

Bogoliubov Many-Body Perturbation Theory For Open-Shell Nuclei

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INPC 2019
Glasgow – 2nd August 2019

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

H : A-body Hamiltonian

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

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- 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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- Link to QCD?
- 3-body, ..., up to A-body forces?



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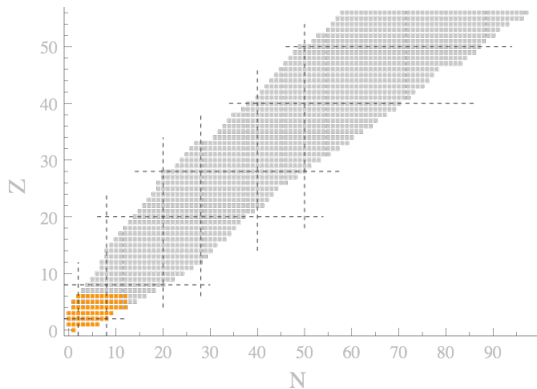


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Schrödinger equation

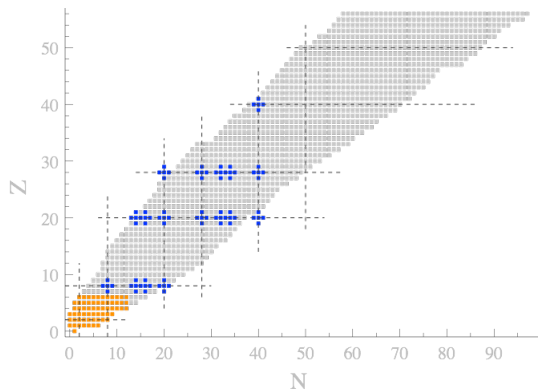
- Accuracy of the SE solving?
- Doable for nuclei up to $A \sim 300$?
- Need more effective approaches?



Courtesy of V. Soma, T. Duguet

"Exact" methods (80's)

- GFMC, NCSM, FY



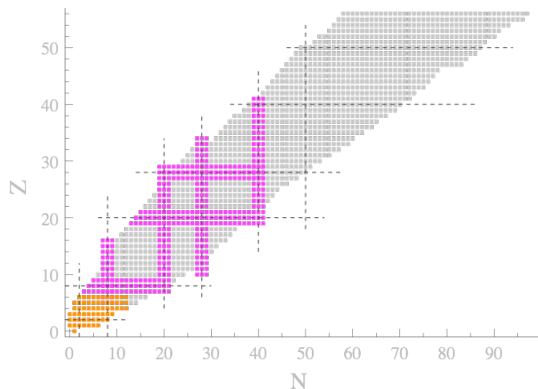
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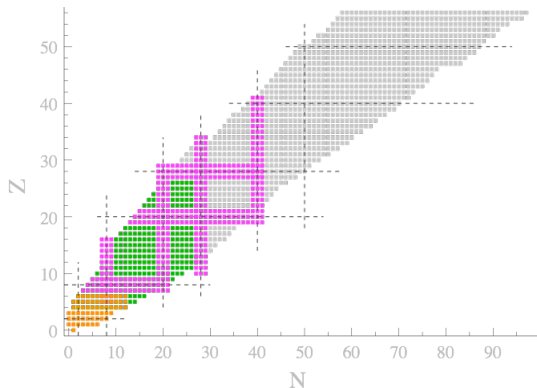
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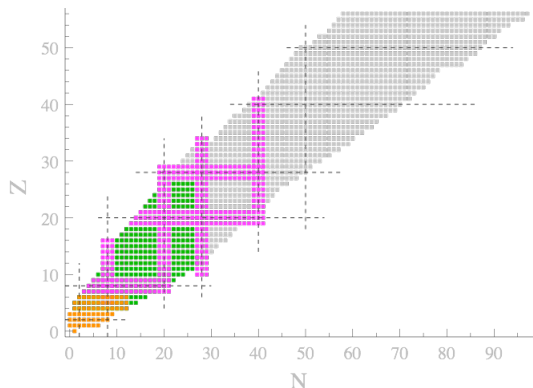
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Ab initio shell model (2014)

- EI via CC, IMSRG, NCSM...



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- 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

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



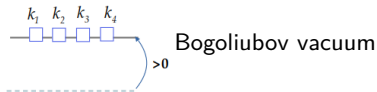
➔ Expansion breakdown signals non-dynamical correlations (superfluidity, ...)

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



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Symmetries to be restored eventually

- 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

$$\beta_k = \sum_p U_{pk}^* c_p + V_{pk}^* c_p^\dagger \quad \beta_k^\dagger = \sum_p U_{pk} c_p^\dagger + V_{pk} c_p$$

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Bulk correlation from second-order correction

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

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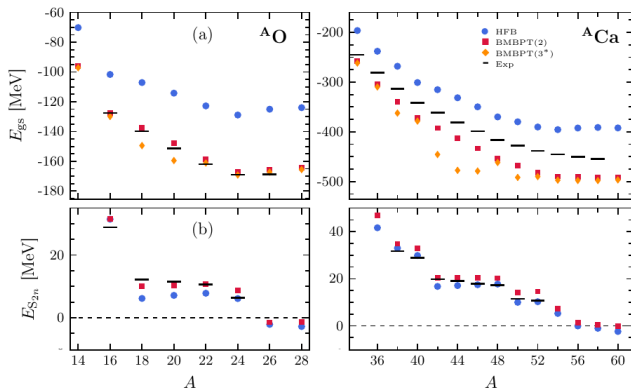
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Beyond the basics

- Automated tool for automatic diagram & expression generation [Arthuis, Duguet, Tichai, Lasserri, 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



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

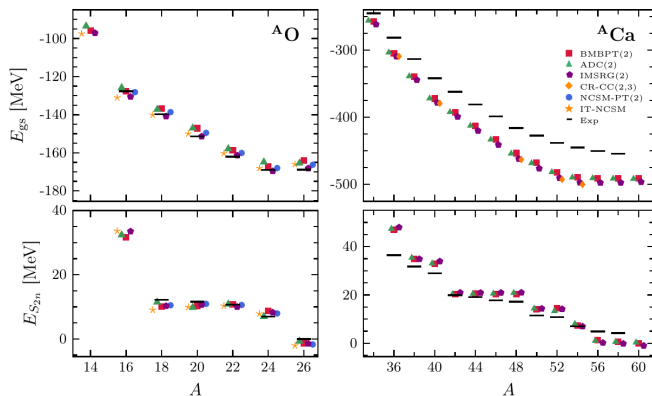
Hamiltonian

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

Basis parameters

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

- 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



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

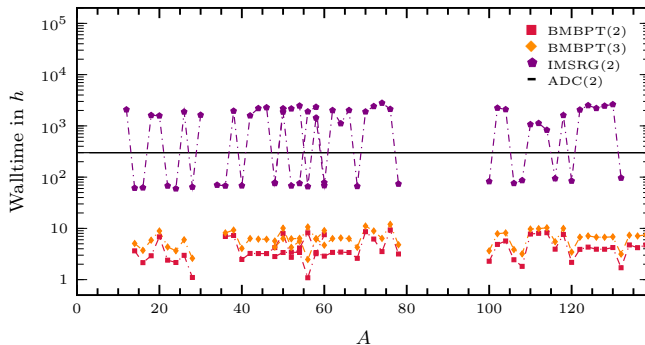
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- **Very good agreement with non-perturbative approaches ($\leq 2\%$)**
 - ◇ Agree with exact results for O
 - ◇ Consistent with other methods for Ca
- **Effects of particle-number breaking**
 - ◇ Little overall effect (similar to GGF)
 - ◇ **Particle-number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



[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

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)]

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, to be submitted]

Move towards symmetry-restored BMBPT

- ✓ Automated diagram generation/derivation
- ✓ Numerical implementation



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M. Drissi
J. Keeble
C. McIlroy
A. Rios



R. Roth



T. Duguet
J.-P. Ebran
M. Frosini
R.-D. Lasserri
F. Raimondi
J. Ripoché
V. Somà
A. Tichai



H. Hergert

 KU LEUVEN

P. Demol

Thank you for your attention!