AMBiT: methods, applications, tips and tricks

Julian Berengut

CompAS / Lund / 13 June 2025

UNSW SYDNEY

MAX-PLANCK-INSTITUT FÜR KERNPHYSIK

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ÅMBiT: methöds, åpplicatiöns, tïps and tricks 🤘

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Motivation

- The most accurately measured numbers in physics are ratios of atomic clock transition frequencies:
  - $\nu_{Al+}/\nu_{Hg+} = 1.0528718331489904 38\ (55)$ [1]
    (NIST; fractional uncertainty 5.2×10^{-17})
  - $\nu_{Yb}/\nu_{Sr} = 1.2075070393433774 9\ (55)$ [2]
    (RIKEN; fractional uncertainty 4.6×10^{-17})
  - $\nu_{E3}/\nu_{E2} = 0.9328294045309653 76\ (32)$ [3]
    (PTB; fractional uncertainty 3.4×10^{-17})
  - $\nu_{In+}/\nu_{Yb+} = 1.9737735915572157 89\ (9)$ [4]
    (PTB; fractional uncertainty 4.4×10^{-18})
- These are sensitive to everything, but we cannot calculate the spectrum below around 1% accuracy.

So what can we do with these?

[1] *Rosenband et al. Science 319, 1808 (2008)*
[2] *Nemitz et al. Nat. Photonics 10, 258 (2016)*
[3] *Lange et al. PRL 126 011102 (2021)*
[4] *Hausser et al. arXiv: 2402.16807 (2024)*

Differential measurements

- Atomic parity violation
  - Limits running of $\sin^2\theta_W$ at low energy; limits on extra Z boson.
- Searches for eEDM, nEDM
- Tests of Lorentz symmetry, local position invariance, CPT
- Limits on time variations of α, μ
- Coupling of fundamental constants to gravity; axion or scalar axion-like particle searches (dark matter candidate)
- Searches for new bosons using isotope shift

Review: Safronova, Budker, DeMille, Kimball, Derevianko, Clark, RMP 90, 025008 (2018)

Why is atomic structure hard?

- We already know the formulas
- Non-relativistic; atomic units ($\hbar = m_e = e = 1$):

$$\hat{H}\Psi = E\Psi$$

$$\hat{H} = \sum_i \frac{p_i^2}{2m_e} - \frac{Ze^2}{r_i} + \sum_{i<j} \frac{e^2}{|\boldsymbol{r}_i - \boldsymbol{r}_j|}$$

$$\Psi = \Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)$$

- So what's the problem?
- Let each $\boldsymbol{r}_i$ sit on a 10^3 point radial grid (rather coarse!) then Ψ is 10^{3N} dimensional.
- Can represent it using 10^{3N} real numbers.
  There are 10^{80} atoms in the universe.

The original sin

(of atomic structure theory)

- Solution: independent-particle approximation.
- Forget about this awful two body $e^2/|\boldsymbol{r}_i - \boldsymbol{r}_j|$ term.
- The wavefunction is made up of electrons in orbitals

$$\Psi(\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N) = \psi_{1s\uparrow}(\boldsymbol{r}_1)\psi_{1s\downarrow}(\boldsymbol{r}_2)\psi_{2s\uparrow}(\boldsymbol{r}_3)\ldots$$

- Don't forget to antisymmetrise.
- Then the approximate energy is

$$E^{(0)} = \varepsilon_{1s\uparrow} + \varepsilon_{1s\downarrow} + \varepsilon_{2s\uparrow} + \cdots$$

- Leaving out two-body term entirely is a bad idea: we need to start with good orbitals. Use relativistic Hartree-Fock

$$\hat{h}_0 = c\boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta c^2 - Z/r + \hat{V}_{dir} + \hat{V}_{exch}$$

- Spend the rest of your life fixing what you just did.

Redemption

- Bring back $e^2/|\boldsymbol{r}_i - \boldsymbol{r}_j|$!
- More methods than there are theorists. Including:
  - Hartree Fock (or relativistic Dirac-Fock)
  - Multiconfiguration Hartree-Fock (or MCDF)
  - Many-body perturbation theory (so many flavours)
  - Coupled-cluster (ditto)
  - Brueckner orbitals
  - Configuration interaction (CI)
  - CI+MBPT
  - MCDF-CI
  - CI+All order
  - CIPT and emu-CI
  - Particle-hole CI+MBPT
- Mix and match with your favourite codes and colleagues!

Don’t forget QED

- Breit interaction (frequency-independent will do)

$$B_{ij} = -\frac{1}{2r_{ij}}\left(\vec{\alpha}_i \cdot \vec{\alpha}_j + \frac{(\vec{\alpha}_i \cdot \vec{r}_{ij})(\vec{\alpha}_j \cdot \vec{r}_{ij})}{{r_{ij}}^2}\right)$$

- Vacuum polarization (Uehling): not too bad, really.
- Self-energy: really bad, actually.

- Approximate QED using an effective potential or model operator approach

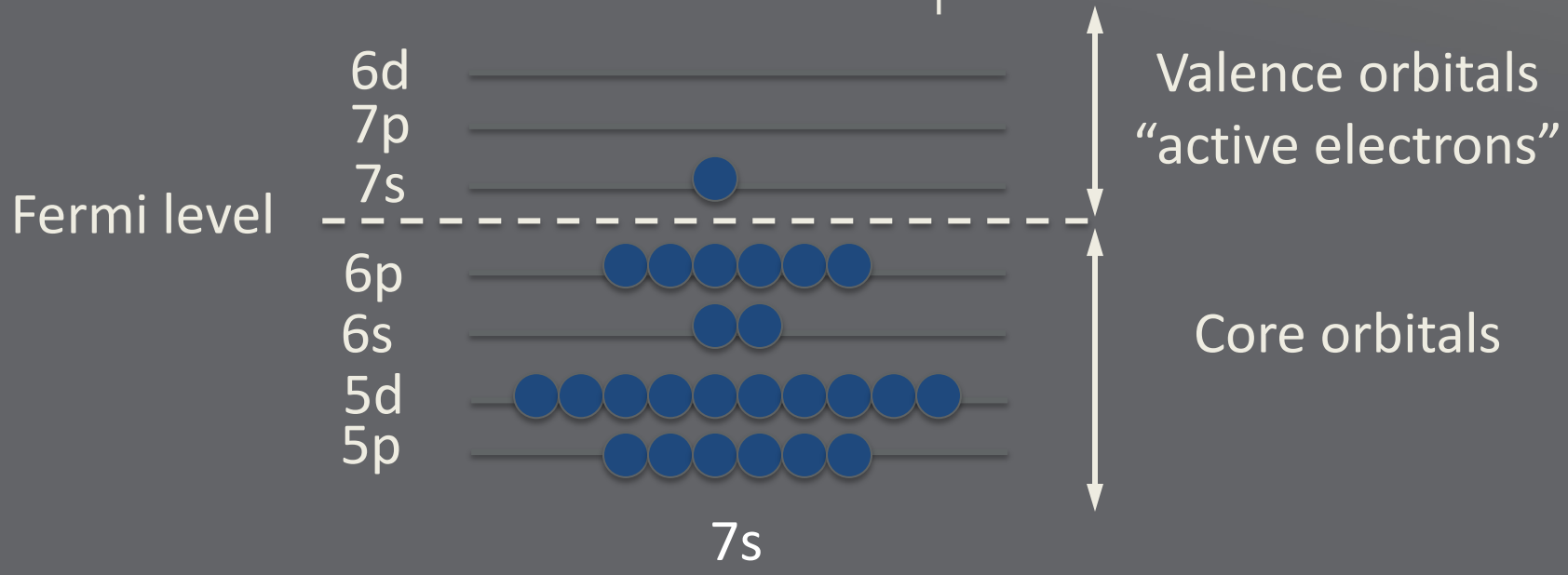
AMBiT – atomic structure code

- Hole-particle CI + MBPT
- Fully relativistic
- Modern C++, parallel, scalable implementation:
  - Optimised on your laptop, workstation, or cluster
- Very flexible, does lots of fancy things (isotope shift, QED, matrix elements, continuum processes …)
- "Nice" interface
- Installation via CMake
- Documentation (!)
- Publicly available at github.com/drjuls/ambit

Kahl and Berengut, CPC 238, 232 (2019)

One valence electron: Fr

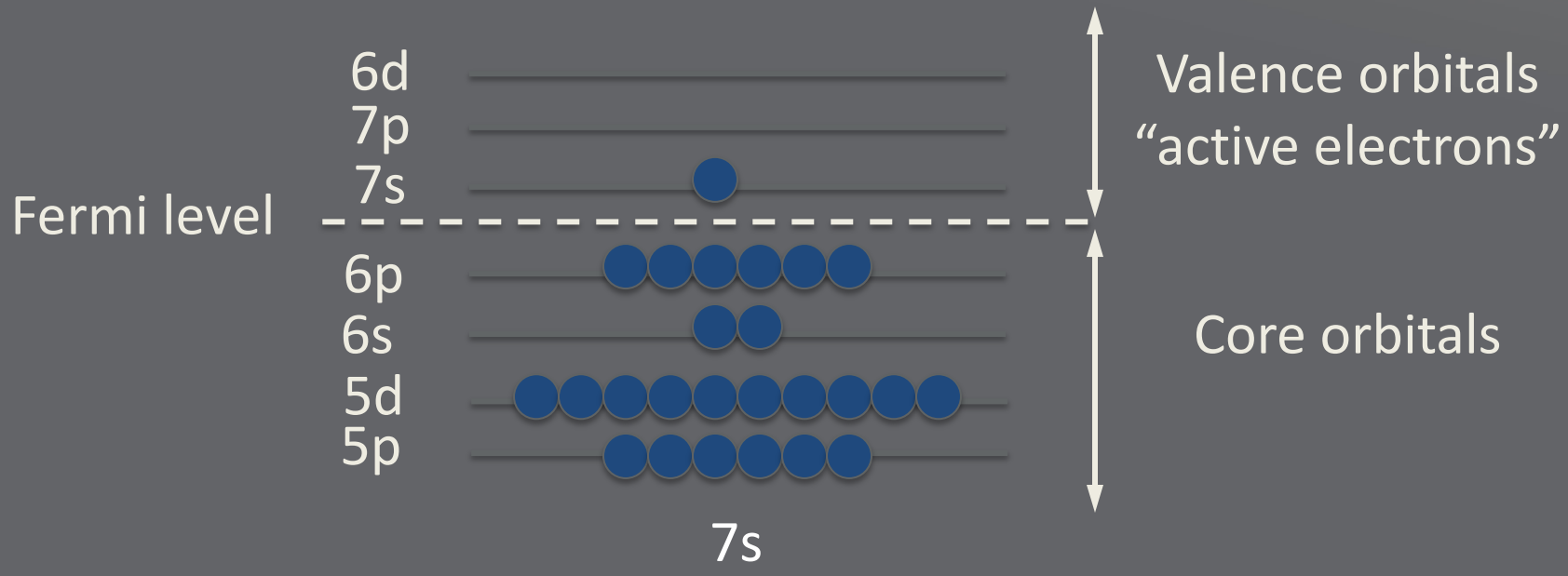
- Single reference Dirac-Hartree-Fock: accuracy ~10%
- Usually use a B-spline basis for valence + virtual states
- Use a log-linear lattice that dynamically resizes as needed
- Continuum orbitals included in HF potential



Dzuba, Flambaum, Sushkov, PLA 140, 493 (1989); PRA 51, 3454 (1995)

One valence electron: Fr

- Single reference Dirac-Hartree-Fock: accuracy ~10%
- Treat core-valence correlations with many-body perturbation theory (MBPT), accuracy ~1%
- Sum leading MBPT diagrams to all orders, ~0.1%



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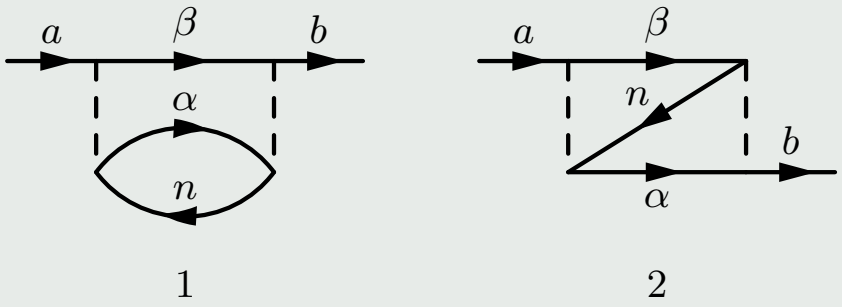
One valence electron

One body diagrams



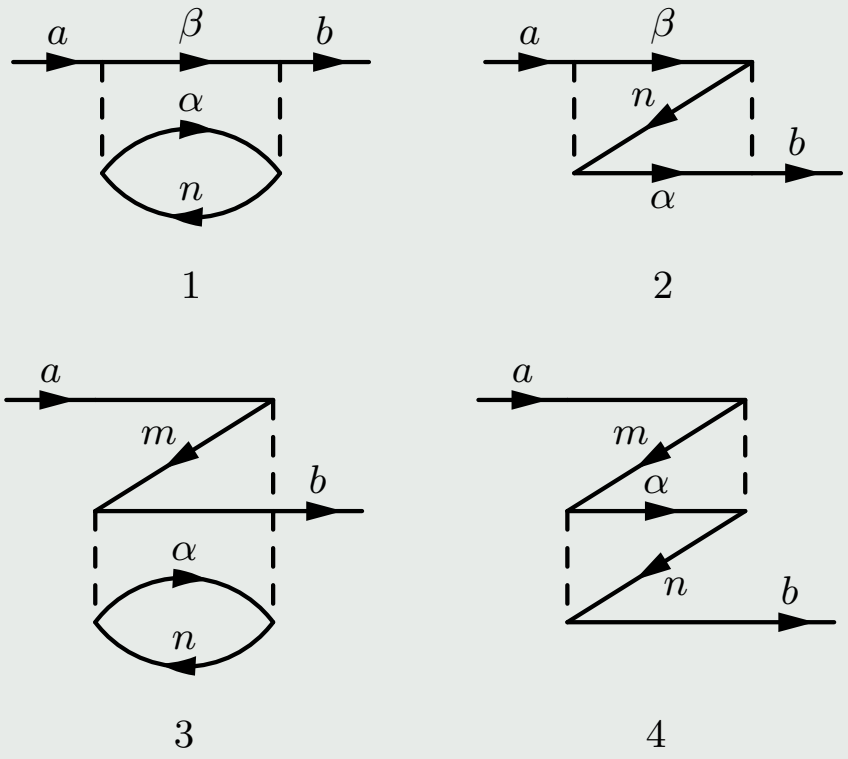
- You can chain these together, for example by making a matrix operator $\hat{\Sigma}$ that expresses these sums and including it in the self-consistent Hartree-Fock procedure:

$$\left(\hat{h}_0 + \hat{\Sigma}\right)\psi_i^{Br} = \varepsilon_i \psi_i^{Br}$$

- Other "all-order" methods include various Fock-space coupled-cluster methods (see Borschevsky talk).

One valence electron

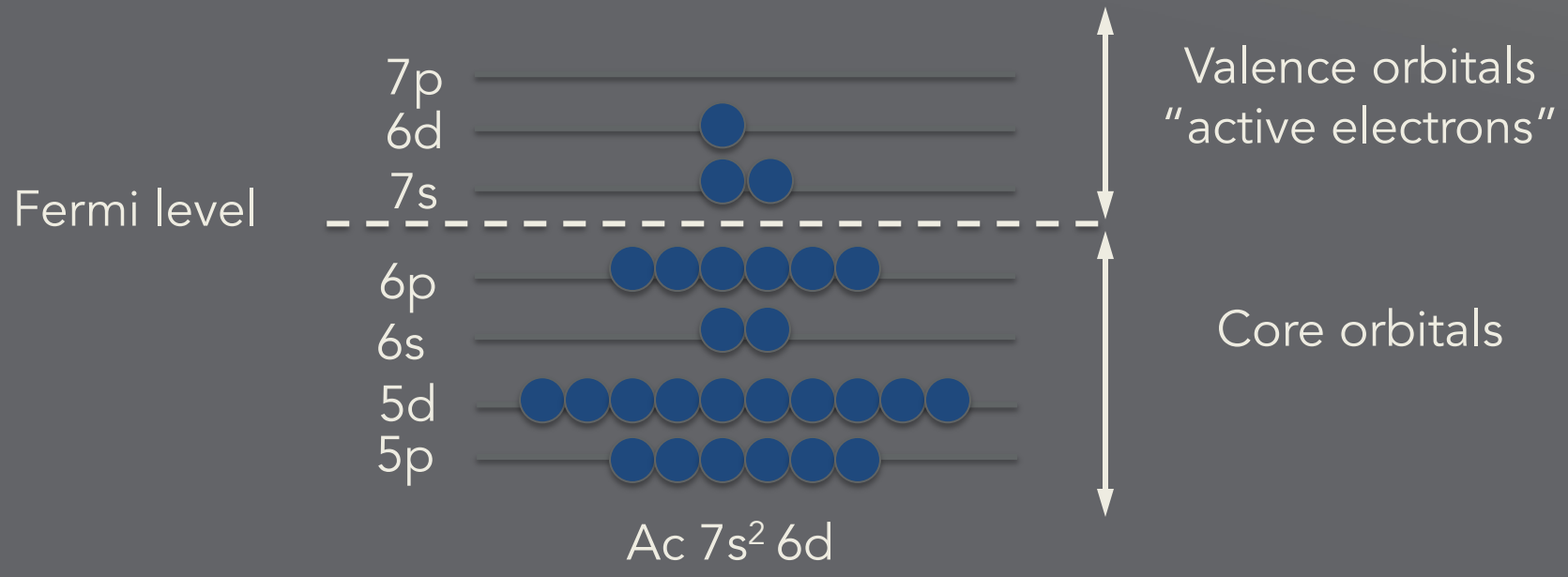
One body diagrams



- In these diagrams α and β lines are summed over an infinite number of valence and virtual states (including the continuum).
- In practice we construct a finite basis. Many options but most common are probably Hartree-Fock, B-splines, and Sturmians.

Multiple valence electrons

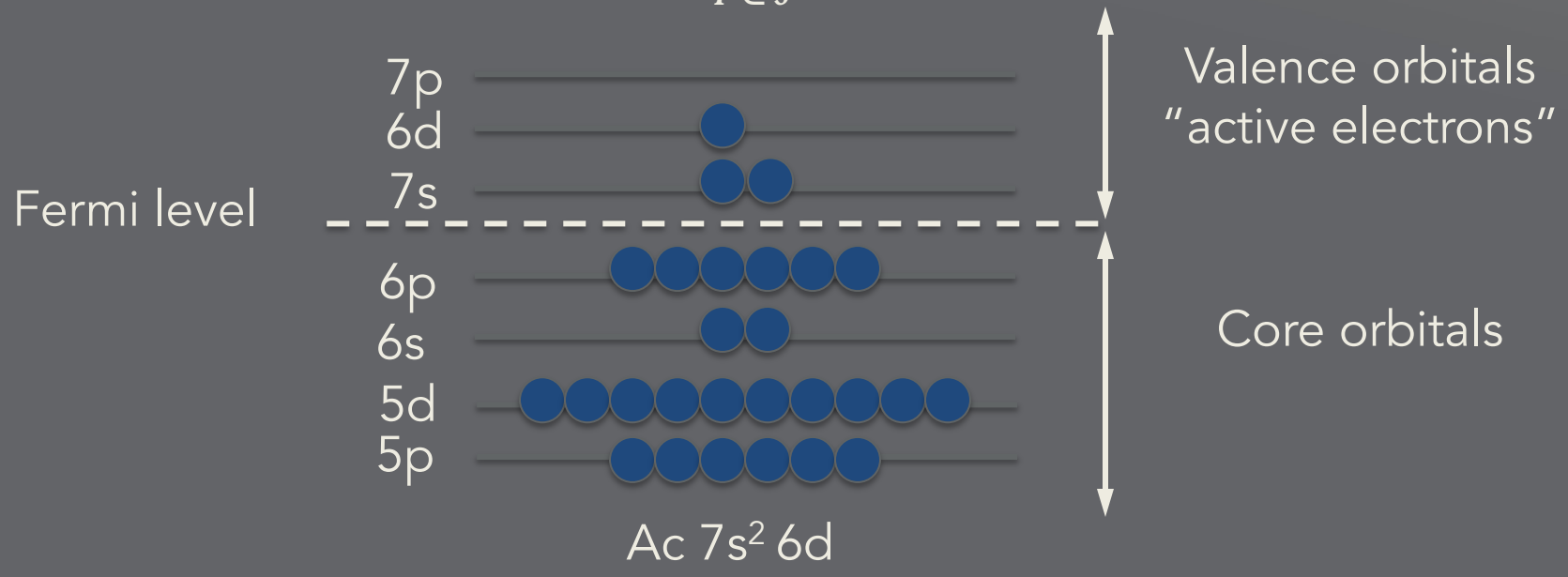
- Configuration interaction (CI) treats valence-valence correlations to all orders
- Accuracy between few % and terrible %.



Configuration Interaction

- Write many-body wavefunction as sum over many-particle "configuration state functions" $|I\rangle$

$$|\Psi\rangle = \sum_{I \in \mathcal{P}} C_I |I\rangle$$



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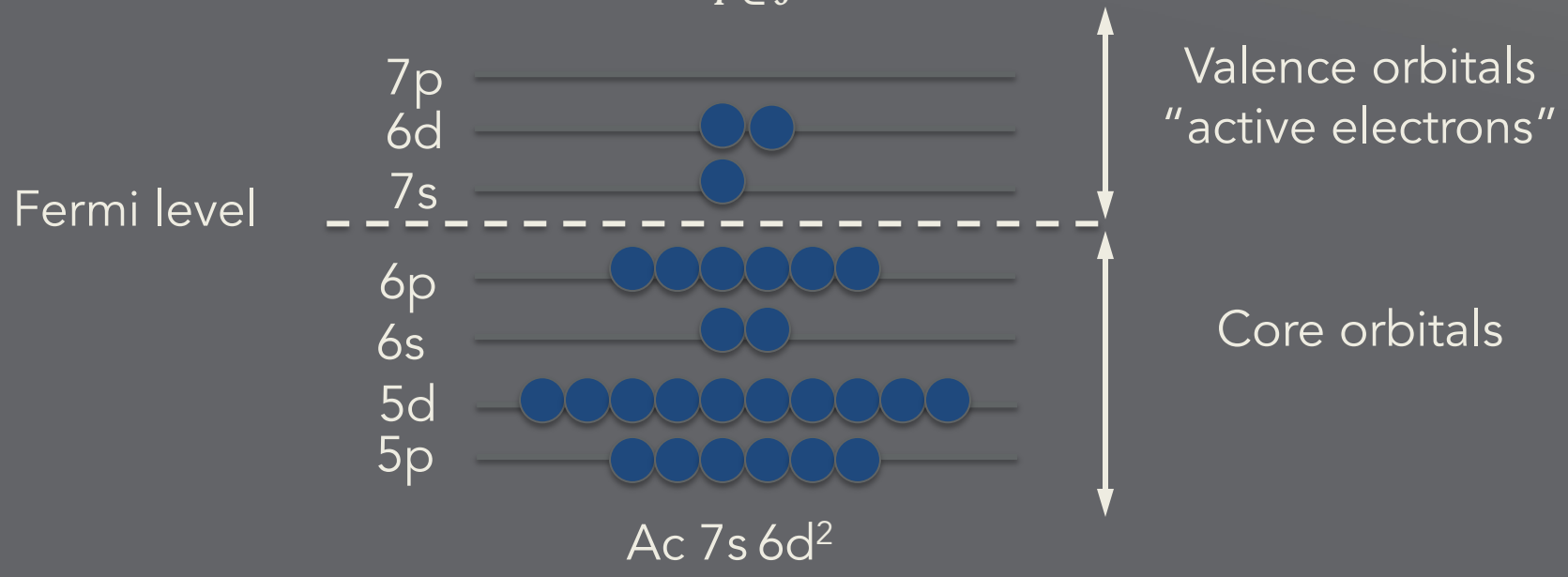
Configuration subspace $\mathcal{P}$



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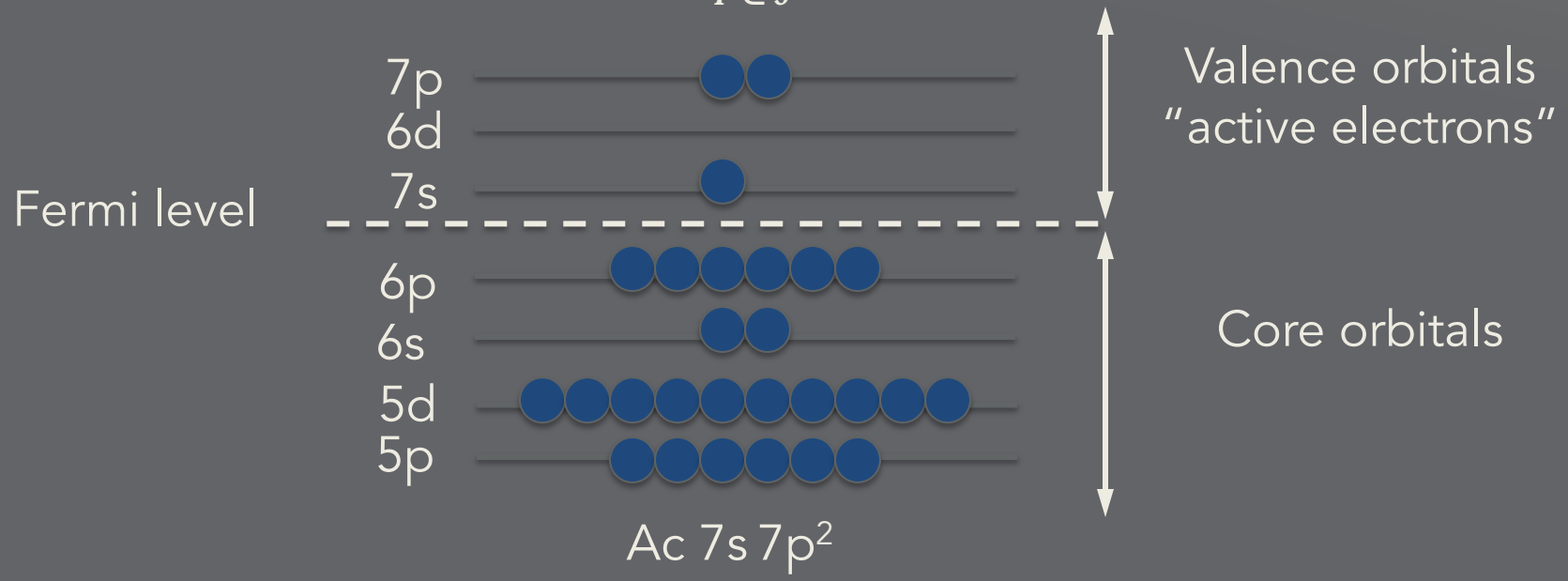


Configuration Interaction

- Reduces to matrix-eigenvalue problem:

$$\sum_J H_{IJ}\, C_J = E C_I$$

with $H_{IJ} = \langle I | \hat{H} | J \rangle$ and $|\Psi\rangle = \sum C_I |I\rangle$.

Configuration Interaction

- Reduces to matrix-eigenvalue problem:

$$\sum_J H_{IJ}\, C_J = E\, C_I$$

  with $H_{IJ} = \langle I | \hat{H} | J \rangle$ and $|\Psi\rangle = \sum C_I |I\rangle$.

- It's always more complicated.
  The CSFs $|I\rangle$ are:
  - Relativistic configurations (j-j coupling), e.g. $7s^2\, 6d_{3/2}$, $7s^2\, 6d_{5/2}$, $7s\, 6d_{3/2}^2$
  - Eigenvalues of projection $\hat{J}_z$
  - Eigenvalues of angular momentum $\hat{J}^2$
  - There are many possible projections of the same relativistic configuration with given $\hat{J}_z$, which are in linear combination in the CSF.

AMBiT: Keep Angular Data

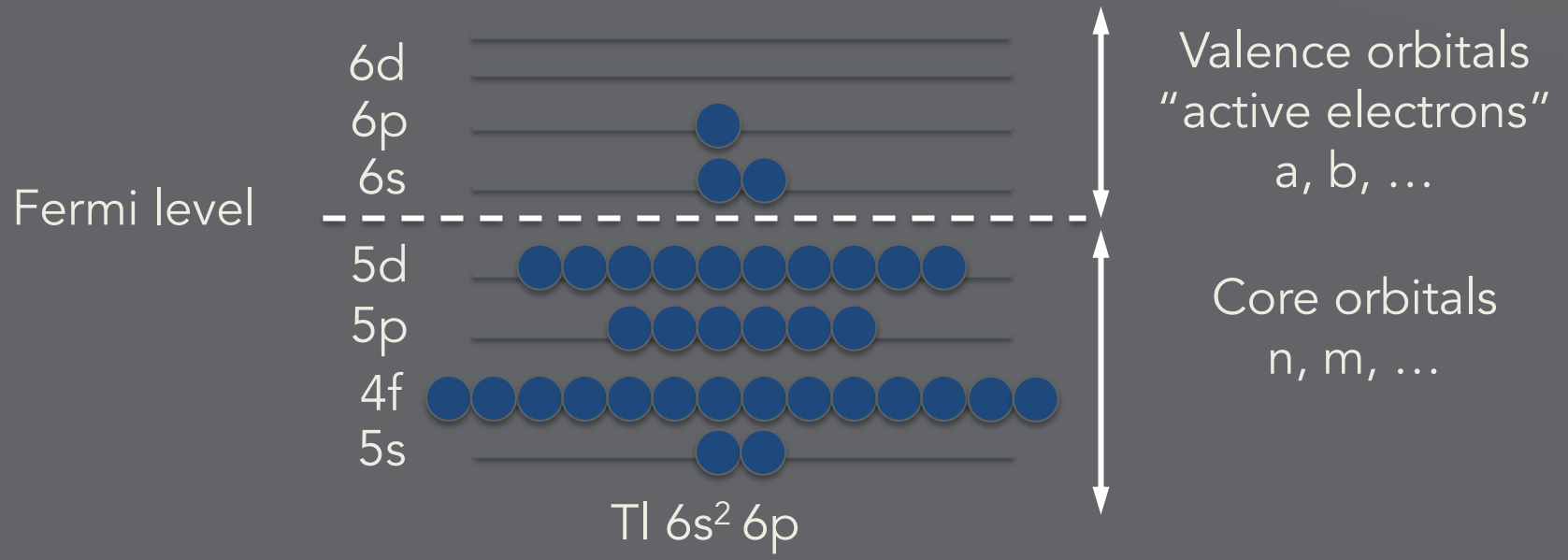
- Take configuration and reduce principal quantum number, e.g. $7s\ 6p_{3/2}\ 7p_{3/2} \rightarrow 1s\ 1p_{3/2}\ 2p_{3/2}$
- Generate set of all "projections" corresponding to a given value of J_z,
  e.g. $1s_{1/2\ (+1/2)} 1p_{3/2\ (+1/2)}\ 2p_{3/2\ (-1/2)}$,
  $1s_{1/2\ (-1/2)}\ 1p_{3/2\ (+3/2)}\ 2p_{3/2\ (-1/2)}$,
  $1s_{1/2\ (-1/2)}\ 1p_{3/2\ (+1/2)}\ 2p_{3/2\ (+1/2)}$, $\cdots$
- Generate the matrix $\hat{J}^2$ for these projections and diagonalise, keeping eigenvectors with desired eigenvalue $J(J+1)$.
- Store these CSFs in an AngularData directory forever.

Configuration Interaction

- **Problem**: Number of CSFs for given symmetry J^{π} grows exponentially (combinatorically? factorially?).
- That's why we can't just do full CI including all core states for heavy atoms.
- And we need to restrict number of excitations (e.g. singles, doubles, important triples and quadruples).
- But we do need to include core-valence correlations.

CI+MBPT

- Designed for few-valence-electron systems, e.g. Tl (3 electron), accuracy between ~0.1% and 1%
- Treat core-valence correlations with MBPT, valence-valence correlations with CI

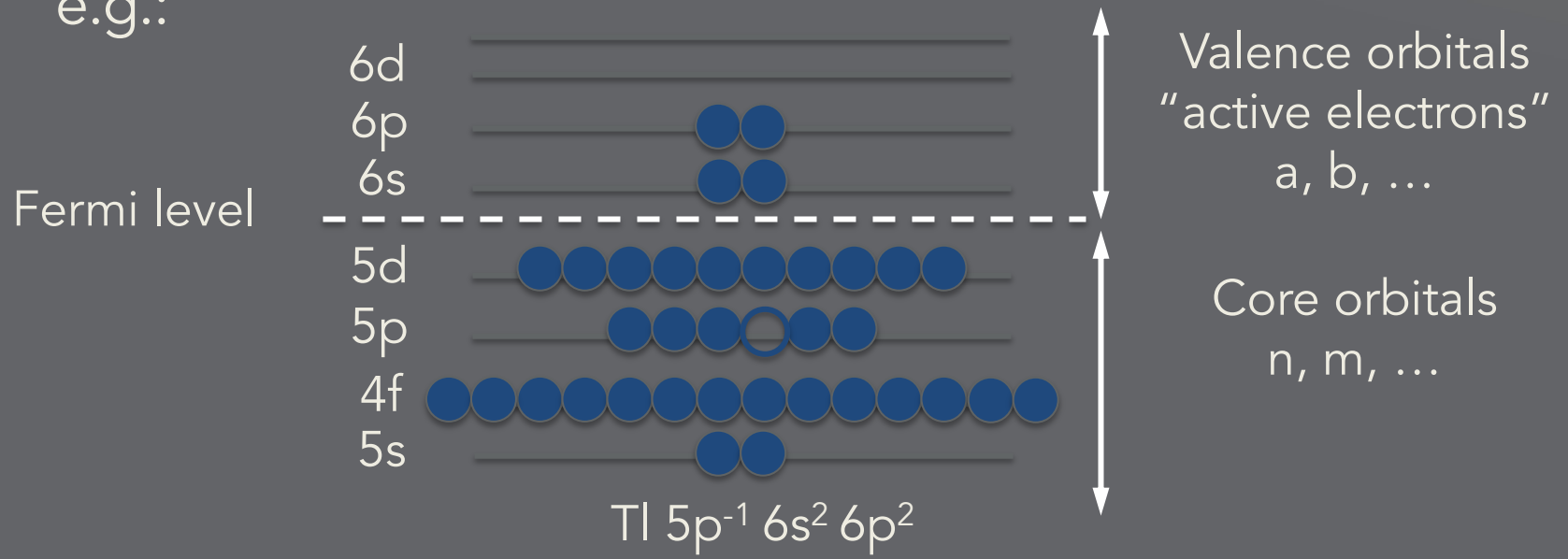


Dzuba, Flambaum, Kozlov, PRA 54, 3948 (1996)

CI+MBPT

$$\sum_{J\in\mathcal{P}}\left(H_{IJ}+\sum_{M\in\mathcal{Q}}\frac{\langle I|\hat{H}|M\rangle\langle M|\hat{H}|J\rangle}{E-E_M}\right)C_J=EC_I$$

- $\mathcal{Q}$ is complementary to $\mathcal{P}$: includes CSFs with core holes, e.g.:



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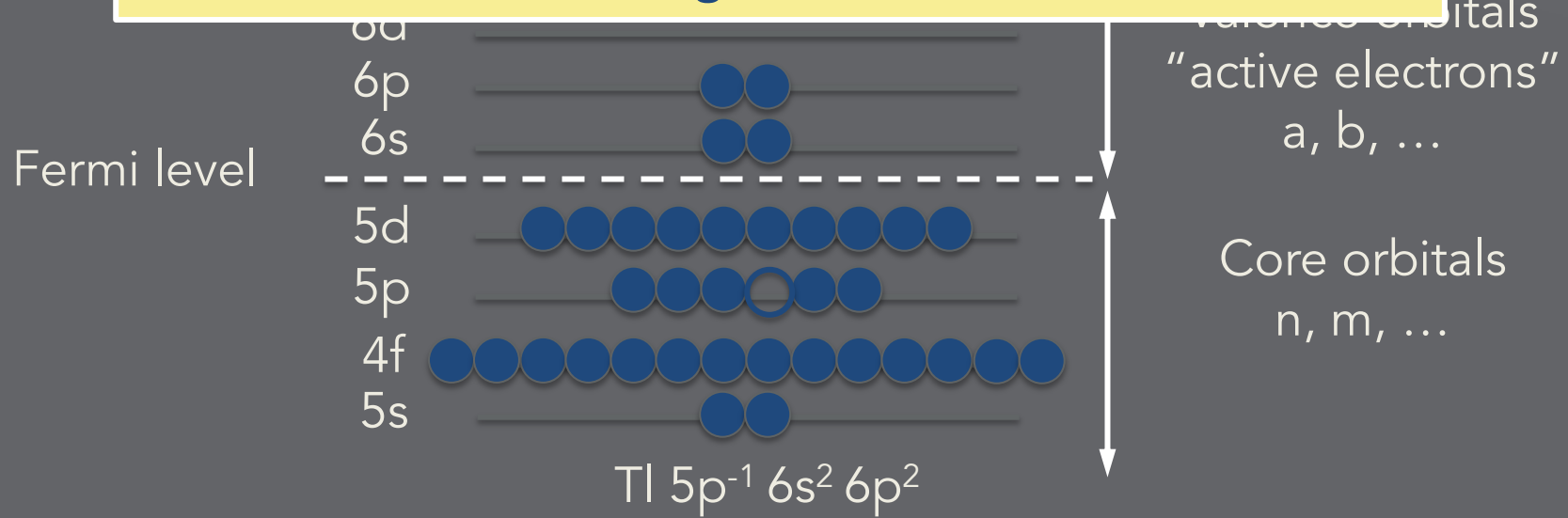
- $\mathcal{Q}$ … es,
  e.g …

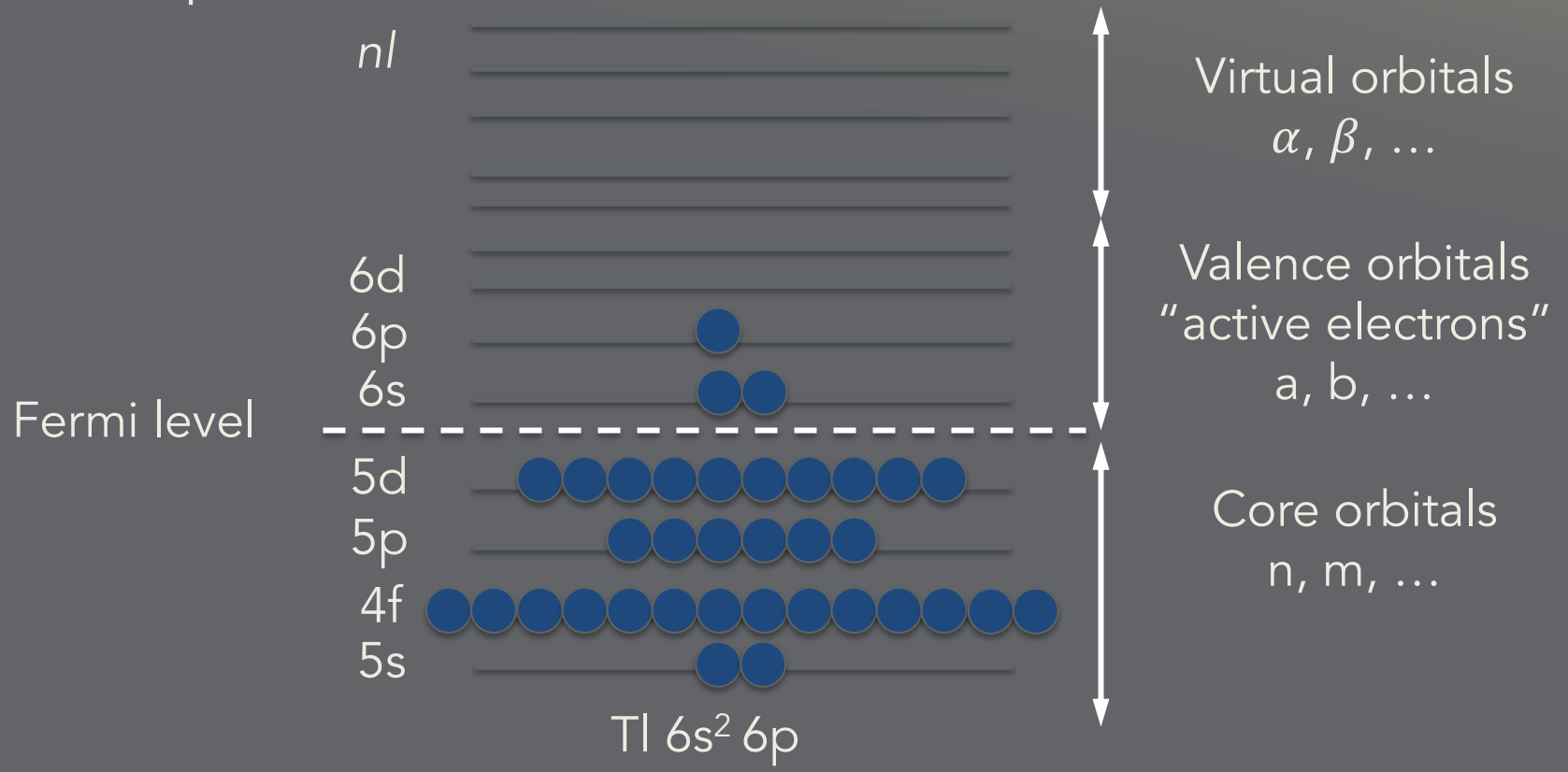
CI+MBPT "trick": modify slater integrals in H_{IJ}: convert sum over configurations to sum over orbitals



Dzuba, Flambaum, Kozlov, PRA 54, 3948 (1996)

CI+MBPT

- MBPT is second-order in residual interaction
- Group orbitals into core, valence, and virtual



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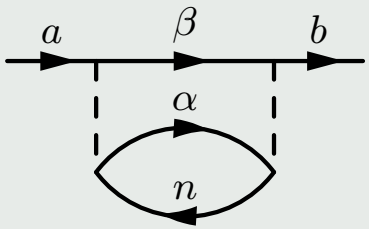
CI+MBPT

One body diagrams



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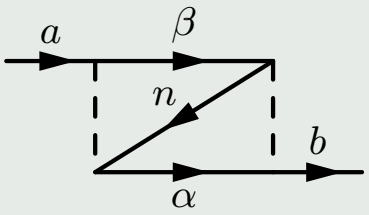

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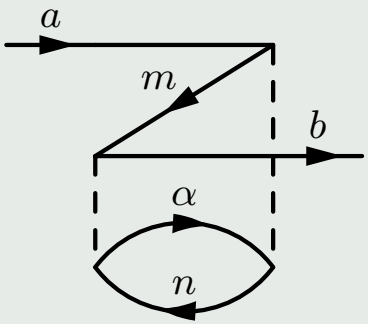

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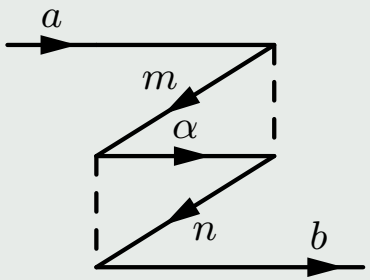

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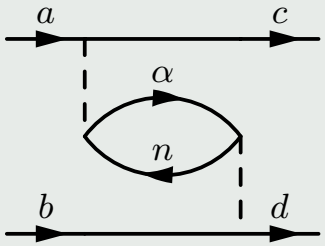
Two body diagrams



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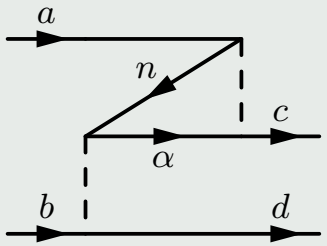

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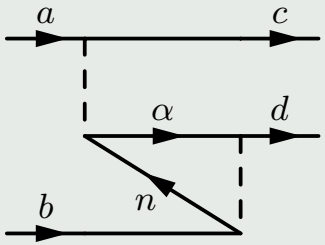

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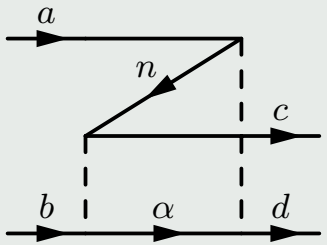

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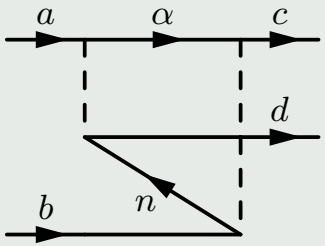

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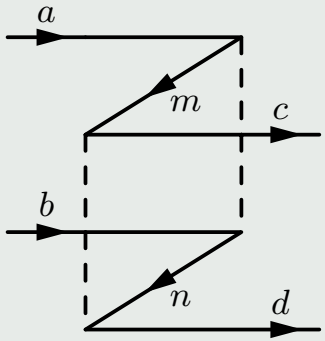

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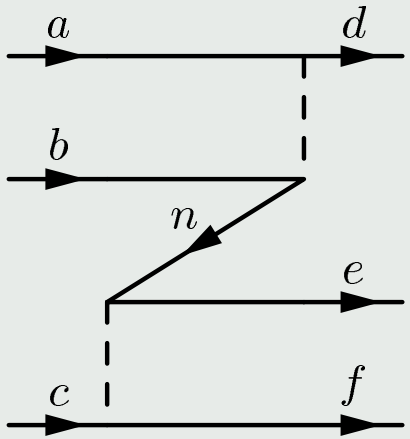
CI+MBPT

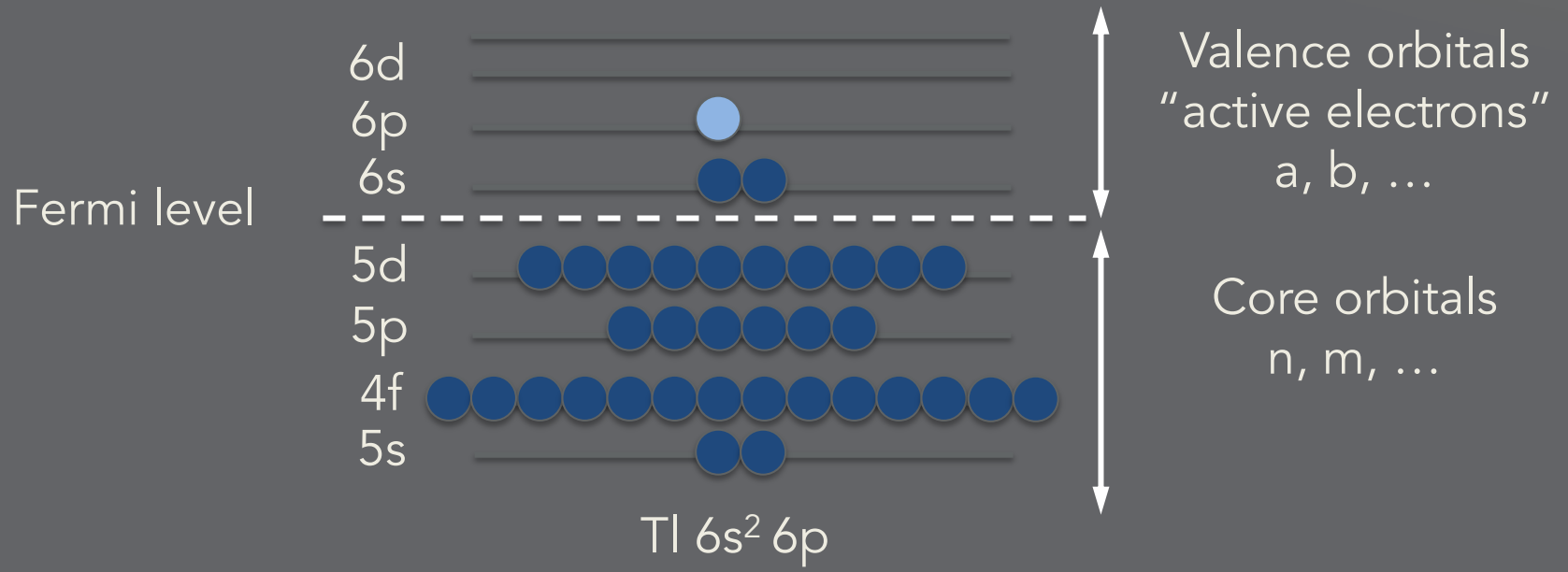
Three body diagram



- Effective three-body term in the Hamiltonian.
- Impossible to store (combinatorics again), need to generate on the fly.

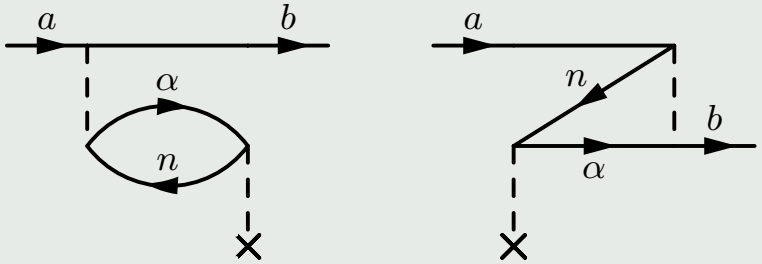
CI+MBPT

- Subtraction diagrams come from using different single-particle operators for creating orbitals (Dirac-Fock) and CI. e.g. Tl basis formed in V^{N-1}, but CI in V^{N-3}



CI+MBPT

Subtraction diagrams



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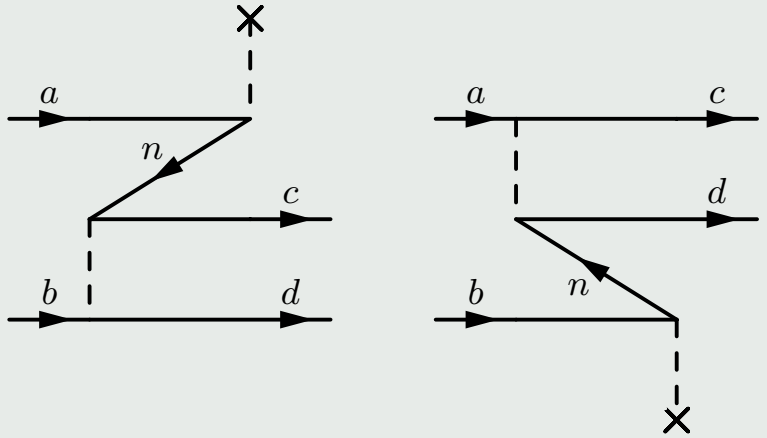

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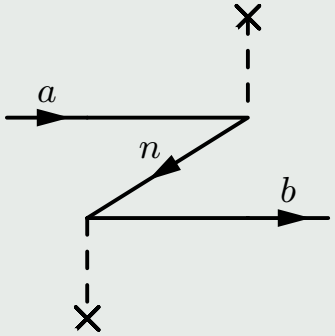
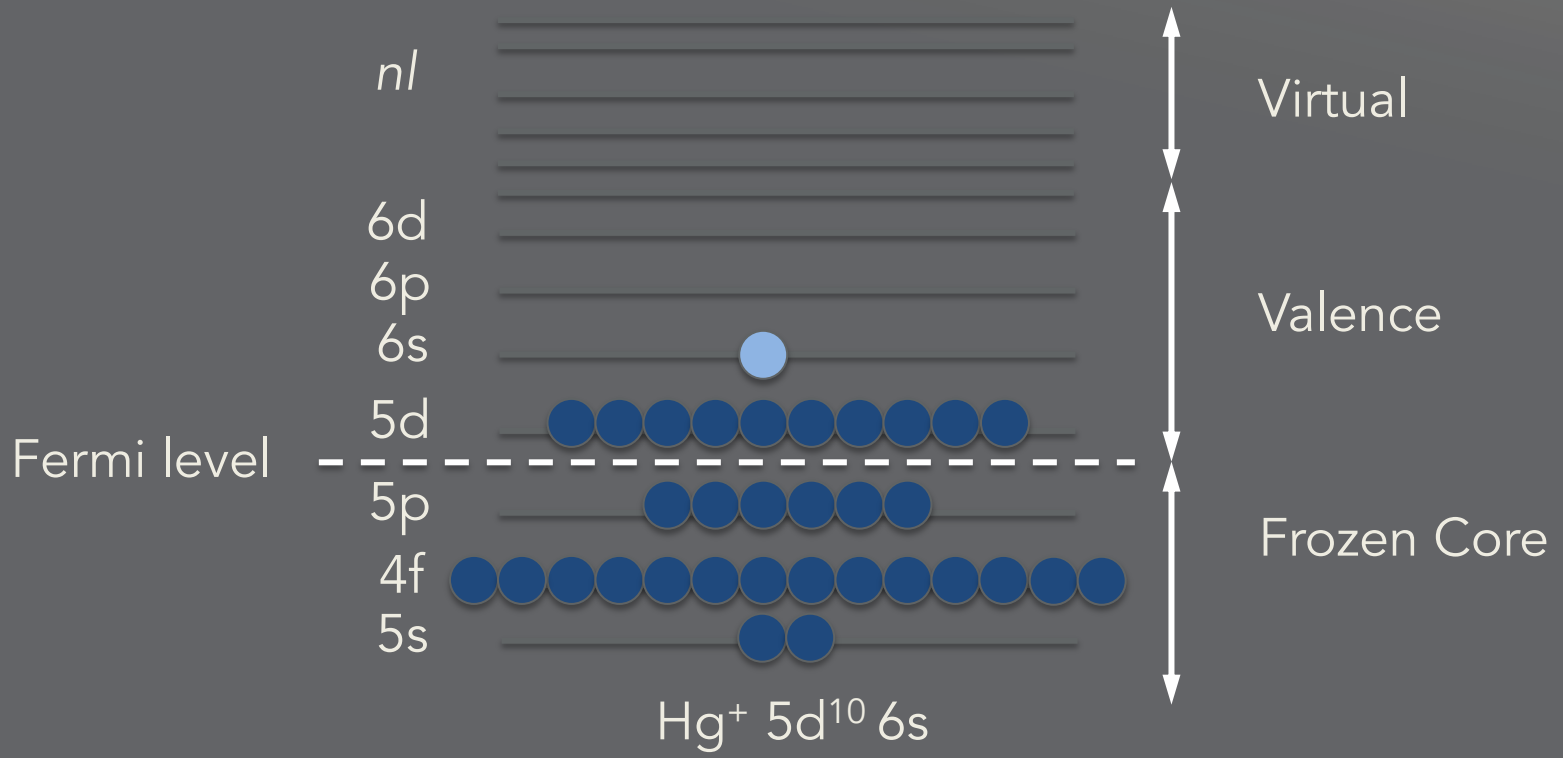


3

These can get quite large for open shell systems: not very perturbative!

Particle-hole CI+MBPT

- Example: Hg^+ has 11 active electrons, which leads to very large subtraction diagrams, making CI+MBPT not work very well.



Berengut, PRA 94, 012502 (2016)

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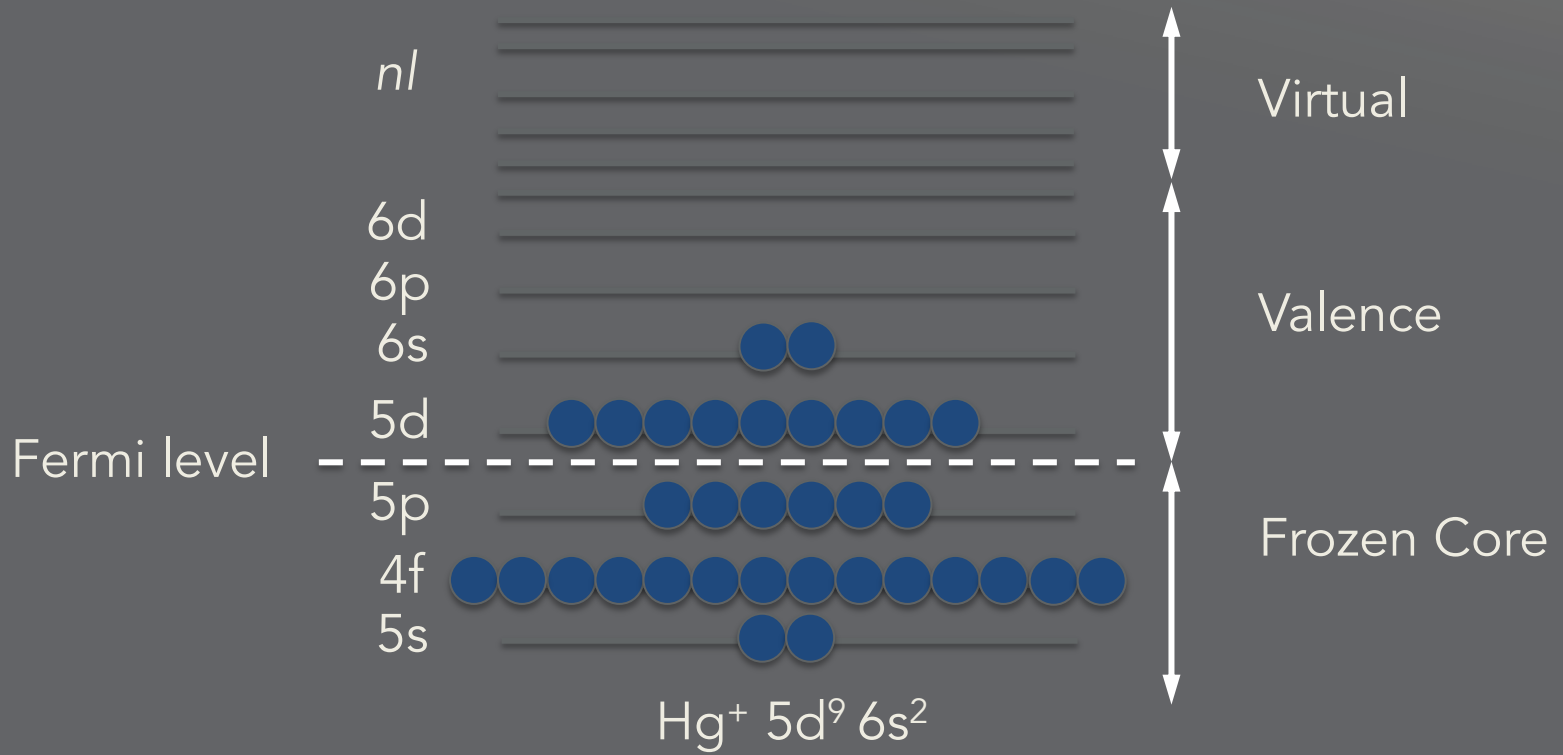
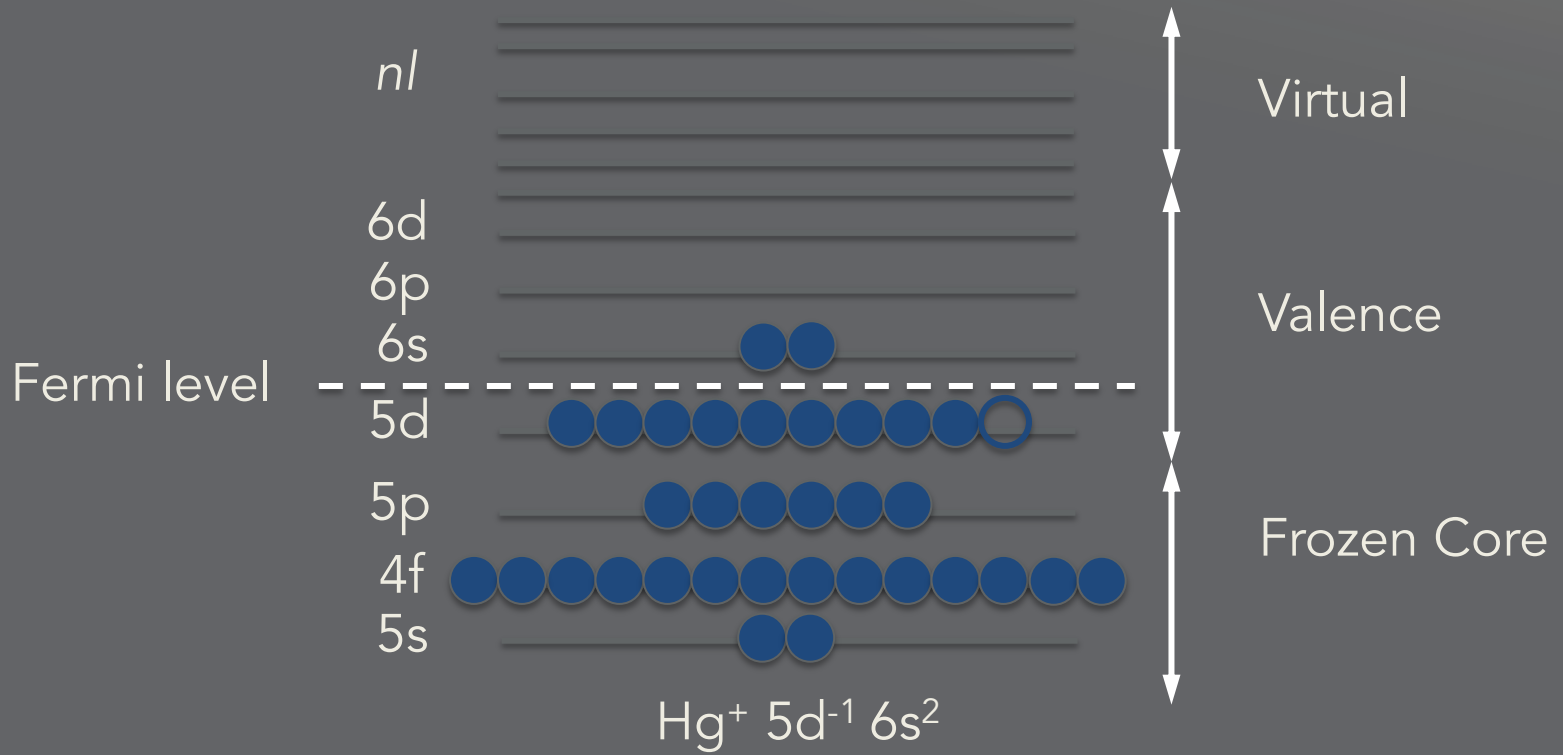


Berengut, PRA 94, 012502 (2016)

Particle-hole CI+MBPT

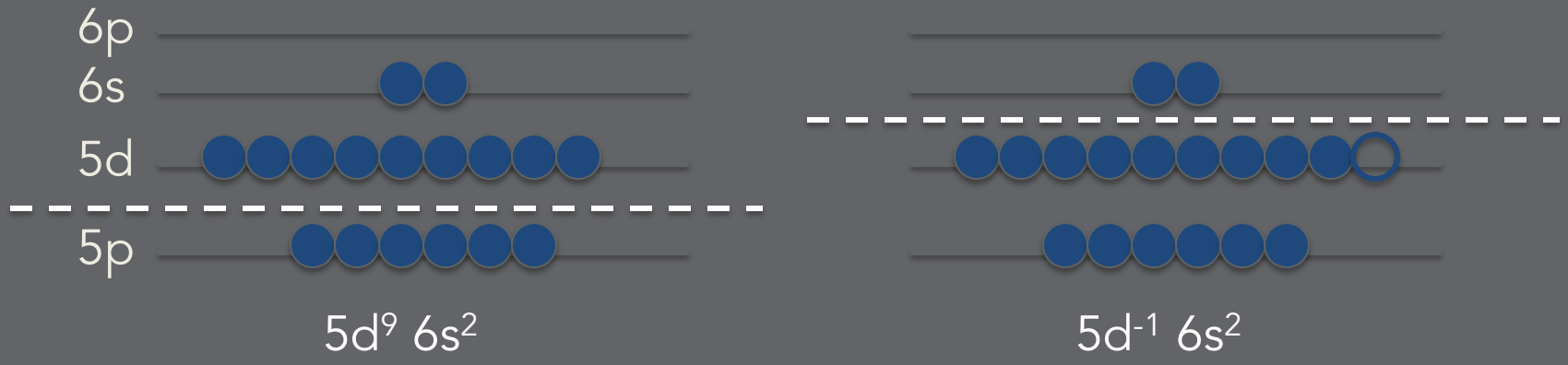
- Particle-hole CI+MBPT:
  - Move the Fermi level
  - Optionally include valence-virtual MBPT in diagrammatic expansion



Berengut, PRA 94, 012502 (2016)

Particle-hole CI+MBPT

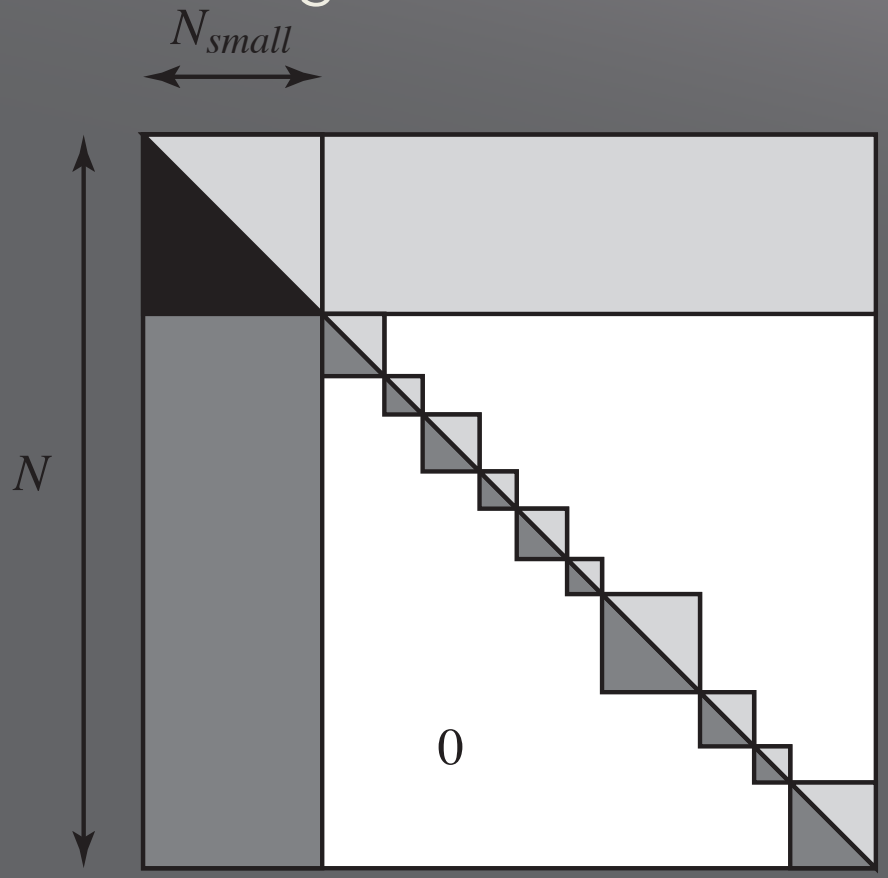
Hg^+ Level	CI+MBPT (cm^{-1})	Particle-hole CI+MBPT (cm^{-1})	Experiment (cm^{-1})
$6s\ ^2S_{1/2}$	0	0	0
$5d^{-1}\ 6s^2\ ^2D_{5/2}$	32305	35121	35515
$5d^{-1}\ 6s^2\ ^2D_{3/2}$	48001	50446	50556



Berengut, PRA 94, 012502 (2016)

Emu CI

- Another way of getting valence-virtual correlations. For when you really just need a lot of configuration interaction.



Emu CI

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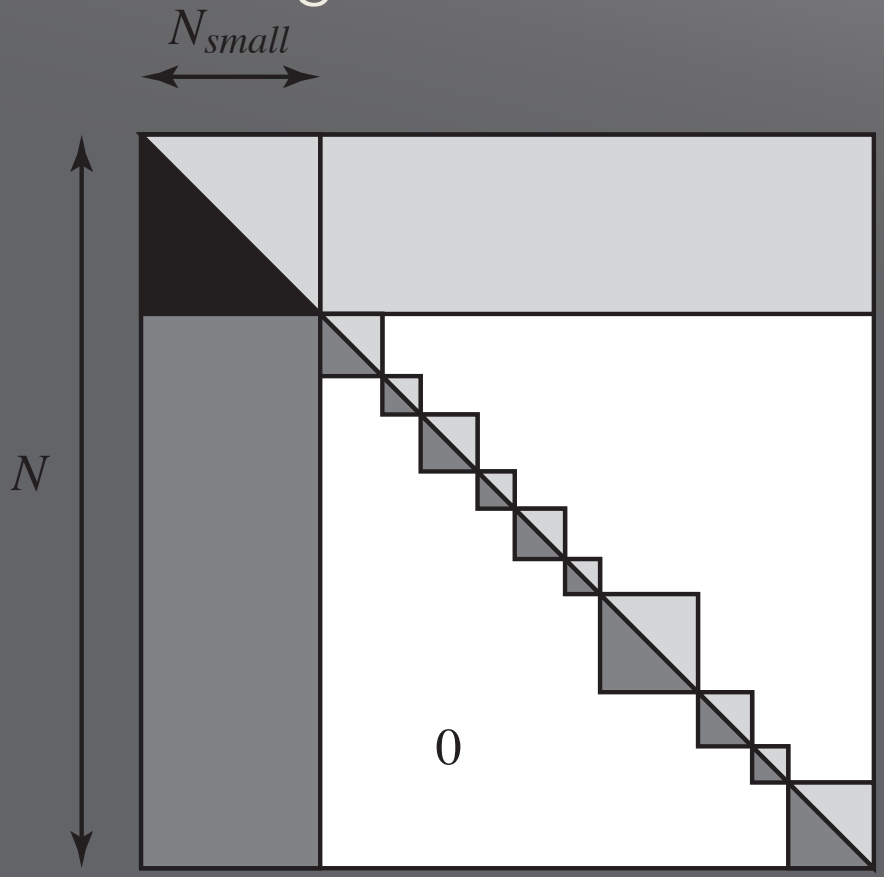
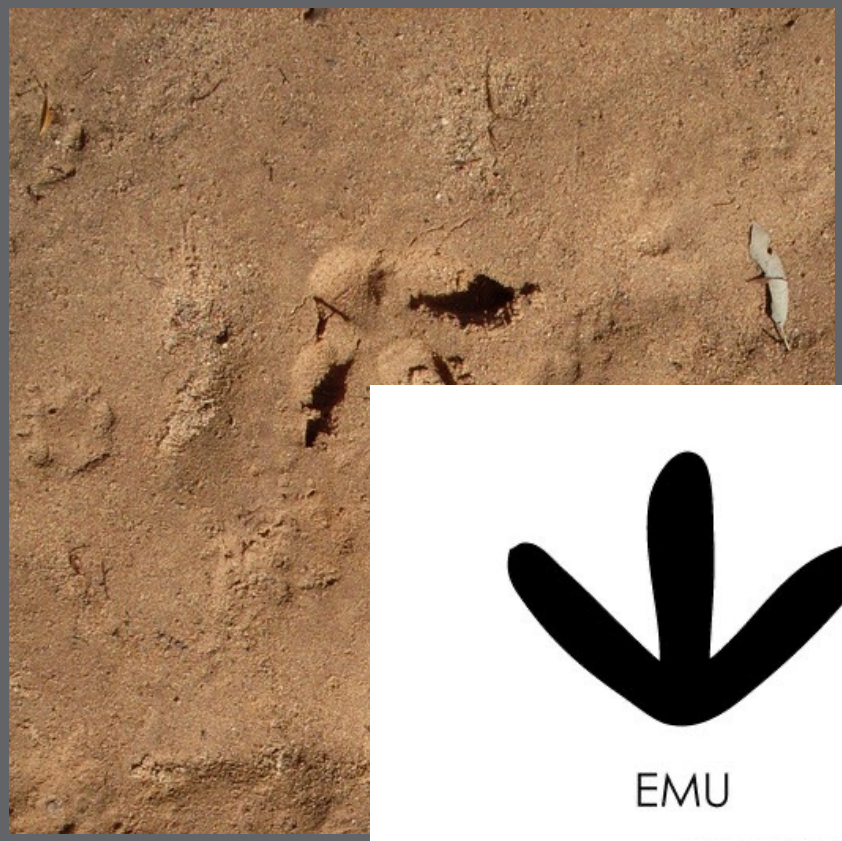
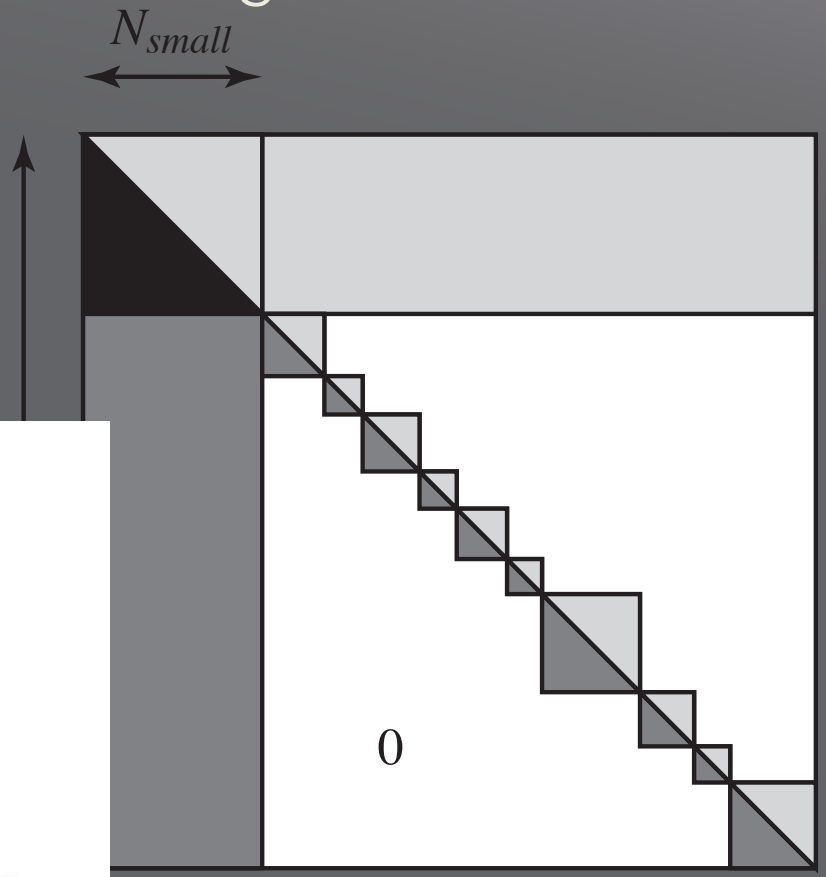


Emu CI

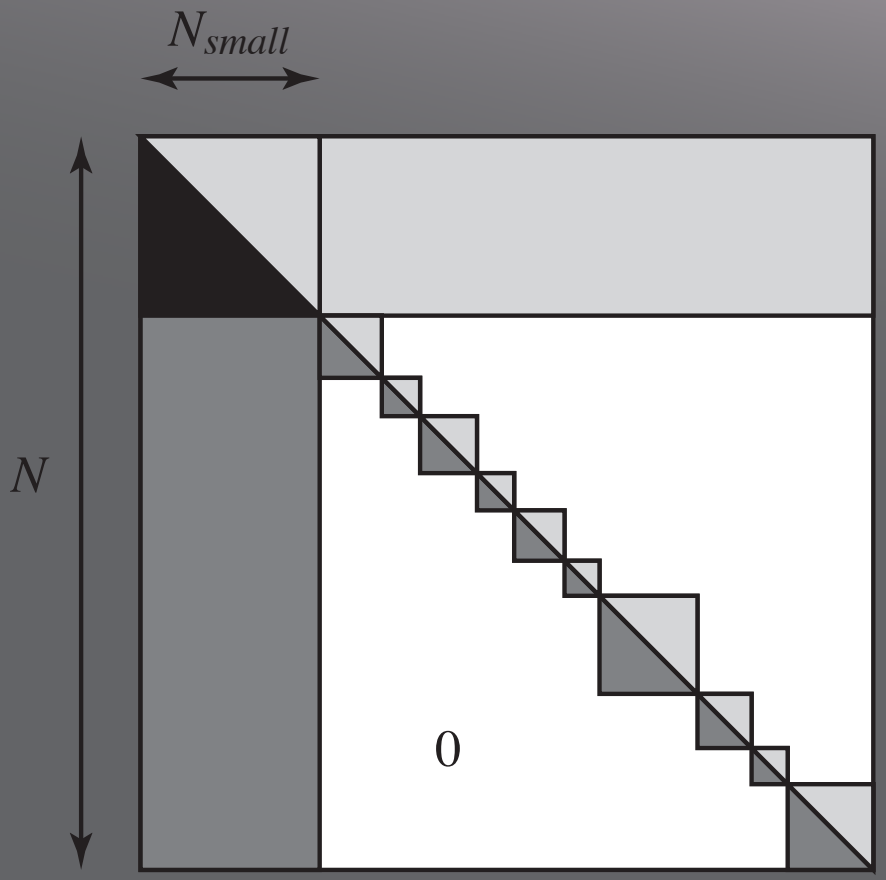
- Another way of getting valence-virtual correlations. For when you really just need a lot of configuration interaction.





Emu CI

- Neglect interaction between high-energy states with small contributions
- Example: Ta, Db
  (5 valence electrons)
  including orbitals up to 21spdf
  for $J^{\pi} = 5/2^{-}$ uses
  N = 952112
  N_{small} = 20462
- Factor 40 reduction in size and speed
- Solve using iterative method (Davidson)



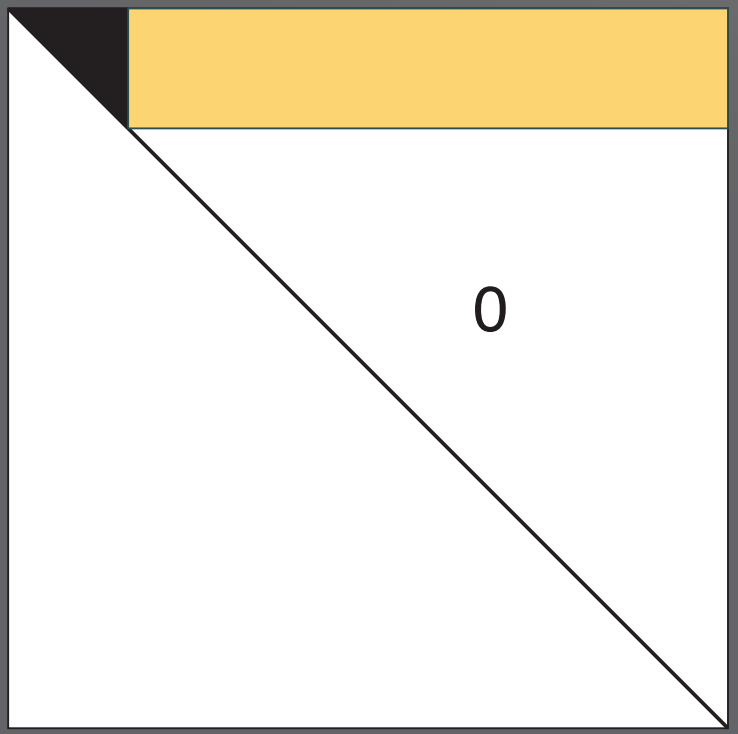
Geddes, Czapski, Kahl, Berengut, PRA 98, 042508 (2018)

CIPT

- Alternative based on perturbation expansion over configurations (but not orbitals as in CI+MBPT).
- Very similar philosophy to emu CI.

$$H_{IJ} \rightarrow H_{IJ} + \sum_K \frac{\langle I|\hat{H}|K\rangle\langle K|\hat{H}|J\rangle}{E - E_K}$$

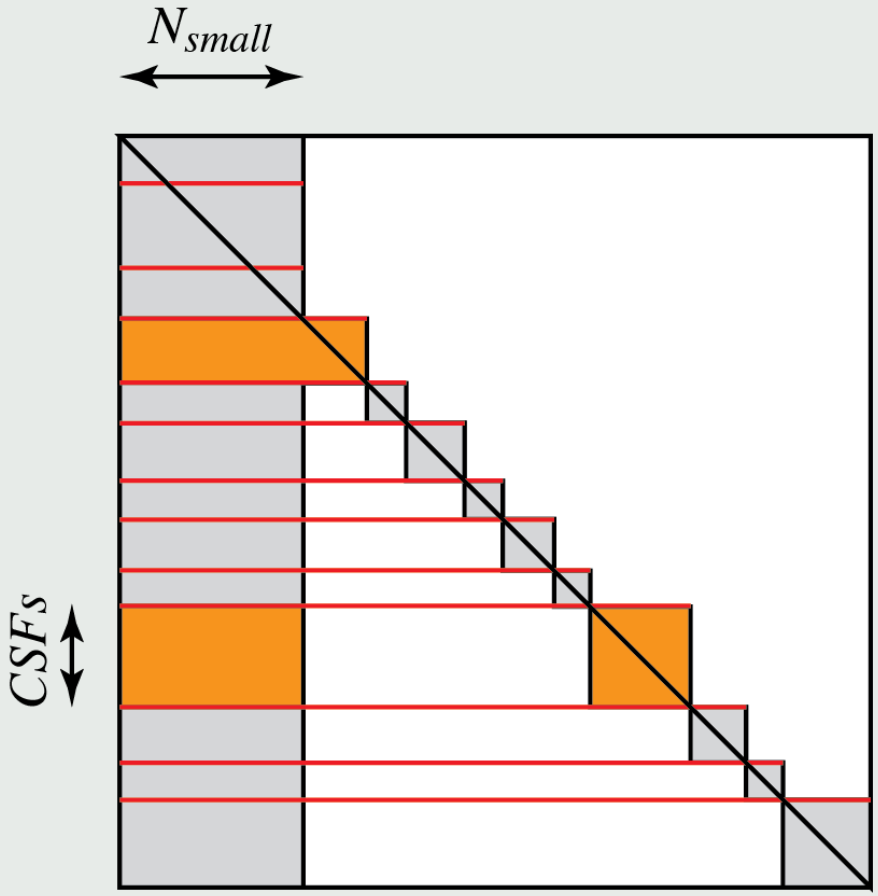
- Need to make sum for all matrix elements – can get expensive.



Dzuba, Berengut, Harabati, Flambaum, PRA 95, 012503 (2017)

AMBiT: CI parallelisation

- CI Matrix is divided into chunks that are distributed amongst MPI processes.
- Workload for a configuration $\sim\mathcal{O}(\#\text{CSFs} \times \#\text{projections}^2)$ and is extremely skewed.
- Each MPI process generates and stores own chunks.
- OpenMP is used to distribute work within each process.



Cartoon showing chunks belonging to a single MPI process.

Atomic structure calculations

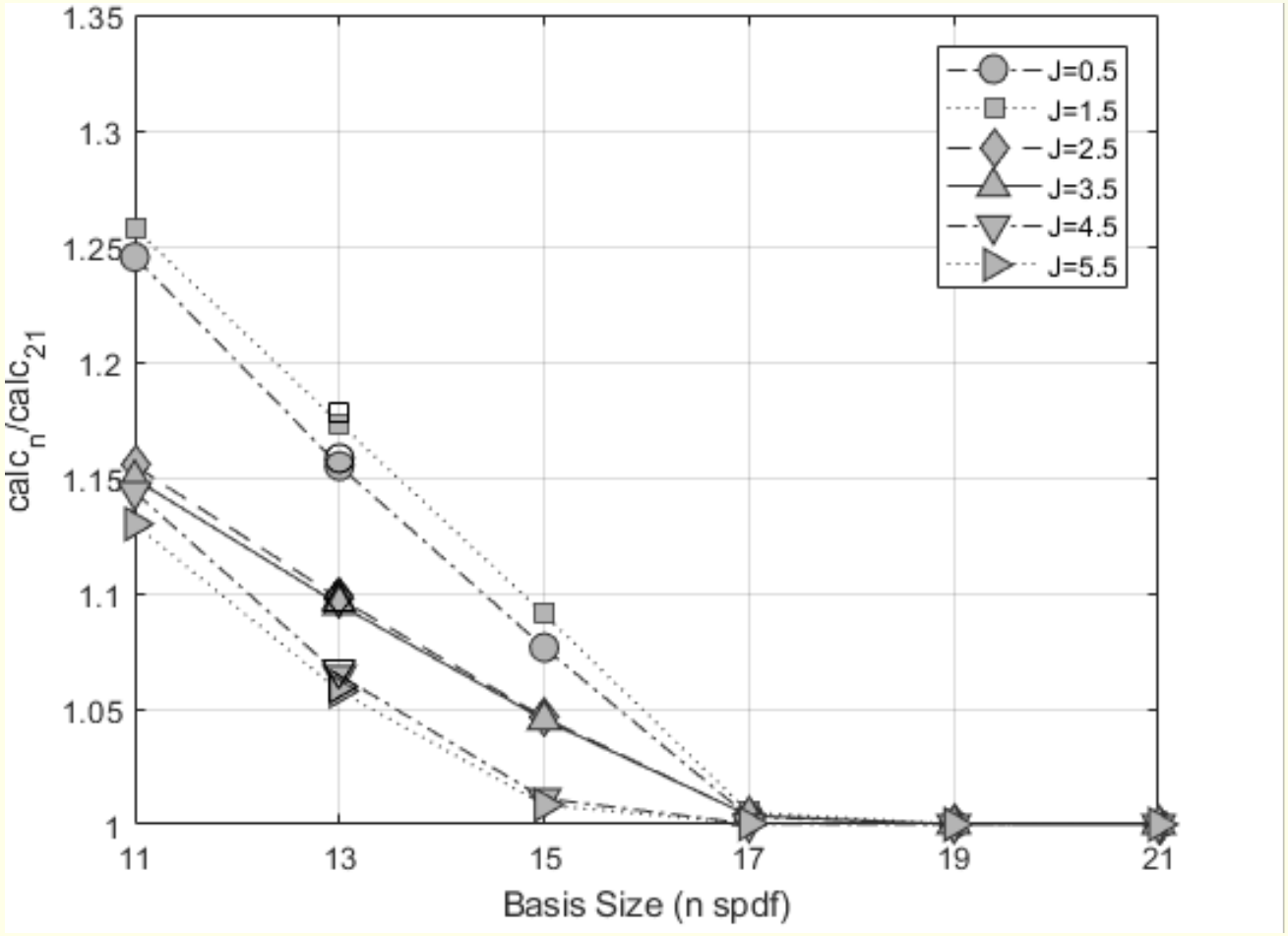
- Regardless of method used, there are still decisions to be made
  - Starting configuration for Dirac-Fock procedure? (V^N, V^{N-1}, …)
  - Create basis: B-splines, L-spinors, Sturmians …?
  - Multiconfiguration Dirac-Fock? Orbitals not orthonormal.
  - How many valence and virtual orbitals to include? Maximum angular momentum of orbitals?
  - Choose configurations: single and double excitations? Hole excitations? Valence triples, quadruples?

Atomic structure calculations

- What about transitions and additional operators? We have the wavefunctions, so why not simply $\langle O \rangle = \langle \Psi | \hat{O} | \Psi \rangle$? But this is only first-order perturbation theory!
- Sometimes can add a term to the Hamiltonian directly, leading to "all order" method, e.g.:
  - Change in fine-structure constant
  - Isotope shift
  - Any scalar operators
- Electronic transitions and hyperfine structure cannot generally be treated in this way.
- Random phase approximation (RPA) models the effect of core polarisation, but is challenging for many valence electron atoms.

Emu CI+MBPT convergence

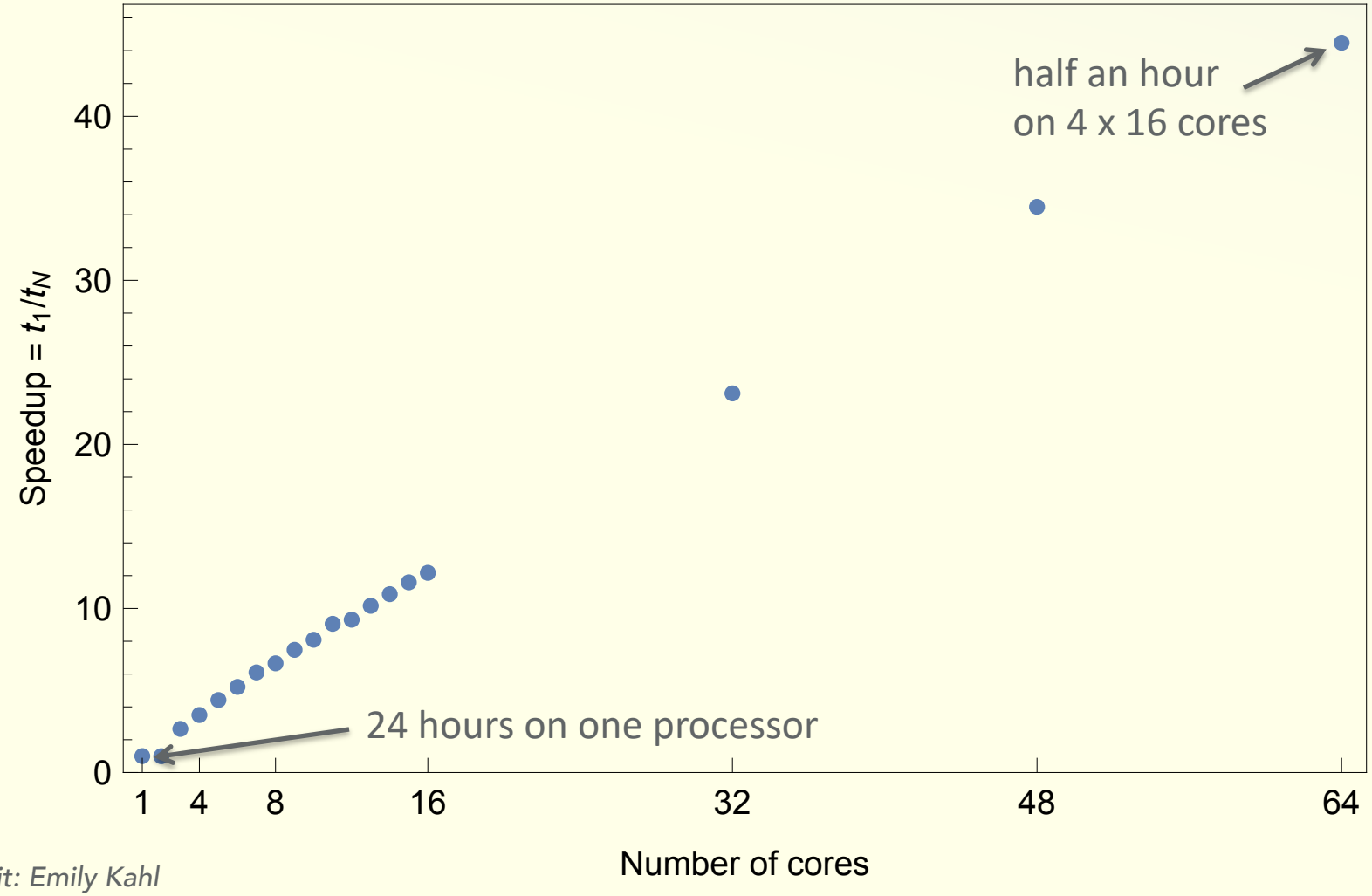
Ta (5 valence electrons): selected even states



Geddes, Czapski, Kahl, Berengut, PRA 98, 042508 (2018)

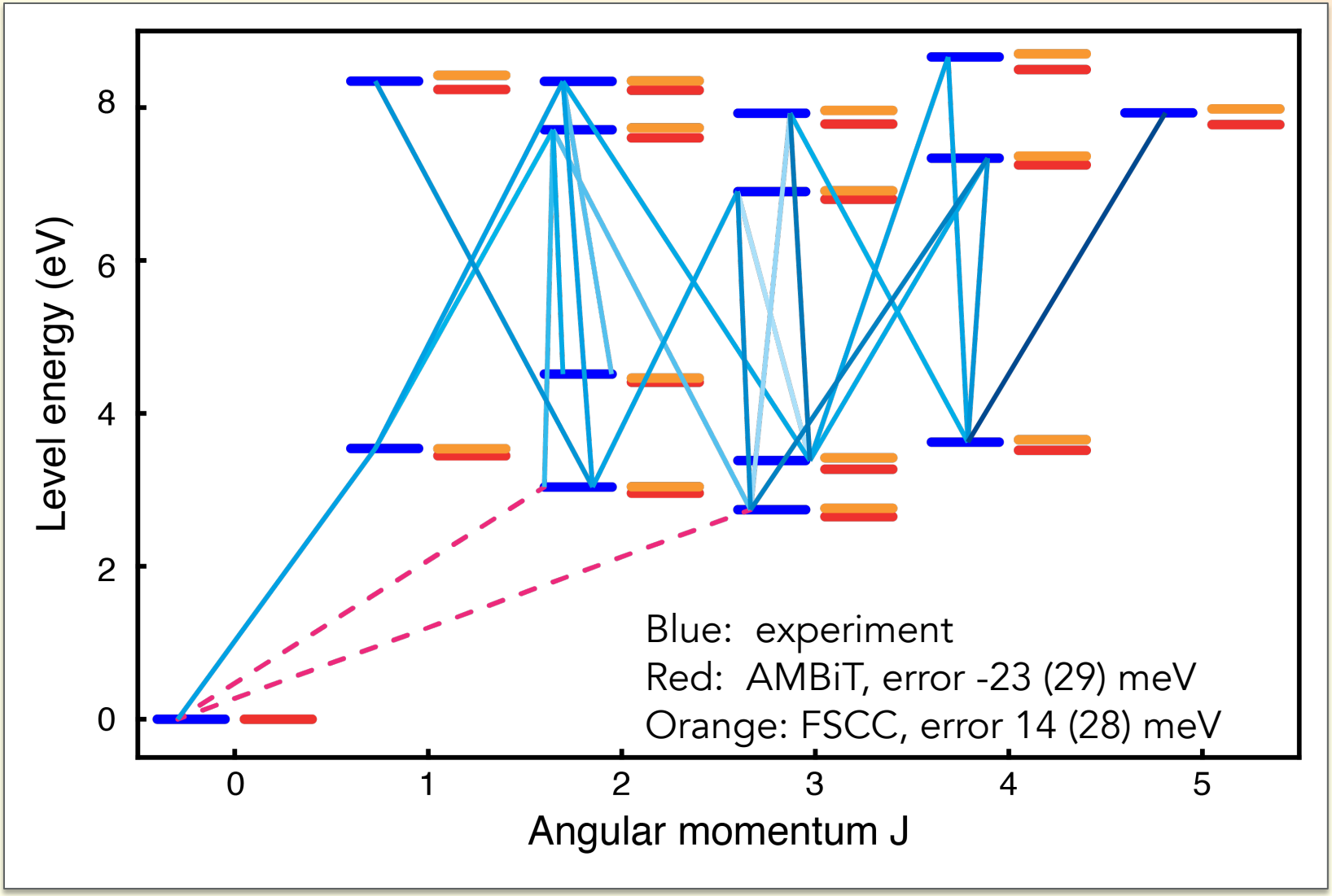
AMBiT Scaling

CI+MBPT scaling in Cr^+ (16 cores/node)



Credit: Emily Kahl

Pr^{9+} experiment and theory



Bekker, Borschevsky, Harman, Keitel, Pfeifer, Schmidt, Crespo, Berengut, Nature Communications 10, 5651 (2019)

Results: Lu^+ (homologue of Lr^+)

- CI+MBPT and FSCC calculations including Breit and QED

State		Energy (cm^{-1})				
		FSCC	Δ QED	CI+MBPT	Δ QED	Expt. [33]
$6s^2$	$^1S_0$ IP	112696	−100			111970
$5d6s$	$^3D_1$	12354	−158	11664	−144	11796
	$^3D_2$	12985	−156	12380	−143	12432
	$^3D_3$	14702	−148	14267	−134	14199
	$^1D_2$	17892	−157	17875	−160	17332
$6s6p$	$^3P_0$	27091	−103	27303	−105	27264
	$^3P_1$	28440	−105	28520	−106	28503
	$^3P_2$	32294	−89	32603	−97	32453
	$^1P_1$	38464	−155	37385	−129	38223

Kahl, Berengut, Laatiaoui, Eliav, Borschevsky, PRA 100, 062505 (2019)

Results: Lr+

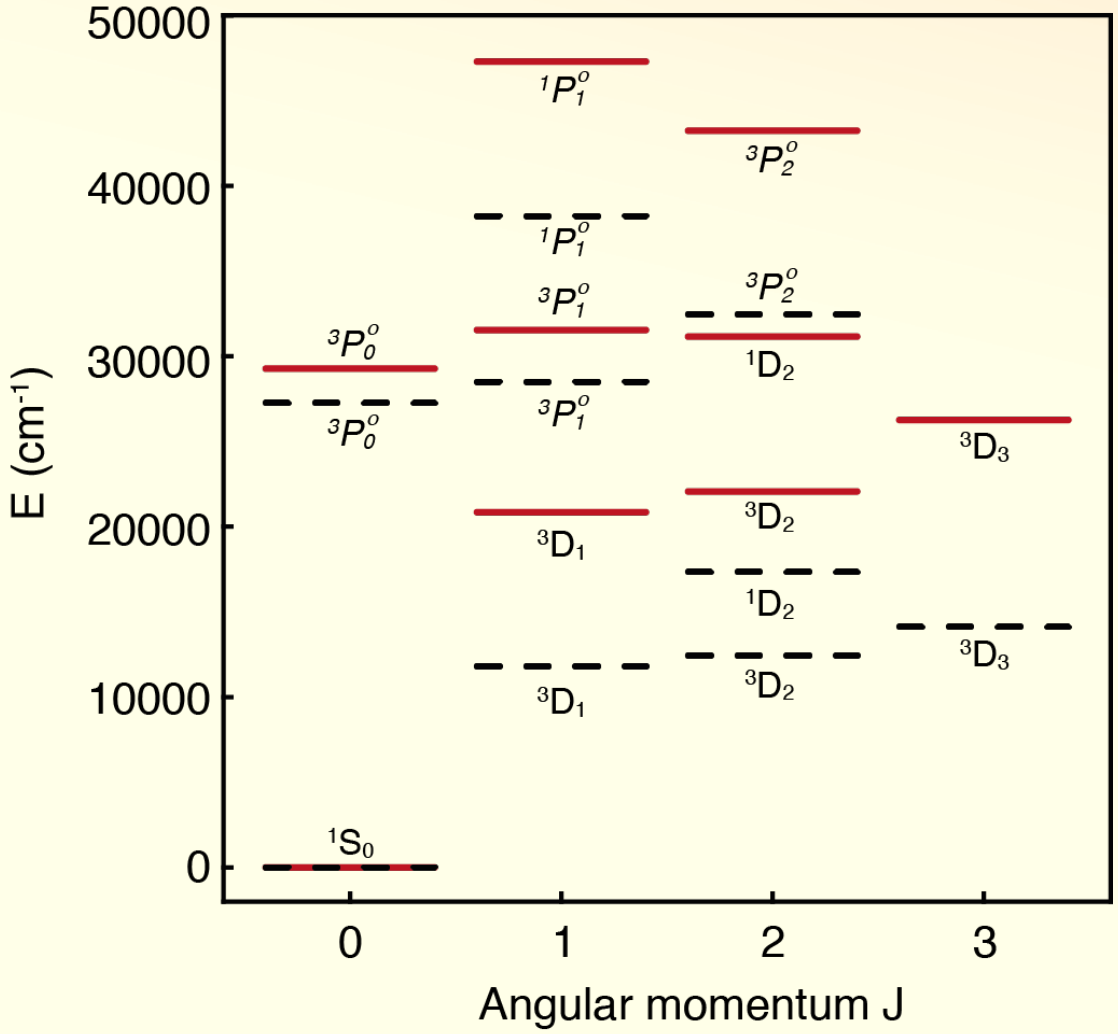
- CI+MBPT and FSCC calculations including Breit and QED

State		Energy (cm^{-1})				
		FSCC	ΔQED	CI+MBPT	ΔQED	Lifetime (s)
$7s^2$	$^1S_0$	116949	−219			
$6d7s$	$^3D_1$	20265	−342	21426	−374	2.23×10^{6}
	$^3D_2$	21623	−344	22507	−373	8.26×10^{-2}
	$^3D_3$	26210	−326	26313	−355	2.97×10^{-2}
	$^1D_2$	31200	−373	30942	−397	1.53×10^{-3}
$7s7p$	$^3P_0$	29487	−167	29059	−306	2.56×10^{-7}
	$^3P_1$	31610	−179	31470	−314	1.45×10^{-8}
	$^3P_2$	43513	−240	42860	−308	2.43×10^{-8}
	$^1P_1$	47819	−260	46771	−376	1.11×10^{-9}

- QED contributions are still below correlation uncertainties

Kahl, Berengut, Laatiaoui, Eliav, Borschevsky, PRA 100, 062505 (2019)

Results: Lu^+ vs Lr^+



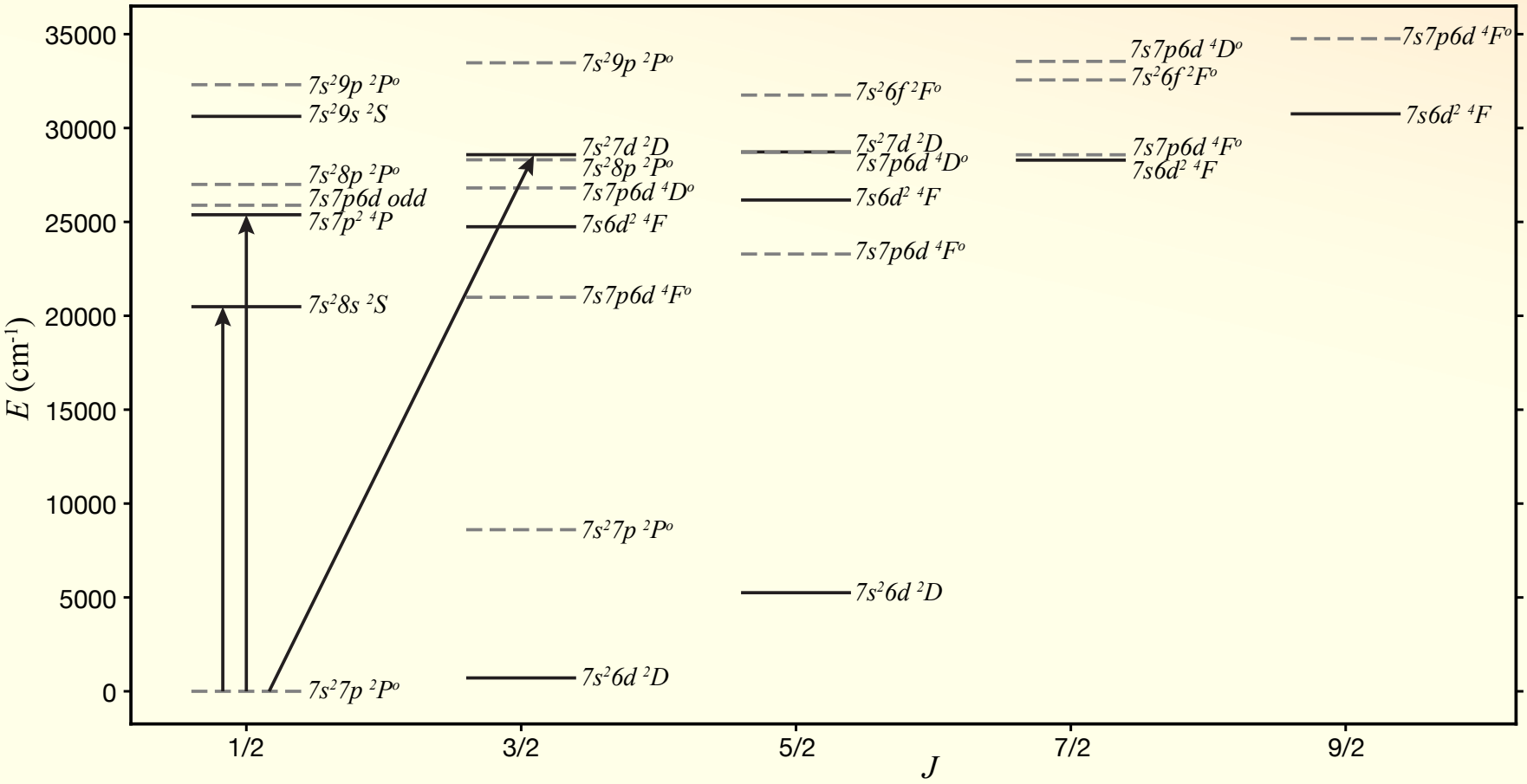
Lr^+ (solid, red)

Lu^+ (dashed, black)

Ground state $7s^2$ of Lr^+ is relativistically stabilised.

Kahl, Berengut, Laatiaoui, Eliav, Borschevsky, PRA 100, 062505 (2019)

Results: Lr



- CI+MBPT calculations shown (FSCC very close)

Kahl, Raeder, Eliav, Borschevsky, Berengut, PRA 104, 052810 (2021)

Summary

- Many methods for finding atomic structure, but fewer for heavy open shell systems.
- Particle-hole CI+MBPT is not terrible.
- It's an atomic physics and computational challenge: need good methods, well coded!

Thanks to many collaborators and to you for listening.

https://github.com/drjuls/ambit

AMBiT

Relativistic Atomic Structure for Everyone

Julian Berengut and Emily Kahl
arXiv:1805.11265 (2018)
https://github.com/drjuls/ambit

UNSW SYDNEY

Now you can access precision atomic structure with AMBiT, a software package for fully relativistic, *ab initio* calculations of electronic structure of atoms and ions. Calculate energy levels, electric and magnetic multipole transition matrix elements, g factors, hyperfine structure, isotope shifts, and much more! AMBiT implements the **particle-hole configuration interaction with many-body perturbation theory** method[1], which extends the CI+MBPT method[2-4] to non-perturbatively include configurations with electron holes below the designated Fermi level. This provides the flexibility required to handle all important configurations, even if the core is unfrozen.

Converged configuration interaction with 'emu CI'

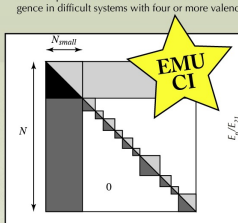
Convergence of atomic calculations with increasing basis size should be at the heart of all atomic structure calculations. Yet in the CI+MBPT framework this has only been possible with few-valence-electron atoms and ions since the configuration interaction grows exponentially fast with increasing basis size. AMBiT implements emu CI[5], a robust method of decreasing the matrix size without undermining the accuracy of the resulting atomic spectra. In this method, matrix elements between high energy configurations are set to zero, with little effect on the accuracy of low lying levels. Emu CI makes it possible to saturate the CI matrix in atoms with many valence electrons, allowing convergence in difficult systems with four or more valence electrons.

Highly accurate energies and wavefunctions

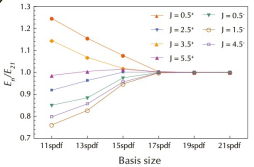
AMBiT is based on the Dirac-Coulomb Hamiltonian with optional Breit and QED. It has been used for many years to calculate low-lying spectra in atomic clock species, astrophys- ically relevant atoms and ions, and highly-charged ions. Recent calculations include

- neutral Ta and Db: highly relativistic atoms with five valence electrons[5];
- tin ions from Sn^{2+} (with three valence holes) to Sn^{10+} (four valence electrons) which are relevant for EUV light generation from laser-produced plasma[6];
- the electron-hole transition in Hg^+ which is the reference for an optical clock at NIST[2].

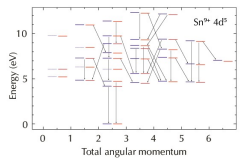
In these **complicated systems**, the particle-hole CI+MBPT method implemented in AMBiT outperforms the competition.



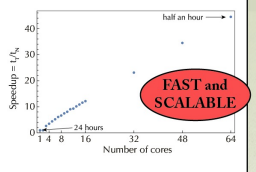
Structure of the CI matrix under the emu CI approximation. The most important configurations are in the upper left corner, while the shaded areas are the effective CI matrix. The unshaded area represents interactions between high energy states which are set to zero.



Convergence of selected states of tantalum when the B-spline basis set used in CI is increased from 11spdf to 21spdf[5]. Emu CI reduces the calculation size by a factor of 40: the largest calculations of Ta in [5] have matrices of size 952112 x 20462.



Measured energy levels (blue) and particle-hole CI+MBPT calculations using AMBiT (red) for the [Kr] $4d^5$ ground state configuration of Sn^{4+}.



Speed up of a large Cr^+ calculation using parallel processing on 16 cores/node Xeon architecture. AMBiT uses OpenMP for shared-memory parallelism within the socket or node, and MPI for inter-node communication.

User-friendly, easy to install, and well documented

Due to the need to have AMBiT optimised for each system, AMBiT is only distributed by source code. To make building easier, we use SCons to find packages automatically and provide flexibility as required. AMBiT is fully documented, with user guides and example input scripts to help users take full advantage of AMBiT's flexibility. All features in AMBiT can be controlled at run-time using input files and the command line.

OPEN SOURCE €0!

Scales on your architecture

Scales up from your laptop to an office workstation or state-of-the-art national cluster. AMBiT is written in modern C++11 and uses both OpenMP and MPI parallelism models to take full advantage of today's computer architectures, which typically consist of large, relatively loosely connected nodes. All time-consuming stages of the CI+MBPT calculation are parallelised, including generation of MBPT diagrams, calculation of angular factors, creation and diagonalisation of the Hamiltonian matrix, and calculation of transition matrix elements from the resulting level structure.

Particle-Hole CI+MBPT

- Start with open-shell Dirac-Hartree-Fock, optionally including Breit, QED, nuclear size and mass-shift corrections, and additional local potentials.
- Choose your Fermi level; this can be below or above any valence electrons or holes.
- Create a basis set using B-splines. Choose your frozen core, below which holes cannot be included in CI. The effect of the frozen core electrons may be included using second-order MBPT.
- Generate configurations by flexibly promoting electrons and from a set of leading configurations.
- Run AMBiT to generate configuration state functions. The resulting angular data is stored for other calculations! Check the size of your CI matrices and adjust for your computer system.
- Generate second-order MBPT diagrams; generate and diagonalise the CI matrix.
- Calculate level properties and transition matrix elements.

References

1. E. V. Kahl and J. C. Berengut, arXiv:1805.11265 (2018)
2. J. C. Berengut, Phys. Rev. A **94**, 012502 (2016)
3. V. A. Dzuba, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A **54**, 3948 (1996)
4. J. C. Berengut, V. V. Flambaum, and M. G. Kozlov, Phys. Rev. A **73**, 012504 (2006)
5. A. J. Geddes, D. A. Czapski, E. V. Kahl, and J. C. Berengut, arXiv:1805.0661 (2018)
6. F. Torretti et al., Phys. Rev. A **95**, 042503 (2017)

Yes, I would like a personalised link to the AMBiT website!
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julian.berengut@unsw.edu.au
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