}{r^{\lambda+1}} \, dr\right) \tag{A.9}$$

then approximations (a) and (b) (see I) for the term F_{n+1}^{LS} on the RHS of (A.7) are given by

(a)

$$I \simeq P_{n+1}\left(\frac{1}{r_{n+1}^{\lambda+1}} \int_0^{r_{n-1}} PF^{LS}r^\lambda \, dr - r_{n+1}^\lambda \int_0^{r_{n-1}} \frac{PF^{LS}}{r^{\lambda+1}} \, dr\right)$$
$$- \frac{h}{3}\frac{P_{n+1}}{r_{n+1}^{\lambda+1}}\left(\frac{P_{n-1}F_{n-1}^{LS}}{r_{n-1}^{\lambda+1}}(r_{n+1}^{2\lambda+1} - r_{n-1}^{2\lambda+1}) + \frac{4P_nF_n^{LS}}{r_n^{\lambda+1}}(r_{n+1}^{2\lambda+1} - r_n^{2\lambda+1})\right) \tag{A.10}$$

(b)

$$I \simeq P_{n+1}\left(\frac{1}{r_{n+1}^{\lambda+1}} \int_0^{r_n} PF^{LS}r^\lambda \, dr - r_{n+1}^\lambda \int_0^{r_n} \frac{PF^{LS}}{r^{\lambda+1}} \, dr\right)$$
$$- \frac{h}{12}\frac{P_{n+1}}{r_{n+1}^{\lambda+1}}\left(\frac{8P_nF_n^{LS}}{r_n^{\lambda+1}}(r_{n+1}^{2\lambda+1} - r_n^{2\lambda+1}) - \frac{P_{n-1}F_{n-1}^{LS}}{r_{n-1}^{\lambda+1}}(r_{n+1}^{2\lambda+1} - r_{n-1}^{2\lambda+1})\right). \tag{A.11}$$

For $k^2 \geqslant 0$, a solution of (A.3) that satisfies (A.5) may be found as in paper I using Percival's method (see Marriott 1958).

For $k^2 < 0$ distinct values of c give rise, in general, to distinct eigenvalues $\varepsilon(=-k^2)$ and we must now search for the values of c and ε which lead to a solution F_ν that satisfies (A.5) and the following asymptotic boundary conditions,

$$F_\nu \underset{r\to 0}{\sim} a_0 r^{l+1} \qquad \text{and} \qquad F_\nu \underset{r\to\infty}{\sim} 0. \tag{A.12}$$

To test programs written for the EDW3 approximation we set

$$b_{\nu\nu} = 1 \qquad h_{\nu\nu}^0 = 1 \qquad h_{\nu\nu}^1 = -1$$

and ${}^{FC}V \equiv 0$ in (A.3) to recover the two-electron problem. We take P to be frozen as a He$^+$ 1s core and F to be a freely varied bound-state radial function. (A.3) are now the prior form of the Hartree–Fock frozen-core equations for He whilst those of Cohen and Kelly (1966) are the post form, there being no post–prior discrepancy. In table A1 we give the values of c and a_0 that generate the required solution, which has been normalised to unity.

Table A1. Parameters c and a_0 for the HFFC approximation for He.

	1^1S	2^3S	2^1S	2^3P	2^1P
c	0.506 22	0.232 59	0.107 70	0.270 57	0.165 68
a_0	3.539 81	1.047 88	0.795 66	0.393 87	0.201 41

The diagonal energy parameters have already been given in table 1, in agreement with Cohen and Kelly (1966), and σ^2 in table 2, in agreement with Cameron *et al* (1970).

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