Pre-processing the Quantum Many-Body Problem

The curse of dimensionality … and how to beat it!

Alexander Tichai

CEA - Saclay

Wise men say ...

$$H\,|\Psi_k^A\rangle = E_k^A\,|\Psi_k^A\rangle$$

'... only fools rush in ... '

Elvis Presley

Wise men say ...

$$H\,|\Psi_k^A\rangle = E_k^A\,|\Psi_k^A\rangle$$

'... only fools rush in ... '

Elvis Presley

'... instead of storing one big file you can store many small files ...'

Kai Hebeler

Tensors and many-body theory

- **Many-body calculations employ mode-*n* tensors and compute tensor networks (TN)**

1) Input

$$H_{\mathrm{nucl}} = \frac{1}{(1!)^2}\sum_{pq} t_{pq} c_p^\dagger c_q + \frac{1}{(2!)^2}\sum_{pqrs} \bar{v}_{pqrs} c_p^\dagger c_q^\dagger c_s c_r + \frac{1}{(3!)^2}\sum_{pqrstu} \bar{w}_{pqrstu} c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s$$

storage cost N^{2k} (here p=2,4,6)

2) Output

CC: $$E_0 = E_0^{\mathrm{HF}} + \frac{1}{2}\sum_{ijab} \bar{v}_{ijab}\, t_i^a\, t_i^b + \frac{1}{4}\sum_{ijab} \bar{v}_{ijab}\, t_{ij}^{ab}$$

IMSRG: $$E_0(s) = \sum_{ab}(n_a - n_b)\eta_b^a f_a^b + \frac{1}{2}\sum_{abcd} \eta_{cd}^{ab} \Gamma_{ab}^{cd} n_a n_b \bar{n}_c \bar{n}_d$$

evaluation cost N^p (here p=4)

Tensors and many-body theory

- Many-body calculations employ mode-*n* tensors and compute tensor networks (TN)

1) Input

$$H_{\text{nucl}} = \frac{1}{(1!)^2}\sum_{pq} t_{pq} c_p^\dagger c_q + \frac{1}{(2!)^2}\sum_{pqrs} \bar{v}_{pqrs} c_p^\dagger c_q^\dagger c_s c_r + \frac{1}{(3!)^2}\sum_{pqrstu} \bar{w}_{pqrstu} c_p^\dagger c_q^\dagger c_r^\dagger c_u c_t c_s$$

storage cost N^{2k} (here p=2,4,6)

2) Output

CC: $$E_0 = E_0^{\text{HF}} + \frac{1}{2}\sum_{ijab} \bar{v}_{ijab}\, t_i^a\, t_i^b + \frac{1}{4}\sum_{ijab} \bar{v}_{ijab}\, t_{ij}^{ab}$$

IMSRG: $$E_0(s) = \sum_{ab}(n_a - n_b)\eta_b^a f_a^b + \frac{1}{2}\sum_{abcd} \eta_{cd}^{ab}\Gamma_{ab}^{cd} n_a n_b \bar{n}_c \bar{n}_d$$

evaluation cost N^p (here p=4)

- Tensors and tensor networks provide the universal language of many-body theory
- Future research will require developments along several frontiers, e.g.,
  - Going to larger model spaces for *3B* operators
  - Relaxing many-body truncations yielding higher-mode tensors
  - Working in deformed basis

Tensors and many-body theory

- Many-body calculations employ mode-*n* tensors and compute tensor networks (TN)

1) Input

$$H_{\text{nucl}} = \frac{1}{(1!)^2}\sum_{pq} t_{pq} c^\dagger_p c_q + \frac{1}{(2!)^2}\sum_{pqrs} \bar{v}_{pqrs} c^\dagger_p c^\dagger_q c_s c_r + \frac{1}{(3!)^2}\sum_{pqrstu} \bar{w}_{pqrstu} c^\dagger_p c^\dagger_q c^\dagger_r c_u c_t c_s$$

storage cost N^{2k} (here p=2,4,6)

2) Output

CC: $$E_0 = E_0^{\text{HF}} + \frac{1}{2}\sum_{ijab} \bar{v}_{ijab}\, t_i^a\, t_i^b + \frac{1}{4}\sum_{ijab} \bar{v}_{ijab}\, t_{ij}^{ab}$$

IMSRG: $$E_0(s) = \sum_{ab}(n_a - n_b)\eta^a_b f^b_a + \frac{1}{2}\sum_{abcd} \eta^{ab}_{cd}\Gamma^{cd}_{ab} n_a n_b \bar{n}_c \bar{n}_d$$

evaluation cost N^p (here p=4)

- Tensors and tensor networks provide the universal language of many-body theory
- Future research will require developments along several frontiers, e.g.,
  - Going to larger model spaces for *3B* operators
  - Relaxing many-body truncations yielding higher-mode tensors
  - Working in deformed basis
- More computational power will not resolve this problem

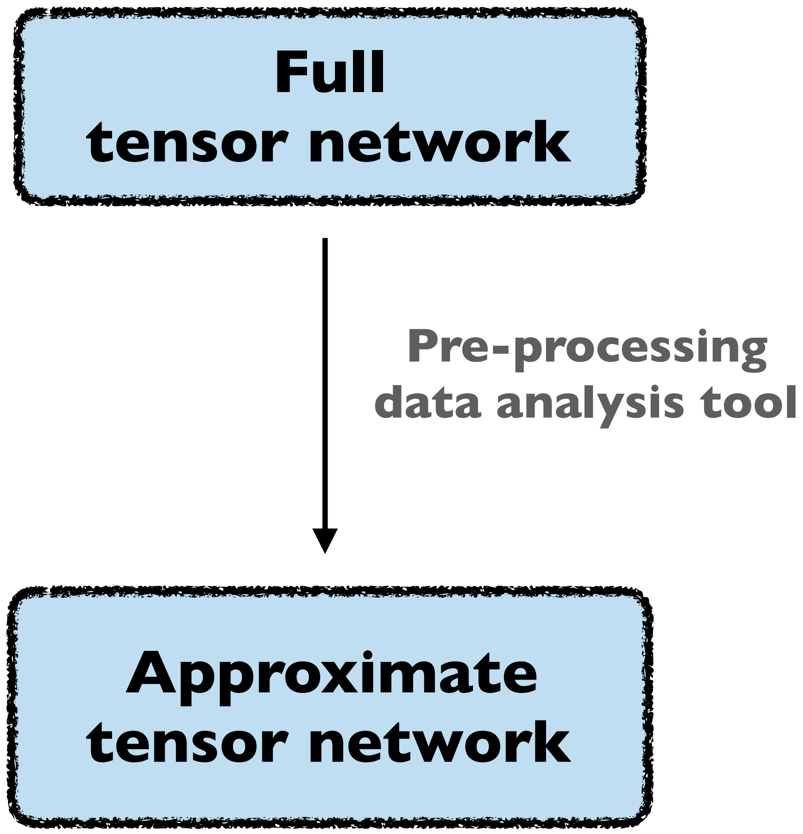
We need new tools to account for such large data!

Two ways of pre-processing data

Full tensor network

Computational scaling might be prohibitive but:
Not all tensor entries are equally important!

Two ways of pre-processing data



Computational scaling might be prohibitive but:

Not all tensor entries are equally important!

Two ways of pre-processing data

Full tensor network

Pre-processing data analysis tool

Approximate tensor network

Computational scaling might be prohibitive but:

Not all tensor entries are equally important!

Tensor factorization (TF)

- Decompose tensor according to a tensor format
- Discard high-rank components in the decomposition
- Factorized TN has possibly lower scaling exponent

Two ways of pre-processing data

Full tensor network

↓ Pre-processing data analysis tool

Approximate tensor network

Computational scaling might be prohibitive but:
Not all tensor entries are equally important!

Tensor factorization (TF)
- Decompose tensor according to a tensor format
- Discard high-rank components in the decomposition
- Factorized TN has possibly lower scaling exponent

Importance truncation (IT)
- IT measure gauges importance of tensor entry
- Discard unimportant entries of the tensor
- IT-TN has lower effective basis size but same exponent

Two ways of pre-processing data

Full tensor network

↓ **Pre-processing data analysis tool**

Approximate tensor network

↓ **Post-processing**

Residual Correction

Computational scaling might be prohibitive but:

Not all tensor entries are equally important!

Tensor factorization (TF)

- Decompose tensor according to a tensor format
- Discard high-rank components in the decomposition
- Factorized TN has possibly lower scaling exponent

Importance truncation (IT)

- IT measure gauges importance of tensor entry
- Discard unimportant entries of the tensor
- IT-TN has lower effective basis size but same exponent

Two ways of pre-processing data

Full tensor network

↓ Pre-processing data analysis tool

Approximate tensor network

↓ Post-processing

Residual Correction

Computational scaling might be prohibitive but:

Not all tensor entries are equally important!

Tensor factorization (TF)

- Decompose tensor according to a tensor format
- Discard high-rank components in the decomposition
- Factorized TN has possibly lower scaling exponent

Importance truncation (IT)

- IT measure gauges importance of tensor entry
- Discard unimportant entries of the tensor
- IT-TN has lower effective basis size but same exponent

Robust medium-mass testbed with open-shell capabilities:

Bogoliubov many-body perturbation theory (BMBPT)

BMBPT in a nutshell

- **MBPT expansion w.r.t. particle-number-broken HFB vacuum:** $\left\{U_k, V_k, E_k > 0\right\}$
- **Hamiltonian replaced by grand potential operator** $\Omega = H - \lambda A$
- **Natural formulation in quasi-particle space (change of algebra!)**

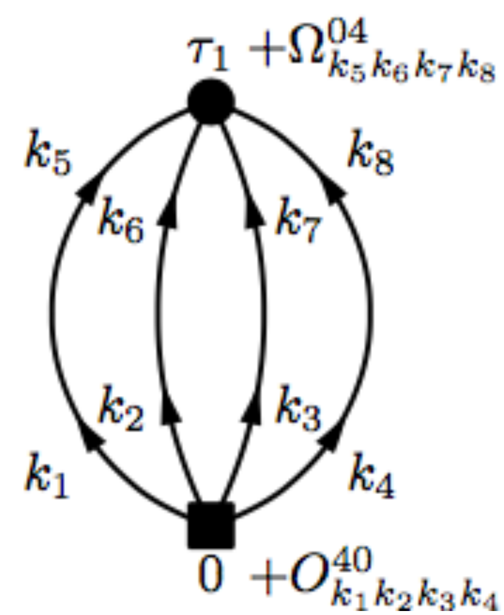
$$\beta_k^\dagger = \sum_p U_{pk} c_p^\dagger + V_{pk} c_p \qquad \beta_k = \sum_p U_{pk}^\star c_p + V_{pk}^\star c_p^\dagger$$

BMBPT in a nutshell

- MBPT expansion w.r.t. particle-number-broken HFB vacuum: $\left\{U_k, V_k, E_k > 0\right\}$
- Hamiltonian replaced by grand potential operator $\Omega = H - \lambda A$
- Natural formulation in quasi-particle space (change of algebra!)

$$\beta_k^\dagger = \sum_p U_{pk} c_p^\dagger + V_{pk} c_p \qquad \beta_k = \sum_p U_{pk}^\star c_p + V_{pk}^\star c_p^\dagger$$

BMBPT(2) Feynman diagram



- Single-reference open-shell technique but all sums run over full basis!
- Bulk correlation from second-order energy correction

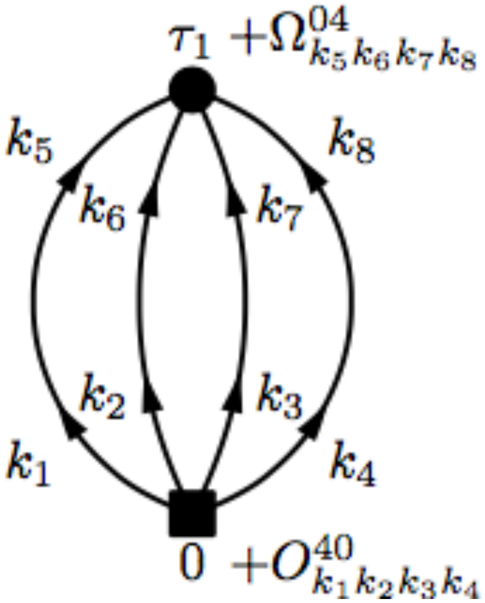
$$\Delta\Omega_0^{(2)} = -\frac{1}{24} \sum_{k_1k_2k_3k_4} \frac{\Omega^{40}_{k_1k_2k_3k_4}\Omega^{04}_{k_1k_2k_3k_4}}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}}$$

BMBPT in a nutshell

- **MBPT expansion w.r.t. particle-number-broken HFB vacuum:** $\left\{U_k, V_k, E_k > 0\right\}$
- **Hamiltonian replaced by grand potential operator** $\Omega = H - \lambda A$
- **Natural formulation in quasi-particle space (change of algebra!)**

$$\beta_k^\dagger = \sum_p U_{pk} c_p^\dagger + V_{pk} c_p \qquad \beta_k = \sum_p U_{pk}^\star c_p + V_{pk}^\star c_p^\dagger$$

BMBPT(2) Feynman diagram



- **Single-reference open-shell technique but all sums run over full basis!**
- **Bulk correlation from second-order energy correction**

$$\Delta\Omega_0^{(2)} = -\frac{1}{24} \sum_{k_1k_2k_3k_4} \frac{\Omega^{40}_{k_1k_2k_3k_4}\Omega^{04}_{k_1k_2k_3k_4}}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}}$$

- **Extension of diagrammatic formalism and development of automised tools**

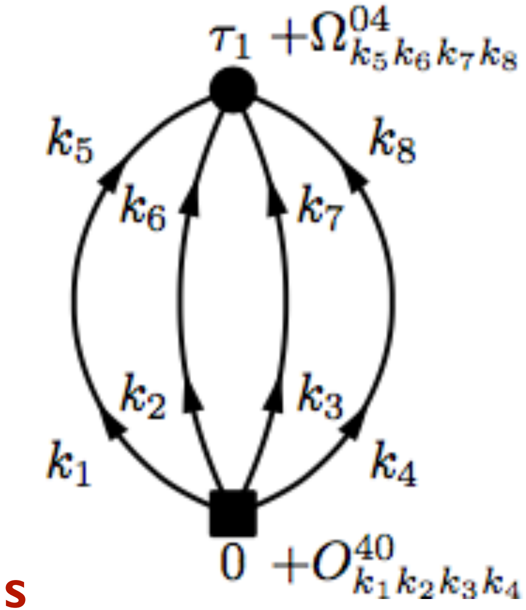
see talk of <u>Pierre Arthuis</u> !

BMBPT in a nutshell

- MBPT expansion w.r.t. particle-number-broken HFB vacuum: $\left\{U_k, V_k, E_k > 0\right\}$
- Hamiltonian replaced by grand potential operator $\Omega = H - \lambda A$
- Natural formulation in quasi-particle space (change of algebra!)

$$\beta_k^\dagger = \sum_p U_{pk} c_p^\dagger + V_{pk} c_p \qquad \beta_k = \sum_p U_{pk}^\star c_p + V_{pk}^\star c_p^\dagger$$

BMBPT(2) Feynman diagram



- Single-reference open-shell technique but all sums run over full basis!
- Bulk correlation from second-order energy correction

$$\Delta\Omega_0^{(2)} = -\frac{1}{24} \sum_{k_1k_2k_3k_4} \frac{\Omega^{40}_{k_1k_2k_3k_4}\Omega^{04}_{k_1k_2k_3k_4}}{E_{k_1} + E_{k_2} + E_{k_3} + E_{k_4}}$$

- Extension of diagrammatic formalism and development of automised tools

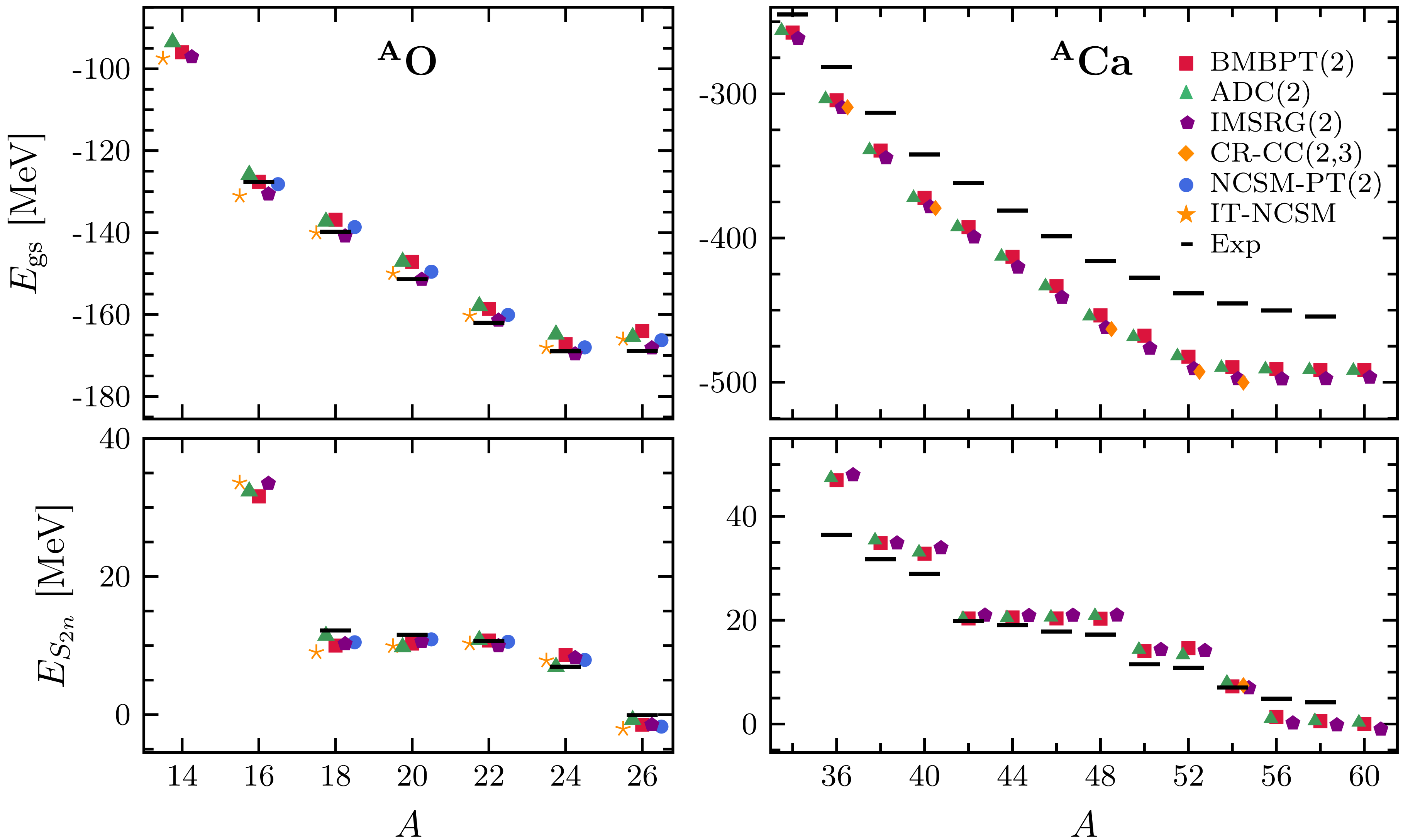
see talk of **Pierre Arthuis** !

- Ultimate restoration of broken symmetry mandatory (work in progress!)

Particle-number projected Bogoliubov coupled cluster theory. Application to the pairing Hamiltonian

Qiu, Henderson, Duguet, Scuseria, arXiv:1810.11245

BMBPT - consistency and complexity



Calculation details

Chiral NN+3N Hamiltonian
NO2B approximation
α = 0.08 fm⁴
13 major shells (1820 s.p. states)
canonical HFB reference

Runtime

NCSM:	20.000 hours
MCPT:	2.000 hours
IMSRG:	1.500 hours
ADC:	400 hours
BMBPT:	**< 1min !**

AT *et al.*, PLB **786** 195 (2018)

- Excellent agreement of all methods with 'exact' results (IT-NCSM)
- Different truncation schemes yield consistent description of open-shell nuclei
- BMBPT is optimal for cheap survey calculations of next-generation chiral Hamiltonians

Tensor decompositions

- **Tensor factorizations require a specific tensor format, here tensor hypercontraction (THC)**

Number of degrees of freedom N^4

$$\hat{T}_{k_1k_2k_3k_4} \approx \sum_{\alpha\beta}^{r_{\mathrm{THC}}} X^1_{k_1\alpha} X^2_{k_2\alpha} W_{\alpha\beta} X^3_{k_3\beta} X^4_{k_4\beta}$$

$r^2_{\mathrm{THC}} + 4 \cdot N \cdot r_{\mathrm{THC}}$

'Super-separable tensor'

Full tensor

$$T^{(\mathrm{sep})}_{k_1k_2k_3k_4} = X^1_{k_1} X^2_{k_2} X^3_{k_3} X^4_{k_4}$$

$r_{\mathrm{THC}} = 1$

Smooth interpolation by choosing THC rank →

$$T_{k_1k_2k_3k_4} = \sum_{\alpha\beta} X^1_{k_1\alpha} X^2_{k_2\alpha} W_{\alpha\beta} X^3_{k_3\beta} X^4_{k_4\beta}$$

$r_{\mathrm{THC}} = N^2$

Tensor decompositions

- Tensor factorizations require a specific tensor format, here tensor hypercontraction (THC)

Number of degrees of freedom N^4

$$\hat{T}_{k_1k_2k_3k_4} \approx \sum_{\alpha\beta}^{r_{\mathrm{THC}}} X^1_{k_1\alpha} X^2_{k_2\alpha} W_{\alpha\beta} X^3_{k_3\beta} X^4_{k_4\beta}$$

$r^2_{\mathrm{THC}} + 4 \cdot N \cdot r_{\mathrm{THC}}$

'Super-separable tensor'

$$T^{(\mathrm{sep})}_{k_1k_2k_3k_4} = X^1_{k_1} X^2_{k_2} X^3_{k_3} X^4_{k_4}$$

$r_{\mathrm{THC}} = 1$

Smooth interpolation by choosing THC rank

Full tensor

$$T_{k_1k_2k_3k_4} = \sum_{\alpha\beta} X^1_{k_1\alpha} X^2_{k_2\alpha} W_{\alpha\beta} X^3_{k_3\beta} X^4_{k_4\beta}$$

$r_{\mathrm{THC}} = N^2$

- Systematically improvable approximation approaching the exact results in a well-defined way

This is (part of) the definition of *ab initio*!

Tensor decompositions

- Tensor factorizations require a specific tensor format, here tensor hypercontraction (THC)

Number of degrees of freedom: N^4

$$\hat{T}_{k_1k_2k_3k_4} \approx \sum_{\alpha\beta}^{r_{\mathrm{THC}}} X^1_{k_1\alpha} X^2_{k_2\alpha} W_{\alpha\beta} X^3_{k_3\beta} X^4_{k_4\beta}$$

$r^2_{\mathrm{THC}} + 4 \cdot N \cdot r_{\mathrm{THC}}$

'Super-separable tensor'

$$T^{(\mathrm{sep})}_{k_1k_2k_3k_4} = X^1_{k_1} X^2_{k_2} X^3_{k_3} X^4_{k_4}$$

$r_{\mathrm{THC}} = 1$

Smooth interpolation by choosing THC rank →

Full tensor

$$T_{k_1k_2k_3k_4} = \sum_{\alpha\beta} X^1_{k_1\alpha} X^2_{k_2\alpha} W_{\alpha\beta} X^3_{k_3\beta} X^4_{k_4\beta}$$

$r_{\mathrm{THC}} = N^2$

- Systematically improvable approximation approaching the exact results in a well-defined way

This is (part of) the definition of *ab initio*!

- Numerical procedure: truncated SVD + least-square minimization of Frobenius norm

$$\Delta T = \frac{\|T - \hat{T}\|}{\|T\|} \qquad \|T\| = \sqrt{T_{k_1k_2\ldots} T^\star_{k_1k_2\ldots}}$$

Tensor decompositions

- Tensor factorizations require a specific tensor format, here tensor hypercontraction (THC)

Number of degrees of freedom N^4

$$\hat{T}_{k_1k_2k_3k_4} \approx \sum_{\alpha\beta}^{r_{\text{THC}}} X^1_{k_1\alpha} X^2_{k_2\alpha} W_{\alpha\beta} X^3_{k_3\beta} X^4_{k_4\beta}$$

$r^2_{\text{THC}} + 4 \cdot N \cdot r_{\text{THC}}$

'Super-separable tensor'

$$T^{(\text{sep})}_{k_1k_2k_3k_4} = X^1_{k_1} X^2_{k_2} X^3_{k_3} X^4_{k_4}$$

$r_{\text{THC}} = 1$

Smooth interpolation by choosing THC rank →

Full tensor

$$T_{k_1k_2k_3k_4} = \sum_{\alpha\beta} X^1_{k_1\alpha} X^2_{k_2\alpha} W_{\alpha\beta} X^3_{k_3\beta} X^4_{k_4\beta}$$

$r_{\text{THC}} = N^2$

- Systematically improvable approximation approaching the exact results in a well-defined way

This is (part of) the definition of *ab initio*!

- Numerical procedure: truncated SVD + least-square minimization of Frobenius norm

$$\Delta T = \frac{\|T - \hat{T}\|}{\|T\|} \qquad \|T\| = \sqrt{T_{k_1k_2\dots} T^\star_{k_1k_2\dots}}$$

- Numerous formats available: CPD, (hierarchical) Tucker, HOSVD, RI, MPS, …

Very active field of research

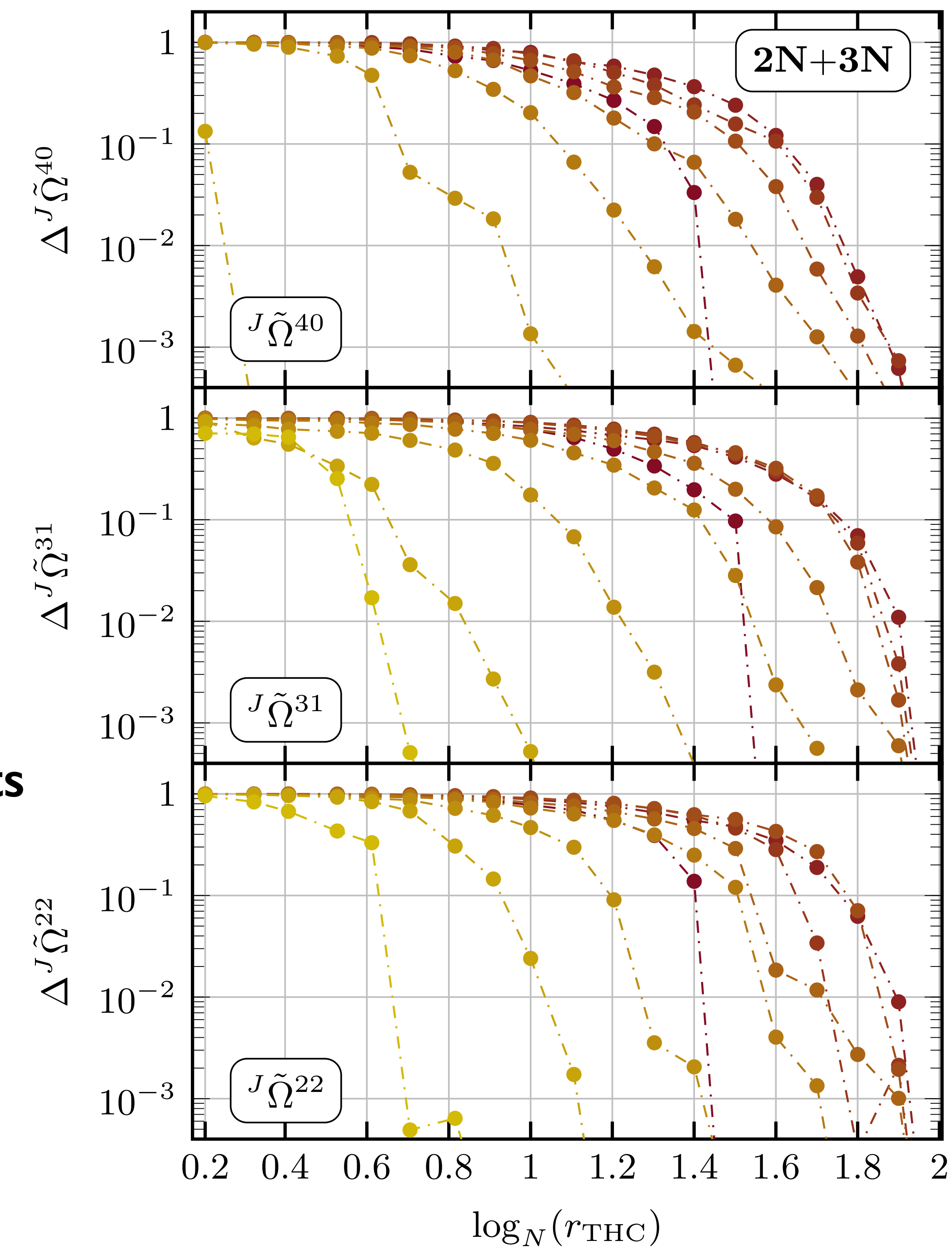
Tensor decomposition of the Hamiltonian

- Better approximation for larger ranks
- Small dependence on normal-ordered component
- THC works independent of target nucleus
- Better compression for sparse *J* channels
  - Parity constraints
  - Isospin constraints
  - Angular-momentum triangle inequalities
- Efficient black-box data compression tool
- Confirms observations for HO and HF matrix elements

AT, Schutski, Scuseria, Duguet, 2018, arXiv:1810.08419

How does THC affect nuclear observables?

SRG-evolved 2N+3N Hamiltonian (NO2B)
quasi-particle basis in 5 major shells



AT, Ripoche, Duguet, arXiv:1902.09043

The BMBPT tensor network

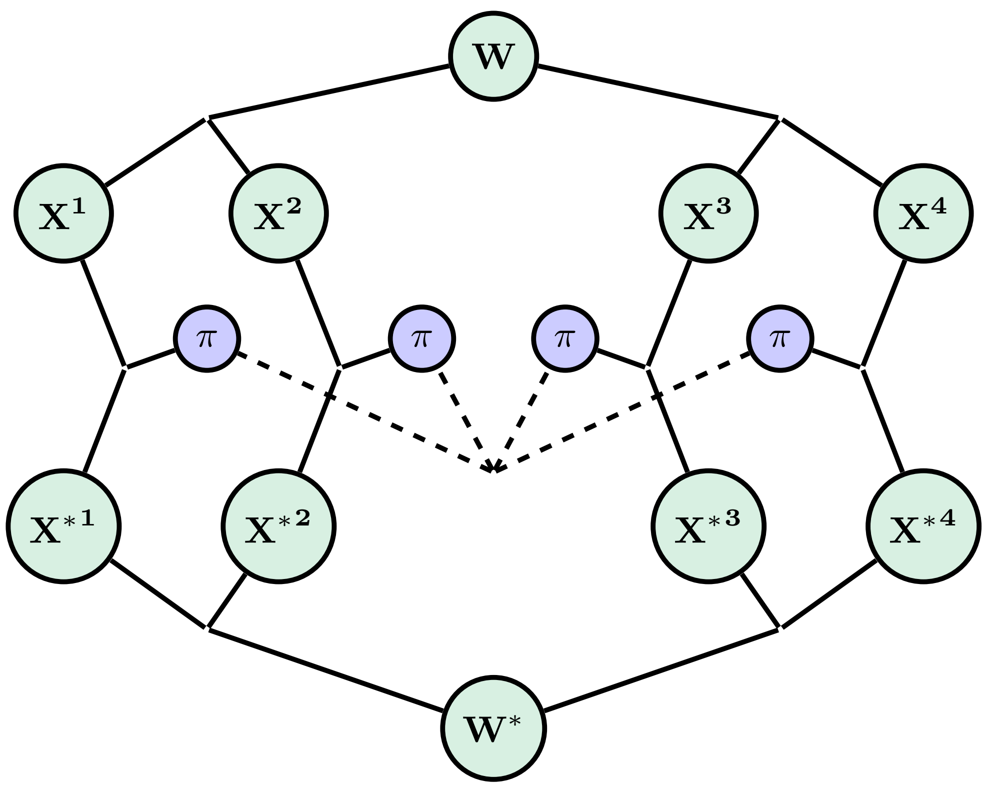
- Second-order energy correction to ground-state correlations

$$\Delta\Omega_0^{(2)} = -\frac{1}{24}\sum_{k_1k_2k_3k_4}\frac{\Omega^{40}_{k_1k_2k_3k_4}\Omega^{04}_{k_1k_2k_3k_4}}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}}$$

- Full-fledged decomposition using
  - Factorized form of nuclear matrix elements
  - Quadrature for decomposition of denominator

$$\frac{1}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}} = \int_0^\infty e^{-t(E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4})}dt$$

The THC-BMBPT(2) tensor network



The BMBPT tensor network

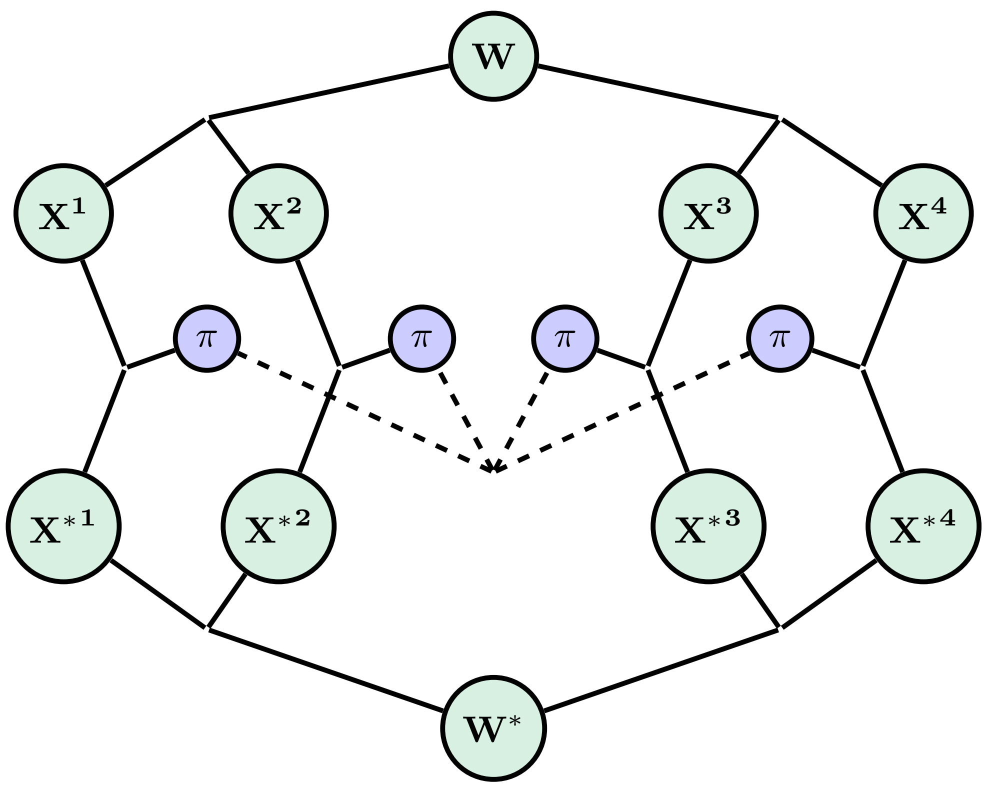
- Second-order energy correction to ground-state correlations

$$\Delta\Omega_0^{(2)} = -\frac{1}{24} \sum_{k_1k_2k_3k_4} \frac{\Omega^{40}_{k_1k_2k_3k_4}\Omega^{04}_{k_1k_2k_3k_4}}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}}$$

- Full-fledged decomposition using
  - Factorized form of nuclear matrix elements
  - Quadrature for decomposition of denominator

$$\frac{1}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}} = \int_0^\infty e^{-t(E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4})}dt$$

The THC-BMBPT(2) tensor network



- Measures for gauging THC performance from error on observable and compression ratio

$$\Delta(\Delta\Omega_0^{(2)}) \equiv \frac{\left|\Delta\Omega_0^{(2)}(\mathrm{THC}) - \Delta\Omega_0^{(2)}\right|}{\left|\Delta\Omega_0^{(2)}\right|}$$

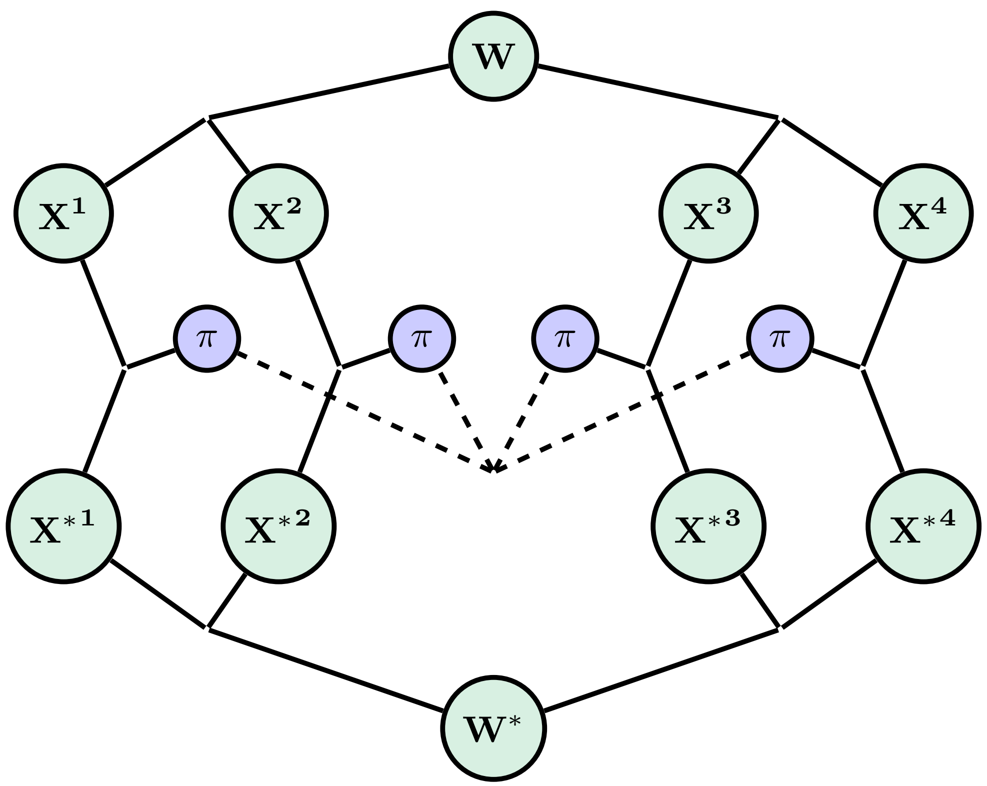
$$R_C = \frac{\#\text{elements of } T}{\#\text{elements of } \hat{T}}$$

The BMBPT tensor network

- Second-order energy correction to ground-state correlations

$$\Delta\Omega_0^{(2)} = -\frac{1}{24}\sum_{k_1k_2k_3k_4}\frac{\Omega^{40}_{k_1k_2k_3k_4}\Omega^{04}_{k_1k_2k_3k_4}}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}}$$

The THC-BMBPT(2) tensor network



- Full-fledged decomposition using
  - Factorized form of nuclear matrix elements
  - Quadrature for decomposition of denominator

$$\frac{1}{E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4}} = \int_0^\infty e^{-t(E_{k_1}+E_{k_2}+E_{k_3}+E_{k_4})}dt$$

- Measures for gauging THC performance from error on observable and compression ratio

$$\Delta(\Delta\Omega_0^{(2)}) \equiv \frac{\left|\Delta\Omega_0^{(2)}(\mathrm{THC}) - \Delta\Omega_0^{(2)}\right|}{\left|\Delta\Omega_0^{(2)}\right|}$$

$$R_C = \frac{\#\text{elements of } T}{\#\text{elements of } \hat{T}}$$

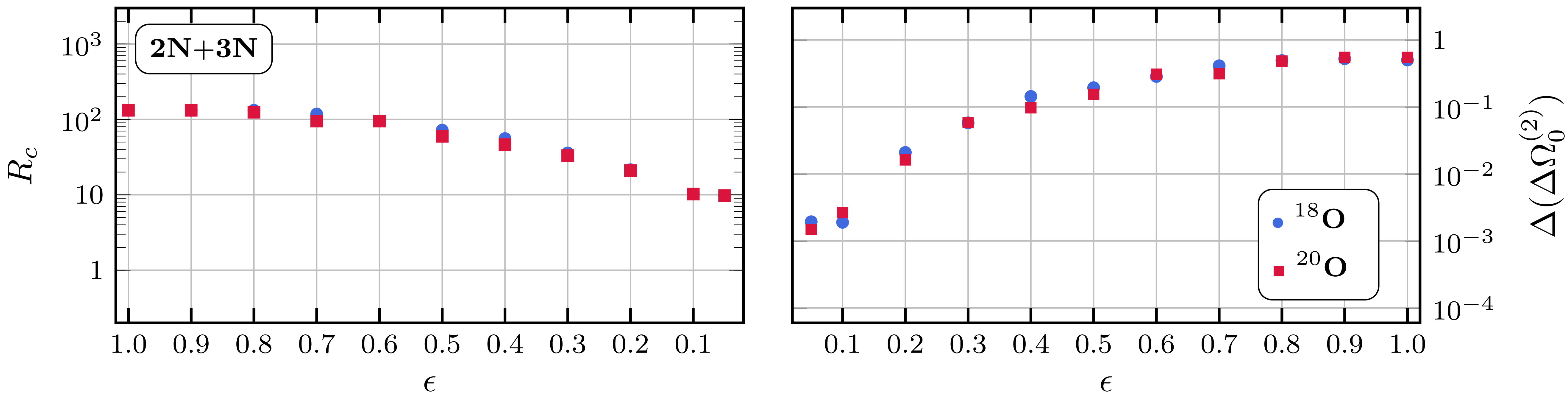
- Using factorisation always requires non-trivial reformulation of many-body formalism

Tensor-structured coupled cluster theory

Schutski *et al.*, JCP **147**, 184113 (2017)

THC - accuracy and compression

Compression ratio and second-order error as function of decomposition error



AT, Ripoche, Duguet, arXiv:1902.09043

Calculation details

Chiral NN+3N Hamiltonian
α = 0.08 fm^4
5 major shells
HFB reference state
BMBPT(2) energy correction

- **Strong correlation between accuracy and data compression**
- **Sub-percent accuracy only for compression ratio R_C < 10**
- **Advantage: flexible tool for compressing many-body tensors**
- **Tradeoff: calculation of decomposition factors is numerically challenging**

Development of parallelized code suite for arbitrary tensors!

Importance truncation

- **Desire:** Non-perturbative open-shell framework with full account of triples in mid-mass nuclei

Bogoliubov CC theory up to triples (BCCSDT)

$$|\Psi\rangle = \exp\left(\mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3\right)|\Phi\rangle\,, \qquad \langle\Phi^{k_1 k_2 \dots}|\left(\Omega e^{\mathcal{T}}\right)_c|\Phi\rangle = 0\,, \qquad \mathcal{T}_n \equiv \frac{1}{(2n)!}\sum_{k_1\dots k_{2n}} t^{2n0}_{k_1\dots k_{2n}}\beta^\dagger_{k_1}\cdots\beta^\dagger_{k_{2n}}$$

Signoracci, Duguet, Hagen and Jansen, PRC **91** 064320

- **Problem:** storage of amplitude tensors requires several TB of memory (in *J*-scheme)

Importance truncation

- **Desire:** Non-perturbative open-shell framework with full account of triples in mid-mass nuclei

Bogoliubov CC theory up to triples (BCCSDT)

$$|\Psi\rangle = \exp\left(\mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3\right)|\Phi\rangle\,, \qquad \langle\Phi^{k_1 k_2 \dots}|\left(\Omega e^{\mathcal{T}}\right)_c|\Phi\rangle = 0\,, \qquad \mathcal{T}_n \equiv \frac{1}{(2n)!}\sum_{k_1\dots k_{2n}} t^{2n0}_{k_1\dots k_{2n}} \beta^\dagger_{k_1}\cdots\beta^\dagger_{k_{2n}}$$

Signoracci, Duguet, Hagen and Jansen, PRC **91** 064320

- **Problem:** storage of amplitude tensors requires several TB of memory (in *J*-scheme)
- Introduction of importance-truncated tensor based on *a priori* measure

$$\mathcal{T}_n(\kappa^{(p)}_{\text{min}}) \equiv \{t^{2n0}_{k_1\dots k_{2n}} \text{ such that } |t^{2n0(p)}_{k_1\dots k_{2n}}| \geq \kappa^{(p)}_{\text{min}}\}$$

Importance truncation

- **Desire:** Non-perturbative open-shell framework with full account of triples in mid-mass nuclei

Bogoliubov CC theory up to triples (BCCSDT)

$$|\Psi\rangle = \exp\left(\mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3\right)|\Phi\rangle\,, \qquad \langle\Phi^{k_1 k_2 \dots}|\left(\Omega e^{\mathcal{T}}\right)_c|\Phi\rangle = 0\,, \qquad \mathcal{T}_n \equiv \frac{1}{(2n)!}\sum_{k_1\dots k_{2n}} t^{2n0}_{k_1\dots k_{2n}} \beta^\dagger_{k_1}\cdots\beta^\dagger_{k_{2n}}$$

Signoracci, Duguet, Hagen and Jansen, PRC **91** 064320

- **Problem:** storage of amplitude tensors requires several TB of memory (in *J*-scheme)
- Introduction of importance-truncated tensor based on *a priori* measure

$$\mathcal{T}_n(\kappa^{(p)}_{\text{min}}) \equiv \{t^{2n0}_{k_1\dots k_{2n}} \text{ such that } |t^{2n0(p)}_{k_1\dots k_{2n}}| \geq \kappa^{(p)}_{\text{min}}\}$$

- Define importance measure based on perturbation theory arguments

$$t^{40(1)}_{k_1k_2k_3k_4} = -\frac{\Omega^{40}_{k_1k_2k_3k_4}}{E_{k_1k_2k_3k_4}}\,, \qquad t^{60(2)}_{k_1k_2k_3k_4k_5k_6} = \mathcal{P}(\dots/\dots)\sum_{k_7}\frac{\Omega^{31}_{k_1k_2k_3k_7}\,\Omega^{40}_{k_7k_4k_5k_6}}{E_{k_7k_4k_5k_6}E_{k_1k_2k_3k_4k_5k_6}}$$

Importance truncation

- **Desire:** Non-perturbative open-shell framework with full account of triples in mid-mass nuclei

Bogoliubov CC theory up to triples (BCCSDT)

$$|\Psi\rangle = \exp\left(\mathcal{T}_1 + \mathcal{T}_2 + \mathcal{T}_3\right)|\Phi\rangle\,, \qquad \langle\Phi^{k_1 k_2 \dots}|\left(\Omega e^{\mathcal{T}}\right)_c|\Phi\rangle = 0\,, \qquad \mathcal{T}_n \equiv \frac{1}{(2n)!}\sum_{k_1\dots k_{2n}} t^{2n0}_{k_1\dots k_{2n}} \beta^\dagger_{k_1}\cdots\beta^\dagger_{k_{2n}}$$

Signoracci, Duguet, Hagen and Jansen, PRC **91** 064320

- **Problem:** storage of amplitude tensors requires several TB of memory (in *J*-scheme)
- Introduction of importance-truncated tensor based on *a priori* measure

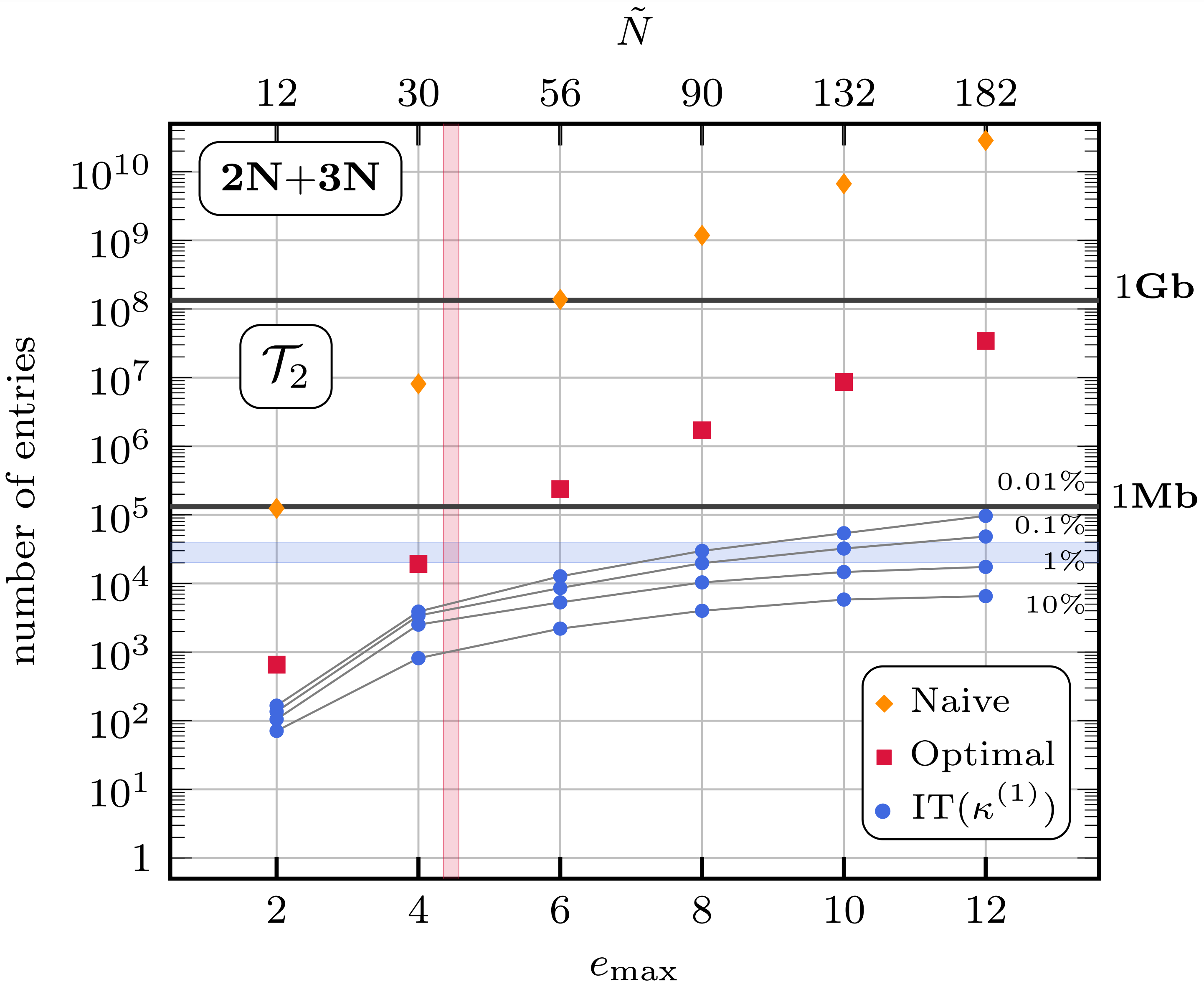
$$\mathcal{T}_n(\kappa^{(p)}_{\text{min}}) \equiv \{t^{2n0}_{k_1\dots k_{2n}} \text{ such that } |t^{2n0(p)}_{k_1\dots k_{2n}}| \geq \kappa^{(p)}_{\text{min}}\}$$

- Define importance measure based on perturbation theory arguments

$$t^{40(1)}_{k_1k_2k_3k_4} = -\frac{\Omega^{40}_{k_1k_2k_3k_4}}{E_{k_1k_2k_3k_4}}\,, \qquad t^{60(2)}_{k_1k_2k_3k_4k_5k_6} = \mathcal{P}(\dots/\dots)\sum_{k_7}\frac{\Omega^{31}_{k_1k_2k_3k_7}\,\Omega^{40}_{k_7k_4k_5k_6}}{E_{k_7k_4k_5k_6}E_{k_1k_2k_3k_4k_5k_6}}$$

- Store only IT tensor and restrict all summations in tensor network to ‘IT-allowed’ states
- Practitioners of other frameworks may feel free to replace CC amplitudes by:
  - Flowing Hamiltonian and generator (IMSRG)
  - Intermediate-state configurations and coupling matrices (Green’s function theory)

Analysis of double amplitudes



Calculation details

Chiral NN+3N Hamiltonian

$\alpha = 0.08\ \text{fm}^4$

13 major shells (1820 s.p. states)

canonical HFB reference

BCC T_2 amplitude

^{18}O

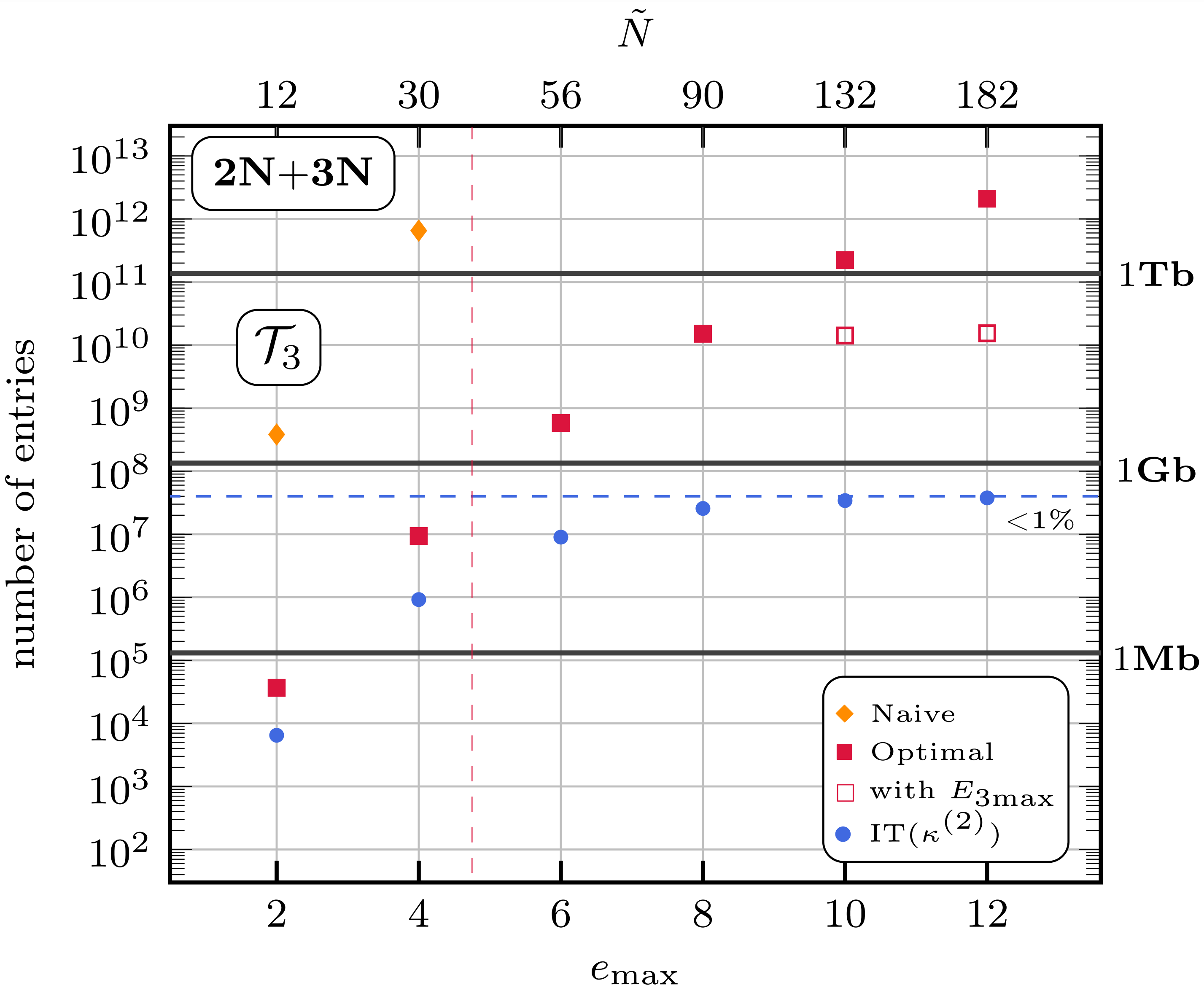
1st pre-processing paradigm:
'Make hard calculations routine'

AT, Ripoche, Duguet, arXiv:1902.09043

$$E^{(2)} = -\frac{1}{24} \sum_{k_1k_2k_3k_4} t^{40(1)}_{k_1k_2k_3k_4} \Omega^{04}_{k_1k_2k_3k_4}$$

- Storage requirements by three orders of magnitude lowered at 1% accuracy
- Estimate error on observable from 2nd-order energy correction in CC-like form
- Essentially all physics are recovered from a selected model space with $e^{(eff)}_{\max} \in [4, 5]$

Analysis of triple amplitudes



Calculation details

Chiral NN+3N Hamiltonian

α = 0.08 fm^4

13 major shells (1820 s.p. states)

canonical HFB reference

BCC T_3 amplitude

^{18}O

2nd pre-processing paradigm:
'Make impossible calculations feasible'

AT, Ripoche, Duguet, arXiv:1902.09043

- **Explosion of storage requirements without data compression (> 10 Tb)**
- **Estimate error on observables via BCCSD[T] correction**

$$\Delta\Omega_0^{[4T]} = \sum_{k_1k_2k_3k_4k_5k_6} |t^{60(2)}_{k_1k_2k_3k_4k_5k_6}|^2 E_{k_1k_2k_3k_4k_5k_6}$$

- **Storage of pre-processed amplitudes possible: full IT-BCCSDT in reach!**

Theoretical perspectives

Solving the *A*-body Schrödinger equation

- Fully consistent restoration of broken *U(1)* gauge symmetry
- Doubly open-shell nuclei from simultaneously breaking *SU(2)* symmetry
- Going to heavier systems: treatment of *3B* forces is a computational bottleneck
- Systematic account of spectroscopy and electromagnetic response

Pre-processing the many-body problem …

- What is the optimal tensor format for a given many-body tensor?
- Extension of tensor factorizations to large model spaces and higher-mode tensors
- Non-perturbative IT measures (QMC was used in quantum chemistry)
- Application of TF/IT to non-perturbative frameworks (CC, IMSRG, SCGF)

… and going beyond

- Is it possible to construct tensor-decomposed chiral matrix elements?
- Tensor-decomposed reformulation of (free-space) SRG evolution

Epilogue

- CEA group
  - P. Demol, T. Duguet, M. Frosini, F. Raimondi, V. Somà
    CEA Saclay, France

- Collaborators
  - P. Arthuis, C. Barbieri
    University of Surrey, UK
  - J.-P. Ebran, J. Ripoche
    CEA DAM DIF, France
  - H. Hergert
    Michigan State University, USA
  - J. Müller, R. Roth, K. Vobig
    Technische Universität Darmstadt, Germany
  - G. Scuseria, J. Zhao
    Rice University, USA
  - R. Schutski
    Skoltech, Russia