Inelastic scattering of electrons from the 2³S state of helium

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Abstract. A distorted-wave approximation is used to calculate differential and total cross sections for the electron excitation of helium from the metastable 2³S state to the 2³P, 3³S and 3³P states for electron energies from 10 to 30 eV. Values of the asymmetry parameter for the scattering of spin-polarised electrons from spin-polarised metastable helium atoms are also given. The present results are compared with previous calculations and recent experimental measurements of the differential cross sections.

1. Introduction

The study of electron impact excitation of atomic systems in the ground state has received considerable attention in the literature. Less work has been reported for scattering from atoms initially in an excited state. The knowledge of electronic collision processes involving excited atomic systems is of importance in astrophysics and plasma physics. It is also of use in the understanding of gaseous discharges and in the development of lasers. Also, because of their long radiative lifetimes, metastable helium atoms play an important role in Penning ionisation processes.

There has been very little theoretical work reported on the excitation of metastable helium. Flannery and McCann (1975) calculated the differential and total cross sections for the excitation of the 2^{1,3}P, 3^{1,3}S, 3^{1,3}P and 3^{1,3}D states from the 2^{1,3}S states of helium using a ten-channel eikonal approximation. Flannery *et al* (1975) also examined the above excitations in the Born and the Vainshtein, Presnyakov and Sobelman approximations. Khayrallah *et al* (1978) calculated differential and total cross sections for the excitation of the 3³S state from the 2³S state in the Glauber and Born approximations. Gupta and Mathur (1980) and Sharma *et al* (1980) reported differential cross sections at energies above 50 eV for excitation from the metastable 2³S state to the 3³S state and from the 2¹S state to the 3¹S and 4¹S states in the two-potential modified Born approximation. Fon *et al* (1981) and Berrington *et al* (1985) published *R*-matrix calculations for the total cross sections at low energies for a number of these processes. Similarly, total cross section results have been given by Badnell (1984) using a distorted-wave approximation.

On the experimental side, total scattering cross sections (elastic plus inelastic) from excited helium atoms have been measured by Neynaber et al (1964), Wilson and Williams (1976) and Khakhaev et al (1977). Recently, Müller-Fiedler et al (1984) performed a crossed-beam experiment to measure the differential cross sections for

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excitation from the metastable 2³S state to the 2³P state as well as all triplet states with principal quantum number 3 or 4 in the energy range from 15 to 30 eV. Measurements of the asymmetry parameter for the excitation of the 3³P state are also planned for the near future (Raith 1986).

In this work we report on a theoretical study of the excitation of the 2³P, 3³S and 3³P states from the metastable 2³S state of helium within the framework of a distorted-wave approximation. We present results for the total and differential cross sections for these transitions for energies up to 30 eV. We also give values for the asymmetry parameter for the excitation of spin-polarised helium atoms in the 2³S state by spin-polarised electrons. In § 2 we give the theoretical expressions used, while the numerical results are given in § 3 along with comparisons with experiment and other calculations.

2. Theory

The T matrix for the excitation of helium from an initial state i to a final state f is given by

$$T = \langle \Phi_f(\mathbf{r}_1 \sigma_1; \mathbf{r}_2 \sigma_2, \mathbf{r}_3 \sigma_3) | V | \Psi_i^+(\mathbf{r}_1 \sigma_1, \mathbf{r}_2 \sigma_2, \mathbf{r}_2 \sigma_3) \rangle$$
 (1)

where the total interaction potential V is

$$V = -\frac{2}{r_1} + \frac{1}{r_{12}} + \frac{1}{r_{13}}. (2)$$

Here r_1 , σ_1 denote the space and spin coordinates of the incident electron, while r_2 , σ_2 and r_3 , σ_3 denote those of the bound atomic electrons. The functions Φ and Ψ satisfy the following Schrödinger equations:

$$(H_0 - E)\Phi = 0 \tag{3a}$$

$$(H - E)\Psi = 0 \tag{3b}$$

where the total Hamiltonian of the system is $H = H_0 + V$. Here H_0 is the unperturbed Hamiltonian and E is the total energy of the system. If the interaction potential is divided according to

$$V = U + \dot{W} \tag{4}$$

then the T matrix may be written as (Taylor 1972)

$$T = \langle \Phi_f(\mathbf{r}_1 \sigma_1; \mathbf{r}_2 \sigma_2, \mathbf{r}_3 \sigma_3) | U | \bar{\chi}_i^+(\mathbf{r}_1 \sigma_1; \mathbf{r}_2 \sigma_2, \mathbf{r}_3 \sigma_3) \rangle$$

$$+ \langle \bar{\chi}_f^-(\mathbf{r}_1 \sigma_1; \mathbf{r}_2 \sigma_2, \mathbf{r}_3 \sigma_3) | W | \Psi_i^+(\mathbf{r}_1 \sigma_1, \mathbf{r}_2 \sigma_2, \mathbf{r}_3 \sigma_3) \rangle$$
(5)

where the functions $\bar{\chi}$ satisfy

$$(H_0 + U - E)\bar{\chi} = 0. \tag{6}$$

Furthermore, if the potential U is chosen to depend on the coordinates of the incident electron only, then the solution of equation (6) (as well as that of equation (3a)) is the product of an unperturbed atomic wavefunction and a scattering function which depends only on the coordinates of the scattered particle. Thus the first term on the right-hand side of (5) vanishes for inelastic transitions. The total wavefunction

 Ψ_i^+ , which must be fully antisymmetrised to take exchange scattering into account, can be written as

 $\Psi_i^+(\mathbf{r}_1\sigma_1,\mathbf{r}_2\sigma_2,\mathbf{r}_3\sigma_3)$

$$= \psi_i^+(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}_3) S(\sigma_1, \sigma_2, \sigma_3) + \psi_i^+(\mathbf{r}_2; \mathbf{r}_3, \mathbf{r}_1) S(\sigma_2, \sigma_3, \sigma_1) + \psi_i^+(\mathbf{r}_3; \mathbf{r}_1, \mathbf{r}_2) S(\sigma_3, \sigma_1, \sigma_2)$$
(7)

where ψ denotes the spatial part and S the spin part of the wavefunction. Similarly we can write

$$\tilde{\chi}_{f}^{-}(\mathbf{r}_{1}\sigma_{1}; \mathbf{r}_{2}\sigma_{2}, \mathbf{r}_{3}\sigma_{3}) = \chi_{f}^{-}(\mathbf{r}_{1}; \mathbf{r}_{2}, \mathbf{r}_{3})S(\sigma_{1}, \sigma_{2}, \sigma_{3}).$$
 (8)

When the helium atom is initially in a triplet state the total spin of the system can be either $\frac{1}{2}$ (doublet state) or $\frac{3}{2}$ (quartet state). Using the explicit form of the spin functions we obtain

$$T^{(4)} = T_{\rm D}^{(4)} + 2T_{\rm E}^{(4)} \tag{9a}$$

for the quartet state and

$$T^{(2)} = T_{\rm D}^{(2)} - T_{\rm E}^{(2)} \tag{9b}$$

for the doublet state, where

$$T_{\rm D} = \int \chi_f^{-*}(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}_3) W \psi_i^{+}(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}_3) \, \mathrm{d}\mathbf{r}_1 \, \mathrm{d}\mathbf{r}_2 \, \mathrm{d}\mathbf{r}_3$$
 (10)

and

$$T_{\rm E} = \int \chi_f^{-*}(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}_3) W \psi_i^{+}(\mathbf{r}_2; \mathbf{r}_3, \mathbf{r}_1) \, \mathrm{d}\mathbf{r}_1 \, \mathrm{d}\mathbf{r}_2 \, \mathrm{d}\mathbf{r}_3. \tag{11}$$

We now make the usual distorted-wave approximation by replacing ψ_i^+ by χ_i^+ . Thus we can write

$$\psi_i^+(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}_3) = F_i^+(\mathbf{r}_1) v_i(\mathbf{r}_2, \mathbf{r}_3) \tag{12a}$$

and

$$\chi_f^-(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}_3) = F_f^-(\mathbf{r}_1) v_f(\mathbf{r}_2, \mathbf{r}_3)$$
 (12b)

where F_i^+ and F_f^- are the scattered-electron wavefunctions in the initial and final channels respectively and v_i and v_f are the bound-state atomic wavefunctions for the initial and final states. For these bound states we use numerical frozen-core Hartree-Fock functions, which can be expressed as

$$v(\mathbf{r}_{2}, \mathbf{r}_{3}) = 2^{-1/2} (R_{1s}(\mathbf{r}_{2}) Y_{00}(\hat{\mathbf{r}}_{2}) R_{nl}(\mathbf{r}_{3}) Y_{lm}(\hat{\mathbf{r}}_{3}) - R_{1s}(\mathbf{r}_{3}) Y_{00}(\hat{\mathbf{r}}_{3}) R_{nl}(\mathbf{r}_{2}) Y_{lm}(\hat{\mathbf{r}}_{2}))$$
(13)

where n, l, m denote the quantum numbers of the initial or final atomic state. In particular, R_{1s} is just the radial function for He^+ . Thus the scattered wavefunctions satisfy

$$(\nabla_1^2 - 2U_i + k_i^2)F_i^+(\mathbf{r}_1) = \rho(S) \int K(\mathbf{r}_1, \mathbf{r}_2)F_i^+(\mathbf{r}_2) d\mathbf{r}_2$$
 (14)

and

$$(\nabla_1^2 - 2U_f + k_f^2)F_f^-(\mathbf{r}_1) = 0 ag{15}$$

where the exchange kernel is given by

$$K(\mathbf{r}_1, \mathbf{r}_2) = \int v_i(\mathbf{r}_2, \mathbf{r}_3) (\nabla_1^2 - 2V + k_i^2) v_i(\mathbf{r}_3, \mathbf{r}_1) d\mathbf{r}_3$$
 (16)

with $k^2 = 2(E - E_A)$, where E_A is the energy of the atomic state. Also $\rho(S) = 1$ for a doublet state and -2 for a quartet state. The potentials U_j are the distorting potentials in channel j and are expressed as $U_j = V_j + V_j^{\text{pol}}$. Here

$$V_i = \langle v_i(\mathbf{r}_2, \mathbf{r}_3) | V | v_i(\mathbf{r}_2, \mathbf{r}_3) \rangle \tag{17}$$

is the static potential and the polarisation potential is given by

$$V_i^{\text{pol}} = \langle v_i(\mathbf{r}_2, \mathbf{r}_3) | V | v_i^{\text{pol}}(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}_3) \rangle \tag{18}$$

where, following the polarised-orbital formulation of Stone (1966), we write the first-order perturbed wavefunction for S states as

$$v_{ns}^{\text{pol}}(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}_3) = \beta_{ns}(\mathbf{r}_1) \sum_{m} Y_{lm}^*(\hat{\mathbf{r}}_1) v_{npm}(\mathbf{r}_2, \mathbf{r}_3)$$
 (19a)

and for P states as

$$v_{npm}^{\text{pol}}(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}_3) = \beta_{np}(\mathbf{r}_1) Y_{lm}(\hat{\mathbf{r}}_1) v_{ns}(\mathbf{r}_2, \mathbf{r}_3). \tag{19b}$$

Each function $\beta_i(r)$ is obtained by solving the pair of equations

$$\langle v_{ns}(\mathbf{r}_2, \mathbf{r}_3) | H_A + V - E | v_i(\mathbf{r}_2, \mathbf{r}_3) + v_i^{\text{pol}}(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}_3) \rangle = 0$$
 (20a)

$$\langle v_{npm}(\mathbf{r}_2, \mathbf{r}_3) | H_A + V - E | v_j(\mathbf{r}_2, \mathbf{r}_3) + v_j^{\text{pol}}(\mathbf{r}_1; \mathbf{r}_2, \mathbf{r}_3) \rangle = 0$$
 (20b)

where j represents the quantum numbers ns or npm. Here H_A represents the atomic Hamiltonian and (20) follows from minimising the energy of the atom in the field of a static electron. This formulation gives the dominant contribution to the dipole part of the polarisation potential. Expanding the scattering functions in partial waves, we have

$$F_{j}(\mathbf{r}) = \left(\frac{2}{\pi}\right)^{1/2} \frac{1}{k_{i}r} \sum_{lm} i^{l} u_{lk_{j}}(r) Y_{lm}(\hat{\mathbf{r}}) Y_{lm}^{*}(\hat{\mathbf{k}}_{j}). \tag{21}$$

By substituting this expression into (14) and (15) we obtain equations for the radial functions $u_{lk_j}(r)$; details are given in the appendix. From (10) and (11) we obtain the following expressions for the T matrices for excitation to the 3S states:

$$T_{\rm D} = \frac{1}{4\pi^2 k_i k_f} \sum_{l} (2l+1) t_{l,l}^{\rm D} P_l(\cos \theta)$$
 (22)

$$T_{\rm E} = \frac{1}{4\pi^2 k_i k_f} \sum_{l} \left((2l+1) t_{l,l}^{\rm E} P_l(\cos \theta) + \delta_{l0} (I_1 - I_2 + I_3 - I_4) \right). \tag{23}$$

Here the $P_l(\cos \theta)$ are the usual Legendre polynomials. Detailed expressions for the partial-wave T matrices and the other terms appearing in (22) and (23) are given in the appendix. Similarly, for excitation to the 3P states we have

$$T_{D,m=0} = \frac{-i\sqrt{3}}{4\pi^2 k_i k_f} \sum_{l} \left((l+1) t_{l,l+1}^D P_{l+1}(\cos \theta) - l t_{l,l-1}^D P_{l-1}(\cos \theta) \right)$$

$$T_{D,m=1} = \left(\frac{3}{2}\right)^{1/2} \frac{\mathrm{i} \,\mathrm{e}^{-\mathrm{i}\phi}}{4\pi^2 k_i k_f} \sum_{l} \left(t_{l,l+1}^D P_{l+1}^1(\cos\theta) + t_{l,l-1}^D P_{l-1}^1(\cos\theta)\right)$$

$$T_{E,m=0} = \frac{-\mathrm{i}\sqrt{3}}{4\pi^2 k_i k_f} \sum_{l} \left((l+1) t_{l,l+1}^E P_{l+1}(\cos\theta) - l t_{l,l-1}^E P_{l-1}(\cos\theta) + \delta_{l0} P_1(\cos\theta)(I_1 + I_3) + \delta_{l1}(I_2 + I_4)\right)$$
(24)

$$T_{E,m=1} = \left(\frac{3}{2}\right)^{1/2} \frac{\mathrm{i} \, \mathrm{e}^{-\mathrm{i}\phi}}{4\pi^2 k_i k_f} \sum_{l} \left(t_{l,l+1}^E P_{l+1}^1(\cos\theta) + t_{l,l-1}^E P_{l-1}^1(\cos\theta) + \delta_{l0} P_1^1(\cos\theta)(I_1 + I_3)\right)$$

where m is the quantum number of the final state and $P_l^1(\cos \theta)$ is the associated Legendre polynomial. Matrix elements with m = -1 are the complex conjugates of the elements with m = 1. Finally, the differential cross section is obtained by averaging over the spin states to yield

$$\frac{d\sigma}{d\Omega}(i \to f) = \frac{k_f}{k_i} 16\pi^4 (\frac{1}{3}|T^{(2)}|^2 + \frac{2}{3}|T^{(4)}|^2). \tag{25}$$

If the final state f is a P state then we sum (25) over the quantum number m to obtain the differential cross sections reported here. Total cross sections $\sigma(i \to f)$ are obtained by integrating over the angles θ and ϕ .

The asymmetry parameter is measured by scattering spin-polarised electrons from spin-polarised atoms, in this case metastable helium atoms with a magnetic spin quantum number equal to one. Thus we define the asymmetry parameter as

$$A = \frac{\sigma(2^{3}S, m_{s} = 1, \mu_{s} = -\frac{1}{2} \rightarrow n^{3}L) - \sigma(2^{3}S, m_{s} = 1, \mu_{s} = \frac{1}{2} \rightarrow n^{3}L)}{\sigma(2^{3}S, m_{s} = 1, \mu_{s} = -\frac{1}{2} \rightarrow n^{3}L) + \sigma(2^{3}S, m_{s} = 1, \mu_{s} = \frac{1}{2} \rightarrow n^{3}L)}$$
(26)

where m_s and μ_s are the magnetic spin quantum numbers for the atom and electron respectively and L is the orbital angular momentum of the final atomic state. This reduces to

$$A = \frac{\sigma^{(2)}(2^{3}S \to n^{3}L) - \sigma^{(4)}(2^{3}S \to n^{3}L)}{\sigma^{(2)}(2^{3}S \to n^{3}L) + 2\sigma^{(4)}(2^{3}S \to n^{3}L)}$$
(27)

where $\sigma^{(2)}$ and $\sigma^{(4)}$ represent the cross sections for the doublet and quartet states respectively.

3. Results

We have used equation (25) to evaluate the differential cross sections for excitation from the 2^3S state to the 2^3P , 3^3S and 3^3P states. Equation (A1) for the scattered radial wavefunction was solved via a non-iterative integral equation method as given in McEachran and Stauffer (1983). The integration that was required to evaluate the various contributions to the T matrices as given in (A5) was carried out on a fixed mesh over the range of the bound-state wavefunctions. However, the direct terms $t_{l,l'}^D$ have a long-range r^{-2} contribution in the case of excitation to the P states. This contribution was evaluated by transforming the integral in question into one containing a decaying exponential and using a Gaussian integration scheme (see Parcell *et al* 1987 for details).

The infinite sum over l in (24) can be performed by the Born subtraction technique (see equation (10) of Parcell *et al* 1983 for details), which is equivalent to replacing the matrix elements for high l values by the corresponding first Born values. In the

present calculation, distorted-wave values for $t_{l,l'}$ were used for l values as high as 50 in some cases in order to obtain converged results. It was found that for l > 6 we could drop the exchange contribution from (A1) without affecting the accuracy of our results. (In the case of excitation to the 3^3 S state at 30 eV we had to retain these exchange terms up to l = 9.) Dropping the exchange terms leads to a potential scattering equation of the form (A4), which is considerably easier to solve.

Our main criterion for these various approximations was that the differential cross section at 180° had converged to within one part in 10^{-4} .

In figures 1, 2 and 3 we show our results for the differential cross sections for final electron energies of 15, 20 and 30 eV, along with the experimental data of Müller-Fiedler et al (1984). We also include results from the ten-channel eikonal calculation of Flannery and McCann (1975), which were calculated with an incident electron energy of 20 eV, as well as the results of an improved version of this approximation (Mansky and Flannery 1985, Mansky 1986) at all three energies.

For the 2³S-2³P transition shown in figure 1 our results agree very well in shape with the experimental data, but lie somewhat below them except in the angular range 30-40° at 15 and 20 eV, where we lie within the experimental error bars. Our results are in generally good agreement with the results of Flannery and McCann (1975) and Mansky and Flannery (1985) for this transition, although their values lie slightly below

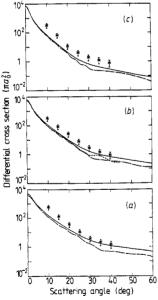


Figure 1. Differential cross sections for the 2^3S-2^3P transition at final electron energies of (a) 15, (b) 20 and (c) 30 eV: ____, present work; ---, Flannery and McCann (1975); _____, Mansky and Flannery (1985); $\frac{x}{2}$, experimental results of Müller-Fiedler et al (1984).

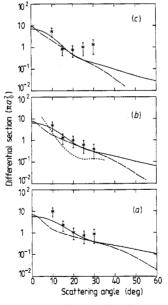


Figure 2. As figure 1 but for the 2^3S-3^3S transition.

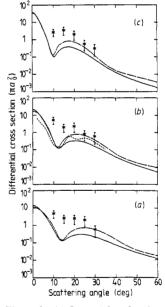


Figure 3. As figure 1 but for the 2³S-3³P transition.

ours and the experimental points. Since the energy at which they performed their calculations is below ours we would have expected their values to be above ours in general.

Figure 2 displays our results for the 2³S-3³S transition. In this case they agree very well with the experimental data at 15 and 20 eV, and for small angles at 30 eV. However, at this latter energy the experimental results show a rise at larger angles, whereas our values decrease monotonically, as was the case at lower energies. The results of Flannery and McCann lie considerably below both the present work and the experimental data, except for angles less than 10°. The results of Mansky and Flannery are closer to our results but in general lie below them and the experimental data. The Glauber approximation results of Khayrallah et al (1978) also lie much below the present ones, except for very small angles. They also exhibit a deep minimum at about 20° which is not present in the other calculations or the experiment.

In figure 3 we present the results for the 2³S-3³P transition. All three sets of calculations show a maximum in the cross section at approximately 20°. The experimental data show some evidence of a slight maximum in this angular neighbourhood, but lie considerably above all the theoretical results presented here. Above the angles at which the maxima occur the results of Flannery and McCann and Mansky and Flannery lie above ours and are within the experimental error bars at 25 and 30°.

As a check on our results, we have compared our Born cross sections with those of Kim and Inokuti (1969), who used elaborate correlated wavefunctions for their calculations. Our total cross sections agree with theirs to within 2% for the 2³S-2³P and 2³S-3³S transitions, and to within 7% for the 2³S-3³P transition. There are somewhat larger discrepancies between the differential cross sections, but they are very comparable in shape and magnitude for all the transitions studied.

Total cross sections were obtained by performing a numerical integration over the angles of the differential cross section. These results are given in table 1. Separate cross sections are shown for the doublet and quartet cases since they are needed in calculating the asymmetry parameter given in equation (27). These total cross section

Final energy (eV)	$\sigma^{(2)}$	$\sigma^{\scriptscriptstyle (4)}$	σ
$2^{3}S-2^{3}P$			
10	128.84	105.58	113.34
15	96.19	85.23	88.88
20	77.49	71.18	73.28
30	56.58	53.69	54.66
$2^{3}S-3^{3}S$			
10	3.709	2.798	3.102
15	2.528	2.056	2.214
20	1.915	1.629	1.725
30	1.287	1.150	1.196
$2^{3}S-3^{3}P$			
10	1.1343	0.5771	0.7628
15	0.8995	0.5678	0.6784
20	0.7826	0.5706	0.6413
30	0.6476	0.5405	0.5762

Table 1. Total cross sections in units of πa_0^2 . $\sigma = \frac{1}{3}\sigma^{(2)} + \frac{2}{3}\sigma^{(4)}$.

results are close to our first Born values, which are about 1% below the results shown in table 1 for the 2³S-2³P transition, 10-20% below for the 2³S-3³S transition and a similar amount above for the 2³S-3³P transition. Thus our cross sections lie above those calculated previously by Flannery *et al* (1975), Flannery and McCann (1975) and Khayrallah *et al* (1978). We are in closest agreement with Flannery and McCann; the differences are in the range 10-30%. Since our differential cross sections are in general below the experimental results, this implies that our total cross sections are if anything too low.

We found that dropping the exchange terms in (A1) made a difference of only a few per cent to the values obtained for the total cross sections. Greater differences occur for the differential cross sections at larger angles, especially if one compares the individual doublet and quartet cross sections.

The asymmetry values as defined in equations (26) and (27) are given in table 2. The values for the two transitions to final P states are roughly in the ratio 1:4, indicating that transitions to the 3³P state are more sensitive to the spin states of the system. This can also be seen by considering the relative values for the doublet and quartet cross sections given in table 1. No other results for this parameter have been published to date.

Final energy (eV)	2 ³ S-2 ³ P	2 ³ S-3 ³ S	2 ³ S-3 ³ P
10	0.0684	0.0979	0.244
15	0.0411	0.0711	0.163
20	0.0287	0.0553	0.110
30	0.0176	0.0382	0.062

Table 2. Asymmetry parameter.

4. Conclusions

We have calculated differential and total cross sections for the excitation of the 2³S state of helium to the 2³P, 3³S and 3³P states. Our results are in satisfactory agreement with the experimental data of Müller-Fiedler *et al* (1984) for the first two of these transitions, but somewhat less so for the latter one. Since the calculations of Flannery and McCann (1975) as well as those of Mansky and Flannery (1985) yielded results similar to ours for this latter transition, it would be of considerable interest to have further experimental measurements for this case. Forthcoming measurements of the asymmetry parameter should provide another sensitive test of the details of these calculations.

On the basis of these results it would appear that the distorted-wave approximation is capable of producing reliable cross sections for excitation from the triplet metastable state of helium in the energy range studied.

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Appendix

In this appendix we give details of the solution for the radial scattering wavefunction and the resulting T-matrix elements.

If we substitute (21) into (14) we obtain the following integro-differential equation for u_{lk} :

$$(d^{2}/dr^{2} - l(l+1)/r^{2} - 2(V_{i} + V_{i}^{pol}) + k_{i}^{2})u_{lk_{i}}(r)$$

$$+ \frac{1}{2}\rho(s)\{[(k_{i}^{2} + 4)\langle P_{1s}|u_{lk_{i}}\rangle P_{1s}(r) + (\varepsilon_{2s} + k_{i}^{2})\langle P_{2s}|u_{lk_{i}}\rangle P_{2s}(r)$$

$$+ 2\langle P_{1s}|u_{lk_{i}}\rangle(y_{l}(P_{1s}, P_{2s}; r)P_{2s}(r) - y_{l}(P_{2s}, P_{2s}; r)P_{1s}(r))]\delta_{l0}$$

$$- [2/(l+1)](y_{l}(P_{1s}, u_{lk_{i}}; r)P_{1s}(r) + y_{l}(P_{2s}, u_{lk_{i}}; r)P_{2s}(r))\} = 0$$
(A1)

where

$$y_t(f, g; r) = \frac{1}{r} \left(\int_0^r f(t)g(t) \left(\frac{t}{r} \right)^t dt + \int_r^\infty f(t)g(t) \left(\frac{r}{t} \right)^{t+1} dt \right)$$
 (A2)

and

$$\langle f|g\rangle = \int_0^\infty f(t)g(t) \, \mathrm{d}t.$$
 (A3)

We have also written $P_{nl}(r) = rR_{nl}(r)$, and ε_{2s} is the Hartree-Fock energy parameter for the 2s orbital. Similarly, substitution of (21) into (15) yields

$$(d^2/dr^2 - l'(l'+1)/r^2 - 2(V_f + V_f^{pol}) + k_f^2)u_{l'k_f}(r) = 0.$$
(A4)

We can now derive detailed expressions for the terms in equations (22)-(25). These are

$$t_{l,l'}^{D} = \frac{2}{2l_{f}+1} \int_{0}^{\infty} u_{l'k_{f}}(r) y_{l_{f}}(P_{nl'_{f}}P_{2s}; r) u_{lk_{i}}(r) dr$$

$$t_{l,l'}^{E} = \frac{-1}{2l'+1} \int_{0}^{\infty} u_{l'k_{f}}(r) y_{l'}(u_{lk'_{i}}P_{nl_{f}}; r) P_{2s}(r) dr$$

$$I_{1} = \frac{1}{2l_{f}+1} \langle P_{1s} | u_{sk_{i}} \rangle \int_{0}^{\infty} u_{l_{f}k_{f}}(r) y_{l_{f}}(P_{1s}, P_{nl_{f}}; r) P_{2s}(r) dr$$

$$I_{2} = \langle P_{nl_{f}} | u_{l_{f}k_{i}} \rangle \int_{0}^{\infty} u_{sk_{f}}(r) y_{0}(P_{1s}, P_{1s}; r) P_{2s}(r) dr$$

$$I_{3} = \frac{-1}{2l_{f}+1} \langle P_{1s} | u_{sk_{i}} \rangle \int_{0}^{\infty} u_{l_{f}k_{f}}(r) y_{l_{f}}(P_{2s}, P_{nl_{f}}; r) P_{1s}(r) dr$$

$$I_{4} = -\langle P_{nl_{f}} | u_{l_{f}k_{i}} \rangle \int_{0}^{\infty} u_{sk_{f}}(r) y_{0}(P_{1s}, P_{2s}; r) P_{1s}(r) dr.$$
(A5)

Note that all of the above quantities depend implicitly on n and l_f , the principal and angular momentum quantum numbers of the final state of the atom. These quantities also depend on whether the system is in a doublet or quartet spin state via the scattering function u_{lk_f} , which satisfies different forms of equation (A1) for these different states.

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