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Electron impact excitation cross sections of the $1s2s$ ^3S metastable state of helium

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Abstract. The differential and integral cross sections for the excited states $1s2p$ ^3P, $1s3s$ ^3S, $1s3p$ ^3P and $1s3d$ ^3D of helium from the metastable state $1s2s$ ^3S are calculated using the relativistic distorted wave method. A systematical comparison is made with the available experimental and theoretical results. Better agreement is found when the present results are compared with previous calculations and experiments for the integral cross sections. For differential cross sections, our results are in general agreement with the experimental data compared with the previous theoretical values.

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Key words: relativistic distorted-wave method, electron impact excitation, differential cross sections

1 Introduction

Excitation out of the metastable levels of rare gases is an important mechanism in a wide variety of phenomena. Accurate cross sections for electron impact excitation out of the metastable levels of rare gases are important for modelling and understanding processes that occur in gas discharge lasers, industrial plasmas, astrophysical plasmas, and electron-beam pumped lasers. Besides long lifetimes and the metastable states of rare gas atoms are known for having rather large electron impact excitation cross sections compared with the ground states. The behaviour of the cross sections for excitation out of the metastable levels has been found to be quite different from the behaviour of the cross sections for excitation out of the ground levels. For example, it is well known that excitations out of the ground state of helium corresponding to dipole-allowed transitions generally show large cross section values, whereas excitations corresponding to dipole-forbidden transitions have smaller cross sections. Yet some excitations out of the 2^3S metastable level of helium corresponding to dipole-allowed transitions

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have been shown to have smaller cross sections than excitations corresponding to dipole-forbidden transitions [1–3]. In the case of the 2^3S metastable level of helium, much theoretical [4–14] and experimental [1, 2, 15–19] work has been done on calculating and measuring both differential and integral cross sections for electron excitation out of these excited levels.

On the theoretical side, Flannery *et al.* [4] calculated the differential and total cross sections for the excitations of the states $2^{1,3}P$, $3^{1,3}S$, $3^{1,3}P$ and $3^{1,3}D$ from the metastable states $2^{1,3}S$ of helium using a ten-channel eikonal approximation. Khayrallah *et al.* [5] calculated the differential and total cross sections for the excitation of the state 3^3S from the state metastable 2^3S of helium in the Glauber approximations. Gupta *et al.* [6] reported the differential cross sections of helium from the metastable state 2^3S to the state 3^3S in the two-potential modified Born approximation. Berrington *et al.* [7] calculated total cross sections from the ground state 1^1S and the metastable states 2^3S and 2^1S of helium to the higher $n = 2$, 3 states by 11-state R-matrix. Mathur *et al.* [8], Mansky *et al.* [9] and Franca *et al.* [10] calculated the differential and total cross sections for the excitation of helium from the metastable state 2 ^3S to the states 2^3P, 3^3S, 3^3P and 3^3D using a distorted-wave approximation, the semiclassical multichannel eikonal method and the first-order many-body theory, respectively. Bray *et al.* [11] calculated the differential and total cross sections for the excitation of the states 2^3P, 3^3S, 3^3P, 3^3D, 4^3S, 4^3P, 4^3D and 4^3F of helium from the metastable states 2^1S and 2^3S using the convergent close-coupling method. Cartwright *et al.* [12] reported the differential and total cross sections for excitation from the metastable states 2^1S and 2^3S to the states $2^{1,3}P$, $3^{1,3}S$, $3^{1,3}P$ and $3^{1,3}D$ using the first-order many-body theory and the distorted wave approximation. Verma *et al.* [13] calculated the differential and total cross sections of helium from the metastable state 2^3S to the higher states $n^{1,3}S$ and $n^{1,3}P$ ($n = 2$, 3, 4). Bartschat *et al.* [14] studied electron impact excitation of helium from the ground state 1^1S and the metastable state 2 ^3S to the higher $n = 2$, 3 states using the R-matrix with pseudo-state.

On the experimental side, Muller-Fiedler *et al.* [15] performed a crossed-beam experiment to measure the differential cross sections for excitation from the metastable state 2^3S to the states 2^3P, 3^3S, 3^3P and 3^3D. Rall *et al.* [16] measured the excitation cross sections of the states 3^3S, 3^3P, 3^3D, 4^3S, 4^3D, 5^3D and 6^3D from the metastable state 2^3S of helium. Lagus *et al.* [17] measured the excitation cross sections of the states 3^3S, 3^3P, 3^3D, and 4^3D from the metastable state 2^3S of helium using a fast metastable atomic beam target. Piech *et al.* [1] measured the excitation cross sections out of the metastable state 2^3S of helium into the the states 2^3P, 3^3S, 3^3P, 3^3D, 4^3S, 4^3P, 4^3D, 5^3S and 5^3D using a laser-induced fluorescence technique. Piech *et al.* [2] also used the optical method to measure the excitation cross sections of the states 2^3P, 3^3S, 3^3P, 3^3D, 4^3S, 4^3P, 4^3D, 5^3S, 5^3P, 5^3D, 6^3S, 6^3P, 6^3D, 7^3S, 7^3P, 7^3D, 8^3S, 8^3P and 8^3D from the metastable state 2^3S of helium. Boffard *et al.* [18] measured the excitation cross sections of the states 3^3S, 3^3P, 3^3D, and 4^3D from the metastable state 2^3S of helium at high electron energies. Uhlmann *et al.* [19] performed using a magneto-optical trap technique to measure the excitation cross sections of the state 2^3P from the metastable state 2^3S.

For excitation cross sections of measure, there are some discrepancies among different experimental results because of using different experimental methods. But all experimental values are more consistent comparison with theoretical calculation. The discrepancy of cross sections in different theoretical methods, and the discrepancy between experiment and theory are larger, especially for the differential cross sections calculation, the discrepancy among the different theoretical results are 1–2 order of magnitude for some transitions. For example, Verma *et al.* [13] using distorted wave approximation calculated the differential cross section of the states 3^3S and 3^3P from the metastable state 2^3S at scattered electron energies of 15 eV comparison with other experimental and theoretical values.

As we known, atomic helium is the simplest multielectron closed-shell atomic system of low Z. For e-He(2^3S) impact excitation, the accurate wave functions calculation of the target states are crucial. However, the influence of the accurate wave functions calculation for helium is how to efficacious consider configurations interaction. In this work, we calculate the wave functions of helium based on configurations interaction is considered systematically by using multiconfiguration Dirac-Fork (MCDF) [20] method. The differential and total cross sections for excitation from the metastable state 2^3S to the states 2^3P, 3^3S, 3^3P and 3^3D are reported using the fully relativistic distorted wave method. The present results are compared with the available experiments and the theoretical calculations.

2 Theoretical method

In our calculations, the wave functions of the target states are generated by the widely used atomic structure package Grasp92 [20] The wave functions for both the initial and final states of the impact systems are the antisymmetric wave functions of the total $(N+1)$-electron system including the target ion plus a continuum electron, which can be written as [3,21,22]

$$\Psi=\frac{1}{(N+1)^{1/2}}\sum_{p=1}^{N+1}(-1)^{N+1-p}\sum_{M_t,m}C(J_tjM_tm;JM)\Phi_{\beta_tJ_t}(x_p^{-1})u_{\kappa m\varepsilon}(x_p), \tag{1}$$

where C is Clebsch-Gordon coefficient, J_t, j, and J are the angular momentum quantum numbers of the target ion, continuum electron and the impact system, respectively. $\Phi_{\beta_tJ_t}$ are the target-ion wave functions. β_t represents all other quantum numbers in addition to J_t. x_p designates the space and spin coordinates for electron p and x_p^{-1} is the space and spin coordinates of all the N electrons other than p. $u_{\kappa m\varepsilon}$ is the relativistic distorted-wave Dirac spinor for a continuum electron, and κ is the relativistic quantum number. The continuum orbitals with given electron energy are solutions of the Dirac-Fock equations [3,21], in which the direct and exchange potentials were considered in the total $(N+1)$-electron system.

The electron impact excitation (EIE) scattering amplitude $B_{m_{sf}}^{m_{si}}$ can be written as [21–24]

$$B_{m_{sf}}^{m_{si}}=\frac{2a_0\pi^{\frac{1}{2}}}{k_i}\sum_{\substack{l_i,j_i,m_i,l_f\\ m_{lf},j_f,m_f}}\sum_{J,M}(i)^{l_i-l_f}(2l_i+1)^{\frac{1}{2}}exp[i(\delta_{k_i}+\delta_{k_f})]Y_{lf}^{m_{lf}}C\left(l_i\frac{1}{2}0m_{s_i};j_im_i\right)$$
$$\times C\left(l_f\frac{1}{2}m_{lf}m_{sf};j_fm_f\right)C(J_ij_iM_im_i;JM)C(J_fj_fM_fm_f;JM)R(\gamma_i,\gamma_f), \tag{2}$$

where a_0 is the Bohr radius, C's are Clebsch-Gordan coefficients. γ_i, γ_f, J and M are the quantum numbers corresponding to the total angular momentum of the complect system, target ion plus free electron, and its z component, respectively. m_{si}, l_i, j_i, m_{l_i} and m_i are the spin, orbital angular momentum, total angular momentum, and its z component quantum numbers, respectively, for the incident electron. δ_{k_i} is the phase factor for the continuum electron. κ is the relativistic quantum number, which is related to the orbital and total angular momentum l and j. $R(\gamma_i,\gamma_f)$ is the collision matrix elements, which is given by

$$R(\gamma_i,\gamma_f)=\left\langle \Psi_i \left| \sum_{p,q p<q}^{N+1} (V_{Coul}+V_{Breit}) \right| \Psi_f \right\rangle, \tag{3}$$

where V_{Coul} is the Coulomb operator and V_{Breit} is the Breit operator [25].

The differential cross sections can be written as [26,27]

$$\frac{dQ}{d\hat{k}_f}=\frac{1}{g_i}\sum_{M_i,M_j}\frac{1}{2}\sum_{m_{si},m_{sf}}|B^{m_{si}}_{m_{sf}}|^2, \tag{4}$$

where g_i is the statistical weight of the initial level of the N-electron target ion.

The relativistic distorted wave (RDW) EIE integral cross sections $\sigma_{if}(\varepsilon)$ from an initial state i to final state f can be written as [3,21,23,24]

$$\sigma_{if}(\varepsilon)=\int \frac{dQ}{d\hat{k}_f}d\Omega=\frac{\pi a_0^2}{k_i^2 g_i}\sum_J(2J+1)\sum_{\kappa,\kappa'}|R(\gamma_i,\gamma_f)|^2, \tag{5}$$

where k_i is the relativistic wave number of the incident electron, and κ and κ' are the relativistic quantum number of the initial and final continuum electrons, respectively.

3 Results and discussion

In the calculations of wave functions of the target states, our model includes the $1s^2$, $1s2s$, $1s2p$, $1s3s$, $1s3p$, $1s3d$, $2s^2$, $2s2p$, $2s3s$ and $3s^2$ configurations. In the calculations of the EIE cross sections, to ensure the convergence of the collision strengths, we have included explicitly all partial waves up to $l=40$.

In order to exposit the accuracy of the present calculations, in Table 1 we list the calculated excitation energies, transition probabilities and oscillator strength for the triplet states of $1s2p$, $1s3s$, $1s3p$ and $1s3d$ levels, relative to the metastable state $1s2s\ ^3S$. The excitation energies are compared with the $NIST$ values [30]. It is clearly seen that the agreement between the current excitation energies and the values in $NIST$ atomic spectra database is very good, and the differences are small than 1% in most cases. For the electric dipole (E1) transition the rates from the Coulomb gauge and Babushkin gauge agree to about 10%, the electric quadrupole (E2) transition the rates from the Coulomb gauge and Babushkin gauge agree to within 12%. For the oscillator strength from different gauges are within 15% of each other. From this

Table 1: Excitation energies ($\triangle E$), transition probabilities (A) and oscillator strengths (gf) from the metastable state 1s2s^3S.

Excitation	$\triangle E$ (eV)		Type	$A(s^{-1})$		gf	
	Present	NIST [30]		C	B	C	B
$1s2p\ ^3P_2$	1.09	1.12	E1	7.738(06)	7.914(06)	7.183(-01)	7.469(-01)
$1s2p\ ^3P_1$	1.15	1.15	E1	7.535(06)	7.728(06)	4.073(-01)	4.481(-01)
$1s2p\ ^3P_0$	1.15	1.14	E1	7.444(06)	7.613(06)	1.319(-01)	1.573(-01)
$1s3s\ ^3S_1$	2.92	2.90	E2	1.145(-09)	2.275(-9)	1.087(-17)	1.241(-17)
$1s3p\ ^3P_2$	3.20	3.19	E1	5.133(06)	5.922(06)	6.587(-02)	7.041(-02)
$1s3p\ ^3P_1$	3.20	3.19	E1	5.765(06)	5.875(06)	4.420(-02)	4.938(-02)
$1s3p\ ^3P_0$	3.20	3.19	E1	6.183(06)	6.861(06)	1.576(-02)	1.942(-02)
$1s3d\ ^3D_2$	3.28	3.26	E2	1.486(02)	1.651(02)	1.691(-06)	2.017(-06)
$1s3d\ ^3D_3$	3.28	3.26	E2	1.485(02)	1.653(02)	2.366(-06)	2.824(-06)
$1s3d\ ^3D_1$	3.28	3.26	E2	1.487(02)	1.651(02)	1.014(-06)	1.610(-06)

comparison, it becomes clear that the present calculation can give a accurate description for the corresponding target states.

In Figs. 1 and 2, we show our results for the differential cross sections of the states 2^3P, 3^3S, 3^3P and 3^3D of helium from the metastable state 2^3S for final electron energies of 15, 20 and 30 eV, along with the experimental data of Muller-Fiedler *et al.* [15]. We also include results from the ten-channel eikonal calculation of Flannery *et al.* [4], the 11-state R-matrix results of Berrington *et al.* [7], the convergent close-coupling results of Bray *et al.* [11], the first-order many-body results of *Franca et al.* [10] and Cartwright *et al.* [12], as well as the results of distorted-wave approximation of Mathur *et al.* [8], Mansky *et al.* [9], Cartwright *et al.* [12] and Verma *et al.* [13].

For the $2^3S \rightarrow 2^3P$ transition shown in Fig. 1(a), (b) and (c) our results agree very well in shape with the experimental data. Our results are in generally good agreement with the results of Franca *et al.* [10] at 20 eV, but their results lie slightly below oures and the experimental points in the angular range 40–60° at 15 eV. The results of Berrington *et al.* [11] lie slightly high ours results in the angular range 40–60° at 30 eV. In the large angular range, the present results agree with the distorted-wave approximation values of Cartwright *et al.* [12].

Fig. 1(d), (e) and (f) display our results for the $2^3S \rightarrow 3^3S$ transition. In this case they agree very well with the experimental data at 15 and 20 eV, but small at 30 eV. However, the discrepancy among the different theoretical results are large at 15 and 30 eV. The first-order many-body results of Franca *et al.* [10] and Cartwright *et al.* [12] are closer to the 11-state R-matrix results of Berrington *et al.* [7] but lie below the experimental data in the angular range 20–40° at 15 and 20 eV. The results of distorted-wave approximation of Cartwright *et al.* [12] are closer to our results. The distorted-wave approximation results of Verma *et al.* [13] are small one order of magnitude obviously, compared with the other available theoretical values including our results at 30 eV.

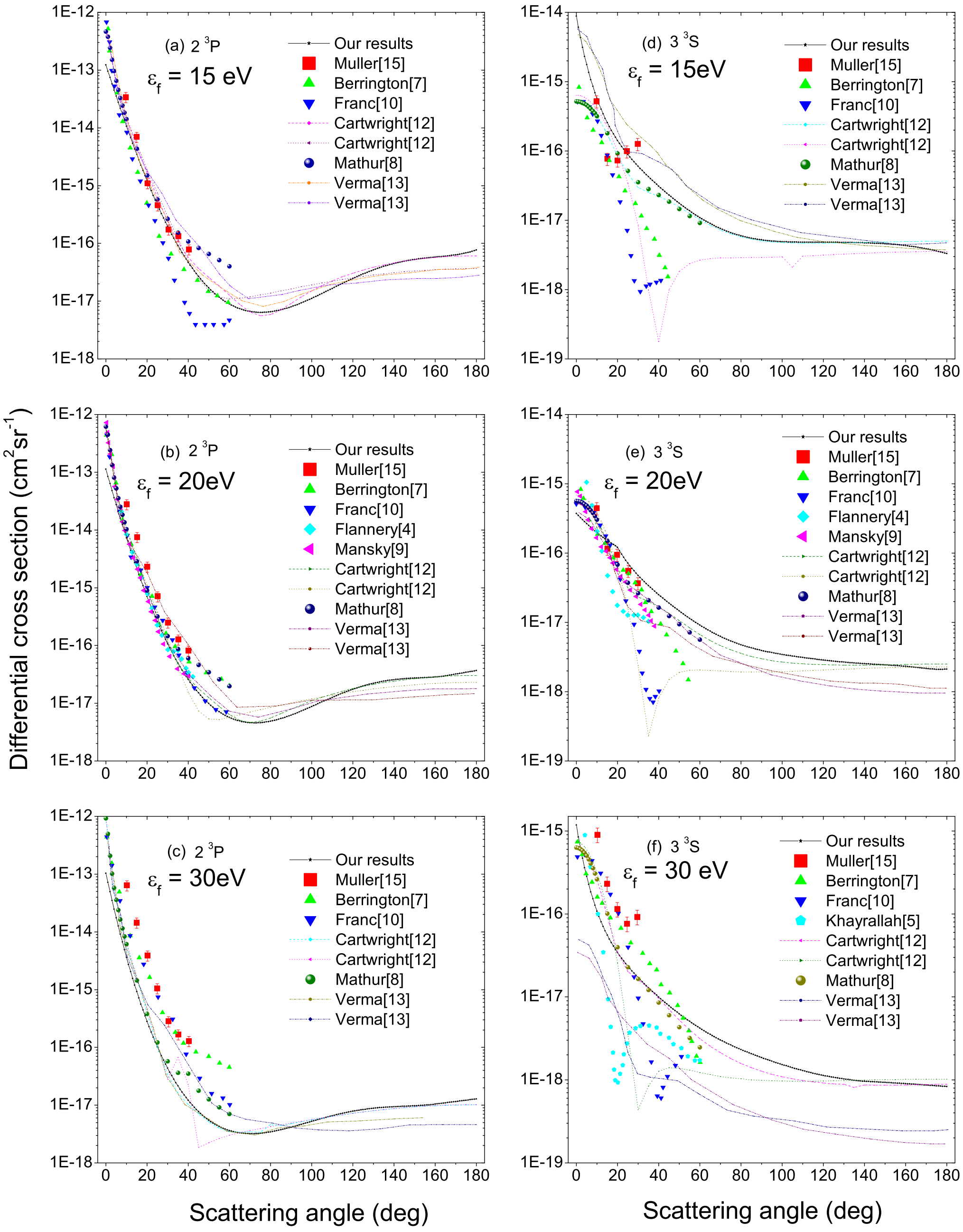

Figure 1: The differential cross sections of the states 2^3P and 3^3S from the metastable state 2^3S of helium (ε_f represents scattered electron energies), compared with the experiments of Muller *et al.* [15], as well as the theoretical calculations of Flannery *et al.* [4], Khayrallah *et al.* [5], Berrington *et al.* [7], Mathur *et al.* [8], Mansky *et al.* [9], Franc *et al.* [10], Cartwright *et al.* [12] and Verma *et al.* [13].

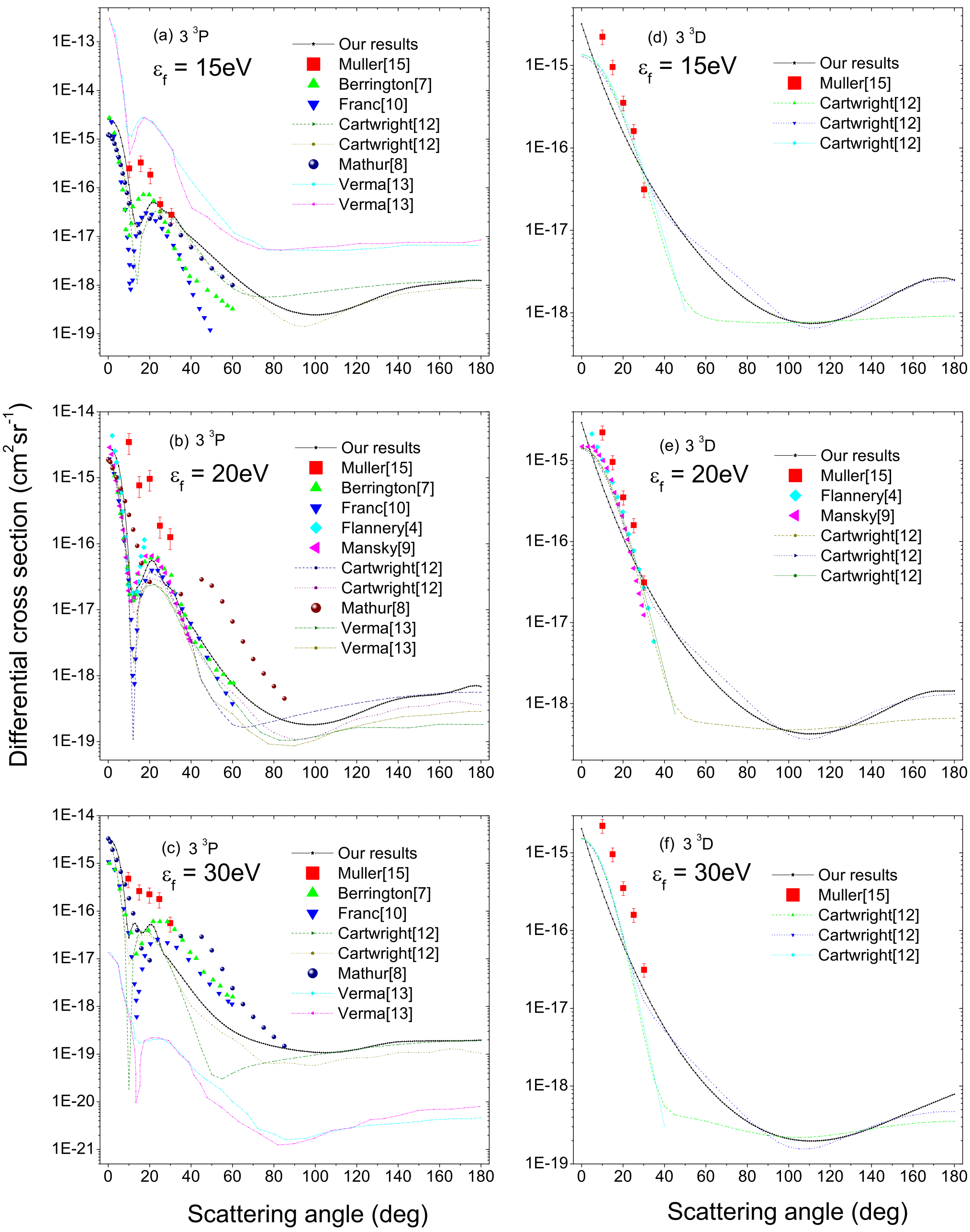

Figure 2: The differential cross sections of the states 3^3P and 3^3D from the metastable state 2^3S of helium (ε_f represents scattered electron energies), compared with the experiments of Muller *et al.* [15], as well as the theoretical calculations of Flannery *et al.* [4], Berrington *et al.* [7], Mathur *et al.* [8], Mansky *et al.* [9], Franca *et al.* [10], Cartwright *et al.* [12] and Verma *et al.* [13].

In Fig. 2(a), (b) and (c) we present the results for the $2^3S \rightarrow 3^3P$ transition. All theoretical calculations including our results show a maximum in the cross section at approximately 20° at 15 and 20 eV. The experimental data show some evidence of a slight maximum in this angular neighbourhood, but lie considerably above all the theoretical results presented here. In general, our results are more closer to the results of distorted-wave approximation of Cartwright *et al.* [12]. However, the distorted-wave approximation results of Verma *et al.* [13] are large one order of magnitude at 15 eV, small two order of magnitude at 30 eV obviously, compared with the other available theoretical values and our results.

Fig. 2(d), (e) and (f) exhibit our results for the $2^3S \rightarrow 3^3D$ transition. For this transition, experimental and theoretical values are rare. Through comparison we found that the first-order many-body results are closer to the Born approximation results of Cartwright *et al.* [12]. The present results are more closer to the results of distorted-wave approximation of Cartwright *et al.* [12].

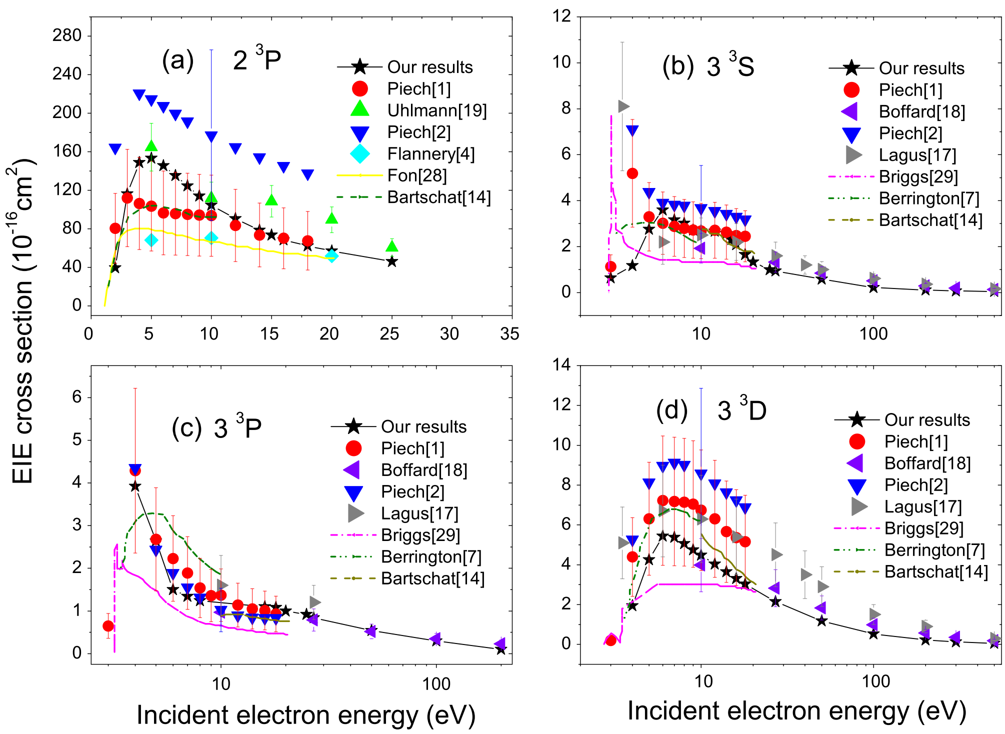

Figure 3: The EIE cross sections of helium from the metastable state 2^3S to the states 2^3P (a), 3^3S (b), 3^3P (c) and 3^3D (d), compared with the experiments of Piech *et al.* [1,2], Lagus *et al.* [17], Boffard *et al.* [18] and Uhlmann *et al.* [19], as well as the theoretical calculations of Flannery *et al.* [4], Berrington *et al.* [7], Bartschat *et al.* [14], Fon *et al.* [28] and Briggs *et al.* [29].

In Fig. 3, we further showed our DWA total cross sections and compared with experimental data [1, 2, 17–19] and theoretical values [4, 7, 14, 28, 29]. Total cross sections are obtained by performing a numerical integration over the angles of the differential cross section. The results for the transition $2^3S \to 2^3P$, $2^3S \to 3^3S$, $2^3S\to 3^3P$ and $2^3S \to 3^3D$ are exhibited Figs. 3(a), (b), (c) and (d). This results are obtained up to 500 eV the incident electron energy. It can be seen from Fig. 3 that there are some discrepancies among different experimental data and the uncertainties of experiment are also large, the present calculations lie closer to the newly experimental values of Uhlmann *et al.* [19].

4 Conclusions

In summary, we have carried out systematic calculations of the differential cross sections and integral cross sections for the electron impact excitation of helium from its metastable state 2^3S to the higher excited states 2^3P, 3^3S, 3^3P and 3^3D. The present results for the $2^3S \to 2^3P$, $2^3S \to 3^3S$, $2^3S \to 3^3P$ and $2^3S \to 3^3D$ excitation are compared with the available experimental data. An overall agreement with those experimental data is generally good. We also compare our cross sections with other theoretical results available so far. Difference in the different calculations is found to be large. Especially for the differential cross sections, the discrepancy between the distorted wave approximation calculated results of Verma *et al.* [13] and the different experimental and theoretical values is 1–2 order of magnitude for $2^3S \to 3^3S$ and $2^3S \to 3^3P$ transitions at scattered electron energies of 15 and 30 eV. The integral cross sections has been calculated up to 500 eV. For the excitations of 2^3P, 3^3S, 3^3P and 3^3D, the newly experimental values of Uhlmann *et al.* [19] lie more closer to the present calculations.

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