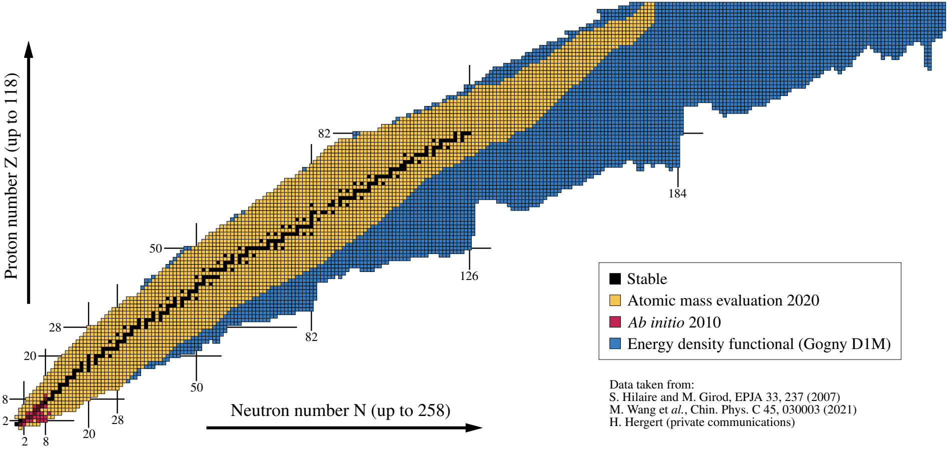
Ab initio Projected Generator Coordinate Method

Benjamin Bally

EMMI RRTF - Heidelberg - 02/06/2022

Progress in *ab initio* methods



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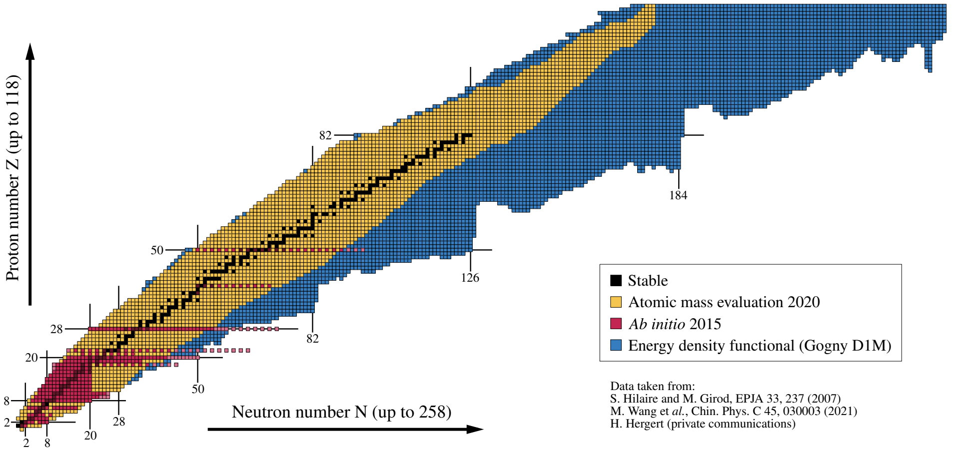

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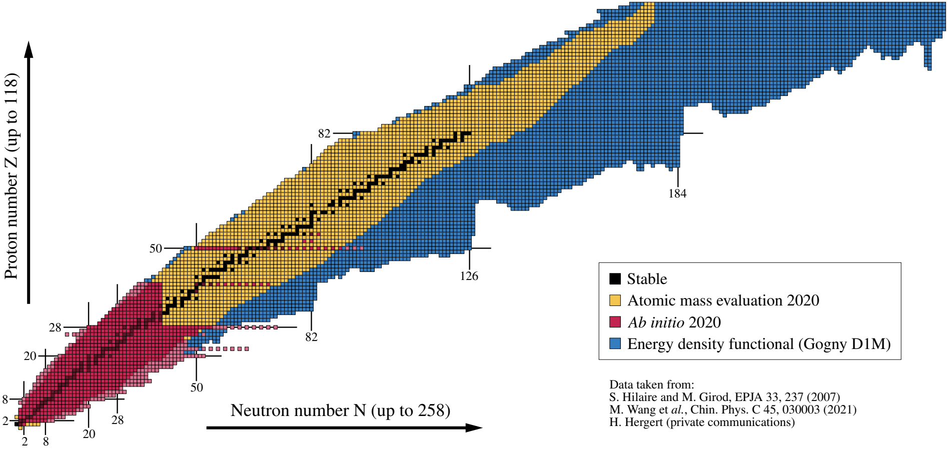

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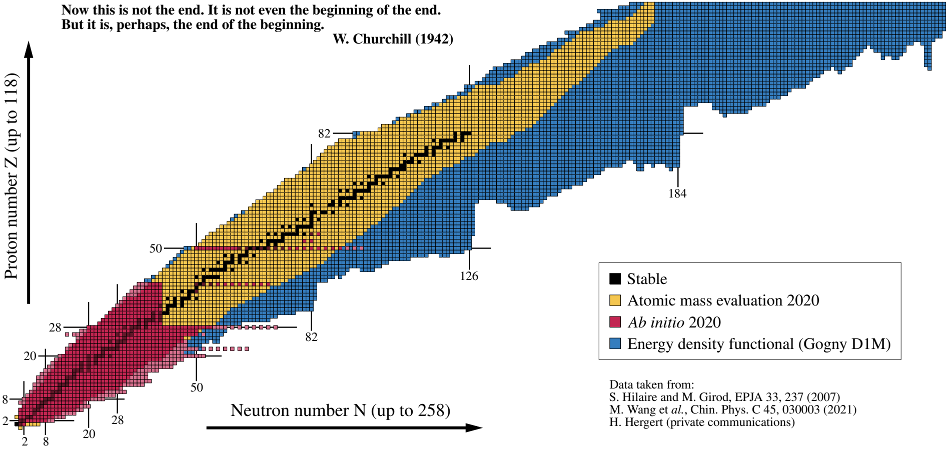
Now this is not the end. It is not even the beginning of the end.
But it is, perhaps, the end of the beginning.
W. Churchill (1942)



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  - Self-consistent Gorkov-Green's Functions
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  - Valence-Space In-Medium Similarity Renormalization Group
  - Projected Generator Coordinate Method + Perturbation Theory

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- Over the past decades: applications based on energy density functionals
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- Nowadays: new developments within the *ab initio* context
  - ◇ Use of chiral-EFT Hamiltonians

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- Allows one to deal with the diversity of emerging phenomena in nuclei

Symmetry group of nuclear Hamiltonian $\hat{H}$

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Rotational inv.	$SU(2)_A$	J, M_J
Parity inv.	Z_{2A}	π
Translational inv.	T_A^3	$\vec{P}$
Exchange of particles	$S_Z \times S_N$	-1, -1
Isospin	$SU(2)_A$	T, M_T

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- Eigenstates of $\hat{H}$ can be characterized: $|\Theta^{NZJM\pi}_{\epsilon}\rangle$

Symmetry-breaking solutions

- Mean-field calculations: $\delta \langle \Phi(q_i) | \hat{H} | \Phi(q_i) \rangle = 0$

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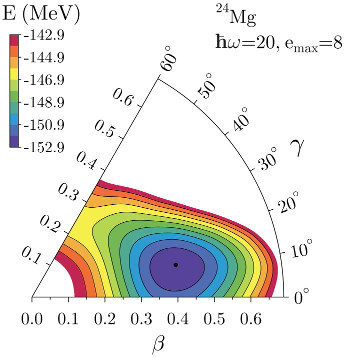
- Symmetry-unrestricted MF calculations favor "deformed" solutions
- Examples: pairing, quadrupole and octupole deformations, ...



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- Problem: deformed solutions break the symmetries of $\hat{H}$

$$|\Phi(q_i)\rangle = \sum_{NZJM\pi} \sum_{\epsilon} c_{\epsilon}^{NZJM\pi} |\Psi_{\epsilon}^{NZJM\pi}(q_i)\rangle$$

$\Rightarrow$ unphysical in nuclei

Symmetry dilemma

- “Symmetry dilemma” of Löwdin

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  - MF ansatz respects the symmetries of $\hat{H}$ but is variationally limited
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- Examples:

Physical symmetry	Group	Quant. numb.	Correlations
Particle-number inv.	$U(1)_Z \times U(1)_N$	N, Z	Pairing, Finite temp.
Rotational inv.	$SU(2)_A$	J, M_J	Deformation (any)
Parity inv.	Z_{2A}	π	Deformation (odd)
Translational inv.	T_A^3	$\vec{P}$	Localization
Isospin	$SU(2)_A$	T, M_T	Pairing n-p

Solution: restoring the symmetries

- Symmetry-breaking MF $\xrightarrow{\text{reference states}}$ Symmetry-restored BMF

  (BMF ≡ beyond mean field)

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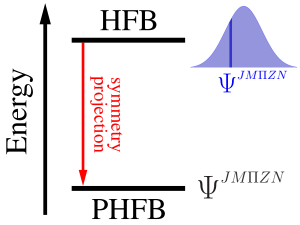
- Projected HFB

  Peierls and Yoccoz *et al.*, Proc. Phys. Soc. A 73, 381 (1957)

- Projected BCC & BMBPT

  Duguet *et al.*, JPG 42, 025107 (2015)

  Duguet and Signoracci *et al.*, JPG 44, 015103 (2017)



- Projection operators

$$\hat{P}^J_{MK} = \frac{2J+1}{16\pi^2} \int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \, \sin(\beta) \int_0^{4\pi} d\gamma \, D^{J}_{MK}{}^{*}(\alpha,\beta,\gamma) \, \hat{R}(\alpha,\beta,\gamma)$$

$$\hat{P}^{NZ} = \frac{1}{4\pi^2} \int_0^{2\pi} d\phi_N \int_0^{2\pi} d\phi_Z \, e^{i\phi_N(\hat{N}-N)} e^{i\phi_Z(\hat{Z}-Z)}$$

$$\hat{P}^{\pi} = \frac{1}{2}(1 + \pi\hat{\Pi})$$

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- Extraction of the components

$$\underbrace{\hat{P}^J_{MK} \hat{P}^{\pi} \hat{P}^{ZN}}_{\text{projection operators}} |\Phi(q_i)\rangle \xrightarrow{\text{projects}} \left\{ \sum_{\varepsilon} c^{NZJK\pi} |\Psi^{NZJM\pi}_{\varepsilon}(q_i)\rangle, K \right\} \xrightarrow{\text{diag. } \hat{H}} \left\{ |\Psi^{NZJM\pi}_{\varepsilon}(q_i)\rangle, \varepsilon \right\}$$

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- Projected states

$$|\Psi^{NZJM\pi}_{\varepsilon}(q_i)\rangle = \sum_K f^{NZJM\pi}_{\varepsilon K}(q_i)\, \hat{P}^J_{MK}\hat{P}^{\pi}\hat{P}^{ZN}|\Phi(q_i)\rangle$$

Symmetry projection: illustration

- Projection operator (angular momentum)

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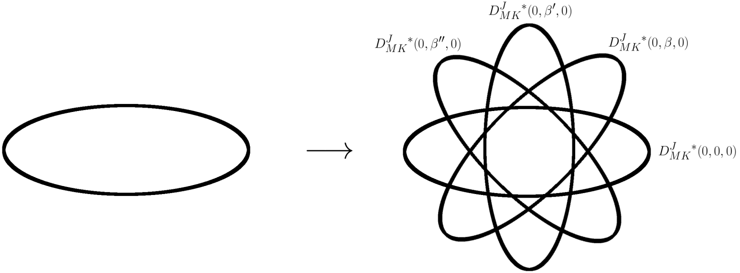
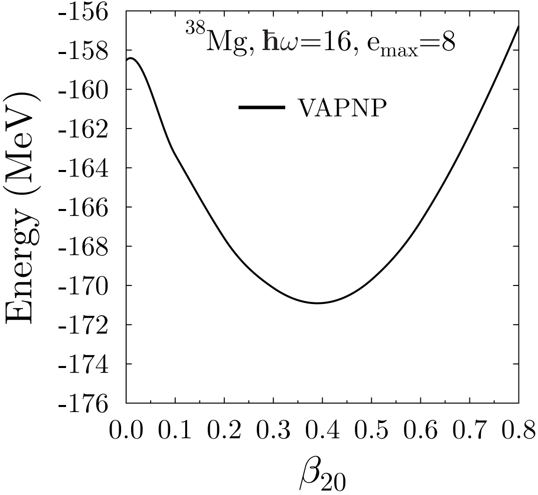


Symmetry projection: example with ^{38}Mg



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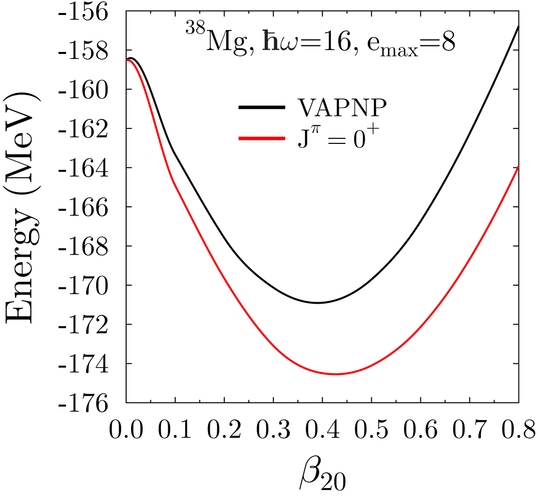

GCM: definition

- Trial wave function depends on continuous variables $q \equiv (p_1, \dots, p_m)$

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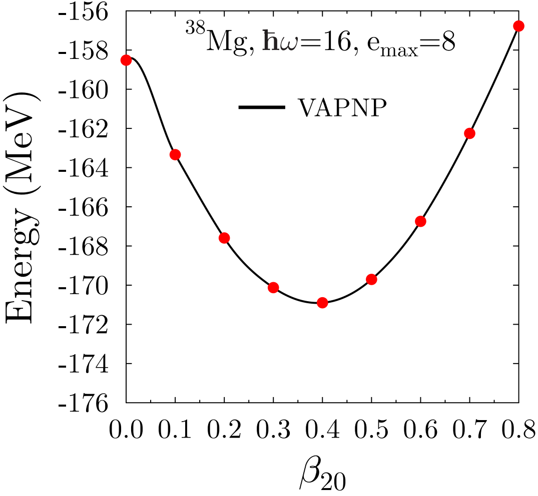
- It translates into solving the generalized eigenvalue problem (GEP)

$$Hf = ENf \quad \text{with} \quad \begin{aligned} H_{ij} &= \langle \Phi(q_i) | \hat{H} | \Phi(q_j) \rangle \\ N_{ij} &= \langle \Phi(q_i) | \Phi(q_j) \rangle \end{aligned}$$



^{38}Mg, ħω=16, e$_{max}$=8
VAPNP
Energy (MeV)
-156
-158
-160
-162
-164
-166
-168
-170
-172
-174
-176
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8
β_{20}

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- The closest we have are the so-called *collective wave functions*

$$Hf = ENf \Leftrightarrow \underbrace{N^{-1/2} H N^{-1/2}}_{\tilde{H}} \underbrace{N^{+1/2} f}_{g} = EN^{+1/2} f \Leftrightarrow \tilde{H} g = Eg$$

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$$g_\mu(q_i) = \sum_j N_{ij}^{1/2} f_\mu(q_j) \quad \text{with} \quad \sum_i g_\mu(q_i) g_{\mu'}(q_i) = \delta_{\mu\mu'}$$

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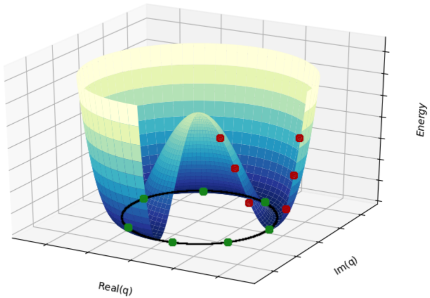
PGCM: unified picture

- Order parameter: $q = |q| e^{i \arg(q)}$



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- Example: quadrupole deformations

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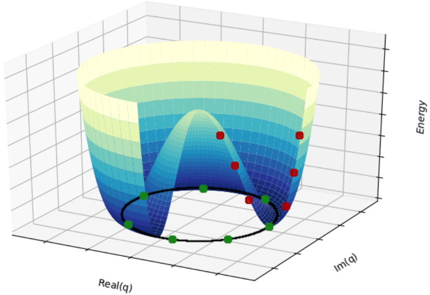
  $\arg(q) \equiv$ Euler angles (α, β, γ)



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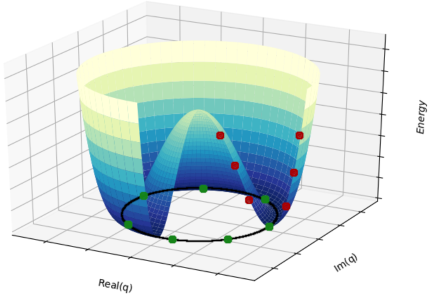

- General ansatz

$$|\Psi_{\mu}^{NZJM\pi}\rangle \equiv \sum_{|q_i|,K} \tilde{f}_{\mu}^{NZJM\pi}(|q_i|, K)\, \hat{P}^J_{MK}\, \hat{P}^{\pi}\, \hat{P}^{ZN} |\Phi(|q_i|)\rangle$$

Nuclear Hamiltonian

$$H = h^{(0)} + \sum_{ij} h^{(1)}_{ij} c^\dagger_i c_j + \frac{1}{(2!)^2} \sum_{ijkl} \overline{h}^{(2)}_{ijkl} c^\dagger_i c^\dagger_j c_l c_k + \frac{1}{(3!)^2} \sum_{ijklmn} \overline{h}^{(3)}_{ijklmn} c^\dagger_i c^\dagger_j c^\dagger_k c_n c_m c_l$$

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- "Full" Hamiltonian

$$\begin{aligned} h^{(0)} &= 0 \\ h^{(1)} &= T^{(1)} \\ \overline{h}^{(2)} &= V^{(2)} \\ \overline{h}^{(3)} &= W^{(3)} \end{aligned}$$

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- In-medium 2-body reduction

Frosini *et al.*, EPJA 58, 63 (2022)

$$\begin{aligned} h^{(0)} &= \frac{1}{3!} W^{(3)} \cdot \rho^{\otimes(3)} \\ h^{(1)} &= T^{(1)} - \frac{1}{2!} W^{(3)} \cdot \rho^{\otimes(2)} \\ \overline{h}^{(2)} &= V^{(2)} + W^{(3)} \cdot \rho \\ \overline{h}^{(3)} &= 0 \end{aligned}$$

- Error ¡ 3% excitation energies

Choice of basis: Spherical Harmonic Oscillator

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  with $m_{j_a} \in [\![-j_a, j_a]\!]$ and $m_{t_a} \in [\![-t_a, t_a]\!]$

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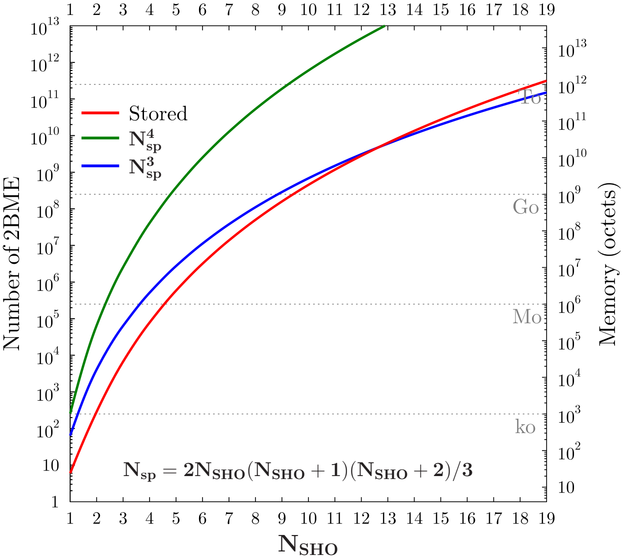
- Limit for three-particle states $|abc\rangle$: $\forall a, b, c,\ e_a + e_b + e_c \leq e_{3\text{max}} \underbrace{< 3e_{\text{max}}}_{\text{generally}}$

  $\Rightarrow$ not all elements $W_{abcdef} = \langle abc|W^{(3)}|def\rangle$ taken into account

Scaling of V_{ijkl} with the basis size

- 4 octets/matrix element

N_{SHO}	N_{sp}
1	4
2	16
3	40
4	80
5	140
6	224
7	336
8	480
9	660
10	880
11	1144
12	1456
13	1820
14	2240
15	2720
16	3264
17	3876
18	4560
19	5320



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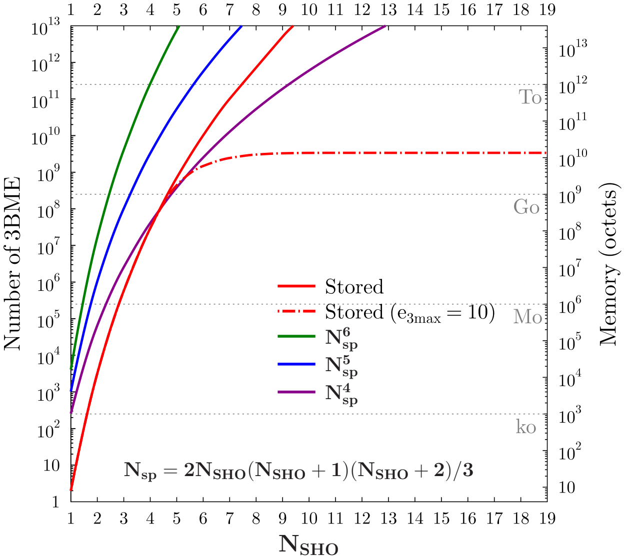


Example of ^{20}Ne: parameters of the calculation

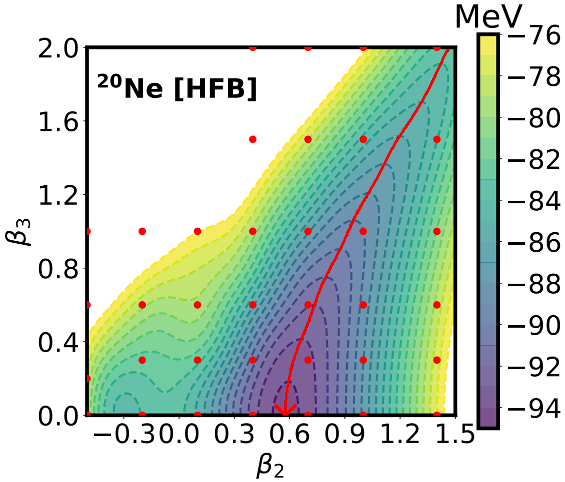
- Chiral-EFT Hamiltonian with NN and NNN interacations
  → NNN reduced to an effective NN
  Frosini *et al.*, EPJA 57, 151 (2021)

- Single-particle basis: spherical HO with $e_{max} = 10$, $e_{3max} = 14$

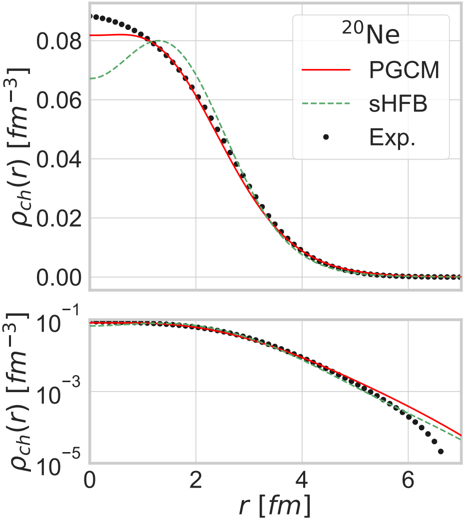
- Collective degrees of freedom explored: $\beta_{20}, \beta_{30}, (\beta_{22})$

- Publication: Frosini *et al.*, EPJA 58, 63 (2022)

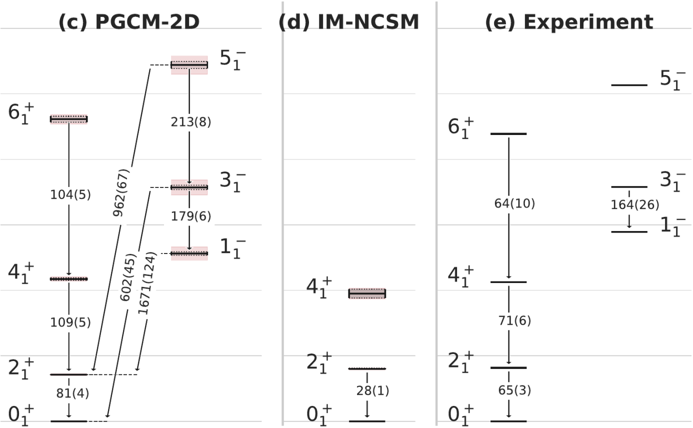
Example of ^{20}Ne: energy surface



Example of ^{20}Ne: charge density

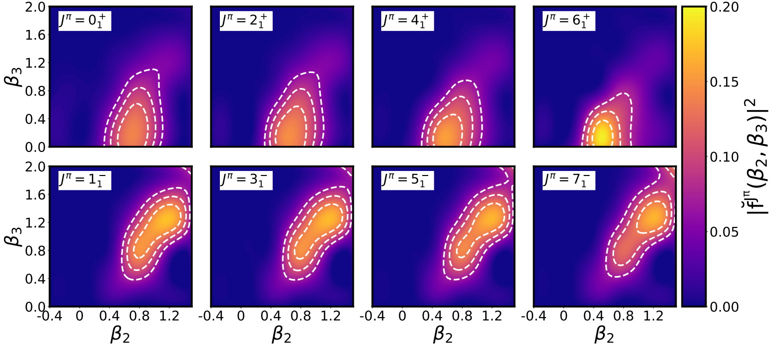


Example of ^{20}Ne: energy spectrum

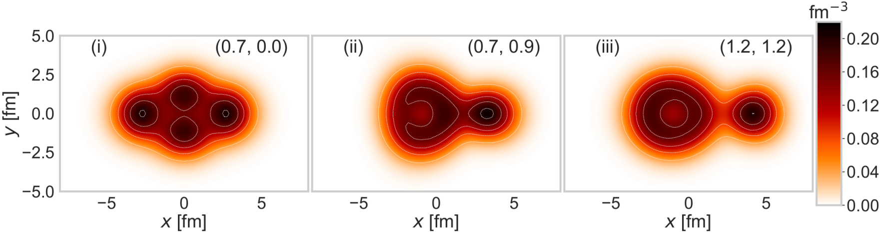


- PGCM-2D: β_{20}, β_{30}
- IM-NCSM: quasi-exact diagonalization

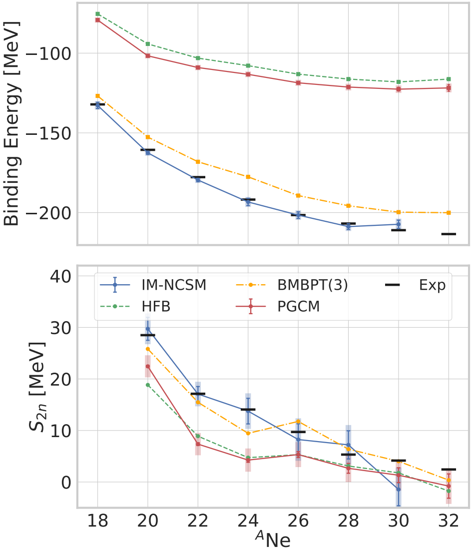
Example of ^{20}Ne: collective wave functions



Example of ^{20}Ne: spatial one-body density



Binding energies of Ne isotopes



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  Yao *et al.*, PRL 124, 232501 (2020)
- Include missing correlations on top of PGCM wave function
  $\rightarrow$ PGCM-PT
  Frosini *et al.*, EPJA 58, 62 (2022)
  Frosini *et al.*, EPJA 58, 63 (2022)
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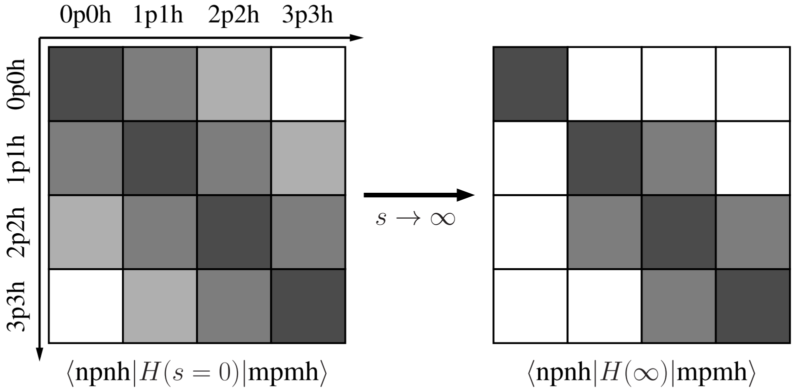
- Calculation of ^{96}Ru and ^{96}Zr
  - Possible at the mean-field level but challenging
  - Not impossible at the PGCM level but **very** challenging

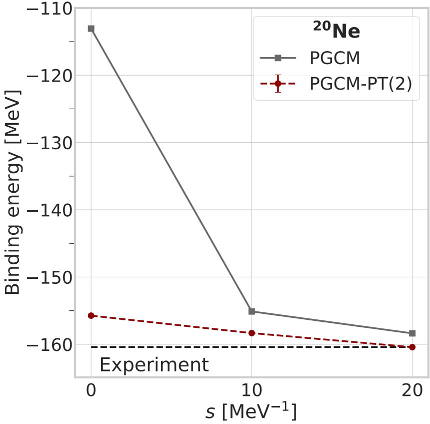
Additional slides

IMSRG: schematic illustration

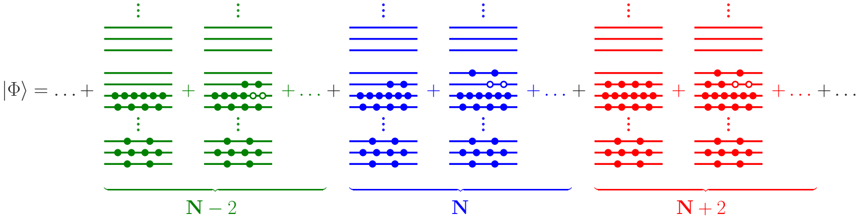
Adapted from H. Hergert



Effects of IMSRG/PT



$(e_{\text{max}} = 6, \hbar\omega = 16 \text{ MeV})$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