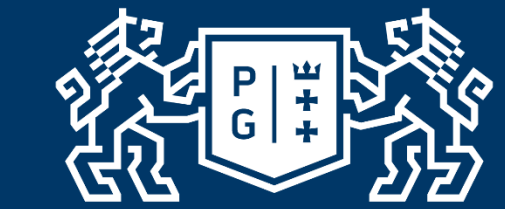

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Current status of the GRASPC development
Calculations for electron-strontium scattering

Paweł Syty
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CompAS annual meeting, Lund, 12/06/2025

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RESEARCH UNIVERSITY EXCELLENCE INITIATIVE

GRASPC – GRASP for calculations of Continuum orbital wave functions

- **As presented at the last CompAS meeting in Lisbon, user-friendly GRASP version for continuum wave function generator has been released at GitHub, and the name has evolved to the GRASPC**

GRASPC - GRASP package adapted for the generation of continuum orbitals wave functions

This repository is a fork of **The General-purpose Relativistic Atomic Structure Package (GRASP)** - a set of Fortran 90 programs for performing fully relativistic electron structure calculations of atoms.

Link to GRASP repository

About this fork

release v1.0 | release date july 2024 | last commit march

This fork is intended to incorporate the scattered (continuum) electron calculations in elastic (single-channel) and inelastic (multi-channel) processes into GRASP.

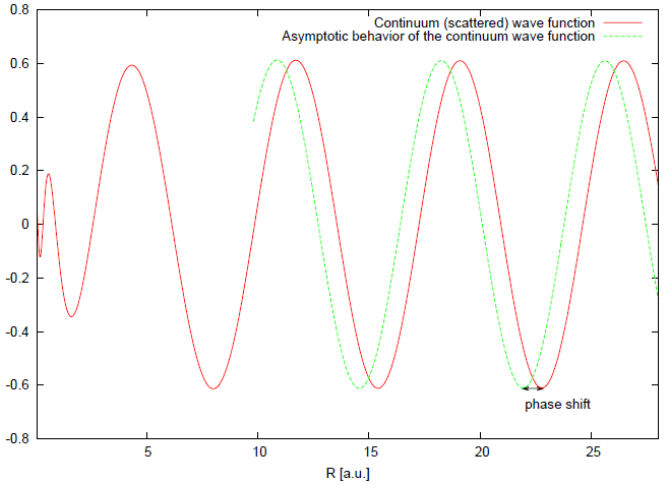
> **Please note:** Currently, only elastic processes are implemented.

The main idea is to use as many computational processes as they are implemented in GRASP, by adapting them to calculate continuum orbitals wave functions.

https://github.com/sylaspg/grasp-continuum

GRASPC – assumptions

- Extension of GRASP with new functionalities, without creating a separate module
  - keeping the original code and computational flow in the case of calculating bound states
  - keeping the original user interface
- Calculate:
  - continuum (normalized or not) orbital wave functions for any partial wave
  - phase shift (NEW since Lisbon)
  - scattering lengths (NEW since Lisbon)
    - using small, but still non-zero energy
    - using zero-energy approach
- Utilize as many computational apparatus from GRASP as possible
  - building the atomic state function and configuration state functions
  - calculating the direct and exchange potentials
  - calculating angular coefficients and integrals
  - constructing the Dirac-Coulomb Hamiltonian
  - performing self-consistent calculations
  - (…)



GRASPC – assumptions

- **Polarization potential**
  - **model**

$$V_{pol}(r) = -\frac{1}{2}\frac{\alpha_d r^2}{\left(r^3 + \langle r_0^3 \rangle\right)^2} - \frac{1}{2}\frac{\alpha_q r^4}{\left(r^5 + \langle r_0^5 \rangle\right)^2} - \frac{1}{2}\frac{\alpha_o r^6}{\left(r^7 + \langle r_0^7 \rangle\right)^2}$$

new since Lisbon

    - **cut-off parameters** $\langle r_0^3 \rangle, \langle r_0^5 \rangle, \langle r_0^7 \rangle$ **are calculated by GRASP for the outermost bound orbital, but the user can replace them with his own**
    - **static polarizabilities** $\alpha_d, \alpha_q, \alpha_o$ **are to be provided by user**
      - **for atoms, recommended** α_d **values are tabulated and may be taken automatically**
  - **numerical values**

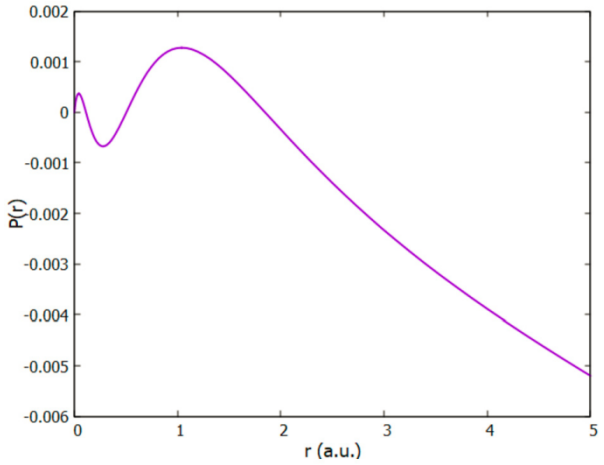
```
1.00000E-05 -5.40690E-08
1.05127E-05 -5.68411E-08
1.10517E-05 -6.28067E-08
1.16183E-05 -6.93969E-08
1.22140E-05 -7.66768E-08
(...)
3.42775E+02 -3.90076E-10
3.60350E+02 -3.19367E-10
3.78825E+02 -2.61476E-10
3.98248E+02 -2.14078E-10
```

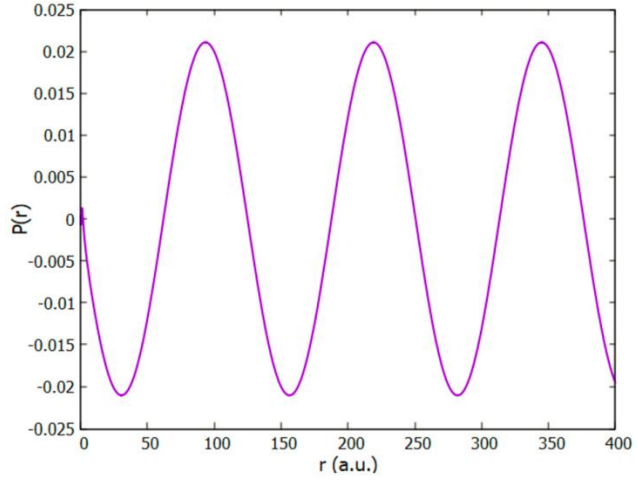
GRASPC – restrictions and limitations

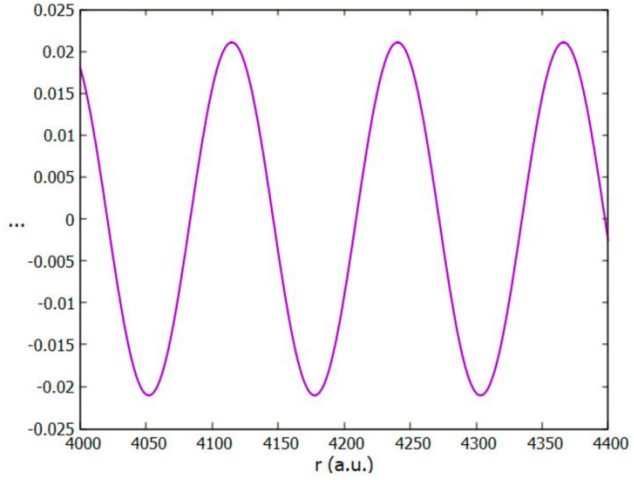
- Only elastic processes
  - work on inelastic processes – in progress
- Frozen-core
  - compensated by using the polarization potential
- Polarization potential relying on static parameters only (model), or independent calculations (numerical)
  - work on including calculation of the polarizabilities or even full polarization by GRASP – in progress
- Normalization not fully tested
  - for phase shift / scattering length determination it is not needed
  - the only reliable method we found is the „per energy” normalization
  - the method was tested by generating the higher and higher Rydberg states and comparing the amplitude with that from continuum state, but generated with the RATIP code
    - need to repeat that test for continuum orbital generated by GRASPC
- The computational grid must be appropriately chosen by the user:
  - linear-logarithmic (constant step at the tail)
  - quite large number of points (usually 5000 is enough)
  - in a future it might be automatically chosen

GRASPC – test cases

- **Electron-argon elastic scattering**
- **Generation of the continuum orbital wave function and phase shift calculation for electron of κ =−1 (s–wave, J = 1⁄2), and energy ϵ = 0.00124997 Hartree = 0.03401334 eV (k = 0.05), using the model polarization potential (dipole term only)**







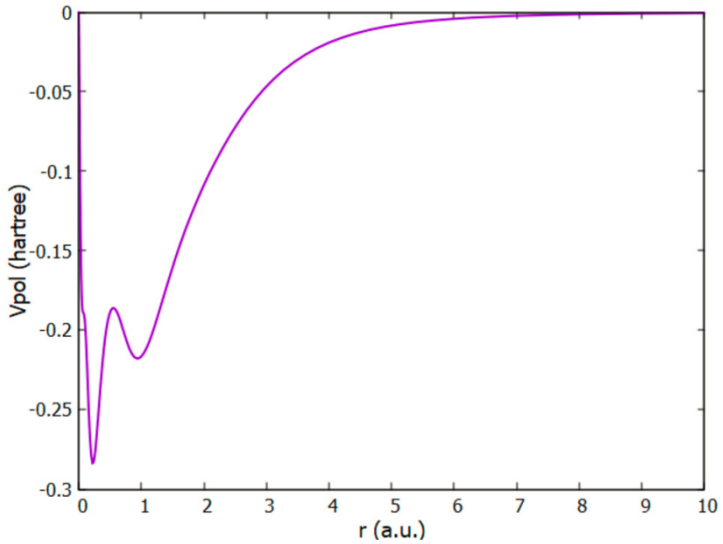

```
Phase shift =    -3.1072761138182852          =     3.4316539771507948E-002
```

Calculated phase shift, δ_0 = 0.03432 stays in good agreement with the result of others, e.g. Cheng et al., 0.03999

Y. Cheng, S. Liu, S.B. Zhang, Y.-B. Tang, Relativistic coupled-cluster-theory study for low-energy electron scattering with argon, Phys. Rev. A 102 (2020) 012824

GRASPC – test cases

- **Electron-argon elastic scattering**
- **Generation of the normalized continuum orbital wave function and phase shift calculation for the electron of $\kappa = 2$ (d–wave, $J = 3/2$), and energy $\epsilon = 0.04499880$ Hartree = 1.22448022 eV ($k = 0.3$), using the polarization potential given in numerical form**

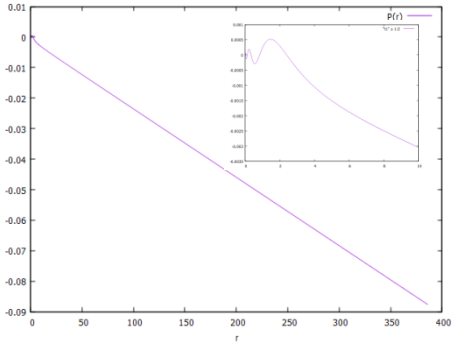



```
Phase shift =     3.2408797325361505E-002
```

Calculated phase shift, $\delta_2^+ = 0.03241$ stays in good agreement with the result of others, e.g. almost perfect with Cheng's result, 0.03253

GRASPC – test cases

- **Electronic scattering lengths for noble gases**
  - **Scattering length as function of the s-wave phase shift:** $a = -\lim_{k\to 0} \frac{\tan(\delta_0)}{k}$
  - **Scattering length and total cross section:** $\sigma_{tot} \overset{k\to 0}{\simeq} 4\pi a^2$
  - **Scattering length for *exactly* zero electron energy:** $P_{\kappa 0}(r) = -\frac{2C}{\alpha} + Dr = D(r-a)$ $\quad a = 2C/\alpha D$



Element	Most recent exp. / theor. / our old theor.	GRASPC, zero energy dipole polarization
Ne	0.214 / 0.227 / -0.021**	0.195
Ar	-1.365 / -1.39 / -1.417*	-1.326
Kr	-3.06 / -3.10 / -3.147*	-2.941
Xe	-5.13 / -4.953 / -5.209*	-5.063
Rn	- / - / -13.315*	-12.553
Og	- / - / 15.098*	15.384

* – using modified RATIP/COWF by Stephan Fritzsche:
P. Syty, M.P. Piłat, J.E. Sienkiewicz,
Calculation of electron scattering lengths on Ar, Kr, Xe, Rn and Og atoms,
J. Phys., B At. Mol. Opt. Phys. 57 (17) (2024) 175202

** – using modified RATIP/COWF by Stephan Fritzsche, unpublished

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GRASPC – publication

Published just before the meeting

(open access)

In the paper:

- **Physical background**
  - **Generation of the continuum orbital wave function**
  - **Polarization potential**
  - **Phase shifts**
  - **Scattering lengths**
- **Computational procedure**
  - **focus on the differences between bound and continuum states calculations**
- **User guide**
  - **step by step manual**
- **Test cases**
  - **as in the previous slides, but scattering lengths only for argon**

Computer Physics Communications 315 (2025) 109691

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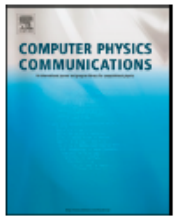
journal homepage: www.elsevier.com/locate/cpc



Computer Programs in Physics

GRASPC – GRASP package adapted for the generation of continuum orbitals wave functions

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ARTICLE INFO

The review of this paper was arranged by Prof. W. Jong

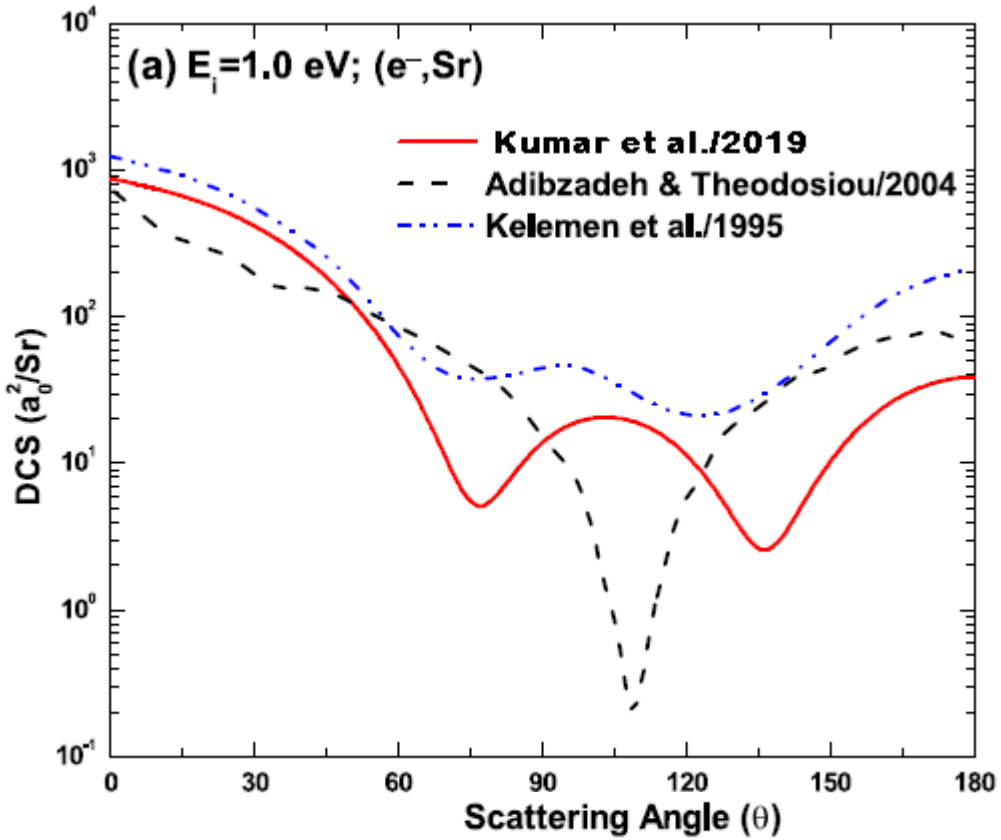
Keywords:
GRASP
Elastic scattering
Continuum orbital
Phase shift
Scattering length

ABSTRACT

The GRASP package (https://github.com/compas/grasp) is a widely used tool for performing fully relativistic bound electron structure calculations of atoms. Its latest official release is GRASP2018, but it has been continuously developed since then.
The presented code, GRASPC, is the adaptation of that package allowing for calculations of the continuum orbital of electrons elastically scattered from atoms and ions. The calculated continuum orbital can be normalized using the per-energy normalization procedure. Then, the phase shifts are calculated by comparing the computed wave function with the free electron wave function in the asymptotic region. Scattering lengths are estimated not only for widely used very low energy scattering but also using an unusual approach with a "zero energy" wave function.
The main idea behind GRASPC is to use as many computational apparatus as they are implemented in GRASP (e.g., building the atomic and configuration state functions, calculating the potentials, angular coefficients and integrals, constructing the Dirac-Coulomb Hamiltonian, performing self-consistent calculations) by adapting them to calculate the wave function of the scattered electron. This adaptation is entirely transparent for usual calculations in GRASP (bound states and their properties). The default flow changes only when calculations involving continuum orbital are requested and different outputs are produced. This approach, combined with the retention of the typical interactive user interface, allows GRASP users to adapt rapidly to the new type of calculation.

GRASPC – electron-strontium scattering

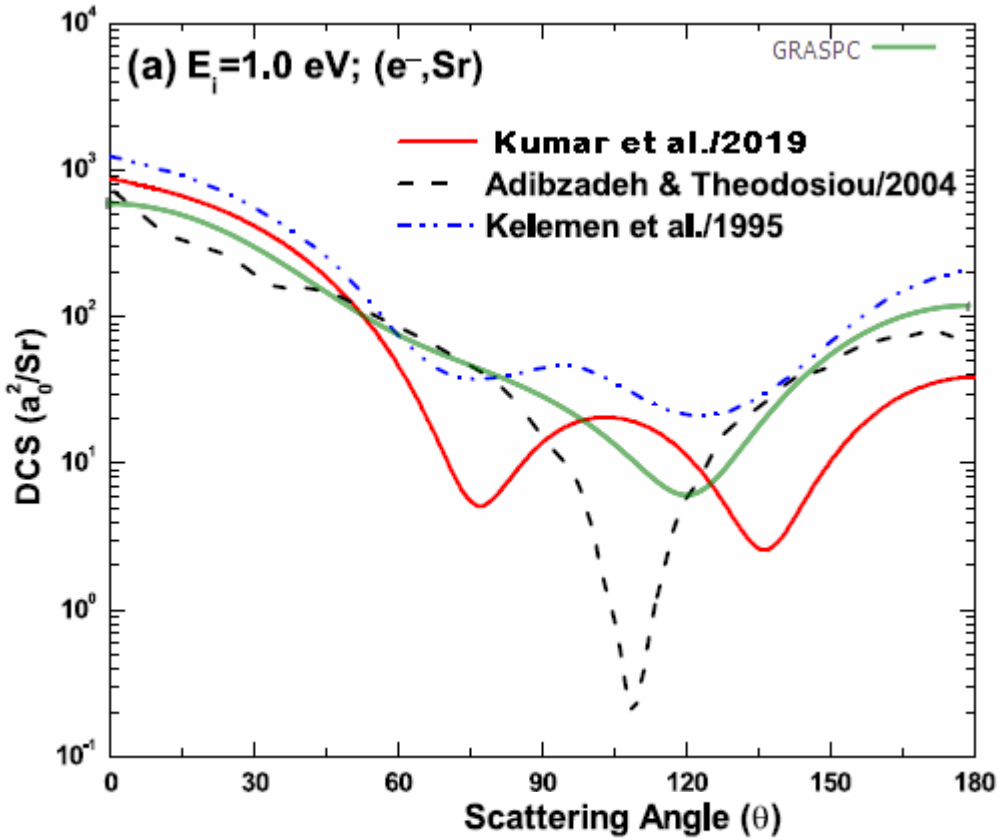
- **Differential cross sections**
  - **Sr: [Kr] 5s(2)**
  - **No experimental data**
  - **Three different methods, three different curves…**



Kumar A et al 2019 J. Phys. Commun. 3 065001
Adibzadeh M and Theodosiou CE 2004 Phys. Rev. A 70 052704
Kelemen V, Remeta E Y and Sabad E P 1995 J. Phys. B: At. Mol. Opt. Phys. 28 1527–46

GRASPC – electron-strontium scattering

- **Differential cross sections**
  - **Fourth method, fourth curve…**
  - **15 partial waves used (up to κ = -8)**



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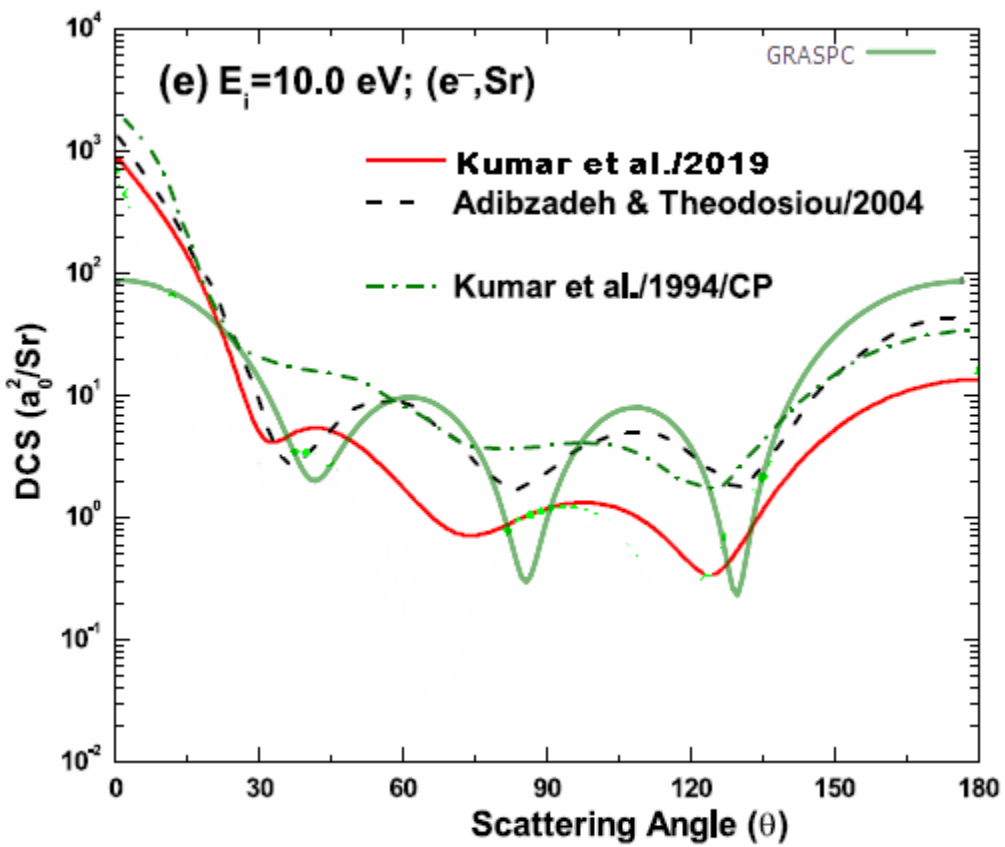

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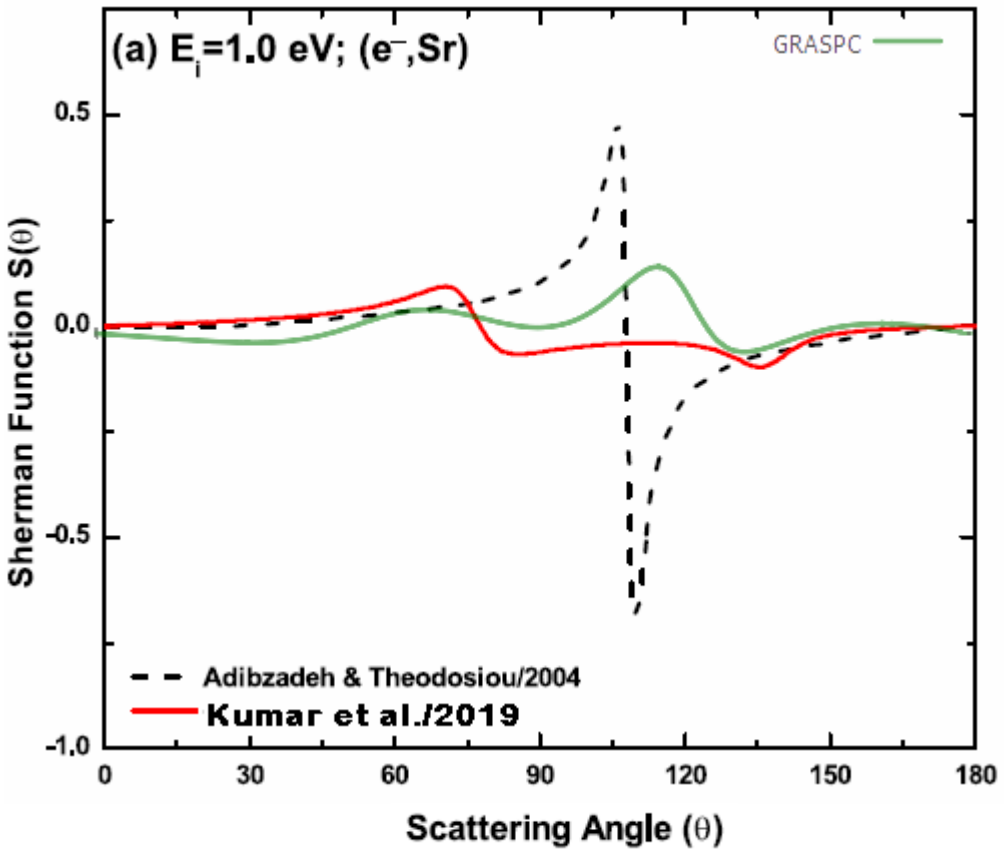
GRASPC – electron-strontium scattering

- **Similar situation for spin-polarization cross section**



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Adibzadeh M and Theodosiou CE 2004 Phys. Rev. A 70 052704

GRASPC – electron-strontium scattering

- **Scattering length**

Result	method, reference
-18	theoretical, non-relativistic R-matrix, Bartschat and Sadeghpour, 2003
-13.2	experimental, DeSalvo et al., 2015
-12.65	theoretical, generalized local frame transformation (semiempirical – fitting phase shifts to the binding energy), Giannakeas, Eiles, Robicheaux and Rost, 2020
-11.61	**GRASPC, zero-energy approach, default parameters of the polarization potential**

Conclusions

- It works
- It will work better

Any feedback would be appreciated!

Thank you!