A partitioned correlation function interaction approach in GRASP

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2025.06.12

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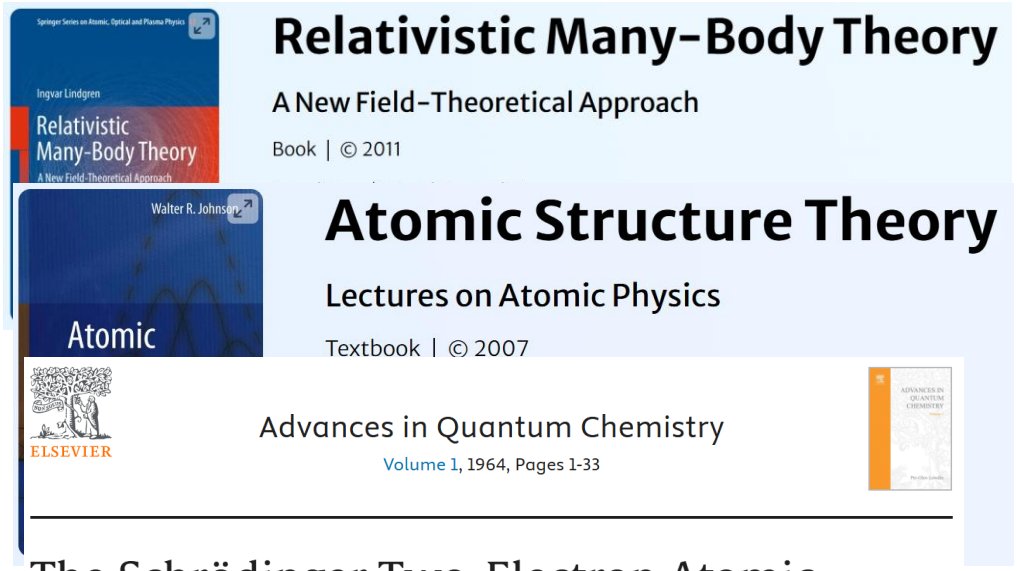
CONTENTS

Background

Accurate description of electron correlation remains a major challenge in atomic structure calculation.



The Schrödinger Two-Electron Atomic Problem

See discussions, stats, and author profiles for this publication at: https://www.researchgate.net/publication/2412780

Ab Initio Methods For Electron Correlation In Molecules

Article · February 2000
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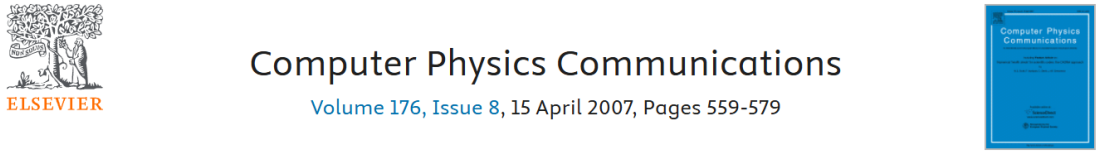

An MCHF atomic-structure package for

roid [c]

CPC 50th anniversary article

GRASP2018—A Fortran 95 version of the General Relativistic Atomic Structure Package ☆

C. Froese Fischer [a], G. Gaigalas [b], P. Jönsson [c], J. Bieroń [d]

Background

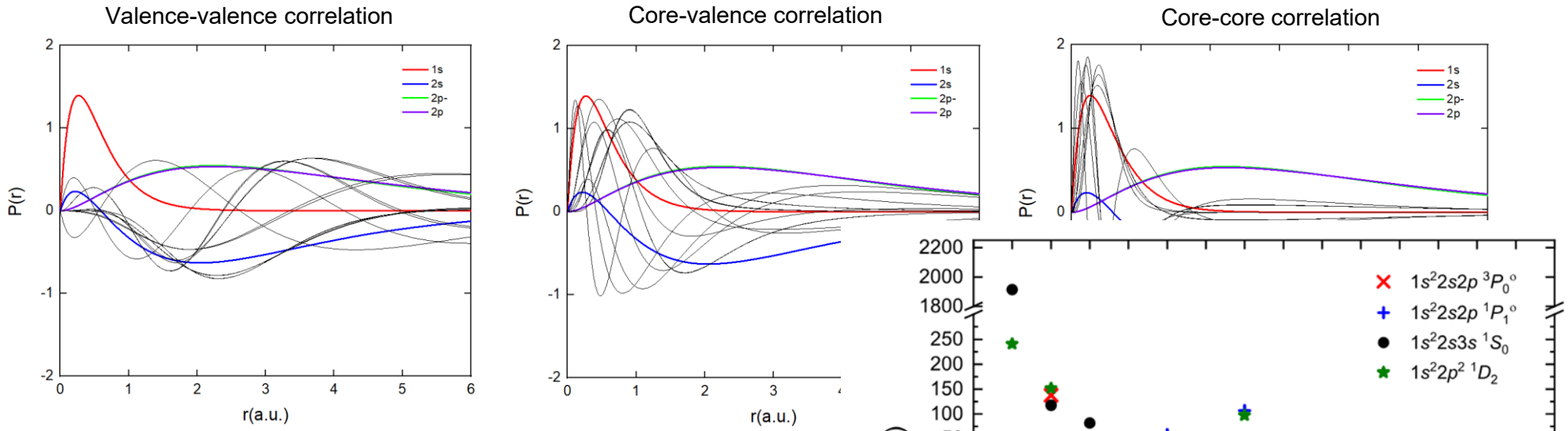

Fig 1. The P(r) of radial orbitals from MCDHI

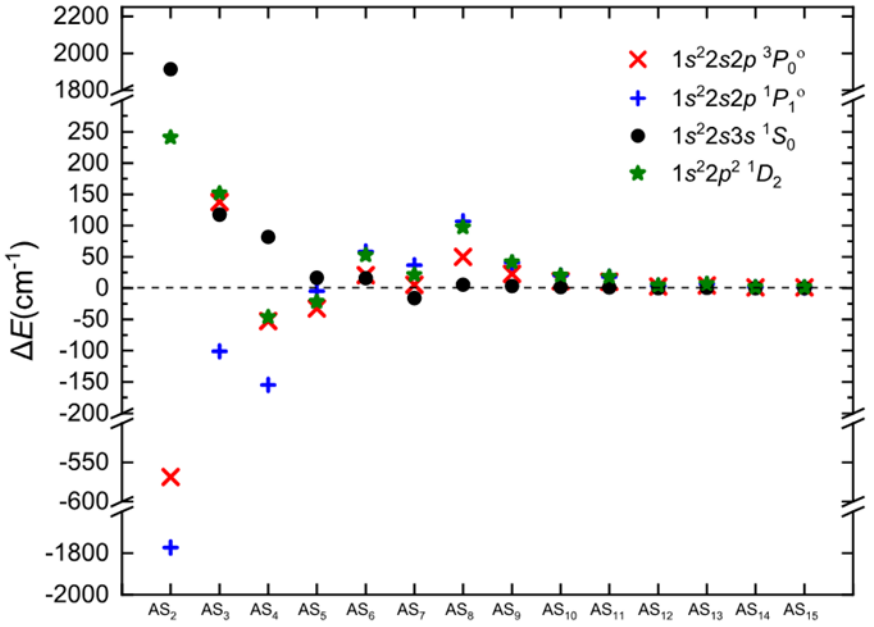

Fig 2. Difference of the excitation energies as a function of AS for Be I

First major problem:

Due to restrictions in the Racah or the Slater determi
required to be orthonormal.

To saturate the pair correlation effects, and properly a
all pairs of electrons, the orbital basis must be extenc
symmetry, leading to **massive CSF expansion**.

$\mathrm{AS}_{15} = \{22s, 22p, 19d, 17f, 16g, 15h, 15i, 13k, 13l, 11m\}$ $N_{\mathrm{CSF}} = 230$ millions

The Breit contributions of $n \geq 12, l \geq 6$ are discarded

Background

Second major problem:
Variational methods are entirely based on the **energy functional**, and properties not strongly coupled to this functional, such as hyperfine structure and transition rates, may be inadequately described by the resulting wave function.
Convergence for expectation values often **irregular** with respect to the increasing active set. (**Oscillation**)

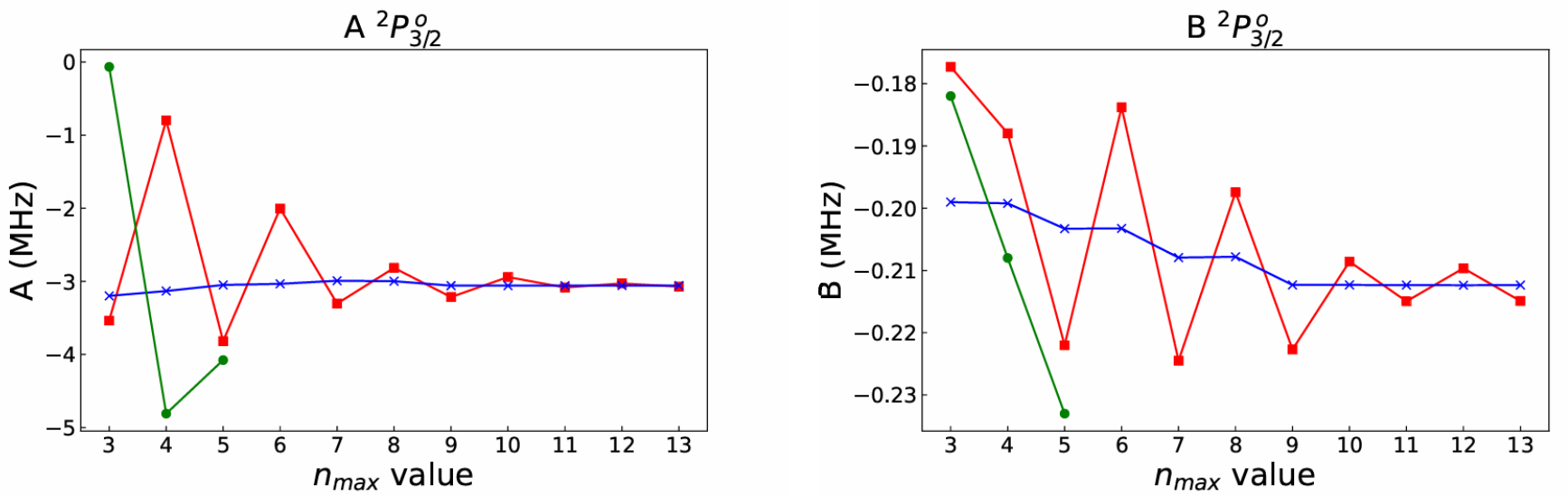

Fig 3. Convergence of hyperfine constants *A* and *B* for $1s^2 2p\ ^2P^o_{3/2}$ of neutral lithium[1]. The red line shows results from the energy-driven layer-by-layer calculations using the GRASP Code.

[1] Independently Optimized Orbital Sets in GRASP—The Case of Hyperfine Structure in Li I. Yanting Li et al. Atoms. (2022)

Theory and program

Partition Correlation Function (PCF): an ASF built on a CSF expansion generated by allowing excitations from specific subshells of the MR CSF expansion to a given orbital active set.

$$|\Psi\rangle = |\Psi^{(0)}\rangle + \sum_{p=1}^{P} |\Lambda_p\rangle$$

Zero-order space:

$$|\Psi^{(0)}\rangle = \sum_{j=1}^{N} a_j |\Phi_j^0\rangle$$

Correlation function space:

$$|\Lambda_p\rangle = \sum_{k=1}^{N_p} c_k^p \, |\Phi_k^p\rangle$$

$$\Longrightarrow \quad |\Psi^{(p)}\rangle = \sum_{j=1}^{N} a_j^p |\Phi_j^0\rangle + \sum_{k=1}^{N_p} c_k^p \, |\Phi_k^p\rangle$$

$$\mathbf{H} = \begin{pmatrix} \langle\Phi_1^{\mathrm{mr}}|\mathcal{H}|\Phi_1^{\mathrm{mr}}\rangle & \cdots & \langle\Phi_1^{\mathrm{mr}}|\mathcal{H}|\Phi_m^{\mathrm{mr}}\rangle & \langle\Phi_1^{\mathrm{mr}}|\mathcal{H}|\overline{\Lambda}_1\rangle & & \langle\Phi_1^{\mathrm{mr}}|\mathcal{H}|\overline{\Lambda}_p\rangle \\ \vdots & \ddots & \vdots & \vdots & & \vdots \\ \langle\Phi_m^{\mathrm{mr}}|\mathcal{H}|\Phi_1^{\mathrm{mr}}\rangle & \cdots & \langle\Phi_m^{\mathrm{mr}}|\mathcal{H}|\Phi_m^{\mathrm{mr}}\rangle & \langle\Phi_m^{\mathrm{mr}}|\mathcal{H}|\overline{\Lambda}_1\rangle & \cdots & \langle\Phi_m^{\mathrm{mr}}|\mathcal{H}|\overline{\Lambda}_p\rangle \\ & & & \langle\overline{\Lambda}_1|\mathcal{H}|\overline{\Lambda}_1\rangle & \cdots & \langle\overline{\Lambda}_1|\mathcal{H}|\overline{\Lambda}_p\rangle \\ & \vdots & & \vdots & \ddots & \vdots \\ & & & \cdots & \cdots & \langle\overline{\Lambda}_p|\mathcal{H}|\overline{\Lambda}_p\rangle \\ & \vdots & & & & \end{pmatrix}$$

Theory and program

Partition Correlation Function (PCF): an ASF built on a CSF expansion generated by allowing excitations from specific subshells of the MR CSF expansion to a given orbital active set.

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$$\mathbf{H} = \begin{pmatrix} \langle \\ \langle \\ \\ \\ \\ \\ \\ \end{pmatrix}$$

- Space divided into a number of sub-spaces. (a divide-and-conquer strategy)
- The CSFs of sub-spaces are independently optimized and built on different active sets.
- No orthogonality requirements between orbitals of active sets of the different sub-spaces.

Theory and program

Partition Correlation Function (PCF): an ASF built on a CSF expansion generated by allowing excitations from specific subshells of the MR CSF expansion to a given orbital active set.

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Theory and program

Non-orthogonal basis

$$\mathbf{Hc} = E\mathbf{Sc}$$

Biorthonormal transformation

Two CSF expansions built on different and mutually non-

$$\Psi_l = \sum_{i=1}^{N_l} c_i^l \Phi_i^l \qquad \Psi_r = \sum_{i=1}^{N_r} c_i^r \Phi_i^r$$

Closed und

$$\Longrightarrow \quad \langle \widetilde{\phi}_{n\kappa}^l | \widetilde{\phi}_{n'\kappa}^r \rangle = \delta_{n,n'} \qquad \Psi_l \equiv \sum_{i=1}^{N_l} \widetilde{c}_i^l \widetilde{\Phi}_i^l$$

a

$$\Longrightarrow \quad \langle \Psi_l | O | \Psi_r \rangle = \sum_{i=1}^{N_l} \sum_{j=1}^{N_r} \widetilde{c}_i^l \widetilde{c}_j^r \langle \widetilde{\Phi}_i^l | O | \widetilde{\Phi}_j^r \rangle$$

```
1s ( 1)   2s ( 1)   3s ( 2)
    1/2       1/2
                    0       0+
1s ( 1)   2s ( 1)   3s ( 1)   4s ( 1)
    1/2       1/2       1/2       1/2
                    0       1/2       0+
1s ( 1)   2s ( 1)   4s ( 2)
    1/2       1/2
                    0       0+
```

Theory and program

Non-orthogonal basis

$$\mathbf{Hc} = E\mathbf{Sc}$$

Biorthonormal transformation

Two CSF expansions built on different and mutually non-orthonormal orbital sets

$$\Psi_l = \sum_{i=1}^{N_l} c_i^l \Phi_i^l \qquad \Psi_r = \sum_{i=1}^{N_r} c_i^r \Phi_i^r$$

Closed under deexcitation (CUD)

$$\Longrightarrow \quad \langle \widetilde{\phi}_{n\kappa}^l | \widetilde{\phi}_{n'\kappa}^r \rangle = \delta_{n,n'} \qquad \Psi_l \equiv \sum_{i=1}^{N_l} \widetilde{c}_i^l \widetilde{\Phi}_i^l \quad \text{and} \quad \Psi_r \equiv \sum_{i=1}^{N_r} \widetilde{c}_i^r \widetilde{\Phi}_i^r.$$

$$\Longrightarrow \quad \langle \Psi_l | O | \Psi_r \rangle = \sum_{i=1}^{N_l} \sum_{j=1}^{N_r} \widetilde{c}_i^l \widetilde{c}_j^r \langle \widetilde{\Phi}_i^l | O | \widetilde{\Phi}_j^r \rangle$$

Theory and program

Biorthonormal weight matrix method

$$\{\Phi_1^p, \ldots, \Phi_{N_p}^p\} \quad \{\Phi_1^q, \ldots, \Phi_{N_q}^q\}$$

$$H_{ij}^{pq} = \langle \Phi_i^p | H | \Phi_j^q \rangle$$

$$\downarrow$$

$$\mathbf{H}^{pq} \equiv (\widetilde{\mathbf{D}}^p)^t \widetilde{\mathbf{H}}^{pq} \widetilde{\mathbf{D}}^q$$

$$\mathbf{D}^p = \underbrace{\begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1 \end{pmatrix}}_{N_p} \longrightarrow \widetilde{\mathbf{D}}^p = \begin{pmatrix} \tilde{d}_{1,1}^p & \tilde{d}_{1,2}^p & \cdots & \tilde{d}_{1,N_p}^p \\ \tilde{d}_{2,1}^p & \tilde{d}_{2,2}^p & \cdots & \tilde{d}_{2,N_p}^p \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{d}_{N_p,1}^p & \tilde{d}_{N_p,2}^p & \cdots & \tilde{d}_{N_p,N_p}^p \end{pmatrix}$$

$$\mathbf{D}^q = \underbrace{\begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1 \end{pmatrix}}_{N_q} \longrightarrow \widetilde{\mathbf{D}}^q = \begin{pmatrix} \tilde{d}_{1,1}^q & \tilde{d}_{1,2}^q & \cdots & \tilde{d}_{1,N_q}^q \\ \tilde{d}_{2,1}^q & \tilde{d}_{2,2}^q & \cdots & \tilde{d}_{2,N_q}^q \\ \vdots & \vdots & \ddots & \vdots \\ \tilde{d}_{N_q,1}^q & \tilde{d}_{N_q,2}^q & \cdots & \tilde{d}_{N_q,N_q}^q \end{pmatrix}$$

$$\underbrace{\begin{pmatrix} \tilde{d}_{1,1}^p & \tilde{d}_{1,2}^p & \cdots & \tilde{d}_{1,k-1}^p & \tilde{d}_{1,k}^p \\ \tilde{d}_{2,1}^p & \tilde{d}_{2,2}^p & & \tilde{d}_{2,k-1}^p & \tilde{d}_{2,k}^p \\ \vdots & & \ddots & \vdots & \\ \tilde{d}_{k-1,1}^p & \tilde{d}_{k-1,2}^p & \cdots & \tilde{d}_{k-1,k-1}^p & \tilde{d}_{k-1,k}^p \\ \tilde{d}_{k,1}^p & \tilde{d}_{k,2}^p & & \tilde{d}_{k,k-1}^p & \tilde{d}_{k,k}^p \end{pmatrix}}_{k \times k} \times \underbrace{\begin{pmatrix} <\tilde{\Phi}_i^p|H|\tilde{\Phi}_j^q> & <\tilde{\Phi}_i^p|H|\tilde{\Phi}_{j+1}^q> & \cdots & <\tilde{\Phi}_i^p|H|\tilde{\Phi}_{j+l-1}^q> & <\tilde{\Phi}_i^p|H|\tilde{\Phi}_{j+l}^q> \\ <\tilde{\Phi}_{i+1}^p|H|\tilde{\Phi}_j^q> & <\tilde{\Phi}_{i+1}^p|H|\tilde{\Phi}_{j+1}^q> & & <\tilde{\Phi}_{i+1}^p|H|\tilde{\Phi}_{j+l-1}^q> & <\tilde{\Phi}_{i+1}^p|H|\tilde{\Phi}_{j+l}^q> \\ \vdots & & \ddots & \vdots & \\ <\tilde{\Phi}_{i+k-1}^p|H|\tilde{\Phi}_j^q> & <\tilde{\Phi}_{i+k-1}^p|H|\tilde{\Phi}_{j+1}^q> & \cdots & <\tilde{\Phi}_{i+k-1}^p|H|\tilde{\Phi}_{j+k-1}^q> & <\tilde{\Phi}_{i+k-1}^p|H|\tilde{\Phi}_{j+l}^q> \\ <\tilde{\Phi}_{i+k}^p|H|\tilde{\Phi}_j^q> & <\tilde{\Phi}_{i+k}^p|H|\tilde{\Phi}_{j+1}^q> & & <\tilde{\Phi}_{i+k}^p|H|\tilde{\Phi}_j^q> & <\tilde{\Phi}_{i+k}^p|H|\tilde{\Phi}_{j+l}^q> \end{pmatrix}}_{k \times l} \times \underbrace{\begin{pmatrix} \tilde{d}_{1,1}^q & \tilde{d}_{1,2}^q & \cdots & \tilde{d}_{1,l-1}^q & \tilde{d}_{1,l}^q \\ \tilde{d}_{2,1}^q & \tilde{d}_{2,2}^q & & \tilde{d}_{2,l-1}^q & \tilde{d}_{2,l}^q \\ \vdots & & \ddots & \vdots & \\ \tilde{d}_{l-1,1}^p & \tilde{d}_{l-1,2}^p & \cdots & \tilde{d}_{l-1,l-1}^q & \tilde{d}_{l-1,l}^q \\ \tilde{d}_{l,1}^p & \tilde{d}_{l,2}^p & & \tilde{d}_{l,l-1}^q & \tilde{d}_{l,l}^q \end{pmatrix}}_{l \times l}$$

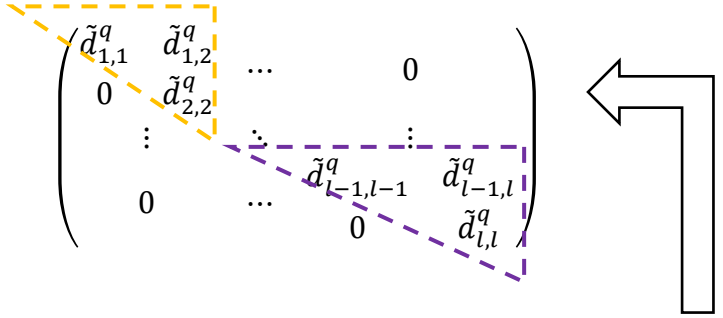
$\Longrightarrow$ Consider an expansion of size N. The computational complexity will be $\mathcal{O}(N^3)$.

Theory and program

Optimization of matrix multiplication

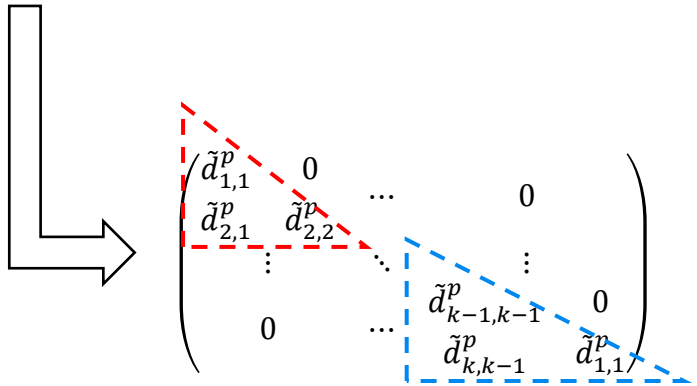
Block-diagonal weight matrix

$$\mathbf{H}^{pq} = ((\tilde{\mathbf{D}}^{p})^{t}\mathbf{H}^{pq}(\tilde{\mathbf{D}}^{q}))$$



$k \times k$ $\quad$ $k \times l$ $\quad$ $l \times l$

$$\begin{pmatrix} \tilde{d}^{p}_{1,1} & 0 & \cdots & 0 \\ \tilde{d}^{p}_{2,1} & \tilde{d}^{p}_{2,2} & & \\ \vdots & & \ddots & \vdots \\ \tilde{d}^{p}_{k-1,1} & \tilde{d}^{p}_{k-1,2} & & \tilde{d}^{p}_{k-1,k-1} \quad 0 \\ \tilde{d}^{p}_{k,1} & \tilde{d}^{p}_{k,2} & \cdots & \tilde{d}^{p}_{k,k-1} \quad \tilde{d}^{p}_{k,k} \end{pmatrix} \times \begin{pmatrix} <\tilde{\Phi}^{p}_{i}|H|\tilde{\Phi}^{q}_{j}> & <\tilde{\Phi}^{p}_{i}|H|\tilde{\Phi}^{q}_{j+1}> & \cdots & <\tilde{\Phi}^{p}_{i}|H|\tilde{\Phi}^{q}_{j+l-1}> & <\tilde{\Phi}^{p}_{i}|H|\tilde{\Phi}^{q}_{j+l}> \\ <\tilde{\Phi}^{p}_{i+1}|H|\tilde{\Phi}^{q}_{j}> & <\tilde{\Phi}^{p}_{i+1}|H|\tilde{\Phi}^{q}_{j+1}> & & <\tilde{\Phi}^{p}_{i+1}|H|\tilde{\Phi}^{q}_{j+l-1}> & <\tilde{\Phi}^{p}_{i+1}|H|\tilde{\Phi}^{q}_{j+l}> \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ <\tilde{\Phi}^{p}_{i+k-1}|H|\tilde{\Phi}^{q}_{j}> & <\tilde{\Phi}^{p}_{i+k-1}|H|\tilde{\Phi}^{q}_{j+1}> & & <\tilde{\Phi}^{p}_{i+k-1}|H|\tilde{\Phi}^{q}_{j+k-1}> & <\tilde{\Phi}^{p}_{i+k-1}|H|\tilde{\Phi}^{q}_{j+l}> \\ <\tilde{\Phi}^{p}_{i+k}|H|\tilde{\Phi}^{q}_{j}> & <\tilde{\Phi}^{p}_{i+k}|H|\tilde{\Phi}^{q}_{j+1}> & \cdots & <\tilde{\Phi}^{p}_{i+k}|H|\tilde{\Phi}^{q}_{j+k-1}> & <\tilde{\Phi}^{p}_{i+k}|H|\tilde{\Phi}^{q}_{j+l}> \end{pmatrix} \times \begin{pmatrix} \tilde{d}^{q}_{1,1} & \tilde{d}^{q}_{1,2} & \cdots & \tilde{d}^{q}_{1,l-1} & \tilde{d}^{q}_{1,l} \\ 0 & \tilde{d}^{q}_{2,2} & & \tilde{d}^{q}_{2,l-1} & \tilde{d}^{q}_{2,l} \\ \vdots & & \ddots & \vdots & \\ & 0 & & \tilde{d}^{q}_{l-1,l-1} & \tilde{d}^{q}_{l-1,l} \\ & & \cdots & 0 & \tilde{d}^{q}_{l,l} \end{pmatrix}$$



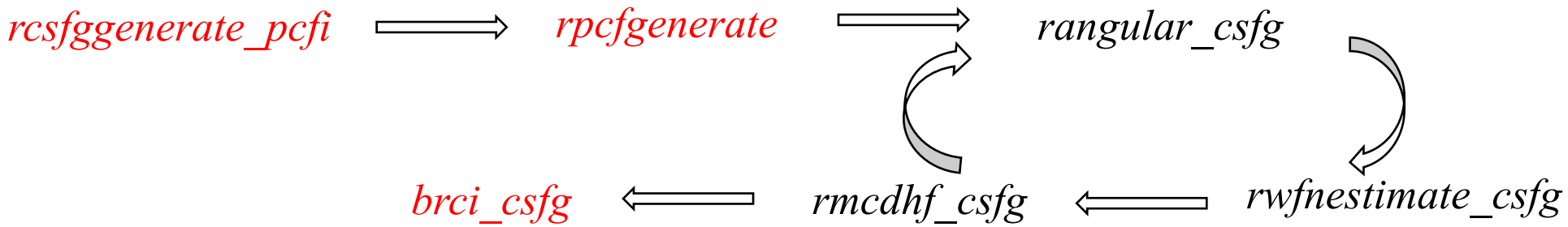
rcfggenerate_pcfi: rearrange

Every part belongs to one CSF generator or two CSF generators according to closed under de-excitation

Computational complexity will be reduced from $\mathcal{O}(N^3)$ to almost $\mathcal{O}(N^2)$

Theory and program

PCFI in GRASP



rcsfggenerate_pcfi: create the whole CSFG space and correctly rearrange the CSFGs, grouping together the CSFGs that need to be placed together to satisfy closed under deexcitation.

rpcfgenerate: divide the original CSF space into multiple PCF spaces and combine them sequentially.

brci_csfg: perform biorthonormal transformation for different wavefunction basis, construct the Hamiltonian matrix elements for different partitioned PCF regions and perform diagonalization calculations.

Calculation of Be I: rotation test

Small example: 7 configurations

```
1s ( 2)  2s ( 2)                  ................MR

                  0+
1s ( 2)  3s ( 2)                  ................VV

                  0+
1s ( 2)  3s ( 1)  4s ( 1)
             1/2       1/2
                          0+
1s ( 2)  4s ( 2)

                  0+
1s ( 1)  2s ( 1)  3s ( 2)         ................CV
    1/2       1/2
                      0       0+
1s ( 1)  2s ( 1)  3s ( 1)  4s ( 1)
    1/2       1/2       1/2       1/2
                      0       1/2       0+
1s ( 1)  2s ( 1)  4s ( 2)
    1/2       1/2
                      0       0+
```

Perform mcdhf calculations for these CSFs

Subshell	e	p0	gamma	P(2)	Q(2)	MTP
1s	4.3071861038D+00	1.434D+01	1.00	3.677D-07	-3.906D-12	332
2s	4.1264187668D-01	3.424D+00	1.00	8.778D-08	-9.324D-13	357
3s	1.1041726949D-01	1.312D+00	1.00	4.757D-08	-5.052D-13	372
4s	5.0335204044D-02	7.211D-01	1.00	-1.071D-08	1.138D-13	382

Rotate 3s and 4s orbitals

Subshell	e	p0	gamma	P(2)	Q(2)	MTP
1s	4.3071861038D+00	1.434D+01	1.00	3.677D-07	7.255D-11	331
2s	4.1264187668D-01	3.424D+00	1.00	8.778D-08	1.732D-11	356
3s	1.1041726949D-01	1.438D+00	1.00	3.685D-08	7.272D-12	381
4s	5.0335204044D-02	-4.179D-01	1.00	2.614D-08	5.158D-12	381

Calculation of Be I: rotation test

Hamiltonian matrix from RCI:

$$\begin{pmatrix} -14.5511 & 1.1921E-2 & 8.5579E-3 & 3.0965E-3 & -2.1566E-3 & -1.6628E-3 & -6.4109E-4 \\ \dots & -13.9869 & -1.1936E-2 & 5.7501E-3 & -8.0319E-2 & 9.6259E-4 & 0.0000 \\ \dots & \dots & -13.9084 & -3.0320E-2 & 9.5210E-4 & -8.1174E-2 & 9.6259E-4 \\ \dots & \dots & \dots & -13.8035 & 0.0000 & 9.5210E-4 & -8.2028E-2 \\ \dots & \dots & \dots & \dots & -9.4775 & -2.9857E-2 & 5.7501E-3 \\ \dots & \dots & \dots & \dots & \dots & -9.3821 & -4.8241E-2 \\ \dots & \dots & \dots & \dots & \dots & \dots & -9.2602 \end{pmatrix}$$

```
RCI
-14.5515746
-13.9898855
-13.9165500
-13.7964744
 -9.4850112
 -9.3895971
 -9.2409794
```

Hamiltonian matrix from PCFI:

$$\left(\begin{array}{cccc|ccc} -14.5511 & 1.1921E-2 & 8.5579E-3 & 3.0965E-3 & -2.5747E-3 & 1.0717E-3 & -2.2307E-4 \\ \dots & -13.9869 & -1.1936E-2 & 5.7501E-3 & -3.9479E-2 & 5.6795E-2 & -4.0840E-2 \\ \dots & \dots & -13.9084 & -3.0320E-2 & -5.6441E-2 & 7.4224E-6 & 5.8356E-2 \\ \dots & \dots & \dots & -13.8035 & -4.0341E-2 & -5.8003E-2 & -4.1687E-2 \\ \hline \dots & \dots & \dots & \dots & -9.4278 & 6.7632E-2 & 9.4778E-3 \\ \dots & \dots & \dots & \dots & \dots & -9.3746 & 8.6016E-2 \\ \dots & \dots & \dots & \dots & \dots & \dots & -9.3174 \end{array}\right)$$

```
PCFI
-14.5515746
-13.9898855
-13.9165500
-13.7964744
 -9.4850112
 -9.3895971
 -9.2409794
```

$$\Longrightarrow \begin{bmatrix} 1.0000 & 0.0000 & 0.0000 & 0.0000 \\ 0.0000 & 0.5000 & 0.0000 & 0.0000 \\ 0.0000 & 0.7071 & 1.0000 & 0.0000 \\ 0.0000 & 0.4999 & 1.4142 & 1.9999 \end{bmatrix} \quad \begin{bmatrix} -2.5747E-3 & -2.5695E-3 & -1.2822E-3 \\ -7.8958E-2 & 1.9252E-3 & 0.0000 \\ -6.0941E-4 & -8.1174E-2 & 1.9252E-3 \\ 0.0000 & -6.0941E-4 & -8.3390E-2 \end{bmatrix} \quad \begin{bmatrix} 1.0000 & -1.4142 & 0.9999 \\ 0.0000 & 1.0000 & -1.4142 \\ 0.0000 & 0.0000 & 1.0000 \end{bmatrix}$$

Calculation of Be I: ground level

Be I: $1s^2 2s^2\ {}^1S_0$

MR: $1s^2\{2s^2, 2p^2\}$

Active space: ⟹ VV, CV and CC

AS_3:$\{3s, 3p, 3d\}$
AS_4:$\{4s, 4p, 4d, 4f\}$
AS_5:$\{5s, 5p, 5d, 5f, 5g\}$
AS_6:$\{6s, 6p, 6d, 6f, 6g, 6h\}$
AS_7:$\{7s, 7p, 7d, 7f, 7g, 7h, 7i\}$
AS_8:$\{8s, 8p, 8d, 8h, 8g, 8h, 8i, 8k\}$

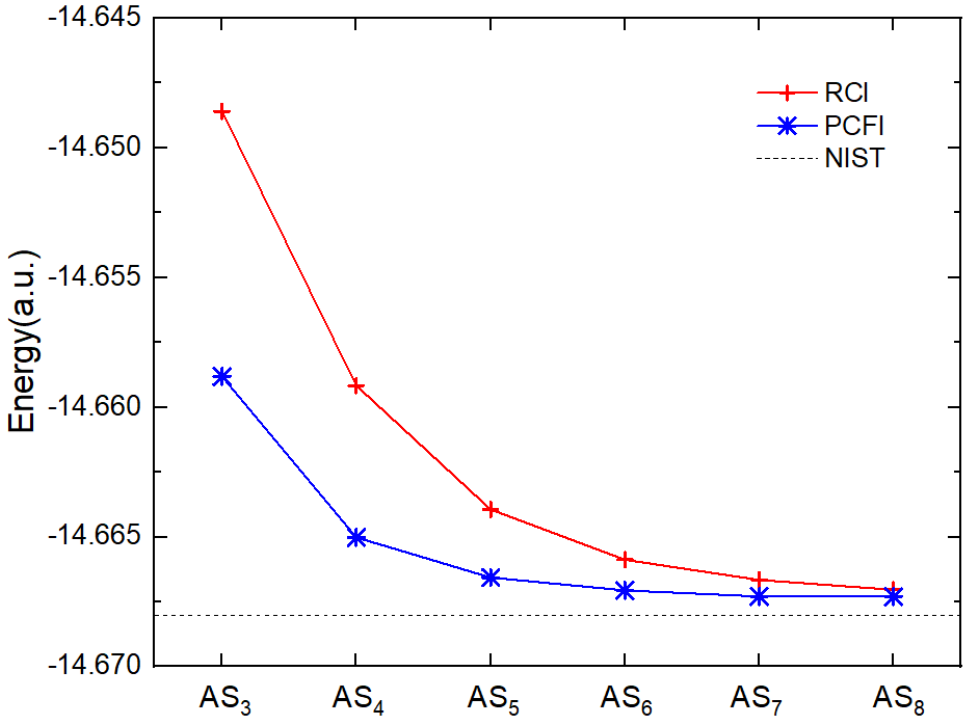


Fig 4. Convergence of the total energy as a function of AS for Be I

Energy (a.u.)	$n = 3$	$n = 4$	$n = 5$	$n = 6$	$n = 7$	$n = 8$
RCI	-14.64859	-14.65916	-14.66394	-14.66588	-14.66666	-14.66704
PCFI	-14.65881	-14.66501	-14.66656	-14.66706	-14.66729	-14.66730

Summary and prospect

Positive things with the PCFI method in GRASP:

- Adhere to a divide-and-conquer strategy and originally big calculation breaks down to a sequence of smaller calculations for the PCFs.
- The PCFs can be built on optimally localized orbitals leading to much faster convergence. The trade-off is the extra matrix multiplication, but it can be efficiently handled and does not significantly increase the computational time.
- PCFs can be specifically targeted to account for electron correlation effects of importance for hyperfine structure and other expectation values.

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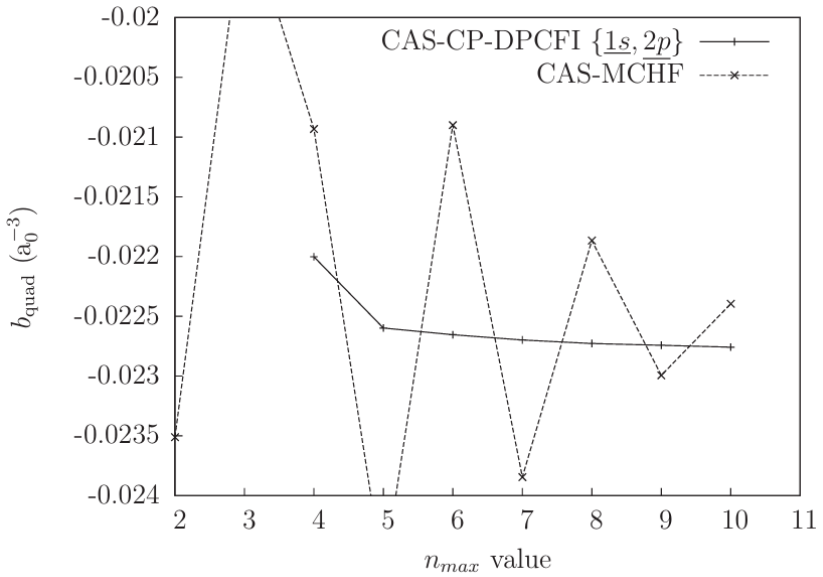

Fig 5. Convergence of the hyperfine parameters (electric quadrupole term) for the first excited state of lithium[2]

[2] A Partitioned Correlation Function Interaction approach for describing electron correlation in atoms. S. Verdebout et al. Journal of Physics B. (2013)

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Prospect:

- Integrate the CSF generator with PCFI
- Realize constrained PCFI method
- Achieve parallelization and structural optimization
- …

Thanks

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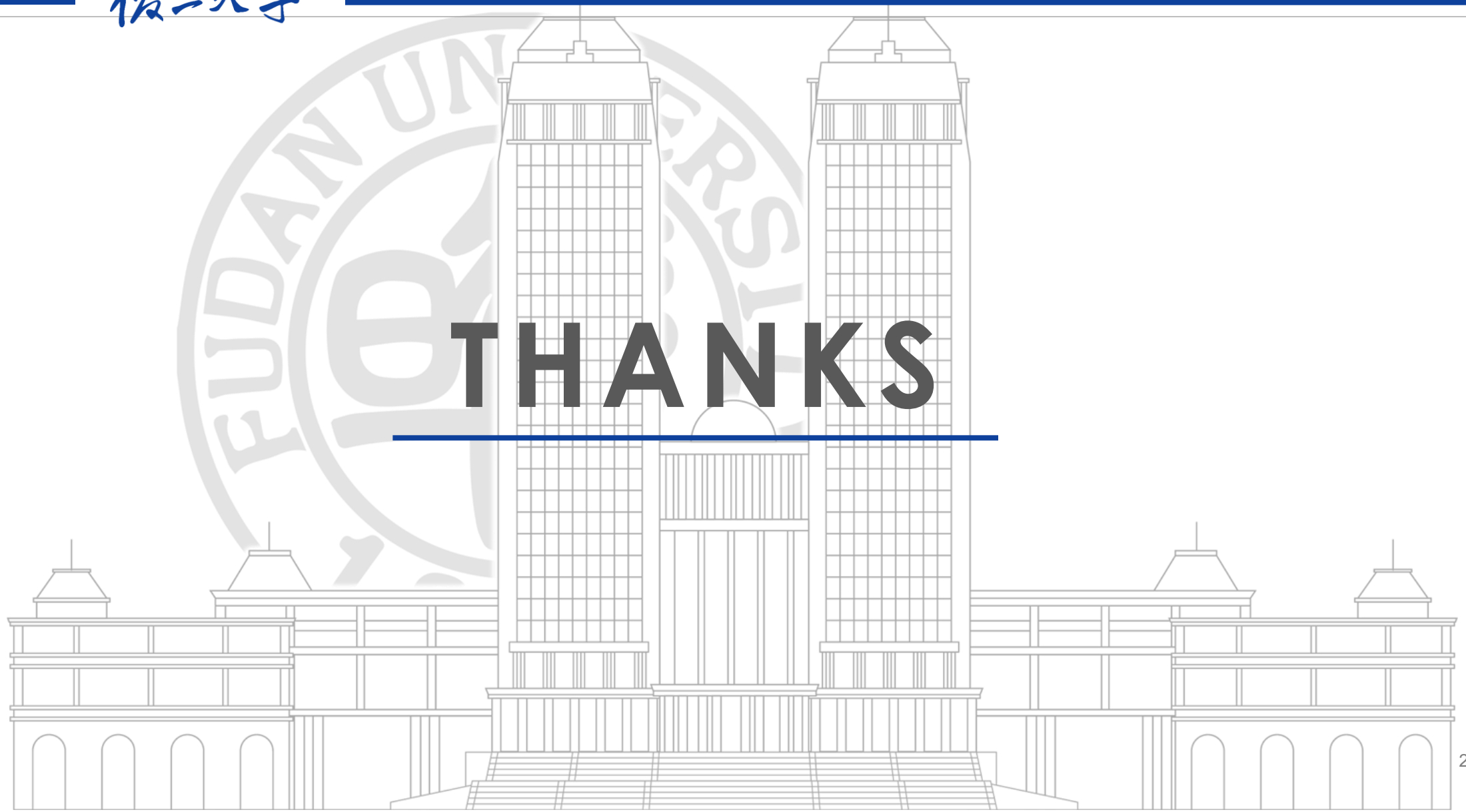

THANKS