Electron-helium S-wave scattering. II. Resonances and cross sections below ionization threshold

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In the preceding J-matrix (JM) paper (referred as Ref. [I]), [D. A. Konovalov *et. al.* Phys. Rev. A **84**, 032707 (2011)], the S-wave e-He scattering problem was solved within the frozen-core (FC) model of helium for the elastic, $2^{1,3}S$-excitation, and single ionization cross sections for impact energies in the range 0.1-1000eV. The reported in Ref. [I] "proof-of-principle" JM calculations were in complete agreement with the convergent-close-coupling (CCC) method, which was also applied to the FC model. In this sequel, the target helium atom is described at much higher level of accuracy by disregarding the FC model. Both target electrons are described within the configuration-interaction (CI) model of helium obtaining accurate first seven bound states of helium. It is found that the theory in Ref. [I] is sufficient to fully solve the S-model below the single ionization threshold. The presented JM results (1-30 eV) are confirmed by the corresponding CCC calculations providing total elastic, $2^{1,3}S$ and $3^{1,3}S$ excitation cross sections with a "benchmark"-level of accuracy for the first time for the considered S-wave model.

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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. Due to technical difficulties working with atomic hydrogen, 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 (TDECS), 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

A. Wave functions

Let the nonorthogonal Laguerre functions used in the original JM method [47, 48] 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 [49]. 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 [47, 48].

III. RESULTS

A. Resonances in e-He S-wave scattering

see the resulting energy levels for two λ_{L} optimized with $n_\gamma = 5$ and $n_\gamma = 7$. Note that $e^{\mathrm{DHIF}}(1s2s,^1S) = -2.14418810$ from [35] is inconsistent and it is likely an error -2.14419810?

TODO Error in exact energy triplet?

[TODO] Atomic unit of energy (or Hartree) was set to 27.21138386 eV [50]. A tabular form of the JM and CCC cross sections is available from jmatrix.googlecode.com.

Cross sections are used to verify the negative-ion eigenstates responsible for resonances. Verification is done by excluding a particular negative-ion state from the JM calculation and observing disappearance of the resonance behavior. Once identified, their radial electron distributions are used to classify the resonances relative to the target eigenstates.

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. $\lambda_{\mathrm{L}} = 4$, $N_c = N_t$

Classification	threshold	e_i or E_i	
		-2.879 028 767 315	Ref. [51]
		-2.879 028 732	Ref. [52]
He($1s^2,^1S$)	0	-2.879 028 569 1	$N_t = 50$
		-2.879 028 504	$N_t = 45$
		-2.879 027 69	Ref. [35]
		-2.879 03	Ref. [39]
		-2.878 95	Ref. [41]
$He^-(1s2s,^2S)$			
He($1s2s,^3S$)	0.704 763 712	-2.174 264 856 2	$N_t = 50$
		-2.174 264 856 2	$N_t = 45$
		-2.174 264 80	
		-2.174 26	
		-2.174 26	
$He^-(1s2s,^2S)$			
He($1s2s,^1S$)	0.734 831 310	-2.144 197 258 7	$N_t = 50$
		-2.144 197 253	$N_t = 45$
		-2.144 188 10	
		-2.144 20	
		-2.144 19	
$He^-(1s3s,^2S)$			
He($1s3s,^3S$)	0.810 538 432	-2.068 490 136 6	$N_t = 50$
		-2.068 490 135	$N_t = 45$
		-2.068 490 12	
		-2.068 49	
		-2.068 48	
$He^-(1s3s,^2S)$			
He($1s3s,^1S$)	0.818 234 531	-2.060 794 037 5	$N_t = 50$
		-2.060 794 025	$N_t = 45$
		-2.060 788 24	
		-2.060 79	
		-2.060 79	
$He^-(1s3s,^2S)$			
He($1s4s,^3S$)	0.842 589 989	-2.036 438 58	Ref. [35]
$He^+(1s)$	0.879 028 569	-2	

IV. CONCLUSIONS

In order to achieve the stated goal we apply the J-matrix (JM) approach to electron-atom scattering, which has been recently revised by merging it with the Fano's multi-configuration interaction matrix elements [45]. In that preceding JM paper [53], the S-wave e-He scattering problem was solved within the frozen-core (FC) model of helium for the elastic, $2^{1,3}S$-excitation, and single ionization cross sections for impact energies in the range 0.1-1000eV. The reported in [53] "proof-of-principle" JM calculations were in complete agreement with the convergent-close-coupling (CCC) method, within the FC model. In this sequel, the scattering target helium atom is described at much higher level of accuracy overcoming the FC model. It is found that the theory in [53] is sufficient to fully solve the S-model below the single ionization threshold. The presented JM results (1-30 eV) are confirmed by the corresponding CCC calculations providing total elastic, $2^{1,3}S$ and $3^{1,3}S$ excitation cross sections with a "benchmark"-level of accuracy for the first time for the considered S-wave model.

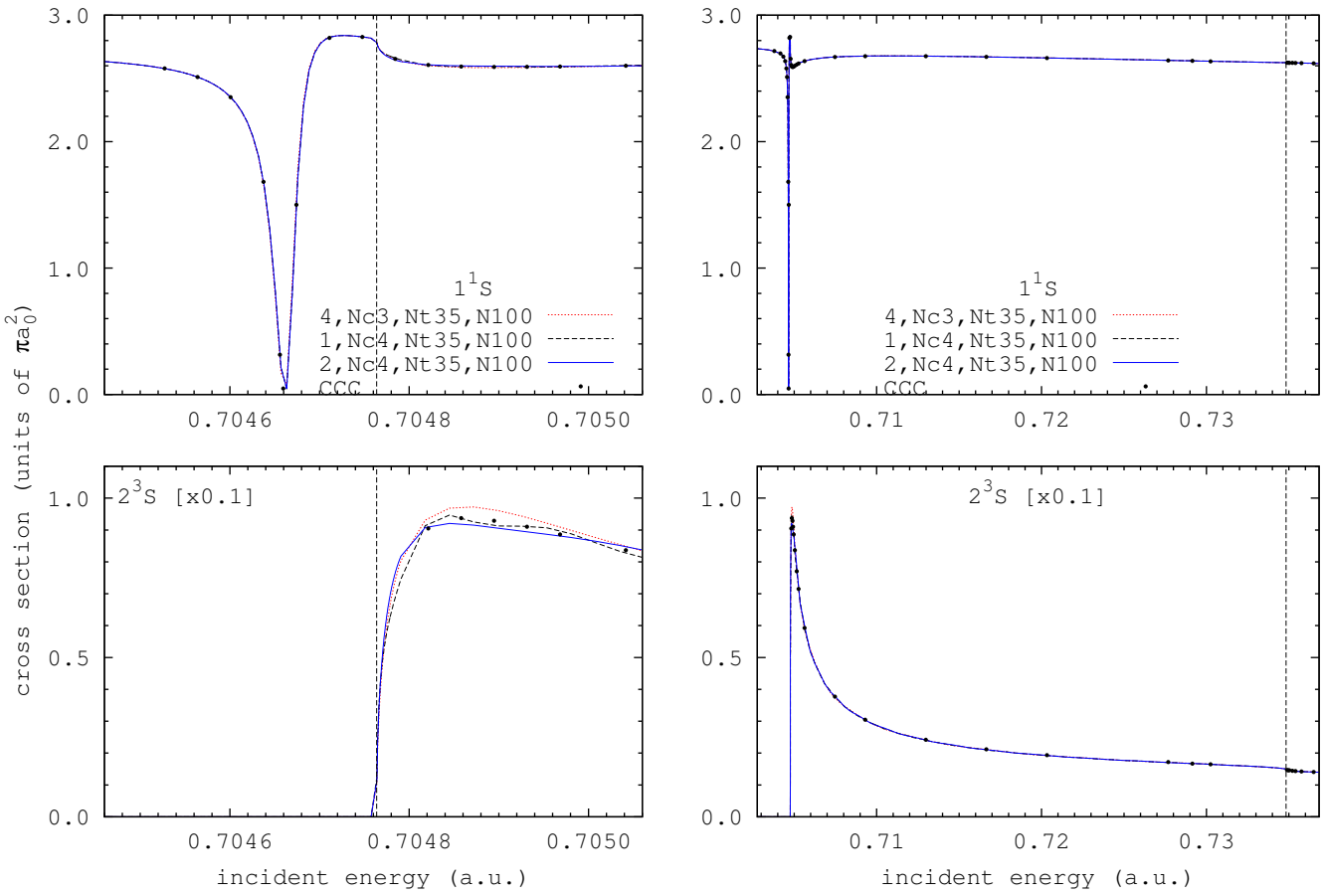

FIG. 1: (Color online) Elastic and excitation cross sections (πa_0^2) for e-He(1^1S) S-wave scattering for the impact energies up to the 2^1S-excitation threshold, see Table I. The first-column sub-figures zoom in on the 2^3S-excitation threshold shown as the vertical line in the middle of the sub-figures. STILL TODO: The $H^-(2s,^1S)$ eigenenergy and $2s$-excitation threshold are shown by the vertical lines labeled "E$_i$" and "2s", respectively. TEST-TODO? denotes JM's result obtained without the $H^-(2s,^1S)$ eigenstate in Eq. (**??**).

Acknowledgments

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[1] G. J. Schulz, Rev. Mod. Phys. **45**, 378 (1973).
[2] S. J. Buckman and C. W. Clark, Rev. Mod. Phys. **66**, 539 (1994).
[3] P. G. Burke and H. M. Schey, Phys. Rev. **126**, 147 (1962).
[4] G. J. Schulz, Phys. Rev. Lett. **10**, 104 (1963).
[5] Y. D. Wang and J. Callaway, Phys. Rev. A **50**, 2327 (1994).
[6] W. C. Fon, K. Ratnavelu, and K. M. Aggarwal, Phys. Rev. A **49**, 1786 (1994).
[7] D. A. Konovalov and I. E. McCarthy, J. Phys. B **27**, L741 (1994).
[8] B. R. Odgers, M. P. Scott, and P. G. Burke, J. Phys. B **29**, 4320 (1996).
[9] K. M. Dunseath, M. Le Dourneuf, M. Terao-Dunseath, and J.-M. Launay, Phys. Rev. A **54**, 561 (1996).
[10] K. M. Dunseath, M. Terao-Dunseath, M. L. Dourneuf, and J.-M. Launay, J. Phys. B **32**, 1739 (1999).
[11] K. M. Dunseath, M. Terao-Dunseath, and J.-M. Launay, J. Phys. B **33**, 3037 (2000).
[12] D. A. Konovalov and I. E. McCarthy, J. Phys. B **28**, L139 (1995).
[13] E. T. Hudson, K. Bartschat, M. P. Scott, P. G. Burke, and V. M. Burke, J. Phys. B **29**, 5513 (1996).
[14] C. A. Nicolaides and N. A. Piangos, J. Phys. B **34**, 99 (2001).
[15] N. A. Piangos and C. A. Nicolaides, Phys. Rev. A **67**, 052501 (2003).
[16] M. Stepanovic, M. Minic, D. Cvejanovic, J. Ju-

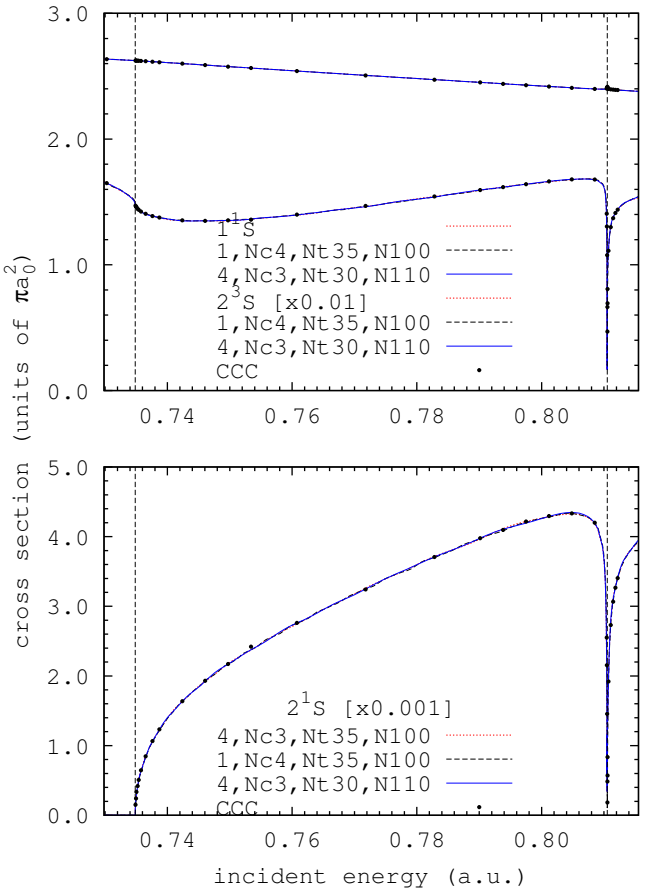

FIG. 2: (Color online) The same as in Fig. 1 but for the impact energies between the 2^1S and 3^3S excitation thresholds (Table I).

reta, J. Kurepa, S. Cvejanovic, O. Zatsarinny, and K. Bartschat, J. Phys. B **39**, 1547 (2006).
[17] A. Temkin, Phys. Rev. **126**, 130 (1962).
[18] E. J. Heller and H. A. Yamani, Phys. Rev. A **9**, 1209 (1974).
[19] R. Poet, J. Phys. B **11**, 3081 (1978).
[20] R. Poet, J. Phys. B **13**, 2995 (1980).
[21] R. Poet, J. Phys. B **14**, 91 (1981).
[22] J. Callaway and D. H. Oza, Phys. Rev. A **29**, 2416 (1984).
[23] I. Bray and A. T. Stelbovics, Phys. Rev. Lett. **69**, 53 (1992).
[24] A. K. Bhatia, B. I. Schneider, and A. Temkin, Phys. Rev. Lett. **70**, 1936 (1993).
[25] D. A. Konovalov and I. E. McCarthy, J. Phys. B **27**, L407 (1994).
[26] W. Ihra, M. Draeger, G. Handke, and H. Friedrich, Phys. Rev. A **52**, 3752 (1995).
[27] M. S. Pindzola and D. R. Schultz, Phys. Rev. A **53**, 1525 (1996).
[28] S. Jones and A. T. Stelbovics, Phys. Rev. A **66**, 032717 (2002).
[29] S. Jones and A. T. Stelbovics, Phys. Rev. Lett. **84**, 1878 (2000).
[30] M. Baertschy, T. N. Rescigno, W. A. Isaacs, and C. W. McCurdy, Phys. Rev. A **60**, R13 (1999).
[31] A. T. Stelbovics, Phys. Rev. Lett. **83**, 1570 (1999).
[32] C. W. McCurdy, D. A. Horner, and T. N. Rescigno, Phys. Rev. A **65**, 042714 (2002).
[33] P. L. Bartlett and A. T. Stelbovics, Phys. Rev. A **69**, 022703 (2004).
[34] A. L. Frapiccini, J. M. Randazzo, G. Gasaneo, and F. D. Colavecchia, J. Phys. B **43**, 101001 (2010).
[35] M. Draeger, G. Handke, W. Ihra, and H. Friedrich, Phys. Rev. A **50**, 3793 (1994).
[36] M. S. Pindzola, D. Mitnik, and F. Robicheaux, Phys. Rev. A **59**, 4390 (1999).
[37] C. Plottke, I. Bray, D. V. Fursa, and A. T. Stelbovics, Phys. Rev. A **65**, 032701 (2002).
[38] C. Plottke, P. Nicol, I. Bray, D. V. Fursa, and A. T. Stelbovics, J. Phys. B **37**, 3711 (2004).
[39] D. A. Horner, C. W. McCurdy, and T. N. Rescigno, Phys. Rev. A **71**, 010701(R) (2005).
[40] D. A. Horner, C. W. McCurdy, and T. N. Rescigno, Phys. Rev. A **71**, 012701 (2005).
[41] P. L. Bartlett and A. T. Stelbovics, Phys. Rev. A **81**, 022715 (2010).
[42] P. L. Bartlett and A. T. Stelbovics, Phys. Rev. A **81**, 022716 (2010).
[43] D. A. Konovalov, D. V. Fursa, and I. Bray, Phys. Rev. A **84**, 032707 (2011).
[44] D. V. Fursa and I. Bray, Phys. Rev. A **52**, 1279 (1995).
[45] U. Fano, Phys. Rev. **140**, A67 (1965).
[46] *The complete Java source code used in this study is freely available from jmatrix.googlecode.com or a relevant link at www.dmitrykonovalov.org for academic use.* .
[47] E. J. Heller and H. A. Yamani, Phys. Rev. A **9**, 1201 (1974).
[48] J. Broad and W. Reinhardt, J. Phys. B **9**, 1491 (1976).
[49] M. Abramowitz and I. A. Stegun, eds., *Handbook of Mathematical Functions* (Dover Publications, Mineola, NY, 1965).
[50] P. J. Mohr, B. N. Taylor, and D. B. Newell, Rev. Mod. Phys. **80**, 633 (2008).
[51] S. P. Goldman, Phys. Rev. Lett. **73**, 2547 (1994).
[52] O. Jitrik and C. F. Bunge, Phys. Rev. A **56**, 2614 (1997).
[53] I. Bray and D. V. Fursa, J. Phys. B **44**, 061001 (2011).

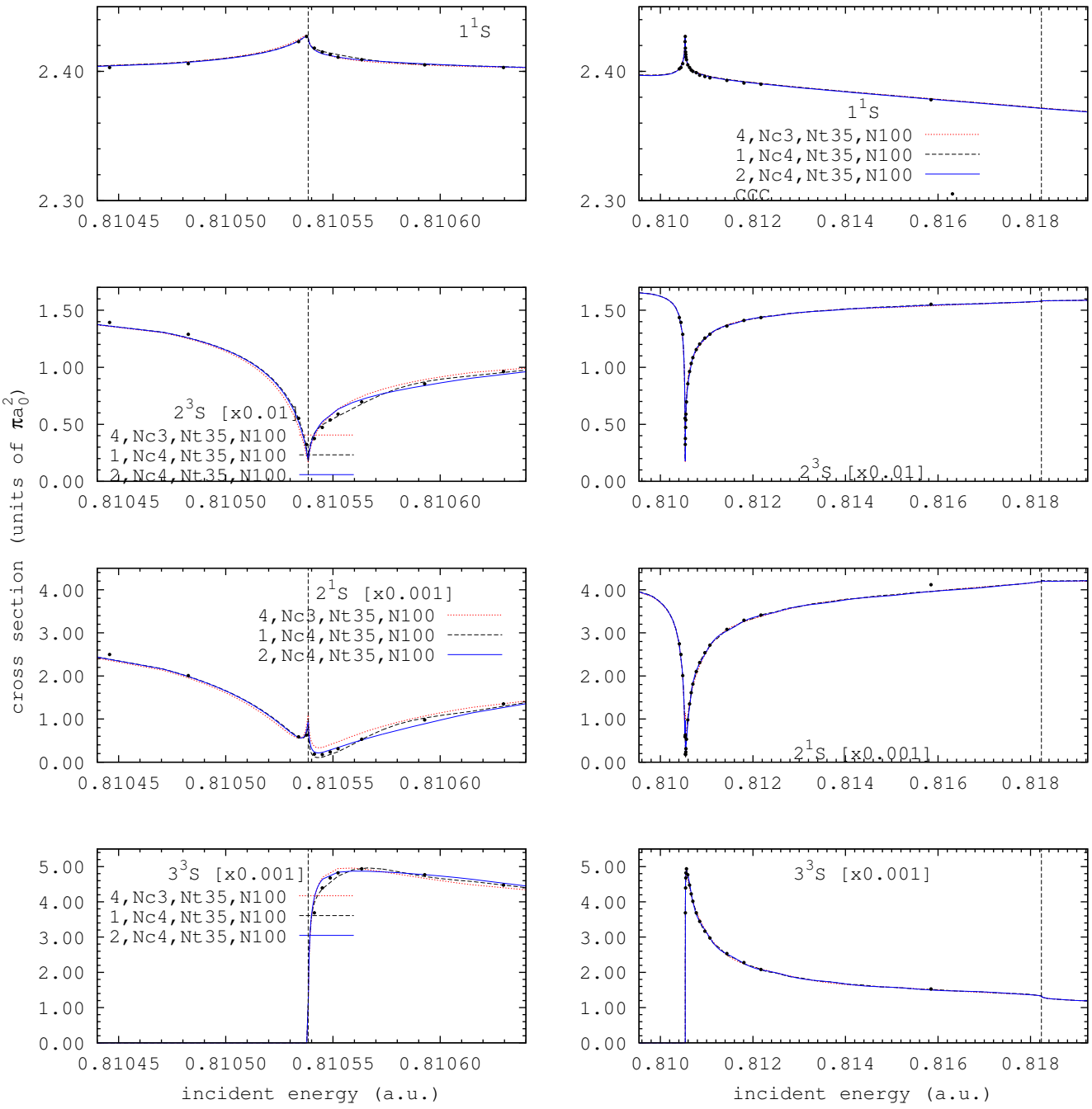

FIG. 3: (Color online) The same as in Fig. 1 but for the impact energies between the 3^3S and 3^1S excitation thresholds (Table I), where the first-column sub-figures zoom in on the 3^3S-excitation threshold.

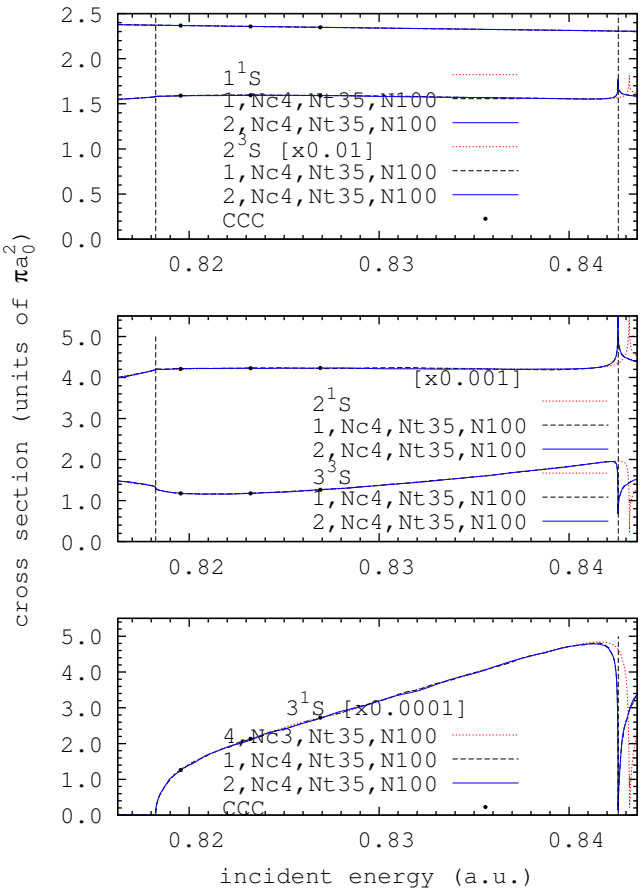

FIG. 4: (Color online) The same as in Fig. 1 but for the impact energies between the 3^1S and 4^3S excitation thresholds (Table I).