Specific computational aspects in nuclear physics

II. Symmetry-breaking calculations

Benjamin Bally

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Basic principles

- Static (or collective) correlations are important in nuclear structure

- Examples: pairing, quadrupole and octupole deformations, ...

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- Static (or collective) correlations are important in nuclear structure

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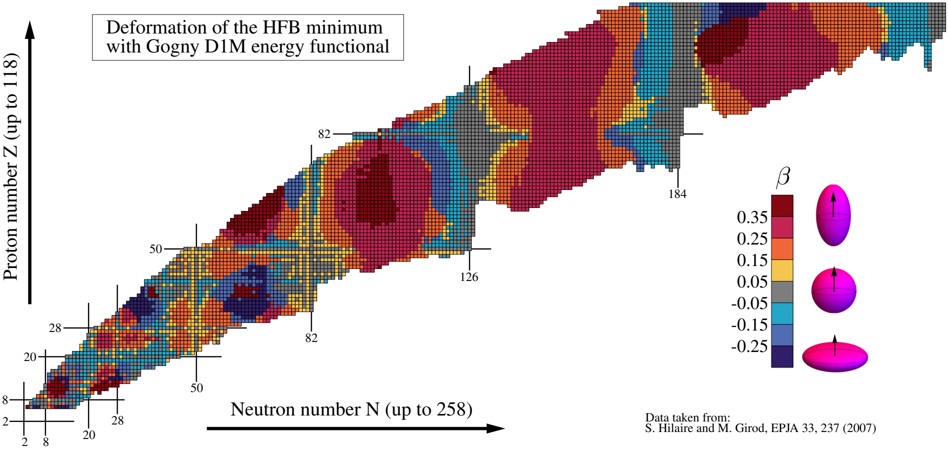
- In most cases, mean-field equations favor "deformed" solutions

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

  (MF ≡ mean field)

  (BMF ≡ beyond mean field)

Example: axial quadrupole deformation



Data taken from:
S. Hilaire and M. Girod, EPJA 33, 237 (2007)

- Problem: deformed solutions break the symmetries of H
  $\Rightarrow$ unphysical in nuclei (finite systems)

Symmetry dilemma

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- "Symmetry dilemma" of Löwdin
  P. Lykos and G. W. Pratt, Rev. Mod. Phys. 35 496 (1963)
  - MF ansatz respects the symmetries of H but is variationally limited
  - MF ansatz is variationally general but breaks the symmetries of H

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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

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Bogoliubov quasiparticle states I

- HFB theory ≡ merges HF and BCS theories into coherent MF framework

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Theory	Variational ansatz
HF	Slater determinants
HFB	Bogoliubov quasiparticle states

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Theory	Variational ansatz
HF	Slater determinants
HFB	Bogoliubov quasiparticle states

- Bogoliubov quasiparticle state $|\Phi\rangle$ defined as vacuum

$$\beta_k|\Phi\rangle = 0$$

for a set of quasiparticle operators $\left\{\beta_k ; \beta_k^\dagger\right\}$ defined as

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} c \\ c^\dagger \end{pmatrix} \equiv \mathcal{W}^\dagger \begin{pmatrix} c \\ c^\dagger \end{pmatrix}$$

with

$$\mathcal{W}\mathcal{W}^\dagger = \mathcal{W}^\dagger\mathcal{W} = 1_{2M} \quad \text{(ensures fermionic CAR)}$$

Bogoliubov quasiparticle states II

- Expanded form of the Bogoliubov transformations

$$\beta_k = \sum_i U^*_{ik} \, c_i + V^*_{ik} \, c^\dagger_i$$

$$\beta^\dagger_k = \sum_i U_{ik} \, c^\dagger_i + V_{ik} \, c_i$$

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- $|\Phi\rangle$ is fully characterzied by the one-body densities

$$\rho_{ij} = \frac{\langle\Phi|c^\dagger_j c_i|\Phi\rangle}{\langle\Phi|\Phi\rangle} = \left(V^* V^T\right)_{ij} \qquad \rho^\dagger = \rho$$
$$\kappa_{ij} = \frac{\langle\Phi|c_j c_i|\Phi\rangle}{\langle\Phi|\Phi\rangle} = \left(V^* U^T\right)_{ij} \qquad \kappa^T = -\kappa$$

Bogoliubov quasiparticle states III

- In its canonical basis $\left\{a_k ; a_k^\dagger\right\}$
  (basis that diagonalizes ρ and puts κ in its canonical form)

$$|\Phi\rangle = \prod_{i=1}^{n} a_i^\dagger \prod_{\substack{j\geq 0 \\ j\neq [\![1,n]\!]}} \left(u_j + v_j a_j^\dagger a_{\bar{j}}^\dagger\right)|0\rangle$$

with $u_j^2 + v_j^2 = 1$ and $\bar{j}$ partner of j.

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- Slater determinants are special cases of Bogoliubov quasiparticle states

  ◇ For occupied single-particle states, set $\begin{cases} u_j = 0 \\ v_j = 1 \end{cases}$

  ◇ For empty single-particle states, set $\begin{cases} u_j = 1 \\ v_j = 0 \end{cases}$

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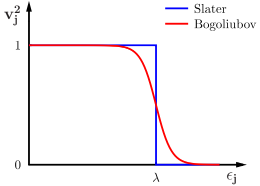

Bogoliubov quasiparticle states IV

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- Trivial example:

$$(u_1 + v_1 a^\dagger_1 a^\dagger_{\bar{1}})(u_2 + v_2 a^\dagger_2 a^\dagger_{\bar{2}})|0\rangle = u_1 u_2 |0\rangle + v_1 u_2 |1\bar{1}\rangle + u_1 v_2 |2\bar{2}\rangle + v_1 v_2 |1\bar{1}2\bar{2}\rangle$$

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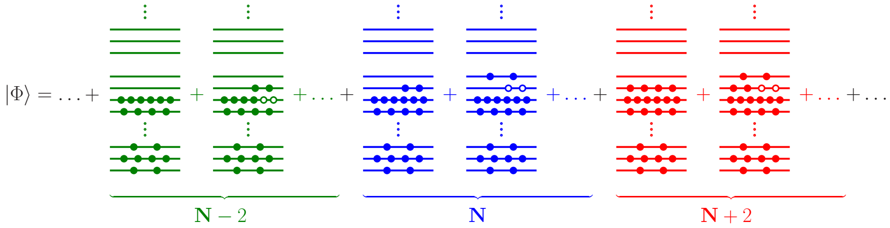
- More generally, we have the superposition



Bogoliubov quasiparticle states V

- Structure of U, V can be chosen to conserve specific symmetries

$$\beta_k = \sum_i U^*_{ik}\, c_i + V^*_{ik}\, c^\dagger_i$$
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$\Rightarrow$ construct U, V that do not mix the $\left\{c_k; c^\dagger_k\right\}$ with $\neq$ quantum numbers

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- Example: separation between protons and neutrons
  - first half: proton single-particle states
  - second half: neutron single-particle states

$$U = \begin{pmatrix} U_n & 0 \\ 0 & U_p \end{pmatrix} \qquad V = \begin{pmatrix} V_n & 0 \\ 0 & V_p \end{pmatrix}$$

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Hartree-Fock-Bogoliubov (HFB) I

- Minimization of the energy in the space of Bogoliubov quasiparticle states

$$\delta \frac{\langle \Phi | \Omega | \Phi \rangle}{\langle \Phi | \Phi \rangle} = 0$$

  where

$$\Omega = H - \lambda_N (N - N_0) - \lambda_Z (Z - Z_0)$$

- N: Neutron number (one-body) operator
  N_0: Number of neutrons in the nucleus
  λ_N: Lagrange multiplier determined such that $\langle \Phi | N | \Phi \rangle = N_0$
- Z: Proton number (one-body) operator
  Z_0: Number of protons in the nucleus
  λ_Z: Lagrange multiplier determined such that $\langle \Phi | Z | \Phi \rangle = Z_0$

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- Z: Proton number (one-body) operator
  Z_0: Number of protons in the nucleus
  λ_Z: Lagrange multiplier determined such that $\langle \Phi | Z | \Phi \rangle = Z_0$
- O_k: additional constraint operator
  O_{0k}: desired average value
  λ_{O_k}: Lagrange multiplier determined such that $\langle \Phi | O_k | \Phi \rangle = O_{0k}$

Hartree-Fock-Bogoliubov (HFB) II

- Let us consider an effective H up to two-body operators

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

- Be careful, if effective: $h^{(0)} \neq 0$, $h^{(1)} \neq T$, $h^{(2)} \neq V$

- They can integrate effects of three-body interaction (nucleus dependent)
  - ◇ Normal-order two-body approximation ⇒ *see Thomas' talk*

    R. Roth *et al.*, Phys. Rev. Lett. 109, 052501 (2012)
  - ◇ In-medium k-body reduction

    M. Frosini, T. Duguet, B. Bally, J.-P. Ebran and V. Somà, to be submitted (2021)

Hartree-Fock-Bogoliubov (HFB) III

- Normal ordering of H with respect to $|\Phi\rangle$

$$
\begin{aligned}
H = H^{00} & \\
&+ \frac{1}{1!}\sum_{k_1 k_2} H^{11}_{k_1 k_2}\beta^\dagger_{k_1}\beta_{k_2} + \frac{1}{2!}\sum_{k_1 k_2}\left\{H^{20}_{k_1 k_2}\beta^\dagger_{k_1}\beta^\dagger_{k_2} + H^{02}_{k_1 k_2}\beta_{k_2}\beta_{k_1}\right\} \\
&+ \frac{1}{(2!)^2}\sum_{k_1 k_2 k_3 k_4} H^{22}_{k_1 k_2 k_3 k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta_{k_4}\beta_{k_3} \\
&+ \frac{1}{3!}\sum_{k_1 k_2 k_3 k_4}\left\{H^{31}_{k_1 k_2 k_3 k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta^\dagger_{k_3}\beta_{k_4} + H^{13}_{k_1 k_2 k_3 k_4}\beta^\dagger_{k_1}\beta_{k_4}\beta_{k_3}\beta_{k_2}\right\} \\
&+ \frac{1}{4!}\sum_{k_1 k_2 k_3 k_4}\left\{H^{40}_{k_1 k_2 k_3 k_4}\beta^\dagger_{k_1}\beta^\dagger_{k_2}\beta^\dagger_{k_3}\beta^\dagger_{k_4} + H^{04}_{k_1 k_2 k_3 k_4}\beta_{k_4}\beta_{k_3}\beta_{k_2}\beta_{k_1}\right\}
\end{aligned}
$$

- Natural NO in Bogoliubov CC (BCC) or Bogoliubov MBPT (BMBPT)

A. Tichai, R. Roth and T. Duguet, Frontiers in Physics 8 164 (2020)

P. Arthuis, PhD Thesis, Université Paris-Saclay (2018)

Hartree-Fock-Bogoliubov (HFB) IV

- $\delta\langle\Omega\rangle = 0 \Rightarrow$ solving the HFB equations

$$\begin{pmatrix} (h^{(1)} + \Gamma - \lambda) & \Delta \\ -\Delta^* & -(h^{(1)} + \Gamma - \lambda)^* \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}_k = E_k \begin{pmatrix} U \\ V \end{pmatrix}_k$$

where we used the fields

$$\Gamma_{ij} = \sum_{kl} h^{(2)}_{ikjl} \rho_{lk} \qquad \Gamma^\dagger = \Gamma$$

$$\Delta ij = \frac{1}{2} \sum_{kl} h^{(2)}_{ijkl} \kappa_{kl} \qquad \Delta^T = -\Delta$$

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- Energy: $E_{\mathrm{HFB}} = h^{(0)} + \mathrm{Tr}\left(h^{(1)}\rho\right) + \frac{1}{2}\,\mathrm{Tr}\left(\Gamma\rho - \Delta\kappa^*\right)$

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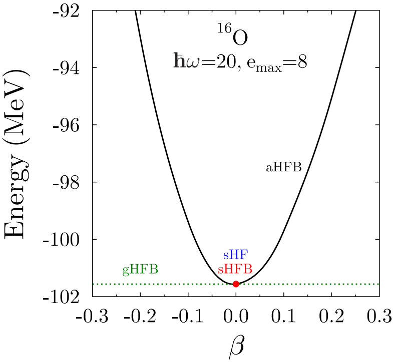
Only part where $h^{(2)}$ is needed

If $h^{(2)}$ large $\rightarrow$ parallelization

- Energy: $E_{\text{HFB}} = h^{(0)} + \text{Tr}\left(h^{(1)}\rho\right) + \frac{1}{2}\,\text{Tr}\left(\Gamma\rho - \Delta\kappa^*\right)$
- Self-consistent problem
  - HFB eq. $\xrightarrow{\text{depend}} \Gamma, \Delta \xrightarrow{\text{depend}} \rho, \kappa \xrightarrow{\text{depend}} U, V$
  - Solved iteratively
  - Diagon. HFB equations or gradient method: $\delta\langle\Omega\rangle = 0 \Rightarrow H^{20} = H^{02} = 0$

Example: $^{16}_{8}$O (doubly closed shell)



E_{exp} = -127.619296(0) MeV

	Symmetries	Constraints	Minimum (MeV)
spherical HF	$J = 0$, Z, N, Π, $\mathcal{T}$, $\mathbb{R}$		-101.6
spherical HFB	$J = 0$, Π, $\mathcal{T}$, $\mathbb{R}$	Z, N	-101.6
axial HFB	$M_J = 0$, Π, $\mathcal{T}$, $\mathbb{R}$	Z, N, β	-101.6
(real) general HFB	$\mathbb{R}$	Z, N	-101.6

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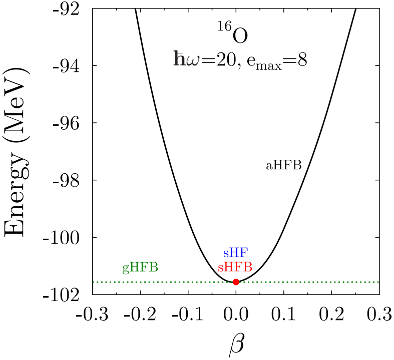

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SCGF ADC(3)	Somà et al. PRC 101 014318 (2020)		-130.81
			-127.27

Example: $^{24}_{12}$Mg (doubly open shell)

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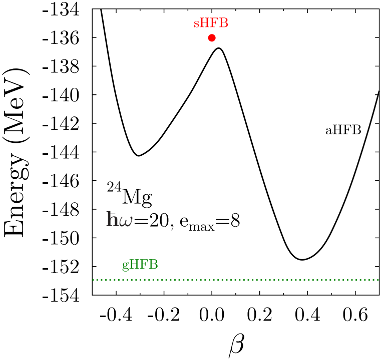

E_{exp} = -198.257016(24) MeV

	Symmetries	Constraints	Minimum (MeV)
spherical HFB	$J = 0$, Π, $\mathcal{T}$, $\mathbb{R}$	Z, N	-136.0
axial HFB	$M_J = 0$, Π, $\mathcal{T}$, $\mathbb{R}$	Z, N, β	-151.5

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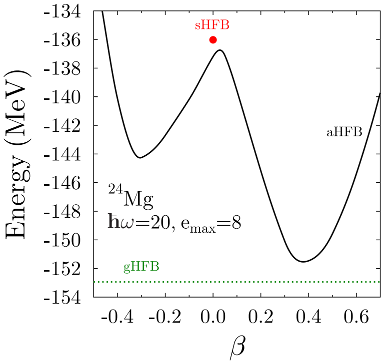

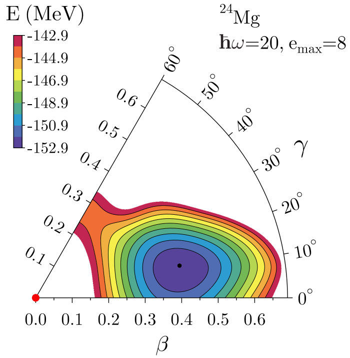

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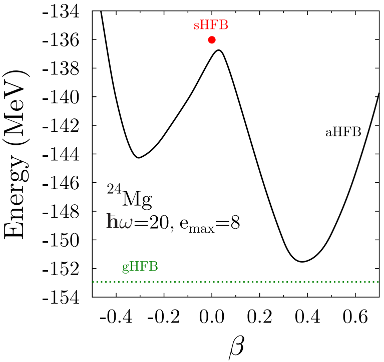

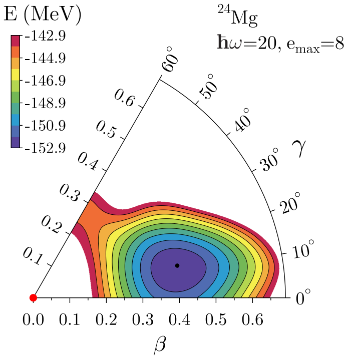

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Choice of basis: Spherical Harmonic Oscillator

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- SHO basis: $|a\rangle \equiv |n_a, l_a, s_a = \frac{1}{2}, j_a, m_{j_a}, t_a = \frac{1}{2}, m_{t_a}\rangle$ $\Rightarrow$ *see Alexander's talk I*

$$|\hat{a}\rangle \equiv \{|a\rangle, \forall\, m_{j_a} \in [\![-j_a, j_a]\!]\} \qquad \text{(multiplet)}$$

- Advantages:
  - Textbook $\Rightarrow$ easy to code and benchmark
  - Commonly used $\Rightarrow$ compare to other solvers, interactions available
  - Flexible $\Rightarrow$ symmetry-restricted and unrestricted calculations

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- Need to uncouple the J-scheme matrix elements to m-scheme

$$V_{abcd} = \sum_{JM_J} \left[\mathcal{N}_{\hat{a}\hat{b}}(J)\mathcal{N}_{\hat{c}\hat{d}}(J)\right]^{-1} (j_a m_{j_a} j_b m_{j_b} | JM_J)(j_c m_{j_c} j_d m_{j_d} | JM_J)\, V^J_{\hat{a}\hat{b}\hat{c}\hat{d}}$$

where

$$\mathcal{N}_{\hat{a}\hat{b}}(J) = \frac{\sqrt{1 + \delta_{\hat{a}\hat{b}}(-1)^J}}{1 + \delta_{\hat{a}\hat{b}}}$$

Choice of basis: Spherical Harmonic Oscillator II

- Need to uncouple the *J*-scheme matrix elements to *m*-scheme

$$V_{abcd} = \sum_{JM_J} \left[\mathcal{N}_{\hat{a}\hat{b}}(J)\mathcal{N}_{\hat{c}\hat{d}}(J)\right]^{-1} (j_a m_{j_a} j_b m_{j_b}|JM_J)(j_c m_{j_c} j_d m_{j_d}|JM_J)\, V^J_{\hat{a}\hat{b}\hat{c}\hat{d}}$$

- Different approaches are possible

Strategy	Storage	Limit
On the fly	$V^J_{\hat{a}\hat{b}\hat{c}\hat{d}}$	CPU
Mixed	$V^J_{\hat{a}\hat{b}\hat{c}\hat{d}}$ + interm. info	Mixed
Storage	V_{abcd}	Memory
Factorization	$\Rightarrow$ *see Alexander's talk II*	

Symmetry reductions of V_{abcd}

- Symmetries of H and SHO basis $\Rightarrow$ reduce the CPU time & storage

Symmetry reductions of V_{abcd}

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- V_{abcd} is non-zero only if

$$[H,\Pi] = 0 \quad \Rightarrow \quad (-1)^{\ell_a+\ell_b} = (-1)^{\ell_c+\ell_d} \tag{1}$$

$$[H,J_z] = 0 \quad \Rightarrow \quad m_{j_a} + m_{j_b} = m_{j_c} + m_{j_d} \tag{2}$$

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[H,T_z] = 0 \quad &\Rightarrow \quad m_{t_a} + m_{t_b} = m_{t_c} + m_{t_d} && (3)
\end{aligned}
$$

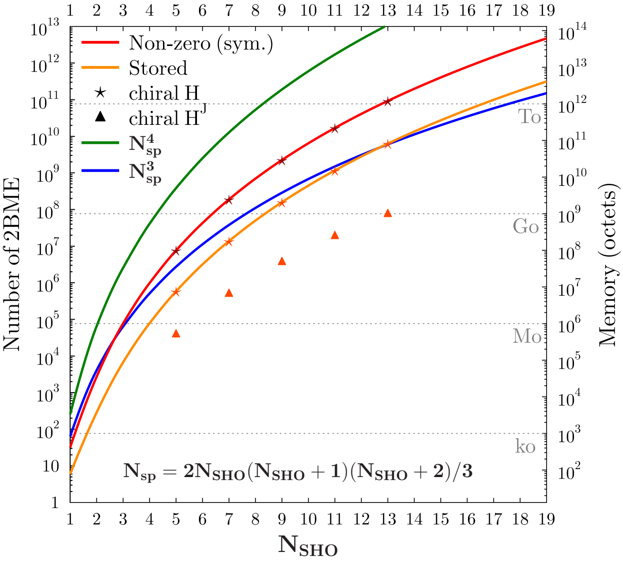
- V_{abcd} has the exchange symmetries

$$
\begin{aligned}
H \in \mathbb{R} \quad &\Rightarrow \quad V_{abcd} = V^*_{abcd} && (4)\\
H^\dagger = H + (1) \quad &\Rightarrow \quad V_{abcd} = V_{cdab} && (5)\\
\text{Fermions} \quad &\Rightarrow \quad V_{abcd} = -V_{bacd} = -V_{abdc} = V_{badc} && (6)\\
(5)+(6) \quad &\Rightarrow \quad V_{abcd} = -V_{bacd} = -V_{abdc} = V_{badc} && (7)\\
&\qquad\qquad\;\; = -V_{cdba} = -V_{dcab} = V_{dcba} &&\\
&\qquad\qquad\;\; = V_{cdab} &&\\
[H,\mathcal{T}] = 0 + (1) \quad &\Rightarrow \quad V_{abcd} = (-1)^{j_a+j_b+j_c+j_d} V_{-a-b-c-d} && (8)
\end{aligned}
$$

Scaling of V_{abcd} with the basis size

- (1-3): green → red ~ CPU
- (4-8): red → orange ~ Memory
- 13 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



Symmetry reductions of W_{abcdef}

- Symmetries of H and SHO basis $\Rightarrow$ reduce the CPU time & storage
- W_{abcdef} is non-zero only if

$$
\begin{aligned}
[H, \Pi] = 0 \quad &\Rightarrow \quad (-1)^{\ell_a+\ell_b+\ell_c} = (-1)^{\ell_d+\ell_e+\ell_f} && (9) \\
[H, J_z] = 0 \quad &\Rightarrow \quad m_{j_a} + m_{j_b} + m_{j_c} = m_{j_d} + m_{j_e} + m_{j_f} && (10) \\
[H, T_z] = 0 \quad &\Rightarrow \quad m_{t_a} + m_{t_b} + m_{t_c} = m_{t_d} + m_{t_e} + m_{t_f} && (11)
\end{aligned}
$$

- W_{abcdef} has the exchange symmetries

$$
\begin{aligned}
H \in \mathbb{R} \quad &\Rightarrow \quad W_{abcdef} = W^*_{abcdef} && (12) \\
H^\dagger = H + (12) \quad &\Rightarrow \quad W_{abcdef} = W_{defabc} && (13) \\
\text{Fermions} \quad &\Rightarrow \quad W_{abcdef} = -W_{bacdef} = \dots \ \text{[36 possiblities]} && (14) \\
(13) + (14) \quad &\Rightarrow \quad W_{abcdef} = \dots \ \text{[72 possiblities]} && (15) \\
[H, \mathcal{T}] = 0 + (12) \quad &\Rightarrow \quad W_{abcd} = (-1)^{j_a+j_b+j_c-j_d-j_e-j_f} W_{-a-b-c-d-e-f} && (16)
\end{aligned}
$$

Reduction through $e_{3\max}$

- Principal quantum number: $e_a = 2n_a + l_a$ $\Rightarrow$ *see Alexander's talk I*

- Limit for single-particle states $|a\rangle$: $\forall a,\ e_a \leq e_{\max}$

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- Limit for two-particle states $|ab\rangle$: $\forall a, b,\ e_a + e_b \leq e_{2\max} \underbrace{= 2e_{\max}}_{\text{generally}}$

  $\Rightarrow$ all elements V_{abcd} taken into account

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  $\Rightarrow$ all elements V_{abcd} taken into account

- 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} taken into account

Scaling of W_{abcdef} with the basis size

- (9-11): green → red ~ CPU
- (12-16): red → orange ~ Memory
- 17 octets/matrix element

N_{SHO}	N_{sp}
1	4
2	16
3	40
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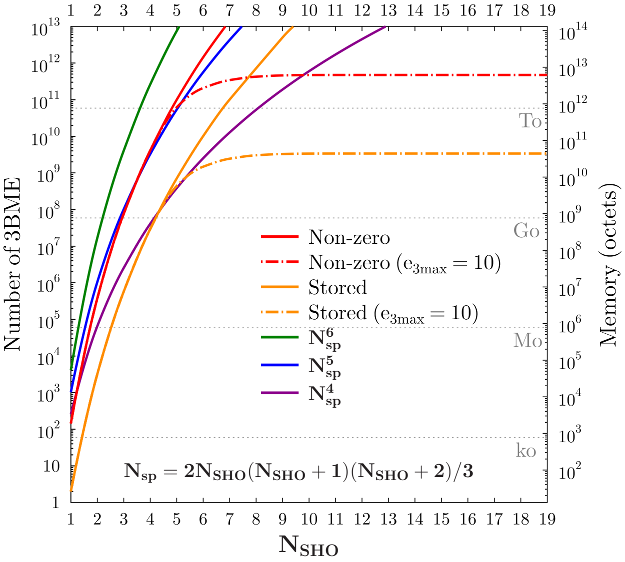

Table of contents

Basic principles

- Symmetry-breaking MF useful but better to restore the symmetries of H
  - Eigenstates of H have good quantum numbers
  - Selection rules for transitions (e.g. electromagnetic)
  - Some correlations are missing

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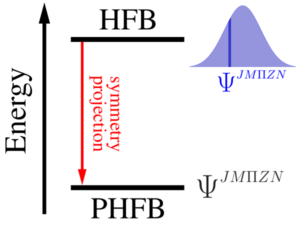
- Symmetry-breaking MF useful but better to restore the symmetries of H
  - Eigenstates of H have good quantum numbers
  - Selection rules for transitions (e.g. electromagnetic)
  - Some correlations are missing

- Symmetry-projected HFB

  B. Bally and M. Bender, arXiv:2010.15224 (2020)/PRC (2021)

  - Obtain symmetry-adapted states (with good quantum numbers)
  - Gain correlation energy (usually)



Symmetry group of H

Definition

Let G be a group with a unitary representation $R(g)$.

$$\forall\, g \in G,\ \left[R(g), H\right] = 0$$

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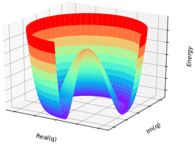
- Consequence: all "rotated" states have same energy

$$\begin{aligned}\langle \Phi(g) | H | \Phi(g) \rangle &\equiv \langle \Phi | R^\dagger(g) H R(g) | \Phi \rangle \\ &= \langle \Phi | H | \Phi \rangle\end{aligned}$$



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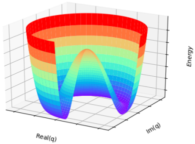

- Consider the vector space

$$\mathrm{span}(G|\Phi\rangle) \equiv \left[\begin{array}{ll} \left\{\sum_G f(g)|\Phi(g)\rangle,\ f(g) \in \mathbb{C}\right\} & \text{(if } G \text{ finite)} \\ \left\{\int_G dv_G(g)\, f(g)|\Phi(g)\rangle,\ f \in L^2(G)\right\} & \text{(if } G \text{ Lie group)} \end{array}\right.$$

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Diagonalization of H in $\mathrm{span}(G_{\mathrm{tot}}|\Phi\rangle)$

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- Decomposition in $\text{span}(G_{\text{tot}}|\Phi\rangle)$

$$|\Phi\rangle = \sum_{JK\Pi ZN} \sum_{\varepsilon} c^{JK\Pi ZN} |\Psi_{\varepsilon}^{JK\Pi ZN}\rangle$$

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- Decomposition in span($G_{\text{tot}}|\Phi\rangle$)

$$|\Phi\rangle = \sum_{JK\Pi ZN} \sum_{\varepsilon} c^{JK\Pi ZN} |\Psi_{\varepsilon}^{JK\Pi ZN}\rangle$$

- Extraction of the components

$$\underbrace{P^J_{MK} P^{\Pi} P^{ZN}}_{\substack{\text{projection}\\ \text{operators}}} |\Phi\rangle \xrightarrow{\text{projects}} \left\{ \sum_{\varepsilon} c^{JK\Pi ZN} |\Psi_{\varepsilon}^{JM\Pi ZN}\rangle, K \right\} \xrightarrow{\text{diag. } H} |\Psi_{\varepsilon}^{JM\Pi ZN}\rangle$$

Symmetry projection: scaling

- Nice but all projection operators involve sums or integrals

$$\langle\Phi|HP^J_{MK}P^\Pi P^{ZN}|\Phi\rangle = \frac{2J+1}{16\pi^2}\underbrace{\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin(\beta) \int_0^{4\pi} d\gamma}_{\text{discret.} \sim 10^{4-5} \text{ points}} D^{J*}_{MK}(\alpha,\beta,\gamma)\ \frac{1}{2}\underbrace{\sum_{p=1,\Pi}}_{2}\pi(p)$$

$$\frac{1}{4\pi^2}\underbrace{\int_0^{2\pi} d\varphi_Z \int_0^{2\pi} d\varphi_N}_{\text{discret.} \sim 10^2 \text{ points}} e^{-i\varphi_Z Z} e^{-i\varphi_N N}\ \underbrace{\langle\Phi|HR(\alpha,\beta,\gamma,p,\varphi_Z,\varphi_N)|\Phi\rangle}_{\sim \mathrm{N}_{\mathrm{sp}}^{3,3}}$$

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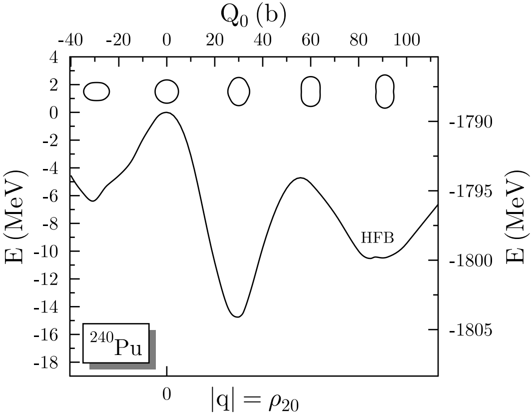
- Scaling: $\sim 10^{6-7}\,\mathrm{N}_{\mathrm{sp}}^{3,3}$

- Fortunately, this is an embarassingly parallel problem

Example: 0^+ state for axially deformed ^{240}Pu



Courtesy of M. Bender

M. Bender, P.-H. Heenen, and P. Bonche, Phys. Rev. C 70, 054304 (2004)

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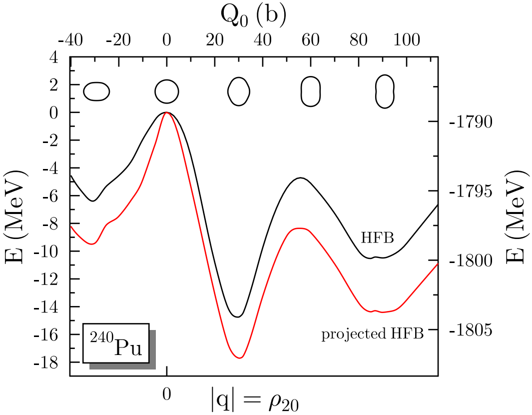

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Better schemes based on projection

- Variation After Projection (VAP): minimizes the projected energy

$$\underbrace{\delta \frac{\langle \Phi | \Omega | \Phi \rangle}{\langle \Phi | \Phi \rangle} = 0}_{\text{HFB}} \quad \longrightarrow \quad \underbrace{\delta \frac{\langle \Phi | \Omega P^S | \Phi \rangle}{\langle \Phi | P^S | \Phi \rangle} = 0}_{\text{VAP}}$$

$\Rightarrow$ but very costly! (can still be done for $S \equiv N, Z, P$)

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- Projected Generator Coordinate Method (PGCM)
  - Build set of reference states

$$\{ |\Phi(q)\rangle, q \} \longrightarrow \{ |\Psi_\varepsilon^{JM\Pi ZN}(q)\rangle, q \}_{JM\Pi ZN}$$

  - Diagonalize H among the projected states (not orthogonal $\Rightarrow$ generalized eigenvalue problem)
  - Final wave function

$$|\Theta_\xi^{JM\Pi ZN}\rangle = \sum_q f_{\xi\varepsilon}^{JM\Pi ZN}(q) |\Psi_\varepsilon^{JM\Pi ZN}(q)\rangle$$

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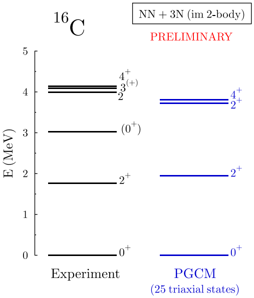

New approaches in *ab initio* nuclear physics

- Development of new approaches that combine
  - symmetry breaking & restoration → includes static correlations
  - expansion scheme → includes dynamic correlations

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- Multi-Reference In-Medium Similarity Renormalization Group (MR-IMSRG)

  H. Hergert, Phys. Scr. 92 023002 (2017)

  J. M. Yao, B. Bally, J. Engel, R. Wirth, T. R. Rodríguez, and H. Hergert, Phys. Rev. Lett. 124, 232501 (2020)

- Projected Bogoliubov Many-Body Perturbation Theory (PBMBPT)

  T. Duguet, J. Phys. G 42 025107 (2015)

  T. Duguet and A. Signoracci, J. Phys. G 44 015103 (2017)

  P. Arthuis, A. Tichai, J. Ripoche and T. Duguet, Comp. Phy. Comm. 261 (2021)

- Projected Bogoliubov Coupled Cluster (PBCC)

  see T. Duguet et al. above

  Y. Qiu, T. Henderson, J. Zhao and G. Scuseria, J. Chem. Phys. 149 164108 (2018)

  Y. Qiu, T. Henderson, T. Duguet and G. Scuseria, Phys. Rev. C 99 044301 (2019)