Challenges for MCMS (Multi-Channel Multiple Scattering) theory in solid state

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Out line of my research

1. Learning Atomic physics and Multi Channel method
   (by R-matrix theory)

~Single electron and Single atom~

2. Training for Multiple Scattering theory and programing by Fortran

~Multi Atoms~

3. Training numerical analysis for solving the differential equation

~For Realization of MCMS~

4. Future tasks

1. single electron - single atom scattering

Schrödinger's equation for an $(N+1)$-electron system

$$H_{N+1}\Psi(\boldsymbol{X}_{N+1}) = E\Psi(\boldsymbol{X}_{N+1})$$

$$H_{N+1} = \sum_{i=1}^{N+1}\left\{-\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i}\right\} + \sum_{j>i}^{N+1}\frac{1}{r_{ij}}$$

$$\Psi_i(\boldsymbol{X}_{N+1}) \underset{r\to\infty}{\sim} \Phi_i(\boldsymbol{X}_N)\chi_{\frac{1}{2}\mu_i}(\boldsymbol{\sigma})\,\mathrm{e}^{\mathrm{i}\boldsymbol{\kappa}_i\cdot\boldsymbol{r}} + \sum_{j\text{ open}}\Phi_j(\boldsymbol{X}_N)\chi_{\frac{1}{2}\mu_j}(\boldsymbol{\sigma})\frac{\mathrm{e}^{\mathrm{i}\kappa_j r}}{r}f_{ji}^{\mathrm{scat}}(\hat{\boldsymbol{\kappa}}_j,\hat{\boldsymbol{\kappa}}_i)$$

$$\frac{\mathrm{d}\sigma_{ji}}{\mathrm{d}\Omega} = \frac{\kappa_j}{\kappa_i}\,|\,f_{ji}^{\mathrm{scat}}(\hat{\boldsymbol{\kappa}}_j,\hat{\boldsymbol{\kappa}}_i)\,|^2$$

Introduction to R-matrix theory

Collisional electron

$e^- \longrightarrow$

Inner region

Atomic / ionic target

Strong interactions Between **all** electrons

Outer region

One collision electron far from atomic target

No exchange with target electrons

Multichannel

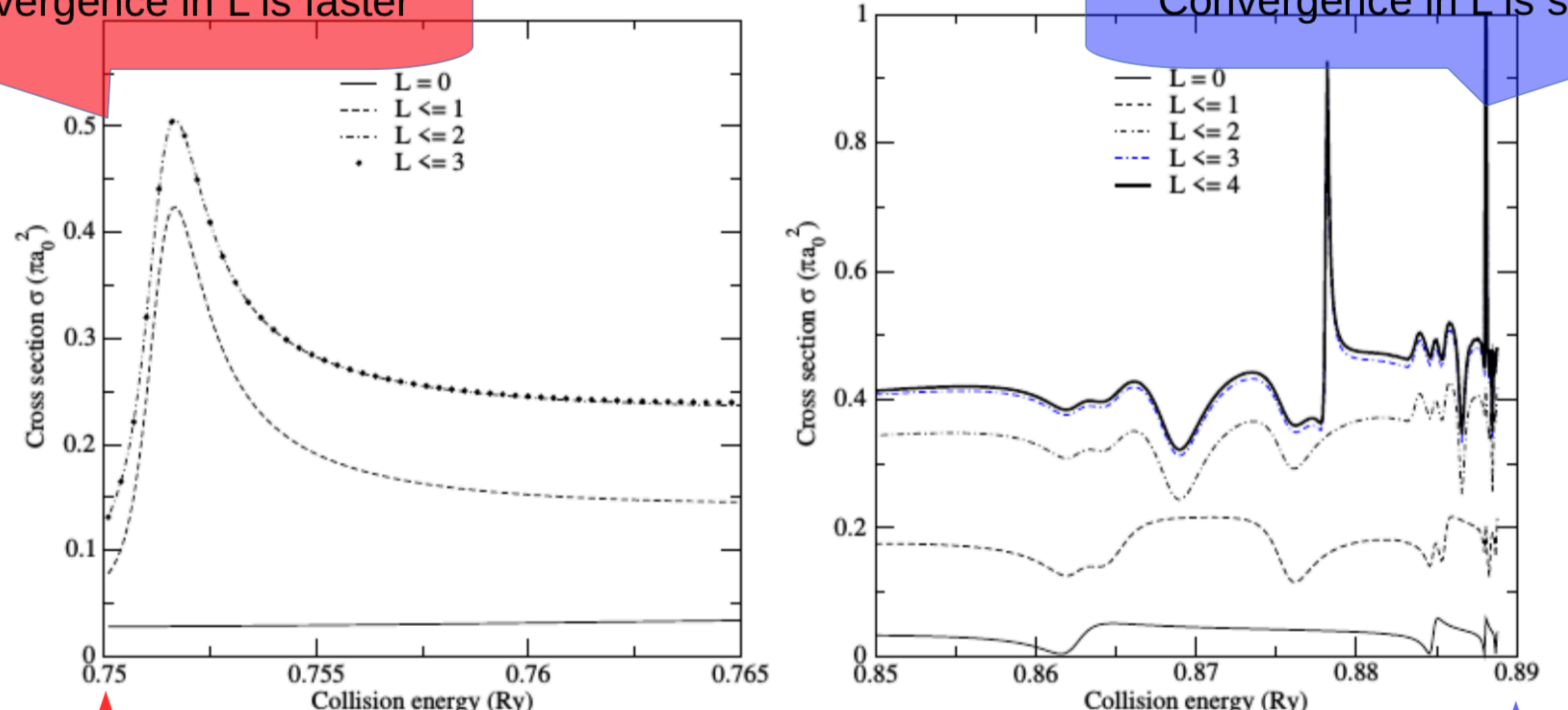
Potential scattering

Match solutions from inner region and outer region with *R-matrix* (inverse log-derivative of solutions) to obtain *phase shifts* and *cross sections*

Computational results of R-matrix method for electron - H

Convergence in L is faster

Convergence in L is slow



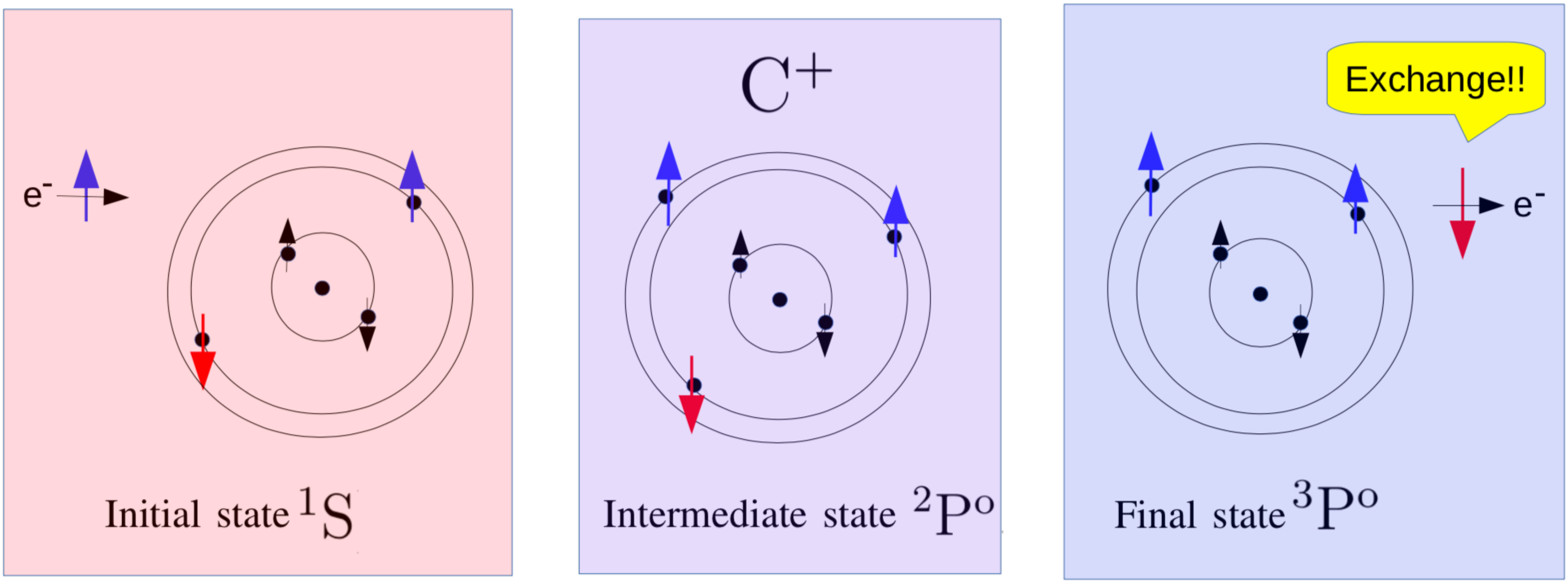
Electron impact excitation of H(1s) to H(2p)

n=2 Threshold = 0.75 Ry

n=3 Threshold = 0.89 Ry

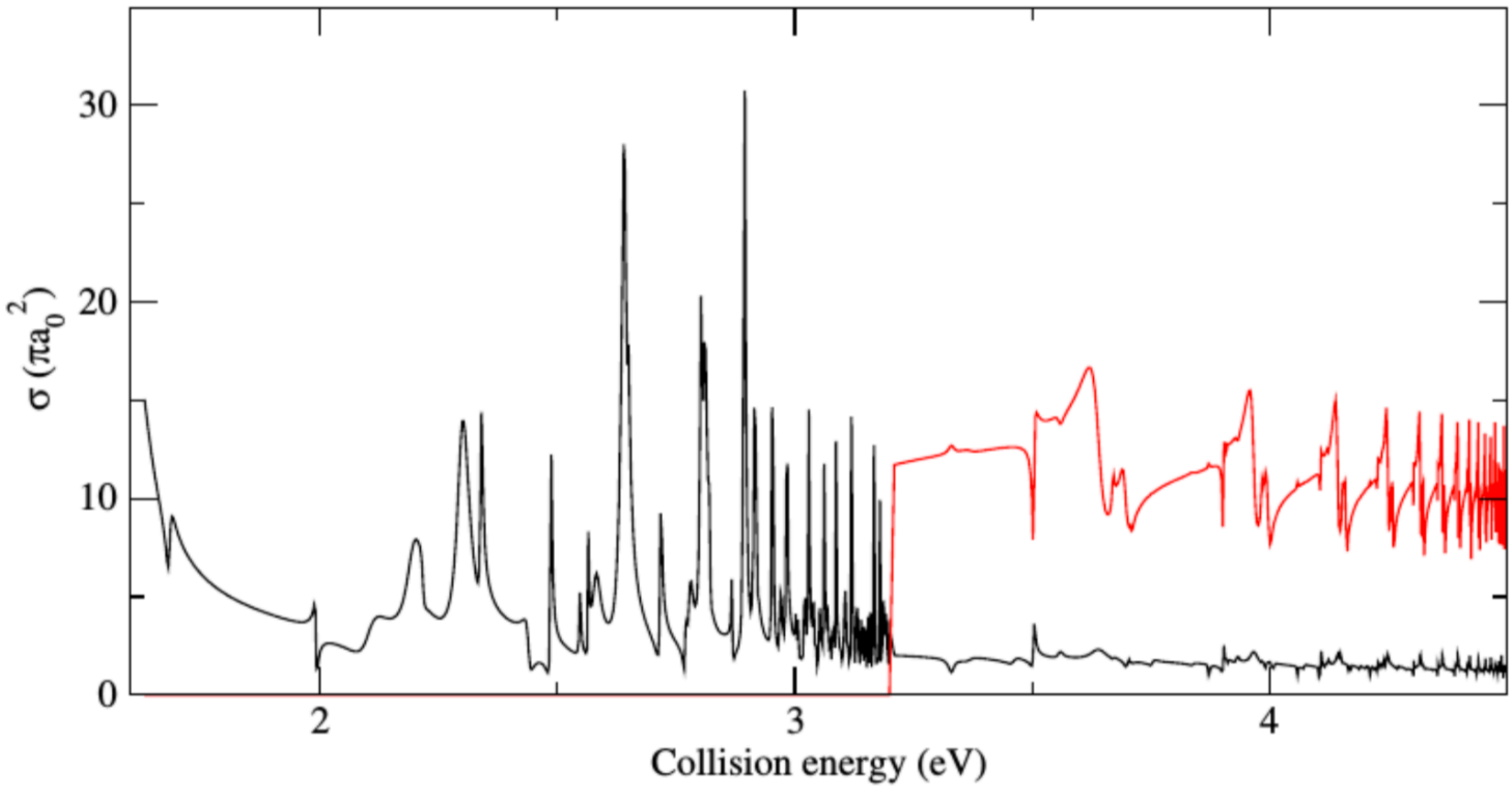
electron - C^{2+} scattering

$$e^- + C^{2+}(1s^2 2s^2\ {}^1S) \rightarrow e^- + C^{2+}(1s^2 2s 2p\ {}^3P^o)$$



Schematic image of the channels change

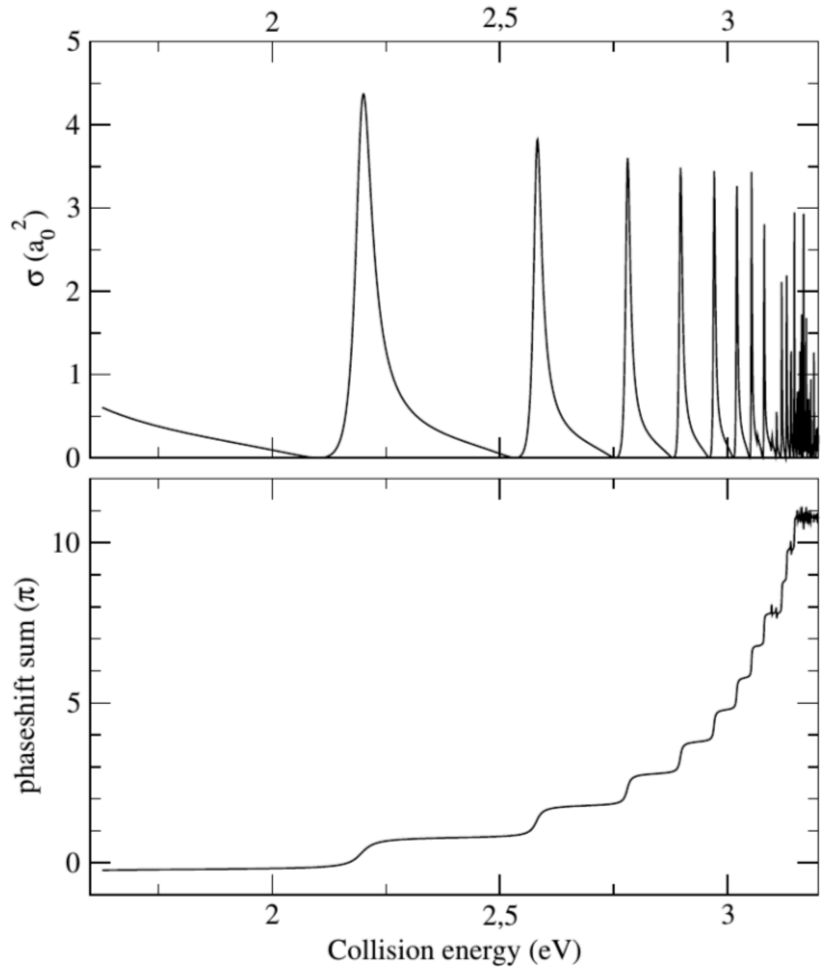
Computational results of R-matrix method for electron - C^{2+}



Cross section σ for electron impact excitation of $C^{2+}(1s^2 2s^2\ ^1S)$.
——: final state $C^{2+}(1s^2 2s2p\ ^3P^o)$; —— final state $C^{2+}(1s^2 2s2p\ ^1P^o)$.

By computing the cross section for each channel
→ we can see regularity

^{2}S



"Regularity"

Fig 1 Contribution of the ^{2}S partial wave to the cross section σ and eigenphase sum for electron impact excitation $e^- + C^{2+}(1s^2 2s^2\ {}^1S) \rightarrow e^- + C^{2+}(1s^2 2s2p\ {}^3P^o)$. At each resonance, the phaseshift in the corresponding channel increases by π. The energy grid is not fine enough to represent the very narrow resonances close to the $C^{2+}(1s^2 2s2p\ {}^1P^o)$ threshold.

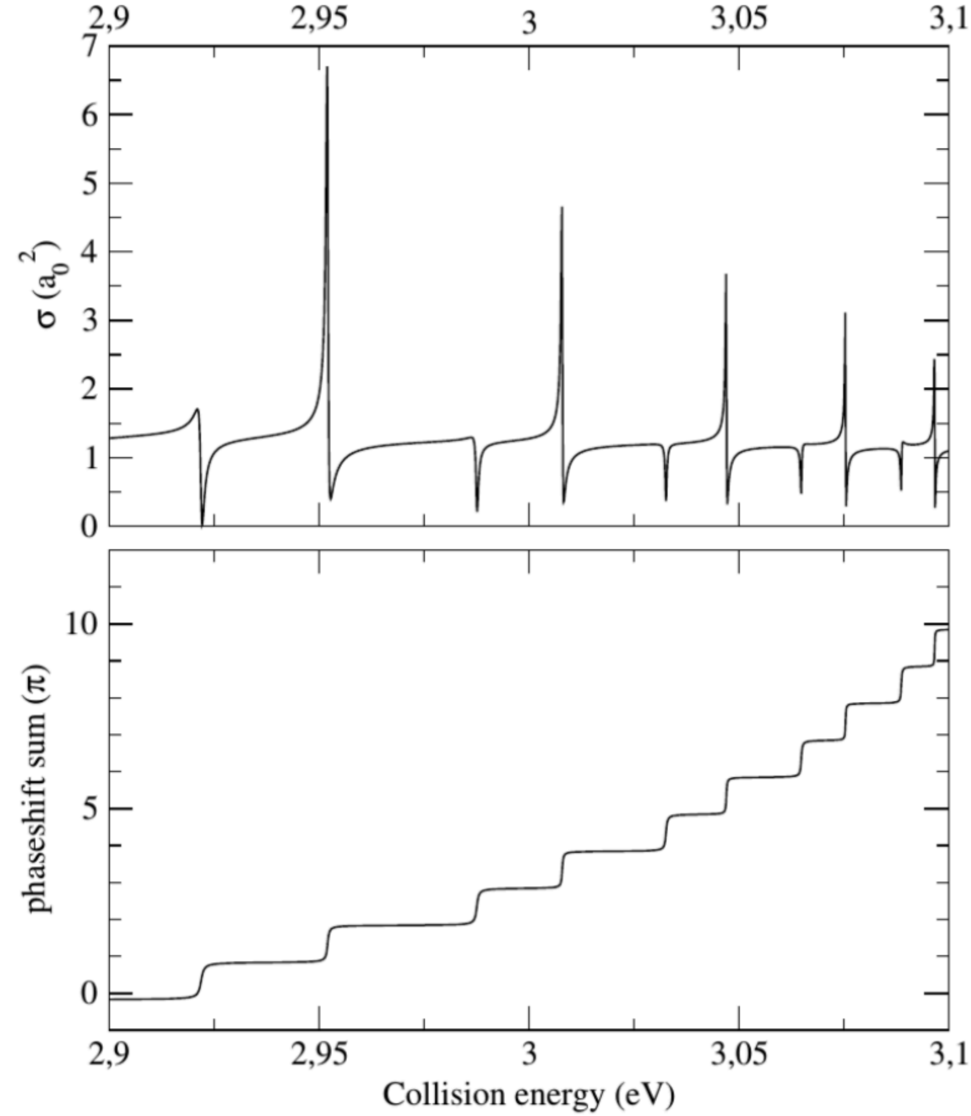


Fig 2 Contribution of the $^2P^o$ partial wave to the cross section σ and eigenphase sum for electron impact excitation $e^- + C^{2+}(1s^2 2s^2\ {}^1S) \rightarrow e^- + C^{2+}(1s^2 2s2p\ {}^3P^o)$. At each resonance, the phaseshift in the corresponding channel increases by π.

Electron scattering by C^{2+} ($1s^2$ $2s^2$)

Main configuration	Total symmetry $^{2S+1}L^{\pi}$	Total energy (Hartree)	Scaled threshold energy (eV)
$1s^22s^2$	^1S	-36.477669	0.0
$1s^22s2p$	$^3P^o$	-36.238542	1.626757
$1s^22s2p$	$^1P^o$	-36.007001	3.201915
$1s^22s3d$	^3D	-35.847916	4.284158
$1s^22s3d$	^1D	-35.810637	4.537762

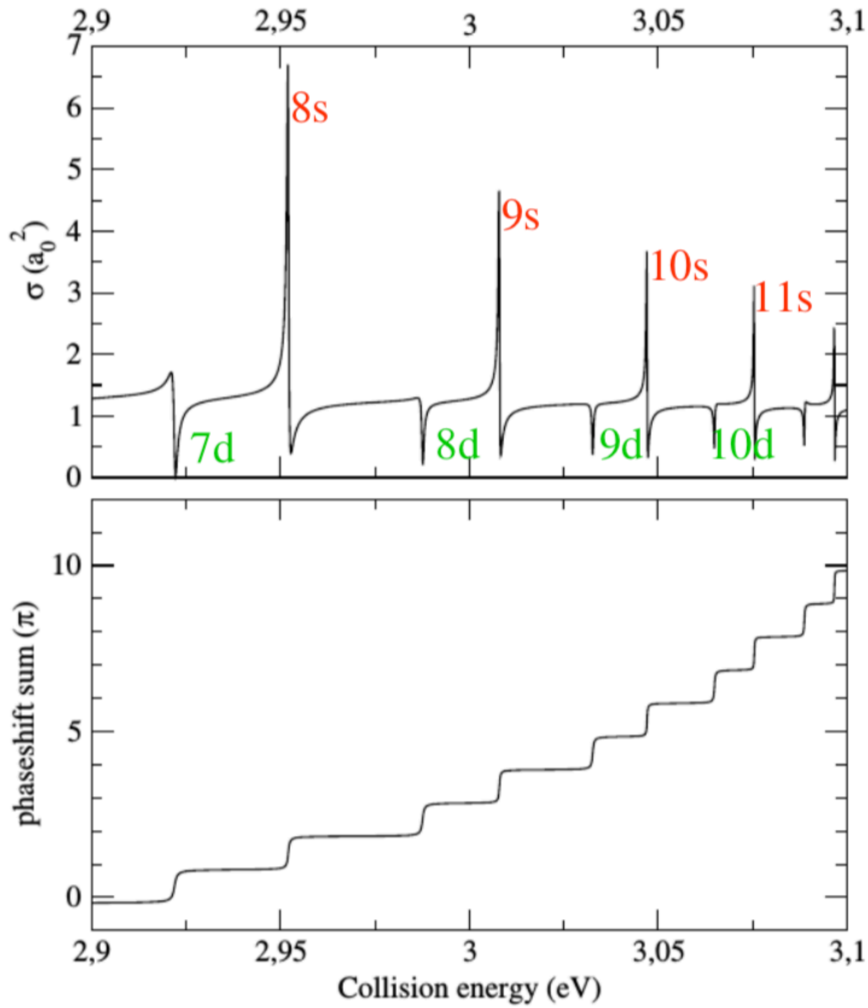
Target states of C^{2+}.

initial target	initial ℓ	final target	final ℓ	total symmetry $^{2S+1}L^{\pi}$	
^1S	0	$^3P^o$,$^1P^o$	1	^2S	Fig 1
	1		0,2	$^2P^o$	Fig 2
	2		2	^2D	
	3		2,4	$^2F^o$	

Table ; Examples of coupled channels for electron impact excitation $e^- + C^{2+}(1s^22s^2\ ^1S) \rightarrow e^- + C^{2+}(1s^22s2p\ ^3P^o,\ ^1P^o)$

Characterization the resonance peaks with partial wave results by help of Quantum Defect Theory.

$^2P^o$



Intermediate state

$C^+(1s^2 2s2p\ ^1P^o\ ns)$

$C^+(1s^2 2s2p\ ^1P^o\ nd)$

Fig 2 Contribution of the $^2P^o$ partial wave to the cross section σ and eigenphase sum for electron impact excitation $e^- + C^{2+}(1s^2 2s^2\ ^1S) \rightarrow e^- + C^{2+}(1s^2 2s2p\ ^3P^o)$. At each resonance, the phaseshift in the corresponding channel increases by π.

2. Learning Multiple Scattering & Fortran

using the renormalization method,
we developed the code.

"***Simple renormalization schemes for scattering series expansion***"

-- Introduce the renormalization method

-- Results of the calculation compared with
Matrix Inversion (direct calculation)

Our motivation

The photoemission cross-section[1] is given by

$$\frac{d\sigma}{d\hat{\boldsymbol{k}}} = 4\pi^2 \alpha \hbar\omega_{\boldsymbol{q}} \sum_{m_c\sigma_c} \left| \sum_L M_{L_cL} \left[B_L^o(\boldsymbol{k})\right]^* \right|^2$$

where the amplitude B is given by

$$B_L^o(\boldsymbol{k}) = \sum_{jL'} \tilde{\tau}_{LL'}^{oj} \mathrm{i}^{\ell'} Y_{L'}(\hat{\boldsymbol{k}}) \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_{jo}} (k/\pi)^{1/2}$$

$$\tau = T(I - G_oT)^{-1}$$

scattering path operator

Takes time, bottle neck of calculation

How can we quickly calculate $(I - G_oT)^{-1}$?

Matrix Inversion (MI)
CPU time $\propto N^3$ $N \equiv Z_{at}(l_{max}+1)^2$

↑ Straight forward

$(I - G_oT)^{-1}$

high energy (EXAFS region)

spectral radius: $\rho(G_oT) < 1$

⇓

Taylor series expansion

$(I - G_oT)^{-1} = \sum_n (G_oT)^n$

3 or 4 terms enough

low energy, large cluster

spectral radius: $\rho(G_oT) > 1$

⇓

Taylor series expansion → diverge …

alternative method

We introduce 2 methods with scaling

[1] D. Sébilleau, K. Hatada, H. Ebert, "Multiple Scattering Theory", *Springer Proceedings in Physics* **204**, Springer (2018).

Introduction to the renormalization method

The renormalized Multiple Scattering (MS) expansions

$$(I - G_o T)^{-1} \equiv (I - K)^{-1}$$

K: kernel matrix

we introduce the auxiliary matrix G[2] by

Hence

$$(I - K)^{-1} = \omega (I - G)^{-1} \quad \dots (1)$$

parameter ω chosen so that $\rho(K) > \rho(G)$.

We should find

whole family of the matrices (G_j) by

$$G_o = K$$

$$G_{j+1} = (1 - \omega) I + \omega G_j$$

iterate this equation, we obtain

$$G_j = (1 - \omega^j) I + \omega^j K$$

$$(I - K)^{-1} = \omega^j (I - G_j)^{-1} \dots \text{(Method 1)}$$

[2] K. B. Janiszowski, *Int. J. Appl.* Math. Comput. Sci. **13**, 199 (2003).

Using the binomial theorem and writing $g_j \equiv \omega^j$,

$$G_j^n = \sum_{n=0}^{\infty} C_n^m (1 - g_j)^{n-m} g_j^m K^m$$

where $C_n^m = \binom{n}{m}$ is the standard binomial coefficient.

the right hand side of Eq. (1) is

$$\omega (I - G)^{-1} = \omega \sum_{n=0}^{\infty} G_j^n \sim \sum_{k=0}^{N_s} R_k(\omega, N_s) K^k$$

N_s : truncation order of the expansion

Summing the G_j matrices, we obtain

$$S_n \equiv \sum_{j=0}^{n} G_j = (n+1) I - \frac{1 - \omega^{n+1}}{1 - \omega} (I - K)$$

$$\Sigma_n \equiv \frac{S_n}{n+1} \quad , \quad s_n = \frac{1}{n+1} \sum_{j=0}^{n} \omega^j$$

$$(I - K)^{-1} = s_n (I - \Sigma_n)^{-1} \dots \text{(Method 2)}$$

Key for better convergence

"spectral radius" ? → Convergence is faster for smaller spectral radius

The Taylor expansion of the matrix inverse is

$$(I - G_oT)^{-1} = I + (G_oT) + (G_oT)^2 + \ldots$$

G_oT : the kernel matrix

As G_oT is diagonalizable,

$$G_oT = SDS^{-1}$$

D: diagonal matrix

$$(I - G_oT)^{-1} = S(I + D + D^2 + \ldots)S^{-1}$$

The expansion converges if the largest element of the diagonal matrix D is smaller than 1,

for any eigenvalue λ_i of D

$$(I - \lambda_i)^{-1} = 1 + \lambda_i + {\lambda_i}^2 + \ldots$$

is convergent.

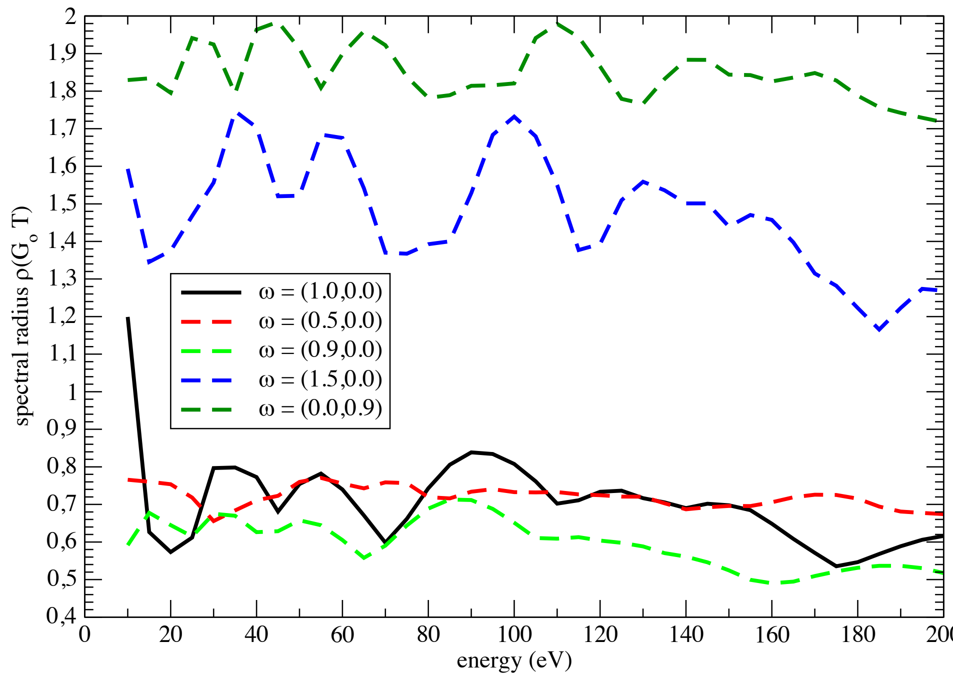
$$\rho(G_oT) \equiv max_i|\lambda_i|$$

spectral radius

∴ We can consider only

$$\rho(G_oT) < 1$$

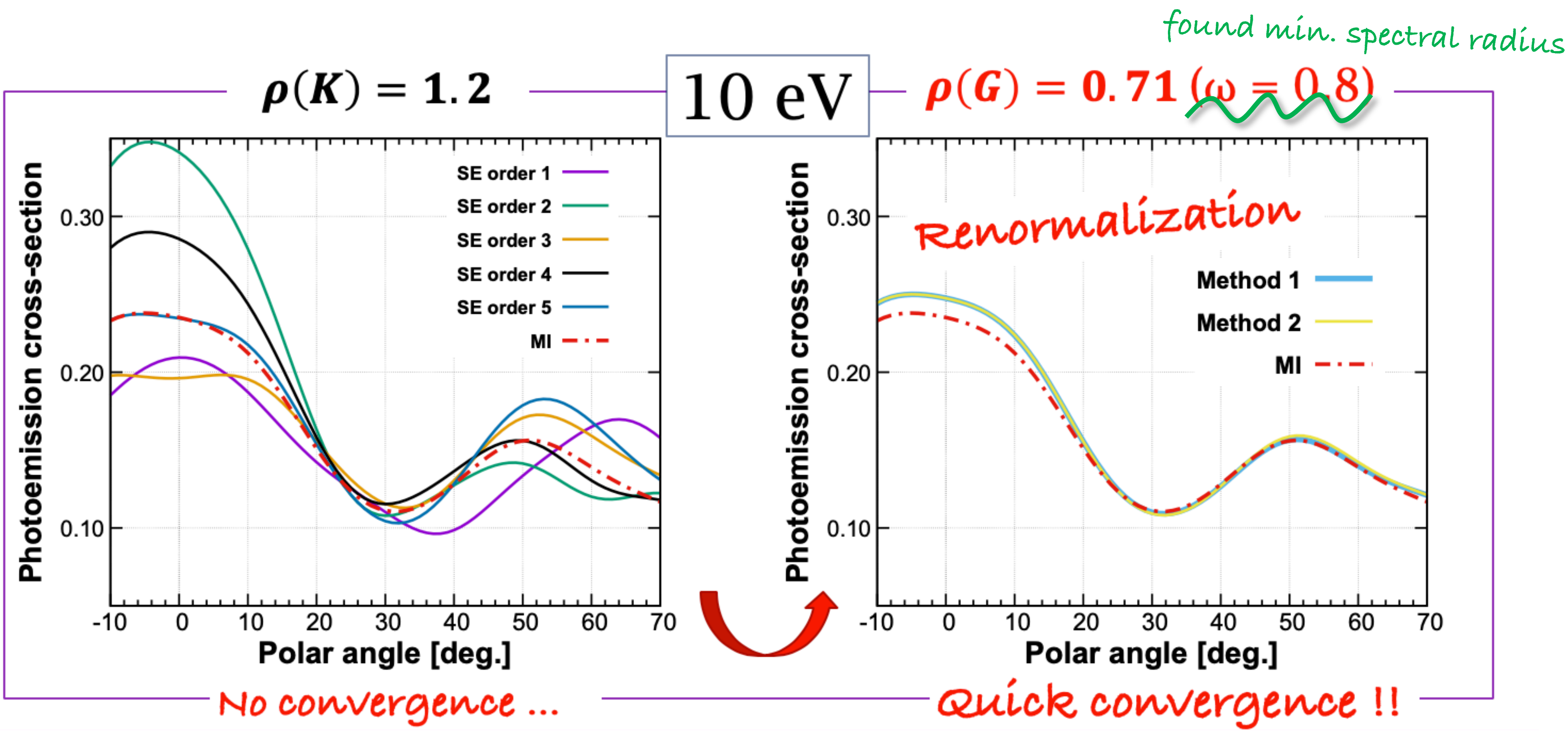
when $(I - G_oT)^{-1}$ is convergent.



Values of the spectral radius of renormalized matrix for different values of the renormalization parameter ω (Cu(111) 50 atom case).[3]

[3] D. Sébilleau, K. Hatada, H. -F. Zhao, C. R. Natoli *e-J. Surf. Sci. Nanotech* **10**, 599-608 (2012).

Results for Cu(111) 50 atom cluster , Kinetic energy: 10eV



- Our results suggest the renormalization 2 methods work well when Taylor like series expansion does not converge (low energy region) for Cu.
- We found the best value of ω empirically.
  → We should establish a relationship between the spectral radius and ω.

3. Training numerical analysis for solving the differential equation

Using numerical analysis { Runge Kutta 4th order method / Numerov method

Started from Schrödinger equation
--- without any potential
--- Coulomb potential

Compared with exact solutions
--- Implement against the numerical errors
--- How to decide the grid

Our ultimate goal is solving this equation

$$\left(\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{\ell_i(\ell_i+1)}{r^2} - V(r) + k_i^2\right) P_i(r) - \sum_j W_{ij}(r, r') P_j(r') + \sum_q \lambda_{iq} P_q(r) \delta_{\ell_i \ell_q} = 0$$

D. Sébilleau, K. Hatada, H. Ebert,
"Multiple Scattering Theory", *Springer Proceedings in Physics* **204**, Springer (2018).

4. Future tasks for realizing MCMS

(・For the renormalization method,
We should establish a relationship between the spectral radius and ω)

・Applying the numerical analysis to more complicated cases
-- the other potentials, especially multi-channel potential
-- the boundary conditions for multichannel wave function

・Learning the solid state physics,
extend the theory for non-single atom cases by multiple-scattering theory

Thank you for your attention