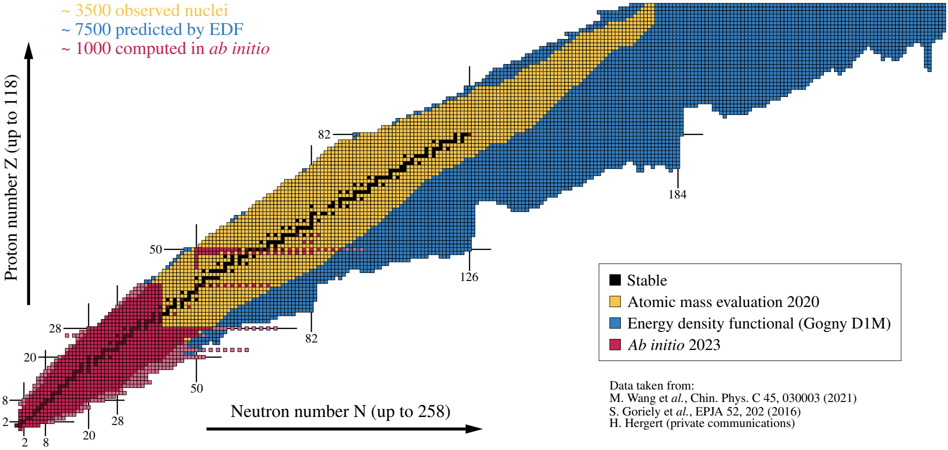
Ab initio Projected Generator Coordinate Method

Benjamin Bally

PAINT workshop - Vancouver - 01/03/2023

The End of the Beginning

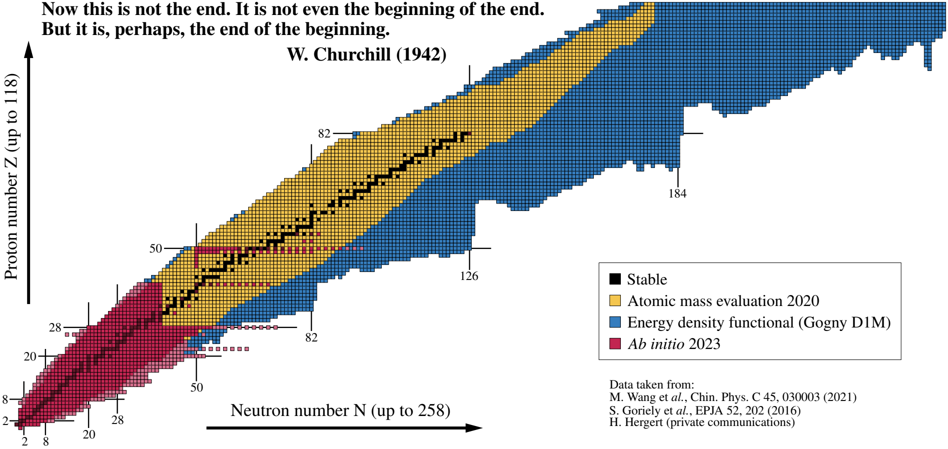


Data taken from:
M. Wang et *al.*, Chin. Phys. C 45, 030003 (2021)
S. Goriely et *al.*, EPJA 52, 202 (2016)
H. Hergert (private communications)

The End of the Beginning

**Now this is not the end. It is not even the beginning of the end.
But it is, perhaps, the end of the beginning.**

W. Churchill (1942)



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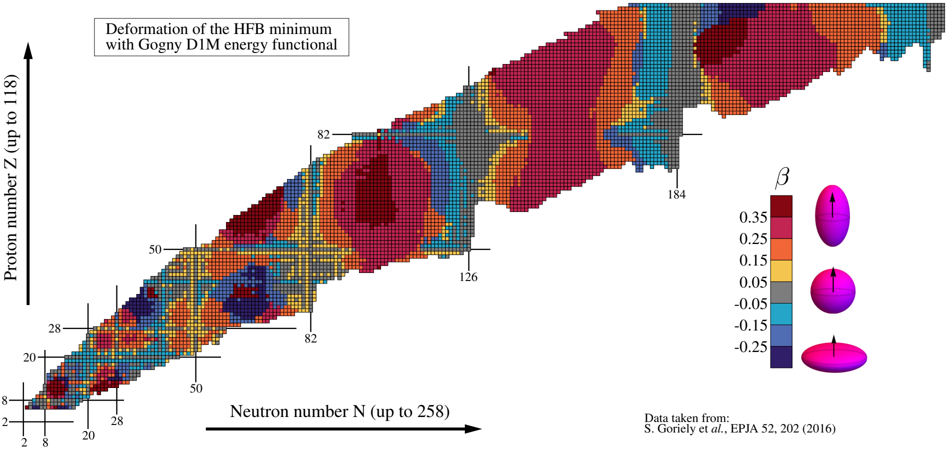
Deformation is (almost) ubiquitous



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Projected Generator Coordinate Method (PGCM)

- Solves HFB equations under a set of constraints $\langle \Phi(q) | Q | \Phi(q) \rangle = q$

  $\Rightarrow$ set of Bogoliubov reference states: $\{ |\Phi(q)\rangle, q \}$

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$$|\Theta_\epsilon^{\sigma M}\rangle = \sum_{qK} f_\epsilon^{\sigma M}(q, K) P_{MK}^\sigma |\Phi(q)\rangle \quad \text{where} \quad \sigma \equiv Z, N, J, \pi$$

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$$\delta \left(\frac{\langle \Theta^{\sigma M}_{\epsilon} | H | \Theta^{\sigma M}_{\epsilon} \rangle}{\langle \Theta^{\sigma M}_{\epsilon} | \Theta^{\sigma M}_{\epsilon} \rangle} \right) = 0$$

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- Pros and cons
  - Strong/static correlations
  - Respects the symmetries of H
  - Access to excited states and various observables
  - Gentle scaling
  - No weak/dynamical correlations
  - Not systematically improvable

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- "Preprocess" the Hamiltonian through IMSRG

$$H(0) \xrightarrow{\text{PGCM}} |\Theta_{\epsilon}^{\sigma M}(0)\rangle \xrightarrow{\text{IMSRG}} H(s) = U(s)H(0)U^{\dagger}(s) \xrightarrow{\text{PGCM}} |\Theta_{\epsilon}^{\sigma M}(s)\rangle$$

Application to $0\nu2\beta$ decay: Yao, Bally, Engel, Wirth, Rodríguez, Hergert, PRL 124, 232501 (2020)

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$\Rightarrow$ Perform perturbative expansion on top of $|\Theta_\epsilon^{\sigma M}(s)\rangle$

Frosini, Duguet, Ebran, Somà, EPJA 58, 62 (2022)

Frosini, Duguet, Ebran, Bally, Mongelli, Rodríguez, Roth, Somà, EPJA 58, 63 (2022)

Frosini, Duguet, Ebran, Bally, Hergert, Rodríguez, Roth, Yao, Somà, EPJA 58, 64 (2022)

Burton, Thom, J. Chem. Theory Comput. 16(4), 5586 (2020)

PGCM - Perturbation Theory (PT)

- Schrödinger equation

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such that

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$$|\Psi_\epsilon^{\sigma M}(s)\rangle = \Omega^{\text{PT}}_{[\sigma,\epsilon,H_1(s)]}|\Theta_\epsilon^{\sigma M}(s)\rangle$$

- Expression for the energy

$$E_\epsilon^\sigma = \frac{\langle\Theta_\epsilon^{\sigma M}(s)|H(s)|\Psi_\epsilon^{\sigma M}(s)\rangle}{\langle\Theta_\epsilon^{\sigma M}(s)|\Psi_\epsilon^{\sigma M}(s)\rangle} = \sum_{k=0}^{\infty} E_\epsilon^{\sigma (k)}(s)$$

Example of ^{20}Ne: description of the calculation

- χEFT Hamiltonian with NN and NNN interactions
  Hüther *et al.*, PLB 808, 135651 (2020)
  → NNN reduced to an effective NN
  Frosini *et al.*, EPJA 57, 151 (2021)

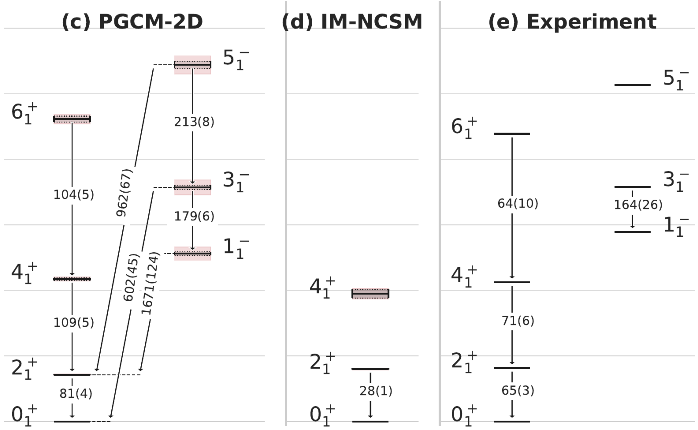
- Collective degrees of freedom explored: $\beta_{20}, \beta_{22}, \beta_{30}$

- Symmetry projections: Z, N, J, M, π

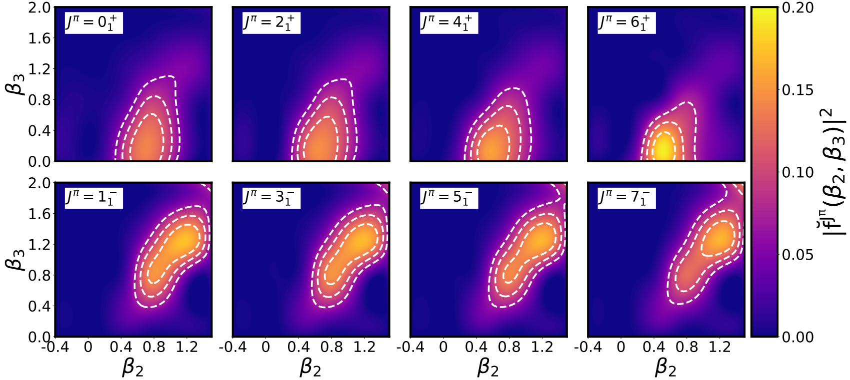
- Model space: SHO basis with $e_{\text{max}} = 10$ or $4, 6$ (PT calc.)

- Use PGCM-PT(2) which scales as $O(n^8)$

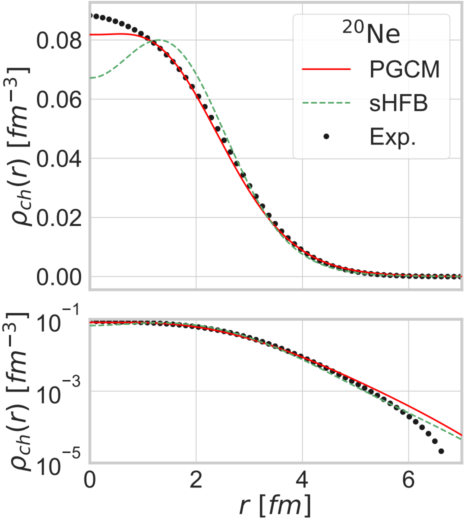
^{20}Ne: energy spectrum



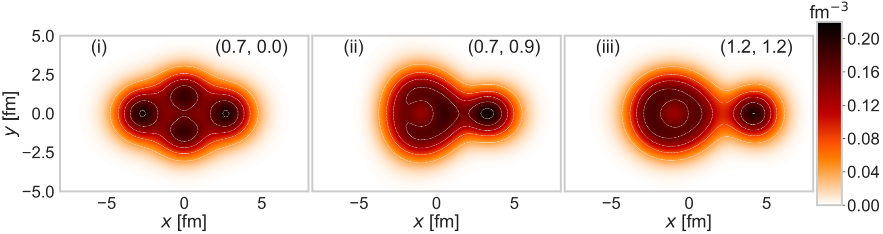
^{20}Ne: collective wave functions



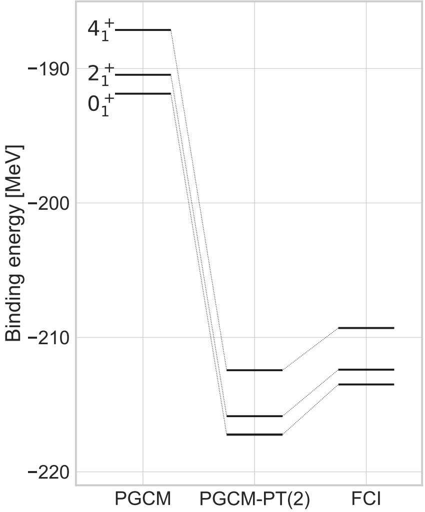
^{20}Ne: charge density



^{20}Ne: spatial one-body density



^{20}Ne: effects of PT(2) for $H(0)$



$e_{\text{max}} = 4$, only β_{20}

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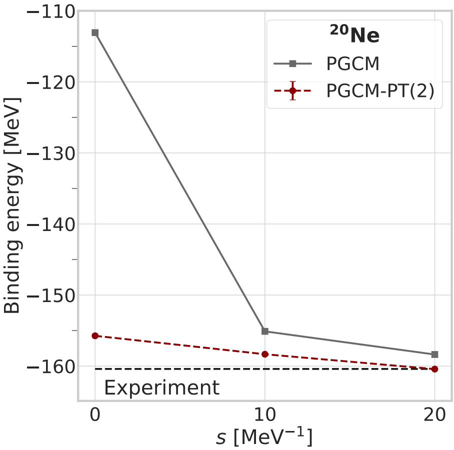

$e_{max} = 6$, only β_{20} (Triax: β_{20}, β_{22})

"Magic" interaction: Hebeler *et al.*, PRC 83, 031301 (2011)

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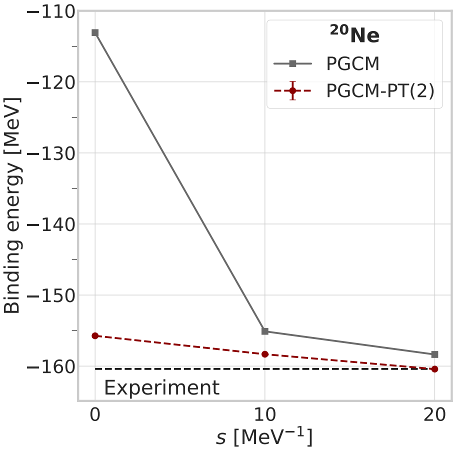

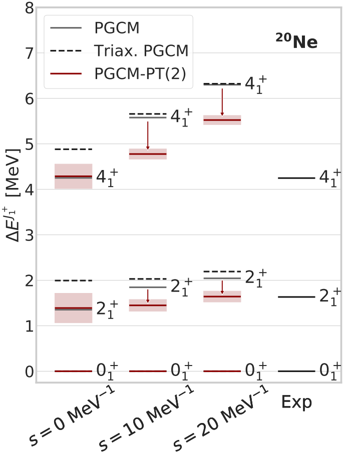

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Application: ultrarelativistic ion collisions

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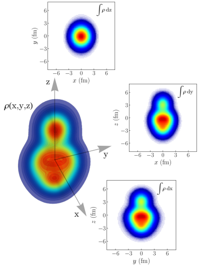
- Provide 1-body densities at PGCM average deformation

  In collaboration with:
  G. Giacalone (ITP Heidelberg)
  W. van der Schee (CERN)
  G. Nijs (MIT)



Bally *et al.* , in preparation (2023)

Conclusions

- PGCM formulated as a proper *ab initio* approach with many advantages
  - Strong/static correlations
  - Weak/dynamical correlations
  - Systematically improvable
  - Respects the symmetries of H
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- Learn how to efficiently distribute the correlations: $H(s)$ vs. PGCM vs. PT

Collaborators (*ab initio* PGCM)

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J. Engel