Symmetries in many-body methods

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2èmes Rencontres PhyNuBE - Aussois - 29/03/2023

Outline of the presentation

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1. Symmetries of the nuclear Hamiltonian
2. Symmetry-conserving schemes
3. Symmetry-guided schemes
4. Symmetry-breaking and -restoration schemes
5. Summary

- Physical symmetry G $\Leftrightarrow$ mathematical group G
  - $G \equiv (\{g\}, \cdot)$, $g_1 \cdot g_2 \in \{g\}$
  - In the Hilbert space $g \xrightarrow{\text{repres.}} R(g)$ (rotation operator)

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Definition

Let H be the Hamiltonian of a system and G a group with unitary representation $R(g)$

If $\forall g \in G$, $R(g) H R^{-1}(g) = H \Rightarrow$ G is a symmetry group of H

(equivalently: $\forall g \in G$, $[H, R(g)] = 0$)

Consequences: quantum numbers and selection rules

- Irreducible represenstations (irreps) of $G \Rightarrow$ good quantum numbers

- Let $|\Psi_\epsilon\rangle$ be an eigenstate of H and λ an irrep of G with dimension d_λ

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- Selection rules for matrix elements of tensor operators

$$\langle\Psi_{\epsilon_1}^{\lambda_1\mu_1}|T^{\lambda_2\mu_2}|\Psi_{\epsilon_3}^{\lambda_3\mu_3}\rangle = \dots$$

Symmetry group of the nuclear Hamiltonian

- In non-relativistic QM, H is invariant under
  - Space-time Galilean transformations
  - Fock-space transformations
  - Exchange of identical particles

- $G \equiv \text{SGal}(3)_A \times U(1)_Z \times U(1)_N \times S_Z \times S_N$

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- For example:

Physical symmetry	Group	Quant. numb.
Fock-space rotations	$U(1)_Z \times U(1)_N$	Z, N
Spatial rotations	$SU(2)_A$	J, M_J
Parity	Z_{2A}	π
Spatial translations	$\mathbb{R}^3_{tA}$	$\vec{P}$
Exchange of particles	$S_Z \times S_N$	-1, -1

Consequences: example of multipole operators

- Expectation value for $T^{\lambda\mu} \equiv Q_{\lambda\mu} = r^{\lambda} Y_{\lambda\mu}(\theta,\phi)$ with $\lambda \in \mathbb{N}$ and $\mu \in [\![-\lambda,\lambda]\!]$

$$\langle \Psi_{\epsilon}^{ZNJM_J\pi} | Q_{\lambda\mu} | \Psi_{\epsilon}^{ZNJM_J\pi} \rangle \neq 0 \Leftrightarrow \begin{cases} J \in [\![|J-\lambda|, J+\lambda]\!] \\ \mu = 0 \\ (-1)^{\lambda} = 1 \end{cases}$$

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- Example of $J = 0$ states
  - If λ or $\mu \neq 0$, $\langle \Psi_\epsilon^{ZNJ=0M_J=0\pi} | Q_{\lambda\mu} | \Psi_\epsilon^{ZNJ=0M_J=0\pi} \rangle = 0$
  - Ground states of all even-even nuclei have $J = 0$

Solving the Schrödinger equation

- Nucleus: A interacting nucleons (Z protons and N neutrons)

- Schrödinger equation: $H|\Psi^{ZNJM_J\pi}\rangle = E^{ZNJ\pi}|\Psi^{ZNJM_J\pi}\rangle$

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  - ◇ Do we want to conserve them at each step of the many-body method?
  - ◇ Can we identify and use additional symmetries?

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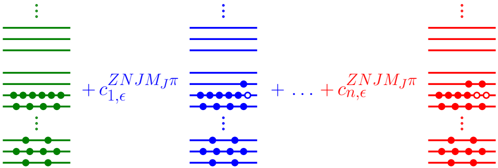
$$|\Theta_{\epsilon}^{ZNJM_J\pi}\rangle = c_{0,\epsilon}^{ZNJM_J\pi} \;[\ldots]\; + c_{1,\epsilon}^{ZNJM_J\pi} \;[\ldots]\; + \ldots + c_{n,\epsilon}^{ZNJM_J\pi} \;[\ldots]\; + \ldots$$



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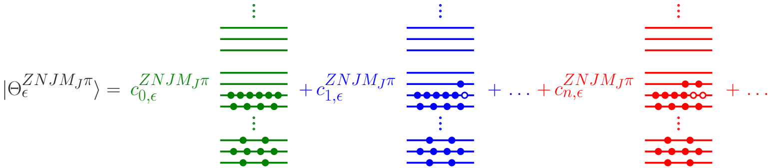

- Examples of CI in nuclear physics:
  - ◇ No-core and valence-space shell models
  - ◇ Spherical Harmonic Oscillator (SHO) single-particle basis: $\phi^{nljm_jsm_stm_t}$

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with

$$T = T_1 + T_2 + T_3 + \dots$$
$$T_n = \sum_{\substack{a_1\dots a_n \\ i_1\dots i_n}} t_{i_1\dots i_n}^{a_1\dots a_n} a_{a_1}^\dagger \dots a_{a_n}^\dagger a_{i_n} \dots a_{i_1}$$

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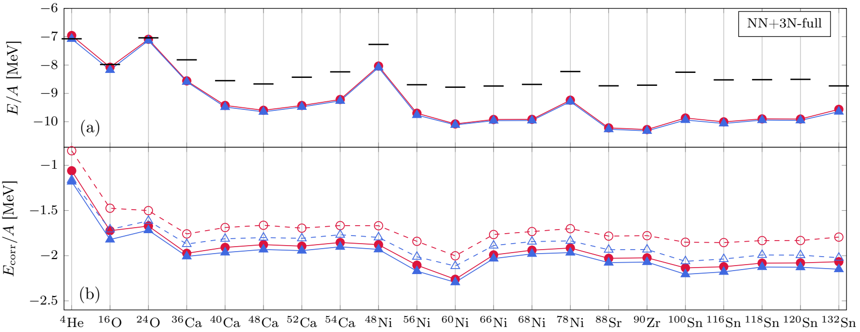
- For example: spherical Hartree-Fock reference state $|\Phi^{ZNJ=0M_J=0\pi=+1}\rangle$
- To learn more about CC → see Pepijn Demol's poster



Tichai, Roth, Duguet, Front. in Phys. 8, 164 (2020)

Symmetry-conserving: advantages/inconvenients

- Advantages
  - Respects the symmetries → good quantum numbers
  - Formalism often simpler
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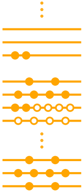
  - Collective phenomena → many-particle many-hole excitations
    → high-order in expansion (expensive)
  - Formal problems (degeneracy of single-particle exc.)
    MBPT(2) $\propto \sum_{abij} \frac{V_{abij} V_{ijab}}{e_a + e_b - e_i - e_j}$



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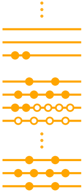

- Application often limited to regions/types of nuclei (e.g. doubly-magic)

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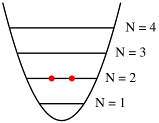
  - $SU(3)$ → see Frédéric's talk
    Symmetry of the Harmonic Oscillator
    Quadrupole operators $Q_{2\mu}$ are part of the generators!



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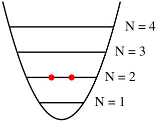
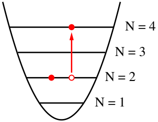
  - ◇ Sympletic $Sp(3,\mathbb{R}) \supset SU(3)$
    Transformations that preserve $[x_{j\alpha}, p_{k\beta}] = i\hbar\delta_{jk}\delta_{\alpha\beta}$
    (with $j, k = 1, \dots, A$, and $\alpha, \beta = x, y, z$)





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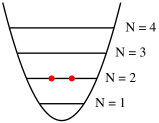

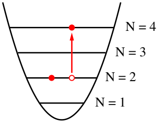

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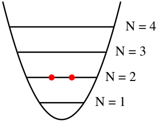

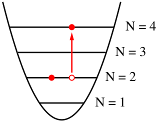

- Contrary to nuclear models, these symmetries are not an end but *a means to an end* $\Rightarrow$ ultimately, broken by H

Symmetry-Adapted No-Core Shell Model (SA-NCSM)

- *Ab initio* CI approach guided by $Sp(3, \mathbb{R})$
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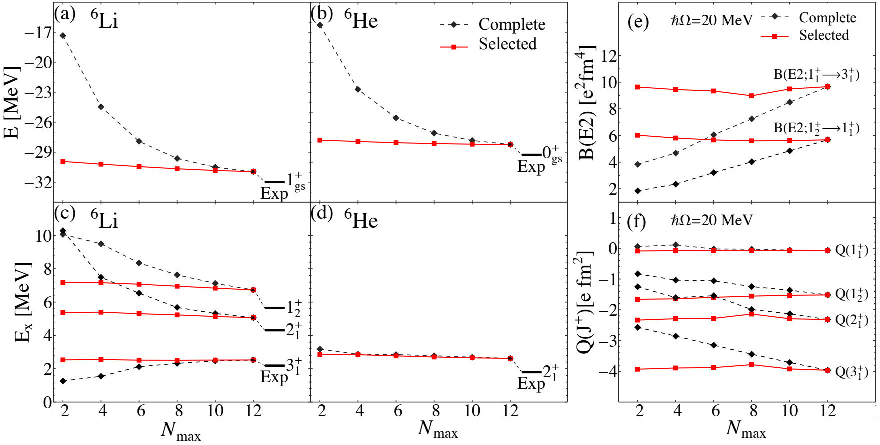
- Diagonalization of H will induce a breaking of $Sp(3,\mathbb{R})$

SA-NCSM: example



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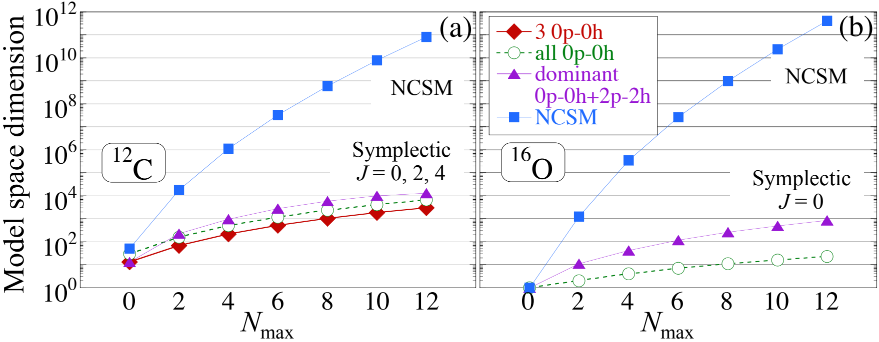

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Nuclear Lattice Effective Field Theory with $SU(4)$

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- Use $SU(4)$ to reduce the sign problem
- Deficiencies have to be corrected
  - Wave function matching
    Elhatisari *et al.*, arXiv:2210.17488 (2022)
  - Perturbation theory

Symmetry-breaking/restoration: principle

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  - Break symmetries in a first step $\Rightarrow$ include correlations in reference states
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- Widespread in nuclear physics
  - Used for a long time in Energy Density Functional
    $\rightarrow$ see Antoine Roux's poster
  - Used also in valence space with phenomenological interactions
  - Gaining popularity in *ab initio* methods
    $\rightarrow$ see Andrea Porro's poster
  - Quantum computing

    Lacroix *et al.*, EPJA 59, 3 (2023)

Symmetry-breaking solutions at the mean-field level

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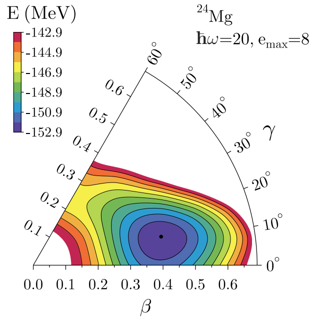
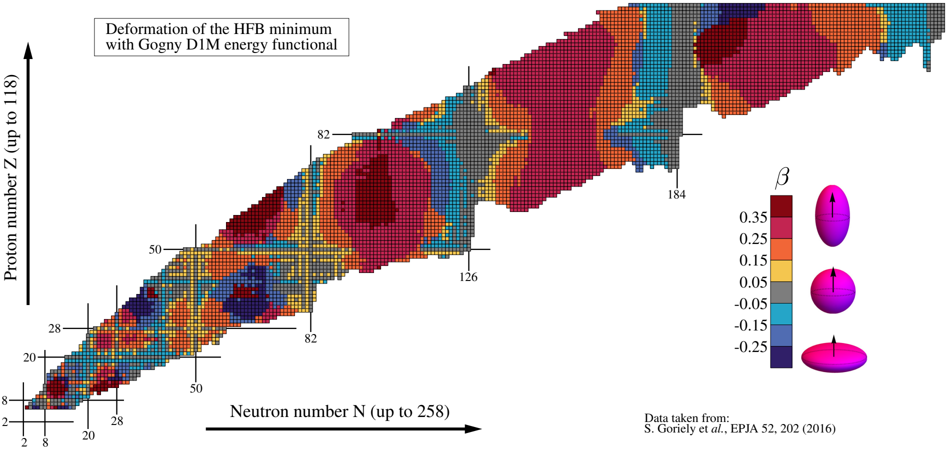
- Mean-field (MF) solution: $\min(\langle\Phi|H|\Phi\rangle, |\Phi\rangle \equiv \text{product states})$
- Symmetry-unrestricted MF calculations favor "deformed" solutions
- Examples: pairing, quadrupole and octupole deformations, ...



Deformation is (almost) ubiquitous



- Problem: deformed solutions break the symmetries of H

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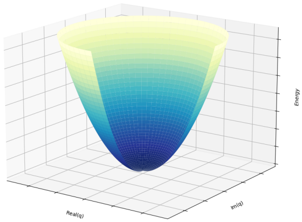
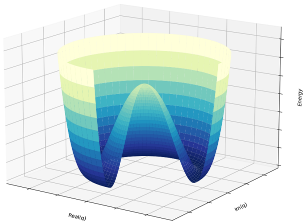
- Dilemma can be bypassed by restoring the symmetries at the beyond MF level

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





Symmetry breaking: order parameter

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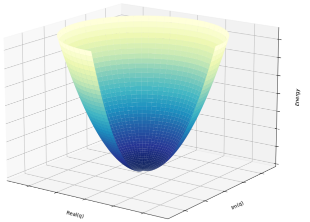
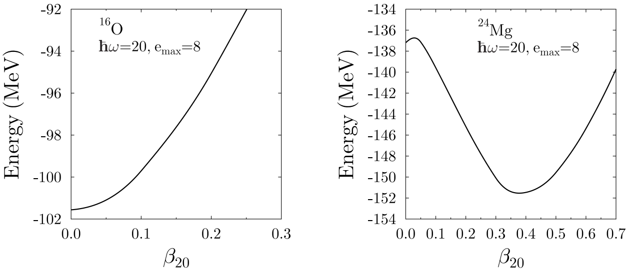
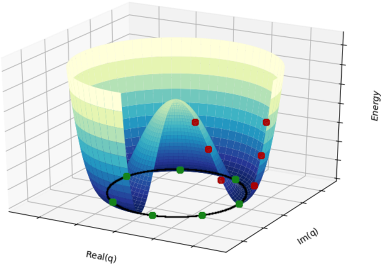


- Example: $|q| = \langle \Phi(q) | Q_{20} | \Phi(q) \rangle$, $\arg(q) \equiv$ Euler angle β_E



- Approximate wave function

$$|\Theta^\Lambda\rangle = \int dq\, f^\Lambda(q)|\Phi(q)\rangle$$
$$\approx \sum_{q_i} f^\Lambda(q_i)|\Phi(q_i)\rangle$$



Symmetry restoration: ansatz

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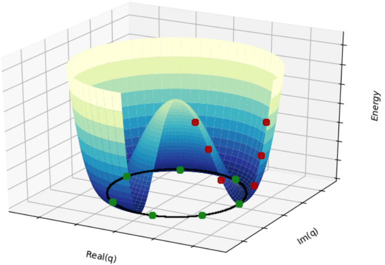

- The weights $f(q)$ are determined minimizing the energy of $|\Theta^{\Lambda}\rangle$

$$\frac{\delta}{\delta f^{\Lambda *}(q)}\left(\frac{\langle\Theta^{\Lambda}|H|\Theta^{\Lambda}\rangle}{\langle\Theta^{\Lambda}|\Theta^{\Lambda}\rangle}\right) = 0$$

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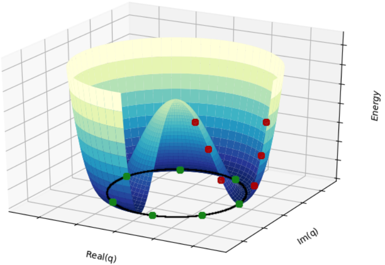

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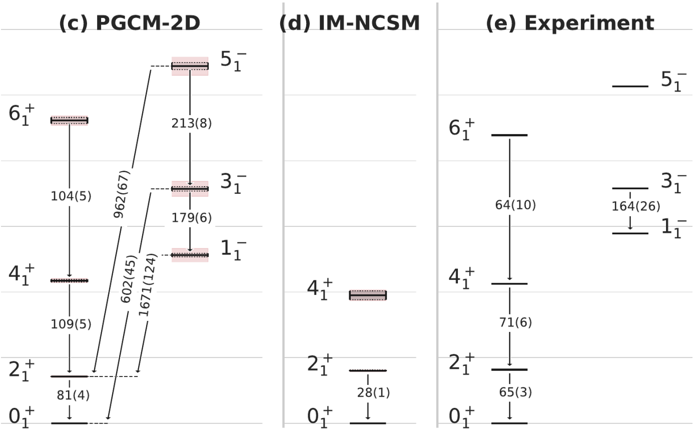
- This the (discretized) Projected Generator Coordinate Method (PGCM)!

$$|\Theta^{ZNJM_J\pi}\rangle \equiv \sum_{q_i} f^{NZJM_J\pi}(q_i) P^{NZJM_J\pi}|\Phi(q_i)\rangle$$

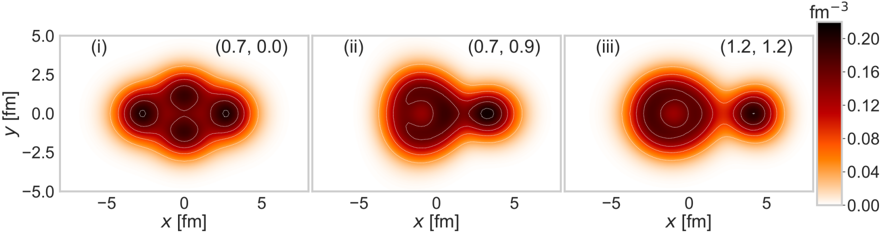
PGCM: example of ^{20}Ne with χEFT interaction



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

- Collective degrees of freedom: $\beta_{20}, (\beta_{22}), \beta_{30}$
- Symmetry projections: Z, N, J, M_J, π

PGCM: example of ^{20}Ne with χEFT interaction



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

- One-body density $\rho(x, y, z)$ for reference states with deformations (β_{20}, β_{30})

Symmetry-breaking/restoration: expansion approach

- Recent developments of expansion schemes using the concept
  - Symmetry-broken reference state → Expansion → Symmetry restoration
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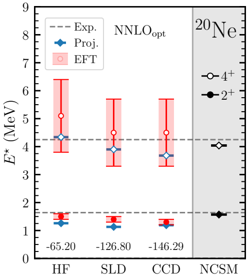
- Projected Coupled Cluster
  Duguet, JPG 42, 025107 (2015)
  Duguet *et al.*, JPG 44, 015103 (2017)



Hagen *et al.*, PRC 105, 064311 (2022)

Outline of the presentation

Summary

- Different approaches to symmetries exist with their advantages/inconvenients
  - Conserve the exact symmetries
  - Exploit extra approximate symmetries
  - Break and restore (selected) symmetries

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  - Break and restore (selected) symmetries

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- Symmetry-breaking and restoration schemes are nice!
  - Applied in EDF context for a long time
  - Also applications in valence space with phenomenological interactions
  - Gaining popularity in *ab initio* context