Bogoliubov Many-Body Perturbation Theory

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24 EFB
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Ab initio many-body scheme

$$H|\Psi_k^{\text{A}}\rangle = E_k^{\text{A}}|\Psi_k^{\text{A}}\rangle$$

H: A-body Hamiltonian

$|\Psi_k^A\rangle$: A-body wave function

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Definitions

- Nucleons as point-like degrees of freedom
- Active in full A-body Hilbert space
- Elementary interactions
- Solve A-body Schrödinger equation (SE)
- Thorough estimate of error

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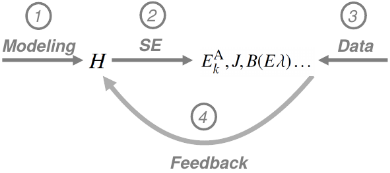

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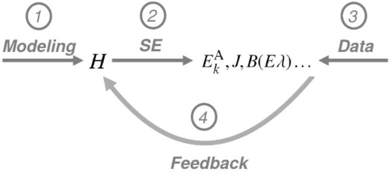

Hamiltonian

- Form of the Hamiltonian?
- Link to QCD?
- 3-body, ..., up to A-body forces?

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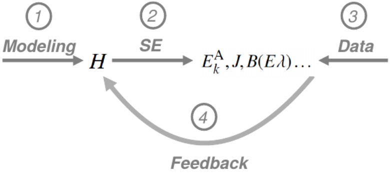

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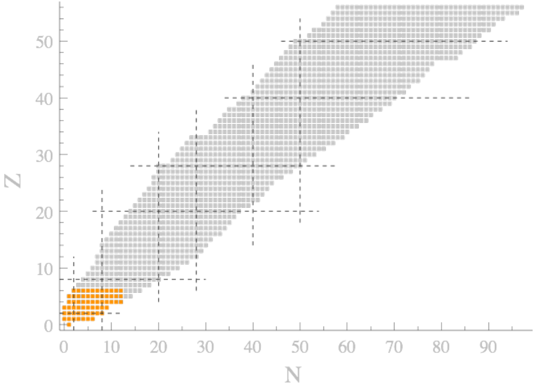
Schrödinger equation

- Accuracy of the SE solving?
- Doable for nuclei up to A $\sim$ 300?
- Need more effective approaches?

Ab initio methods

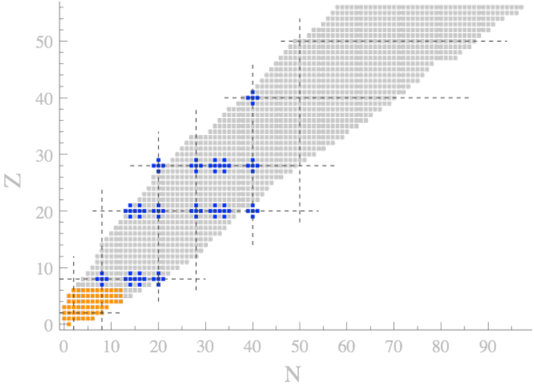


Courtesy of V. Soma, T. Duguet

"Exact" methods (80's)

- GFMC, NCSM, FY, HH...

Ab initio methods



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- DSCGF, CC, IMSRG

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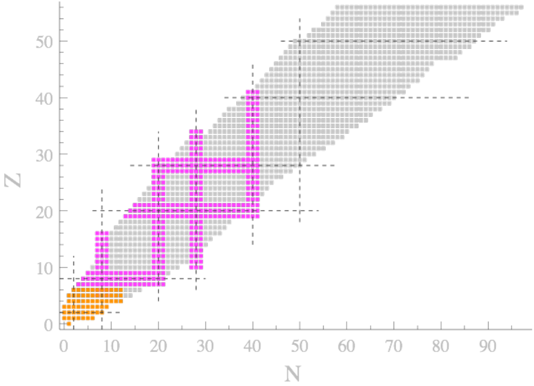

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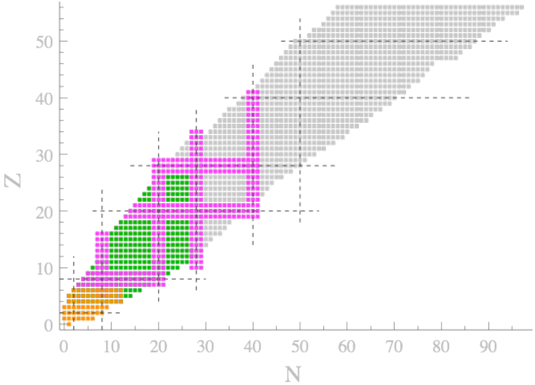

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Ab initio shell model (2014)
- EI via CC, IMSRG, NCSM...

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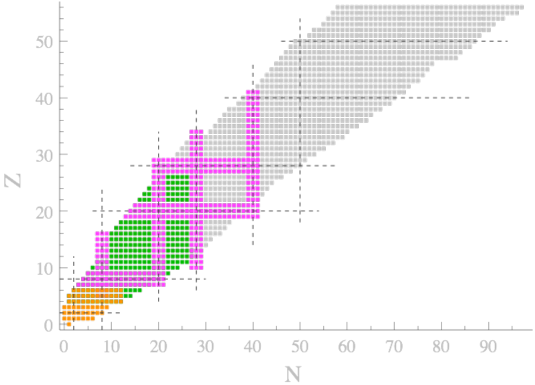

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- Closed-shell MBPT competes with non-perturbative methods for soft interactions [Tichai, Langhammer, Binder, Roth, *PLB* **756** (2016)]

Access open-shell nuclei through SR perturbative expansion method?
- Precise enough at (relatively) low order
- Low computational cost

SR expansion methods vs $U(1)$ symmetry

Operators of interest

- Nuclear Hamiltonian: $H = T + V + W$
- Particle number operator: A
- Grand potential: $\Omega = H - \lambda A$

A-body eigenvalue problem

$$H|\Psi_k^A\rangle = \mathrm{E}_k^A|\Psi_k^A\rangle$$

Particle number conserving

- Split H: $H = H_0 + H_1$

$$[A, H_0] = 0$$

- Introduce reference state

$$|\Psi_0^A\rangle = U^A(\infty)|\Phi^A\rangle$$

Wave operator to be expanded
Reference state solution of the SE

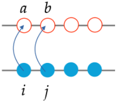
$$H_0|\Phi^A\rangle = \mathrm{E}_0^A|\Phi^A\rangle$$

- Symmetry-conserving method

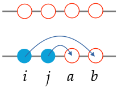
➥ **Slater determinant reference state**

Expansion methods and degenerate systems

- Basic idea: collect dynamical correlations through ph excitations
- Open-shell nuclei are degenerate w.r.t. ph excitations



Closed-shell



Open-shell

➥ Expansion breakdown signals non-dynamical correlations (superfluidity, ...)

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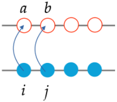

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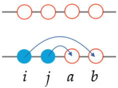

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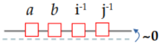
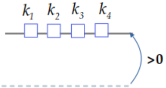
➥ Expansion breakdown signals non-dynamical correlations (superfluidity, ...)

- Various possible approaches
  - ◇ High-order non-pertubative method (if near-degenerate)
  - ◇ Multi-reference/configuration method (MR-MBPT, MR-CC, MR-IMSRG, MCPT)
  - ◇ Use a symmetry-breaking reference state

➥ Lift the degeneracy



Degenerate Slater



Bogoliubov vacuum

Expansion methods and degenerate systems

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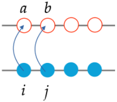

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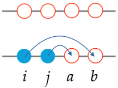

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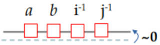

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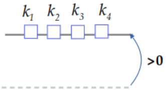

Bogoliubov vacuum

Symmetries to be restored eventually

SR expansion methods vs $U(1)$ symmetry

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Particle number breaking

- Split Ω: $\Omega = \Omega_0 + \Omega_1$

$$[A, \Omega_0] \neq 0$$

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Wave operator to be expanded

Reference state solution of the SE

$$\Omega_0|\Phi\rangle = E_0|\Phi\rangle$$

- Symmetry-breaking method

➥ **Bogoliubov reference state**

BMBPT in a nutshell

- MBPT expansion with respect to a particle-number broken vacuum
- Hamiltonian replaced by grand potential operator $\Omega = H - \lambda A$
- Natural formulation in quasiparticle space

$$\beta_k = \sum_p U^*_{pk} \, c_p + V^*_{pk} \, c^\dagger_p \qquad \beta^\dagger_k = \sum_p U_{pk} \, c^\dagger_p + V_{pk} \, c_p$$

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Bulk correlation from second-order correction

$$\Delta\Omega^{(2)}_0 = -\frac{1}{24} \sum_{k_1 k_2 k_3 k_4} \frac{\Omega^{40}_{k_1 k_2 k_3 k_4} \Omega^{04}_{k_1 k_2 k_3 k_4}}{E_{k_1 k_2 k_3 k_4}}$$

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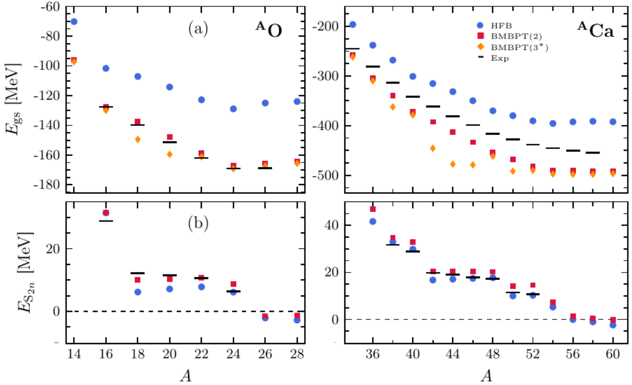
Beyond the basics

- Automated tool for automatic diagram & expression generation
  [Arthuis, Duguet, Tichai, Lasseri, Ebran, *CPC* **40** (2019)]
- Analysis of the perturbative series convergence
  [Demol, Frosini, Tichai, Ripoche, Somà, Duguet, to be published]
- Eventual restoration of broken symmetry mandatory (work in progress!)
  [Qiu, Henderson, Duguet, Scuseria, *PRC* **99** (2019)] for Bogoliubov Coupled-Cluster

Isotopic chains calculations - Energetics



[Tichai, Arthuis, Duguet, Hergert, Somà, Roth, *PLB* **786** (2018)]

Hamiltonian

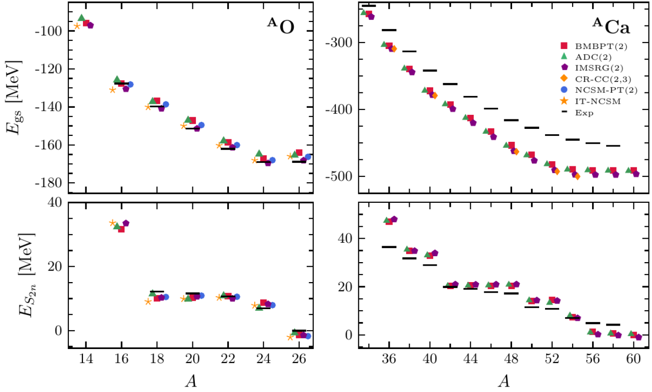
- Chiral EFT
  2NF: N3LO
  3NF: N2LO
- SRG: $\alpha = 0.08$ fm^4
- NO2B approximation

Basis parameters

- $\hbar\Omega = 20$ MeV
- $e_{max} = 12$
- $E_{3max} = 14$

- Closed-shell results agree with established HF-MBPT
- $E^{(3*)}$ **one order of magnitude smaller than** $E^{(2)}$
  - ◇ Well-behaved series at low order
- Reproduction of experimentally observed shell gaps
- Third order without particle number adjustment so far
- Ni chain shows similar results

Isotopic chains calculations - Comparisons



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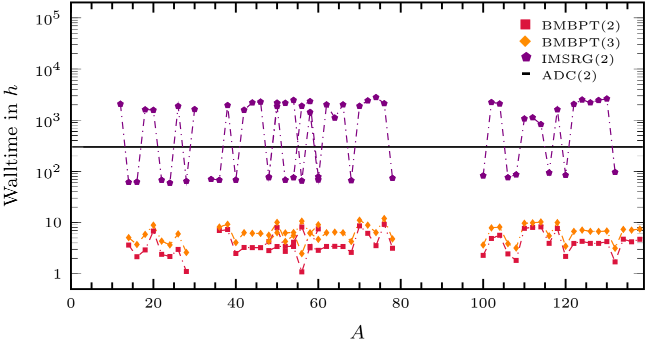
- **Very good agreement with non-perturbative approaches ($\leq 2\%$)**
  - ◇ Agree with exact results for O
  - ◇ Consistent with other methods for Ca
- Effects of particle-number breaking
  - ◇ Little overall effect (similar to GGF)
  - ◇ **Particle-number restoration could impact near magic numbers**

Numerical scaling



[Tichai, Arthuis, Duguet, Hergert, Somà, Roth, *PLB* **786** (2018)]

- **Two orders of magnitude cheaper than non-perturbative *ab initio* methods**
  - Three orders lower than exact result (IT-NCSM) in Oxygen chain
  - **Best accuracy/cost ratio**
- **Method of interest for large-scale *ab initio* calculations**
  - Test of newly developed chiral H
  - Systematic prediction/post-diction of nuclear properties

Conclusion

BMBPT diagrams generated and evaluated automatically

- ✔ Fast and error-safe
- ✔ Open-source code available for BMBPT, HF-MBPT
- ✔ Order 4 to be implemented in BMBPT code in near future
- ✔ Text-format output available for interface with numerical codes

Numerical implementation of BMBPT(2) and BMBPT(3*)

- ✔ Very low-cost correlated method
- ✔ Competes with non-perturbative *ab initio* methods
- ✔ Used as importance estimator for IT-BCC [Tichai, Ripoche, Duguet, *EPJA* **55** (2019)]

Perspectives

Extend the scope of BMBPT

- New observables, e.g. charge radius
- Excited states and transitions
- Resummation method based on low orders
  [Demol, Frosini, Tichai, Ripoche, Somà, Duguet, to be published]

Extend the scope of our automated diagram generator

- ✔ Particle-number-projected BMBPT [Ripoche, Arthuis, Tichai, Duguet, to be submitted]
- Gorkov SCGF at ADC(n) [Raimondi, Arthuis, Barbieri, Somà, Duguet, in prep.]
- ✔ Interface with J-coupling tools on the way [Ripoche, Wirth, Duguet, Tichai, arXiv:1908.00765]

Move towards symmetry-restored BMBPT

- ✔ Automated diagram generation/derivation
- ✔ Numerical implementation

Group and collaborators

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M. Drissi
J. Keeble
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T. Duguet
J.-P. Ebran
M. Frosini
R.-D. Lasseri
F. Raimondi
J. Ripoche
V. Somà
A. Tichai

H. Hergert

P. Demol

Thank you for your attention!