Ab initio description of deformed intermediate-mass nuclei

Benjamin Bally

Exploring nuclear physics across energy scales Beijing - 16/04/2024



#### Nuclear theory: hierarchy of scales

• Nuclear matter made of quarks and gluons



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  - $\diamond$  Impossible except  $A \sim 1$
  - Even if possible, would be very inefficient
  - What would we learn?



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### Nuclear theory: hierarchy of scales

- Nuclear matter made of quarks and gluons
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  - ♦ Impossible except  $A \sim 1$
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  - What would we learn?
- Define appropriate degrees of freedom for the scale
- Connect different scales
  - $\rightarrow$  Tower of Effective Field Theories



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Courtesy of P. Arthuis



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Weinberg, Phys. Lett. B 251, 288 (1990)

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Epelbaum et al., Front. Phys. 8, 98 (2020)



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- Several variants of EFT
  - $\diamond$  With  $\pi$  (pionful) or without  $\pi$  (pionless)
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  ⇒ Evaluate order by order to assess convergence and uncertainty
- Not free of questions or problems!
  - o Original "Weinberg" power counting not renormalizable!
  - $\diamond~$  Interactions not alway built consistently (different orders for 2N and 3N)
  - Need to go at N?LO
  - Multiplication of the number of interactions ("Skyrmization")

• Same strategy can be applied to transition operators (weak, electromagnetic)



### Systematic tool: EFT for decays

- Same strategy can be applied to transition operators (weak, electromagnetic)
- Example: neutrinoless double-beta decay ⇒ see talk by Jiangming



Cirigliano et al., J. Phys. G 49, 120502 (2022)



### Many-body theories

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  - ◊ No-Core Shell Model (NCSM)
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  - Many-Body Perturbation Theory (MBPT)
  - ◊ Coupled Cluster (CC)
  - Self-Consistent Green's Function (SCGF)
  - In-Medium Similarity Renormalization Group (IMSRG)
  - Valence-Space IMSRG (VS-IMSRG)
  - $\diamond~$  Nuclear Lattice EFT (NLEFT)  $\Rightarrow$  see talks by UIf and Dean
  - $\diamond \ \ \mathsf{Projected} \ \ \mathsf{Generator} \ \mathsf{Coordinate} \ \mathsf{Method} \ \ + \ \mathsf{Perturbation} \ \mathsf{Theory} \ (\mathsf{PGCM-PT})$

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  - $\diamond~$  Nuclear Lattice EFT (NLEFT)  $\Rightarrow$  see talks by UIf and Dean
  - $\diamond$  Projected Generator Coordinate Method + Perturbation Theory (PGCM-PT)
- Variants/generalization of these methods to describe
  - $\diamond$  singly open-shell nuclei → pairing (Bogoliubov formalism)
  - $\diamond~$  doubly open-shell nuclei  $\rightarrow~$  deformation





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- Strategy 1: consider only max(i + j + k) = max(l + m + n) = P < 3M</li>
  In general, we consider HO energy quanta → e<sub>3max</sub> = max(e<sub>i</sub> + e<sub>j</sub> + e<sub>k</sub>)



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$$H \longrightarrow \tilde{H} = \tilde{H}^{0\mathsf{N}} + \tilde{H}^{1\mathsf{N}} + \tilde{H}^{2\mathsf{N}}$$

with, e.g., 
$$\tilde{H}^{2N}_{ijlm} = V^{2N}_{ijlm} + \sum_{kn} V^{3N}_{ijklmn} \rho_{kn}$$

• Recent breakthrough in the computation of the effective two-body



Miyagi et al., Phys. Rev. C 105, 014302 (2022)





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• Strategy 3: tensor factorization

Tichai et al., Phys. Rev. C 99, 034320 (2019)

























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- Used deformed  $|\Phi\rangle$  in the description of deformed nuclei
  - $\diamond$  Much better starting point
  - ◊ Collective correlations difficult to include in expansions (many particle-hole)
  - $\diamond~$  Success of symmetry-breaking/restoration within energy functional methods



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- Such deformed states break the symmetries of H
   ⇒ symmetries have to be restored
   Duguet, J. Phys. G 42, 025107 (2015)
   Duguet et al., J. Phys. G 44, 015103 (2017)
   Qiu et al., Phys. Rev. C 99, 044301 (2018)


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- Perturbation theory applied to a many-body reference state Tichai *et al.*, Front. Phys. 8, 164 (2020)
  - ♦ Partition the Hamiltonian:  $H = H_0 + H_1 \rightarrow H_0$  solved exactly  $\rightarrow |\Phi\rangle$

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  - $\langle |\Psi\rangle = \sum_{k=0}^{\infty} (RH_1)^k |\Phi\rangle$
- Method is computationally cheap  $\rightarrow$  large-scale calculations possible
- Does it converge? At least deformed  $|\Phi\rangle$  is a better starting point for deformed nuclei

## Deformed MBPT (dMBPT)

• Application to deformed case ongoing



Alberto Scalesi et al., to be published (2024)



# Deformed CC (dCC)



• Expands the eigenstate as  $|\Psi\rangle = e^{T} |\Phi\rangle$ Hagen *et al.*, Rep. Prog. Phys. 77, 096302 (2014)

 $\diamond \quad T = T_1 + T_2 + T_3 + \ldots + T_A \text{ with, e.g., } T_2 = \frac{1}{4} \sum_{ijkl} t_{ijkl} a_i^{\dagger} a_j^{\dagger} a_l a_k$ 

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  - Exponential ansatz is powerfull
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  - ♦ In nuclear physics, we consider up to CCSDT (= stop at  $T_3$ )
- Extension to deformed reference states with symmetry projection!



Ekström et al., arXiv:2305.06955 (2023)

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- Block diagonalizes H by a unitary transformation Hergert *et al.*, Phys. Rep. 621, 165 (2016)
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0p0h 1p1h 2p2h 3p3h

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Adapted from H. Hergert







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  - $\diamond$  Flow generates higher-body terms  $\rightarrow$  truncation IMSRG(k)

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- Extension to deformed nuclei

Yuan et al., Phys. Rev. C 105, L061303 (2022)





## Valence-Space IMSRG (VS-IMSRG)

• Ab initio re-interpretation of the traditional shell model (SM)

Stroberg et al., Anns. Rev. Nucl. Part. Sci. 69, 307 (2019)



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  - $\diamond~$  Uses IMSRG to decouple a valence space from a core
  - Exact diagonalization within the valence space





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  - $\diamond~$  Uses IMSRG to decouple a valence space from a core
  - Exact diagonalization within the valence space
- Can reuse SM know-how and numerical codes!
  ⇒ Large contribution to recent progress in *ab initio* reach



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· Problems to take into account collectivity



Stroberg et al., Phys. Rev. c 105, 034333 (2022)

## Valence-Space IMSRG (VS-IMSRG)

- Problems to take into account collectivity
  - $\diamond~$  Includes all correlations inside the valence space but  $\ldots$
  - $\diamond \ \ldots$  still depends on  $\mathsf{IMRSG}(\mathsf{k})$  for the decoupling



Stroberg et al., Phys. Rev. c 105, 034333 (2022)

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

Projected Generator Coordinate Method (PGCM)



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- Reference states:
  - Bogoliubov quasiparticle states
  - $\diamond$  Series of constrained HFB minimization, e.g.,  $\langle \Phi(q) | Q | \Phi(q) \rangle = q$
- Advantages:
  - ◊ Multi-reference approach
  - $\diamond~$  Symmetry conserving  $\rightarrow$  good quantum numbers
  - ♦ Scales with A as mean field ... but with a LARGE prefactor

#### PGCM: schematic example









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  - Expansion on top of multi-reference state is more complicated/costly
- Two methods recently developed
  - $\diamond \ \mathsf{IMSRG} + \mathsf{PGCM} \rightarrow \mathsf{In}\text{-}\mathsf{Medium} \ \mathsf{GCM}$

Yao et al., Phys. Rev. Lett. 124, 232501 (2020)

- PGCM + Perturbation Theory (PGCM-PT)
  Frosini *et al.*, Eur. Phys. J. A 58, 62 (2022), Frosini *et al.*, Eur. Phys. J. A 58, 63 (2022), Frosini *et al.*, Eur. Phys. J. A 58, 64 (2022)
- ◊ (the two can be combined!)

Frosini et al., Eur. Phys. J. A 58, 64 (2022)

## In-Medium GCM: application to <sup>76</sup>Ge

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- Workflow:
  - ♦ Perform PGCM calculation  $\rightarrow |\Phi^{ZNJ\pi}\rangle$
  - ♦ Evolve *H* through IMSRG using  $|\Phi^{ZNJ\pi}\rangle$  as reference state →  $H(\infty)$
  - $\diamond~$  Perform new PGCM calculation with  $H(\infty)$

 $\Rightarrow$  see talk by Jiangming

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Belley et al., arXiv:2308.15634 (2023) + Phys. Rev. Lett., in production (2024)

#### PGCM-PT: application to <sup>20</sup>Ne



- Perturbation Theory on top of PGCM state
  - Multi-reference & symmetry conserving
  - ◊ State dependent PT
  - Scaling much worse than PGCM (need better partitioning)



Frosini et al., Eur. Phys. J. A 58, 64 (2022)

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- Perturbation Theory on top of PGCM state
  - Multi-reference & symmetry conserving
  - $\diamond \ \ \mathsf{State} \ \ \mathsf{dependent} \ \mathsf{PT}$
  - Scaling much worse than PGCM (need better partitioning)
- Plain PGCM enough for relative quantities



Frosini et al., Eur. Phys. J. A 58, 64 (2022)

- State-of-the-art PGCM and NLEFT calculations for <sup>16</sup>O and <sup>20</sup>Ne Giacalone *et al.*, arXiv:2402.05995 (2024)
- The two methods agree quite well!





#### Calculations for ion-ion collisions




## Conclusion



• Intrinsic deformation is an important feature of atomic nuclei

⇒ see talks by Peter, Dario, Magda

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- Development of new ab initio schemes to tackle it
- Good strategy for expansion methods:
  - include static deformation correlations in the reference states
  - include dynamic correlations through the expansion
  - ◊ need to restore the symmetries!

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- Development of new ab initio schemes to tackle it
- Good strategy for expansion methods:
  - include static deformation correlations in the reference states
  - include dynamic correlations through the expansion
  - ◊ need to restore the symmetries!
- Collaboration with heavy-ion community started but could be reinforced Summerfield et al., PRC 104, L041901 (2021)
  Mäntysaari et al., PRL 131, 062301 (2023)
  Giacalone et al., arXiv:2402.05995 (2024)