J-matrix calculation of electron-helium S-wave scattering. II. Benchmark cross sections below ionization threshold

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In the preceding paper [D. A. Konovalov *et. al.* Phys. Rev. A **84**, 032707 (2011)], the S-wave e-He scattering (S-e-He) problem was solved within the frozen-core (FC) model of helium for impact energies in the range 0.1-1000eV. In this sequel, both target electrons are described within the configuration-interaction model of helium obtaining significantly more accurate (compared to the FC model) first seven bound states of the helium S-wave model. The presented JM results are confirmed by the corresponding the convergent-close-coupling (CCC) calculations providing total elastic, $2^{1,3}S$, $3^{1,3}S$ excitation cross sections with a benchmark level of accuracy for the considered S-e-He problem below the ionization threshold.

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I. INTRODUCTION

Resonances in electron-atom scattering processes is a striking quantum mechanical phenomenon, which were comprehensively reviewed by Schulz [1] in 1973 and then by Buckman and Clark [2] in 1994. Historically and limiting the scope of this introduction to the helium and atomic hydrogen scattering targets, in 1962 Burke and Schey [3] theoretically predicted a very sharp resonance in the elastic e-H scattering at 9.6 eV with a half-width (Γ) of 0.1 eV. The resonances were confirmed experimentally first for the e-He scattering, when in 1963 Schulz [4] observed the resonance in the elastic e-He scattering at 19.3 eV with Γ=0.06 eV. Since their discovery in the 1960s, the resonances have been and continue to be studied extensively for e-H [5–11] and e-He [12–16] (citing only studies not already referenced in [1, 2]), where it is well understood that the resonances are nothing more (nor less) than the manifestation of the negative-ion metastable states [2].

This study focuses on the resonances in the S-wave e-He (S-e-He) scattering, where the target helium atom is in its ground state before the electron impact, and where only the partial wave with zero angular momentum ($l = 0$) is retained in all calculations and partial-wave expansions. The S-wave model has proven to be a very productive testing ground for scattering theories, see [17–34] for the S-wave e-H scattering (S-e-H) and [35–43] for the S-e-He problem. The main attraction of the S-wave model is that it retains most of the physics complexities of the full scattering problems while simplifying the problems computationally. In particular, it is somewhat expected or implied that if a theoretical method solves the S-wave model, then the remaining partial waves could be solved with additional computational resources, which is in deed the case for the CCC [44] and JM [7, 12] methods.

The main goal of this study is to provide high accuracy total elastic and excitation S-e-He cross sections below the ionization threshold, focusing on their resonant features. The need for such benchmark theoretical data is evident from the existing *ab initio* attempts to solve the S-e-He problem. Reviewing in reverse chronological order, in 2010 Bartlett and Stelbovics [41] developed a four-body propagating exterior scaling (PECS) method and reported results claiming to achieve "benchmark" level of accuracy. However none of their cross sections, including elastic and $2^{1,3}S$ excitation cross sections, displayed any resonances at the accuracy level achieved for the S-e-H problem [19]. In 2005, Horner et al. [40] reported results using time-dependent exterior complex scaling (TD-ECS), which also failed to described resonance behavior of the cross sections. The notable exception is the convergent-close-coupling (CCC) method which in 2002 and 2004 [37, 38] did not examine the resonance regions with sufficiently fine energy grid. This is now corrected to some extent when in 2011 Konovalov et al. [43] reported the CCC and J-matrix (JM) *frozen-core* (FC) results clearly showing the resonances in the elastic and $n = 2$ (2^1S and 2^3S) excitation cross sections.

The stated goal is achieved by applying the CCC method together with the JM method, where the later has been recently revised by merging it with the Fano's multi-configuration interaction matrix elements [45], see [46] for information on availability of the JM source code used in this paper.

II. THEORY

Arguably, the main attraction of the JM method is its computational efficiency, where cross sections could be calculated many thousands of in one calculation.

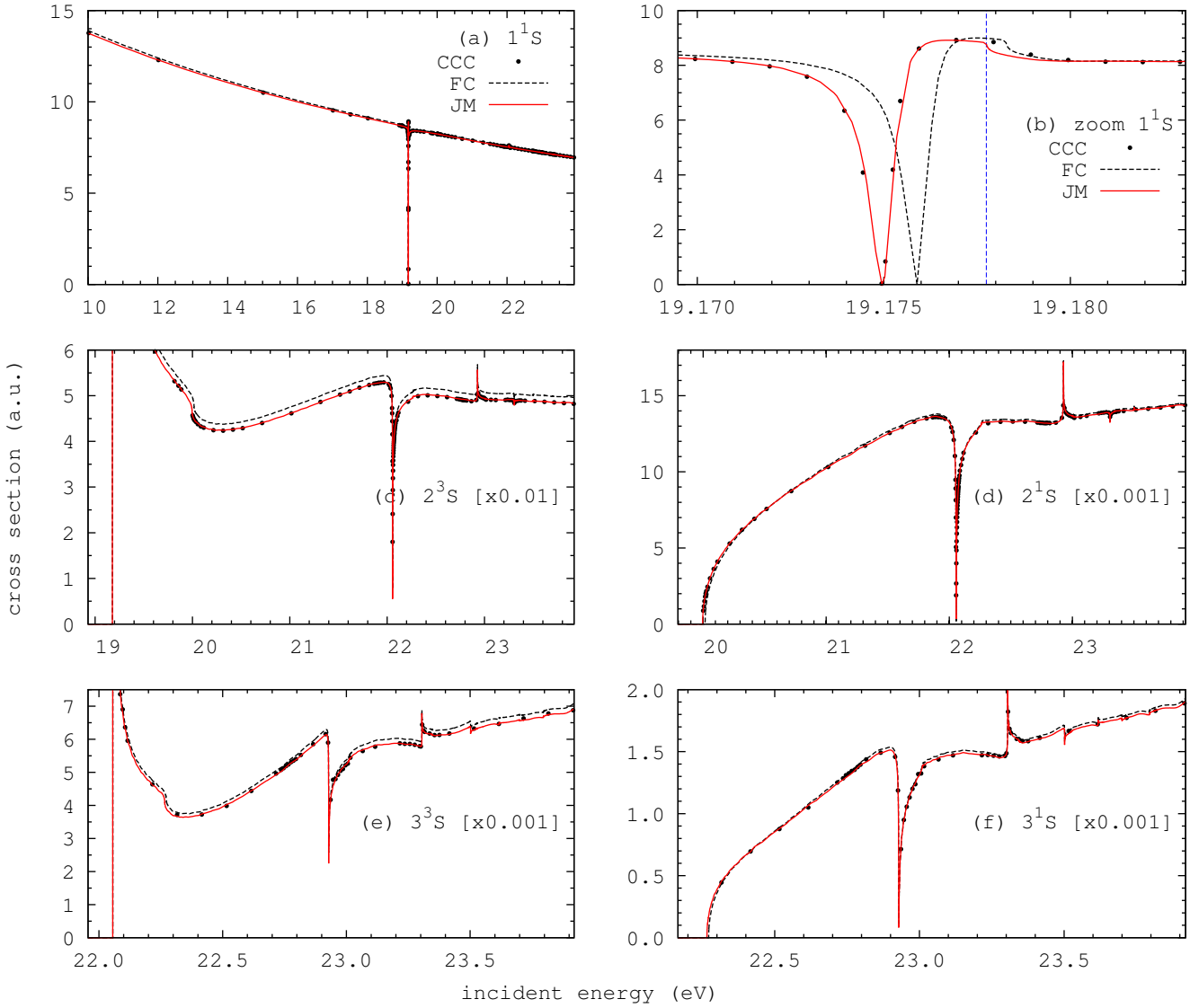

FIG. 1: (Color online) Elastic (1^1S), $n = 2$ (2^3S and 2^1S) and $n = 3$ (3^3S and 3^1S) single-excitation cross sections below the ionization threshold (23.92eV from Table I) for the e-He S-wave scattering model. Sub-figure (b) zooms in on the 2^3S excitation threshold (Table I) shown by the vertical dashed line. Frozen-core (FC), JM and CCC results were shifted by 0.17747eV, 0.0018eV and 0.0018eV (Table I), respectively.

Both JM and CCC methods rely on a

Let the nonorthogonal Laguerre functions used in the original JM method [49, 50] be referred to as the JM functions and denoted by $\{\xi_p(r)\}_{p=0}^{\infty}$,

$$\xi_p(r) = x^{l+1}\mathrm{e}^{-x/2}L_p^{2l+1}(x), \quad p = 0, 1, ..., \infty,$$

where $x = \lambda_{\mathrm{L}} r$, λ_{L} is the Laguerre exponential falloff, $l \equiv 0$ (for the S-model), and $L_p^{\alpha}(x)$ are the associated Laguerre polynomials [51]. The JM method splits the one-electron radial functional space into *inner* $\{\xi_p\}_{p=0}^{N-1}$ and *outer* $\{\xi_p\}_{p=N}^{\infty}$ subsets controlled by the number (N) of JM functions in the inner subset [49, 50].

III. RESULTS

A. Resonances in e-He S-wave scattering

[TODO] Atomic unit of energy (or Hartree) was set to 27.2116 eV. A tabular form of the JM and CCC cross sections is available from jmatrix.googlecode.com .

Again, both CCC and JM methods described the target helium atom , where the target eigenstates were constructed from the first N_t JM functions (**??**). Convergence in the CCC cross sections (Figs. **??** and **??**) was achieved at N_t =?, where the corresponding JM cross sections converged at N_t =? and N =?.

TABLE I: Energies and classifications for S-wave helium electron configurations. Energies e_i and E_i are from Eqs. (**??**) and (**??**), respectively. $\lambda_{\rm L} = 4$, $N_c = N_t$

Classification	threshold	e_i	
		-2.879 028 767 315	Ref. [47]
		-2.879 028 732	Ref. [48]
He($1s^2,^1S$)	0	-2.879 028 569 1	$N_t = 50$
		-2.879 027 69	Ref. [35]
		-2.879 03	Ref. [39]
		-2.878 962 303	$N_c = 7$, $N_t = 30$
		-2.878 95	Ref. [41]
		-2.872 506 673	$N_c = 1$, $N_t = 30$
He($1s2s,^3S$)	0.704 763 712	-2.174 264 856 2	$N_t = 50$
		-2.174 264 618	$N_c = 7$, $N_t = 30$
		-2.174 26	Ref. [41]
		-2.174 245 504	$N_c = 1$, $N_t = 30$
He($1s2s,^1S$)	0.734 831 310	-2.144 197 258 7	$N_t = 50$
		-2.144 191 393	$N_c = 7$, $N_t = 30$
		-2.144 19	Ref. [41]
		-2.143 449 321	$N_c = 1$, $N_t = 30$
He($1s3s,^3S$)	0.810 538 432	-2.068 490 136 6	$N_t = 50$
		-2.068 490 070	$N_c = 7$, $N_t = 30$
		-2.068 48	Ref. [41]
		-2.068 484 660	$N_c = 1$, $N_t = 30$
He($1s3s,^1S$)	0.818 234 531	-2.060 794 037 5	$N_t = 50$
		-2.060 792 356	$N_c = 7$, $N_t = 30$
		-2.060 79	Ref. [41]
		-2.060 573 161	$N_c = 1$, $N_t = 30$
He($1s4s,^3S$)	0.842 589 989	-2.036 438 58	Ref. [35]
		-2.036 438 560	$N_c = 7$, $N_t = 30$
		-2.036 43	Ref. [41]
		-2.036 436 372	$N_c = 1$, $N_t = 30$
He($1s4s,^1S$)			$N_t = 50$
		-2.033 392 203	$N_c = 7$, $N_t = 30$
		-2.033 39	Ref. [41]
		-2.033 300 706	$N_c = 1$, $N_t = 30$
He($1s5s,^3S$)			Ref. [35]
		-2.022 583 695	$N_c = 7$, $N_t = 30$
		-2.022 582 608	$N_c = 1$, $N_t = 30$
		-2.022 58	Ref. [41]
He($1s5s,^1S$)			$N_t = 50$
		-2.021 079 423	$N_c = 7$, $N_t = 30$
		-2.021 07	Ref. [41]
		-2.021 033 007	$N_c = 1$, $N_t = 30$
$He^+(1s)$	0.879 028 569	-2	

IV. CONCLUSIONS

Acknowledgments

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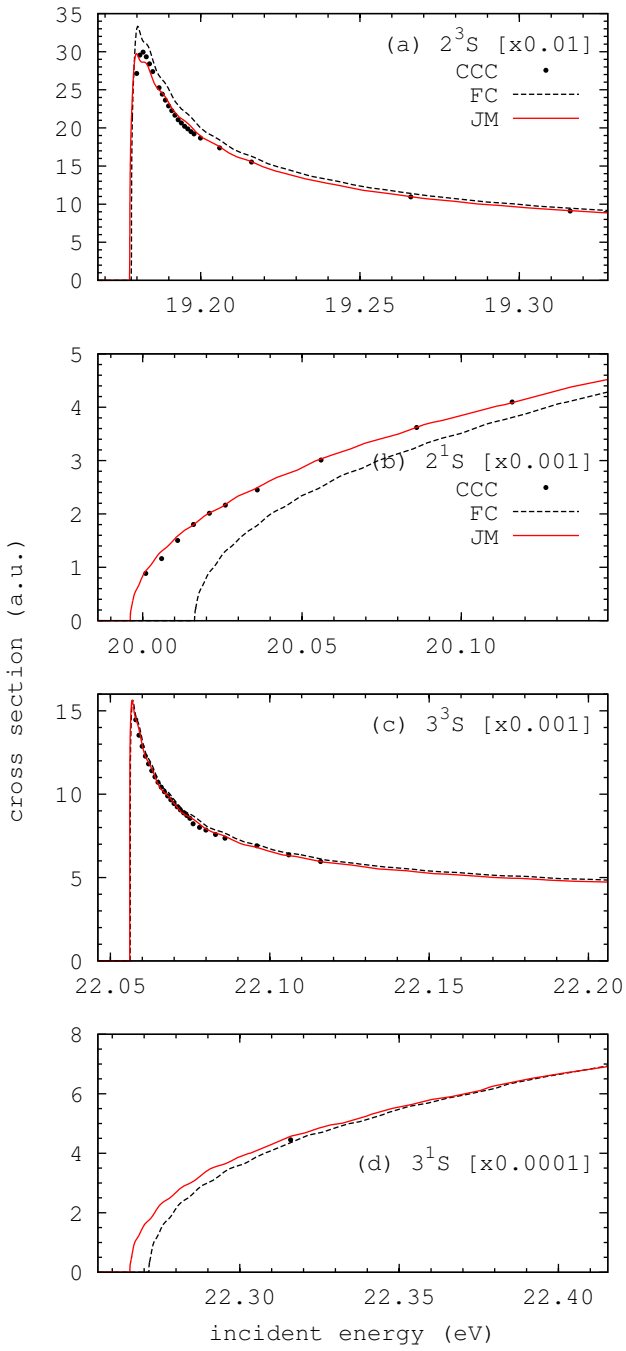

FIG. 2: (Color online) The same as in Fig. 1 but zooming in on the corresponding excitation threshold energies (Table I).

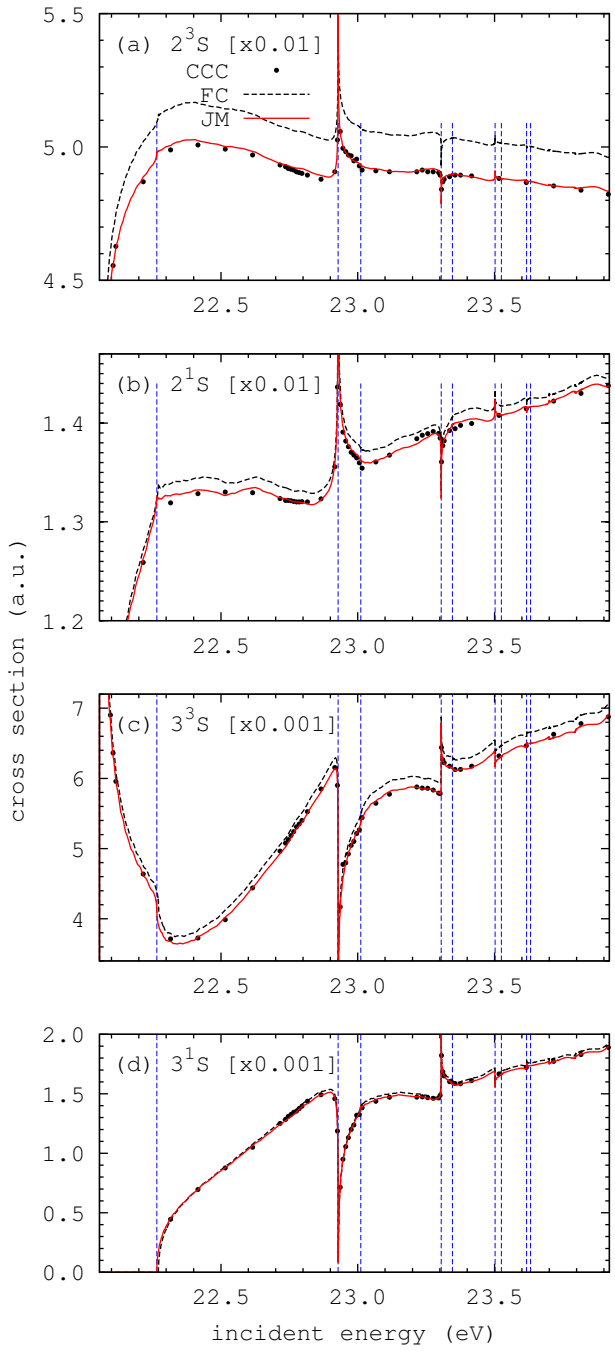

FIG. 3: (Color online) The same as in Fig. 1 but starting from the 3^3S threshold and aligned by incident energies. The 3^1S, $4^{1,3}S$, ..., $7^{1,3}S$, excitation thresholds (Table I) are shown by vertical dashed lines (from left to right).

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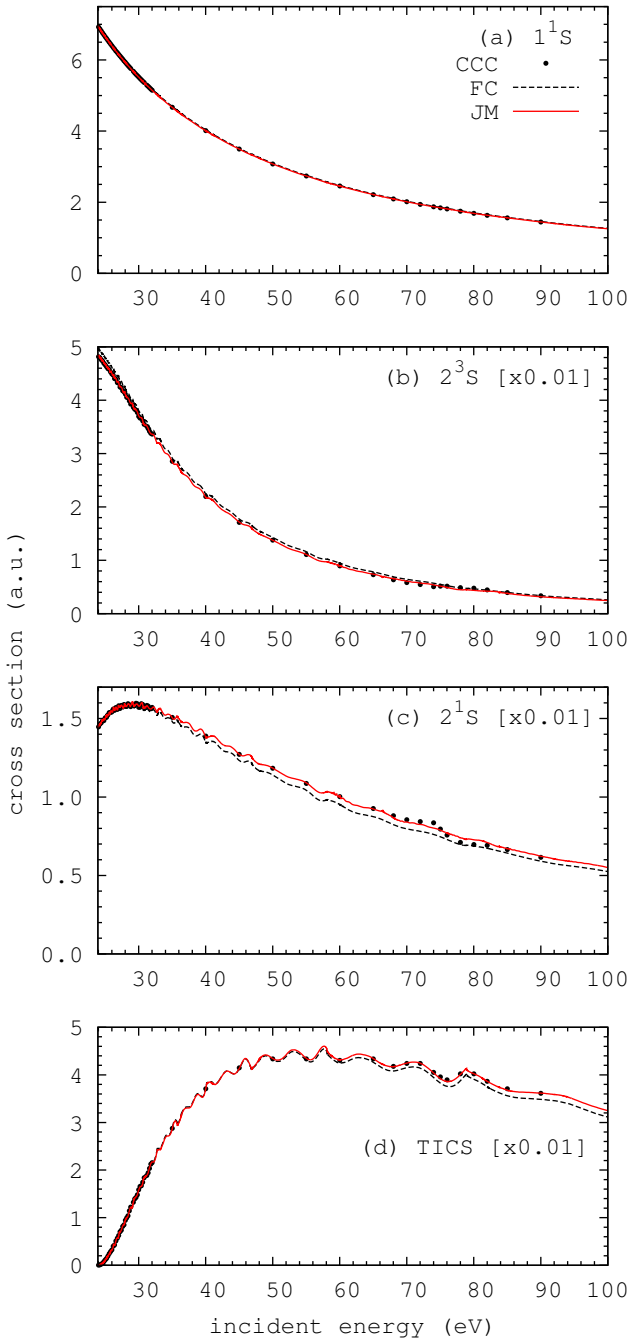

FIG. 4: (Color online) The same as in Fig. 1 but above the ionization threshold.

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