European Nuclear Physics Conference 2022 (EuNPC 2022)

Theoretical tools in low energy nuclear structure: an update

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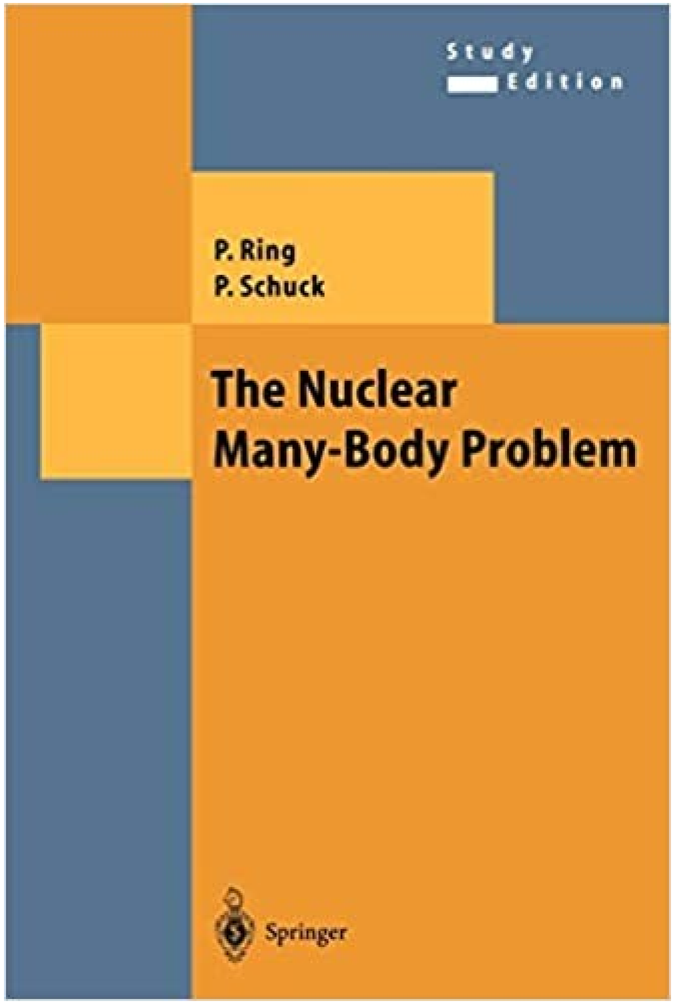


Motivation

Overview of the present status of low energy nuclear structure

Nuclear structure
Bound states
Ground and excited states
And decays

~~Low energy reactions~~
~~Scattering states~~

Discuss some of the recent developments in the theoretical tools used to describe nuclear structure

Nuclear structure at a glance

Nuclear interaction

- Residual interaction of QCD
- Strongly attractive and repulsive
- Spin dependent
- Tensor
- Three, four, etc body
- Strong in-medium effects

Many body methods

- Mesoscopic system (≈ 100)
- Mean field driven (magic numbers)
- Spontaneous symmetry breaking
- Symmetry restoration
- Collective and single particle dof

Current approaches

- Ab-initio
  - Based on Effective Field Theory
  - Inspired by Chiral symmetry (QCD)
  - Requires RG or SRG techniques
- Effective interactions
  - Skyrme, Gogny, covariant EDF
- Shell model in configuration space
- Schematic, residual ints
- Macroscopic (Liquid drop)

Current approaches

- Mean field with constraints
- QRPA (pp, pn)
- Symmetry restoration (N, J, π, I, COM)
- Collective degrees of freedom
  - GCM
  - Collective hamiltonian
- Configuration interaction (MQP, ISM, MSM)
- Boson models (IBM, etc)
- Green functions,
- Coupled cluster
- SRG, perturbation theory
- ...

Where do we stand today ?

Look at last year of **Physical Review C** for new developments and/or relevant aspects of the different methods used in theoretical nuclear structure

Disclaimer: Choices based on my own taste ….

Interacting shell model

IN-BEAM γ-RAY SPECTROSCOPY OF … PHYSICAL REVIEW C **105**, 034318 (2022)

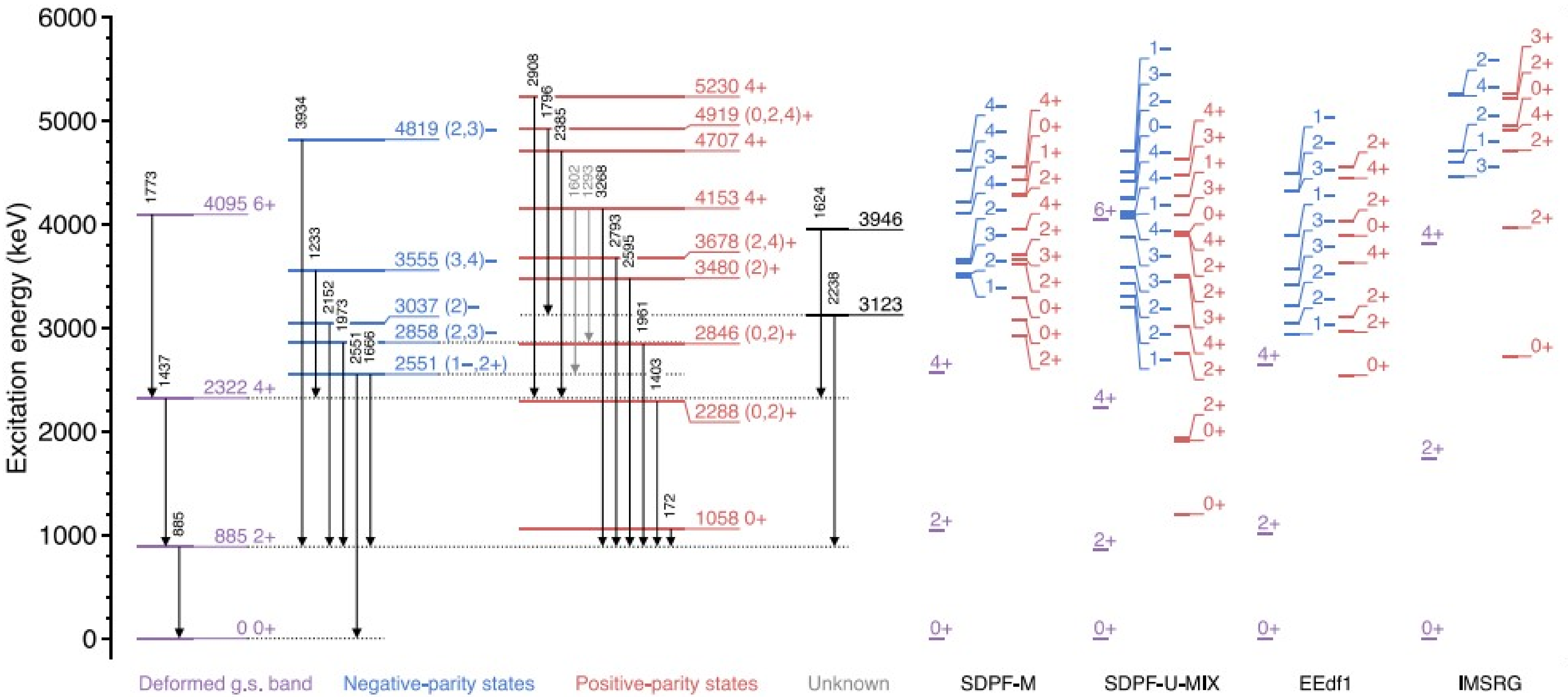


FIG. 3. Level scheme of ^{32}Mg constructed in the present work. Placed transitions are indicated by the arrows. Tentative placements are

Given a good interaction and an appropriate configuration space the ISM is able to reproduce experimental results with an outstanding accuracy

- **Kumar invariants** to introduce the concept of deformation in the lab frame
- Shell model i**nteractions from ab-initio**

- Efforts to create interactions in valence spaces suited for **heavy nuclei**
- Exploring nuclear properties in new nuclei

Mean field, QRPA, Green functions and GCM developments

- Deformed relativistic **Hartree-Bogoliubov theory in continuum** with a point-coupling functional.
  Phys. Rev. C 106, 014316

- Complete solution to the **inverse Kohn-Sham problem**: From the density to the energy
  Phys. Rev. C 105, 034309

- Gamow-Teller transitions charge-exchange subtracted **second random-phase approximation**
  Phys. Rev. C 106, 014319

- Several papers implementing **FAM+QRPA** for different physical situations:
  Phys. Rev. C 105, 044311, Phys. Rev. C 105, 044312, Phys. Rev. C 105, 044314

- **Many-body** approach to **superfluid** nuclei in axial geometry,
  Phys. Rev. C 105, 044326

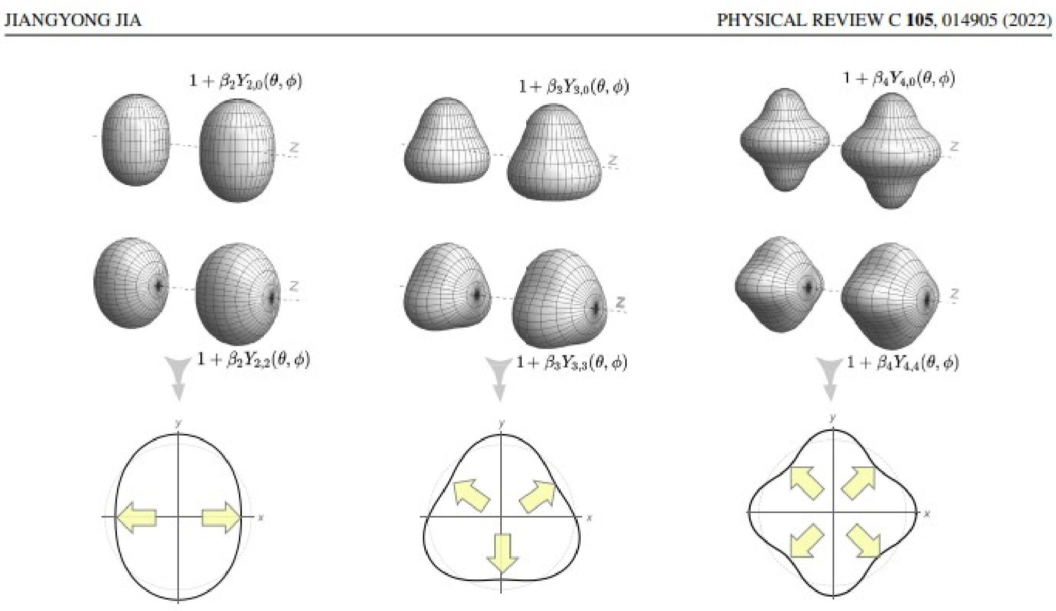
- **Gorkov** algebraic diagrammatic construction formalism at third order,
  Phys. Rev. C 105, 044330

- Microscopic description of cluster decays based on the **generator coordinate method**
  Phys. Rev. C 105, 034326

- Applications of the dynamical **generator coordinate method** to quadrupole excitations
  Phys. Rev. C 105, 064302

Mean field, QRPA, Green functions and GCM developments (2)

- Accessing the shape of atomic nuclei with relativistic collisions of isobars, Phys. Rev. C 104, L041903
- Shape of atomic nuclei in heavy ion collisions Phys. Rev. C 105, 014905
- Description of **isospin mixing** by a generator coordinate method Phys. Rev. C 105, 014311
- New many-body method using cluster expansion diagrams with **tensor-optimized** antisymmetrized molecular dynamics, Phys. Rev. C 105, 014317
- Angular momentum projection in the deformed relativistic Hartree-Bogoliubov theory in **continuum**, Phys. Rev. C 104, 064319
- Translationally invariant **matrix elements** of general one-body operators, Phys. Rev. C 104, 064322



- Nuclear landscape in a **collective Hamiltonian** from covariant density functional theory, Phys. Rev. C 104, 054312
- Ab initio **no-core Monte Carlo shell model calculations** with non local NN interactions, Phys. Rev. C 104, 054315
- Pfaffian formulation for matrix elements of three-body operators in **multiple quasiparticle configurations** Phys. Rev. C 105, 034342
- **Many-body** theory for quasiparticle states in **superfluid** fermionic systems, Phys. Rev. C 104, 044303
- Quantum many-body calculations using **body-centered cubic lattices**, Phys. Rev. C 104, 044304 (2021)

The nuclear mean field often spontaneously breaks symmetries: intrinsic frame.

Symmetry restoration of spontaneously broken symmetries at the mean field level is a technique that is gaining ground in spite of still *unresolved issues with self-energies and density dependent forces*

- **Skyrme, Gogny, covariant**: Angular momentum projection, including parity, triaxiallity and cranking like states. Isospin projection.
- **Shell model like configuration spaces**: an avenue to approach shell model accuracy at a much lower cost (larger configuration spaces): Taurus, etc
- Technical developments to compute **overlaps of operators for not closed basis**: projections with finite basis
- Projection on a **space domain** (fission fragments)

PHYSICAL REVIEW C **104**, 054306 (2021)

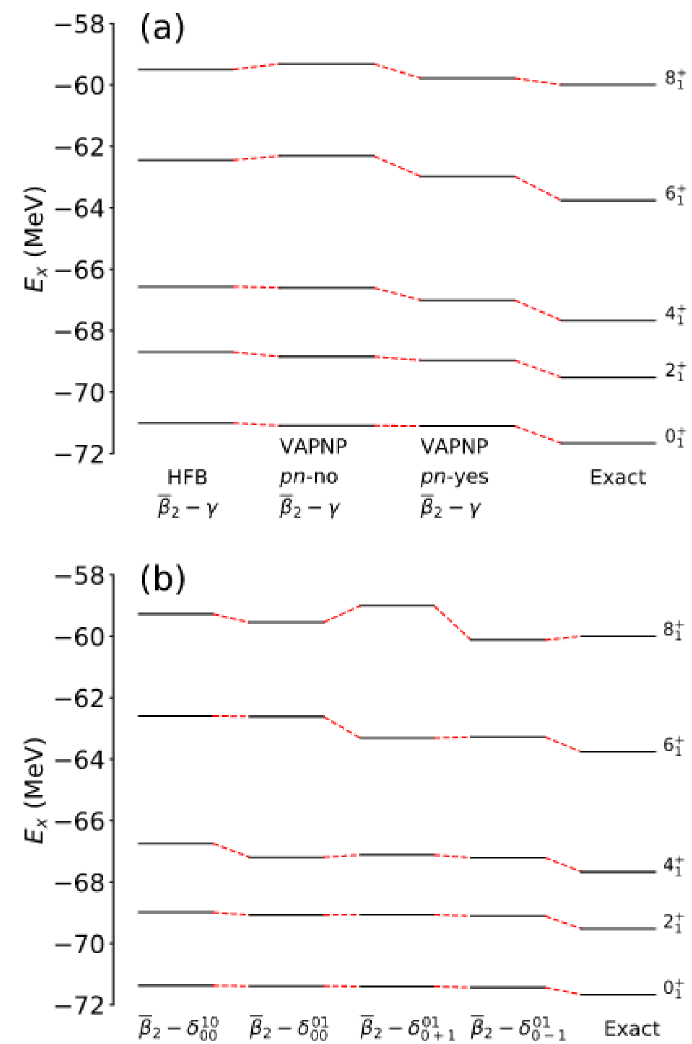


FIG. 12. PGCM and exact energies of the yrast states for ^{24}Ne

Symmetry restoration (2)

NUCLEAR STRUCTURE WITHIN A DISCRETE …

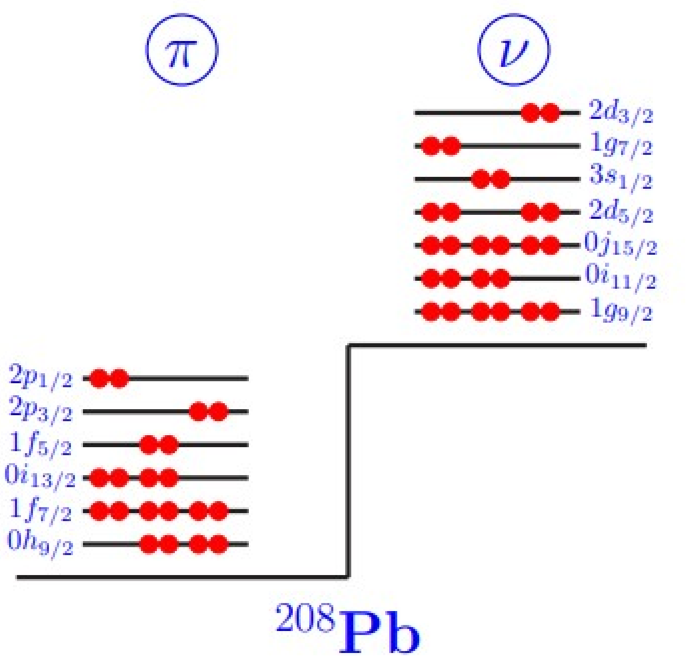


FIG. 11. Valence space above ^{208}Pb.

PHYSICAL REVIEW C 105, 054314 (2022)

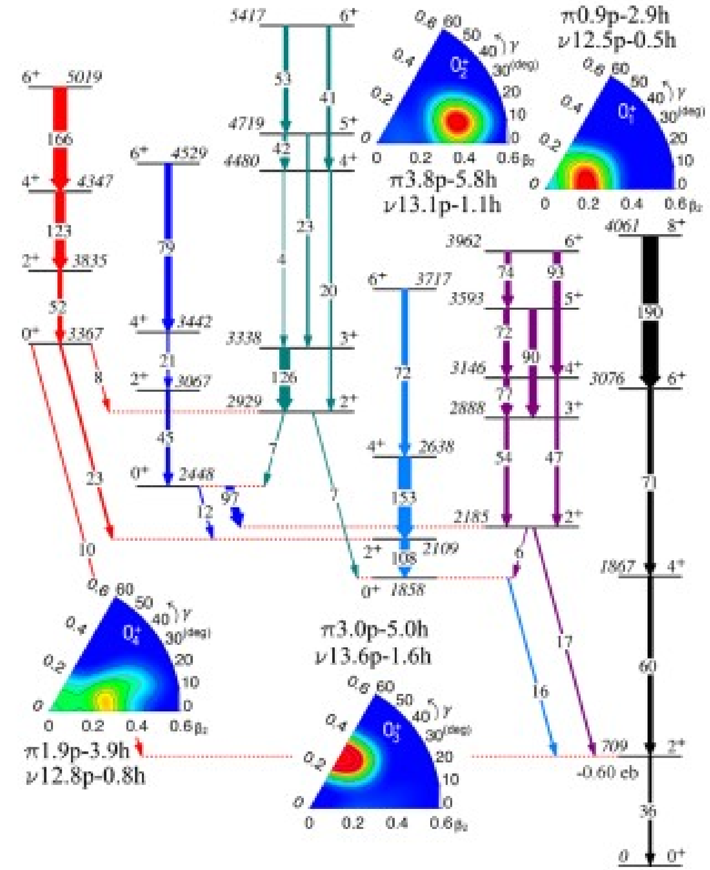
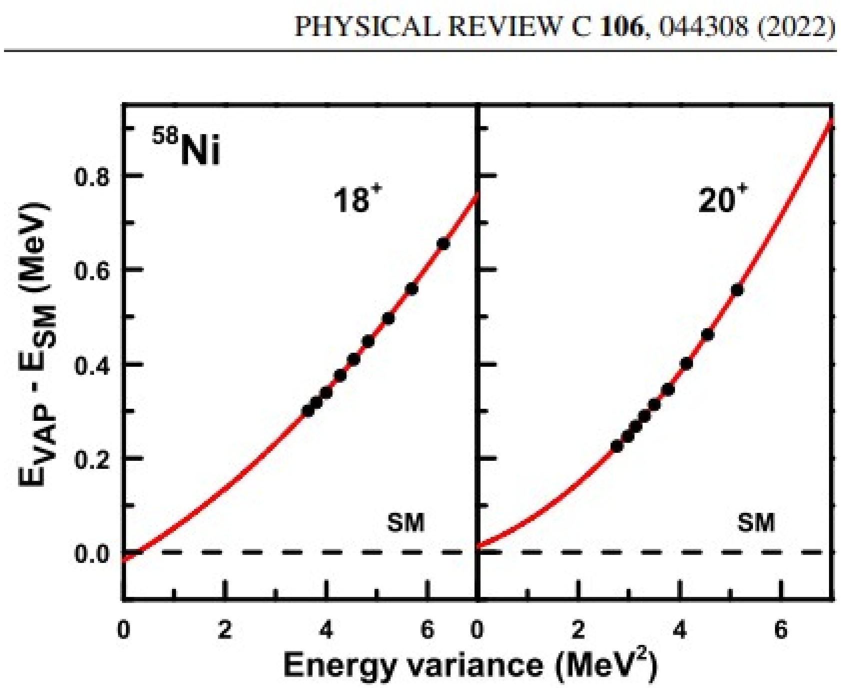


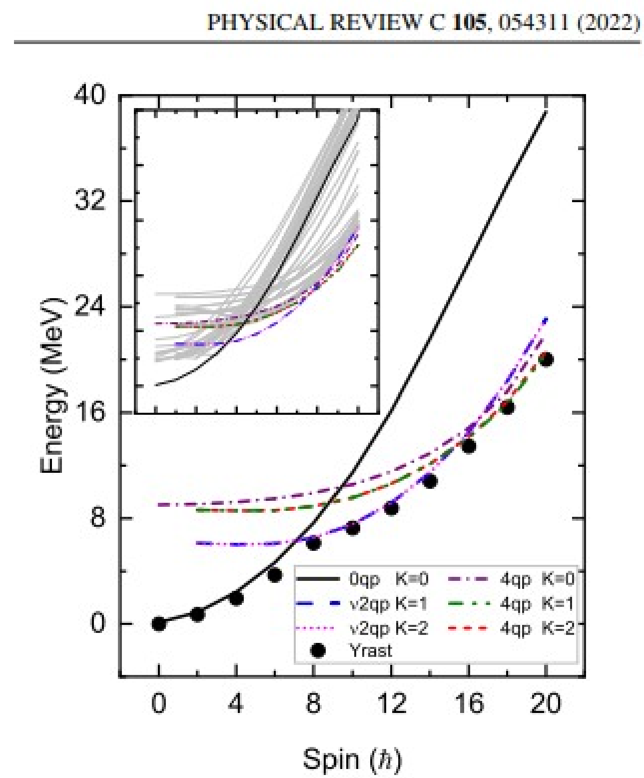
FIG. 2. The partial experimental level scheme deduced for ^{110}Cd (top) and from the BMF calculation (bottom) showing the

PHYSICAL REVIEW LETTERS 123, 142502 (2019)

Symmetry restoration (3)



Energy variance extrapolation

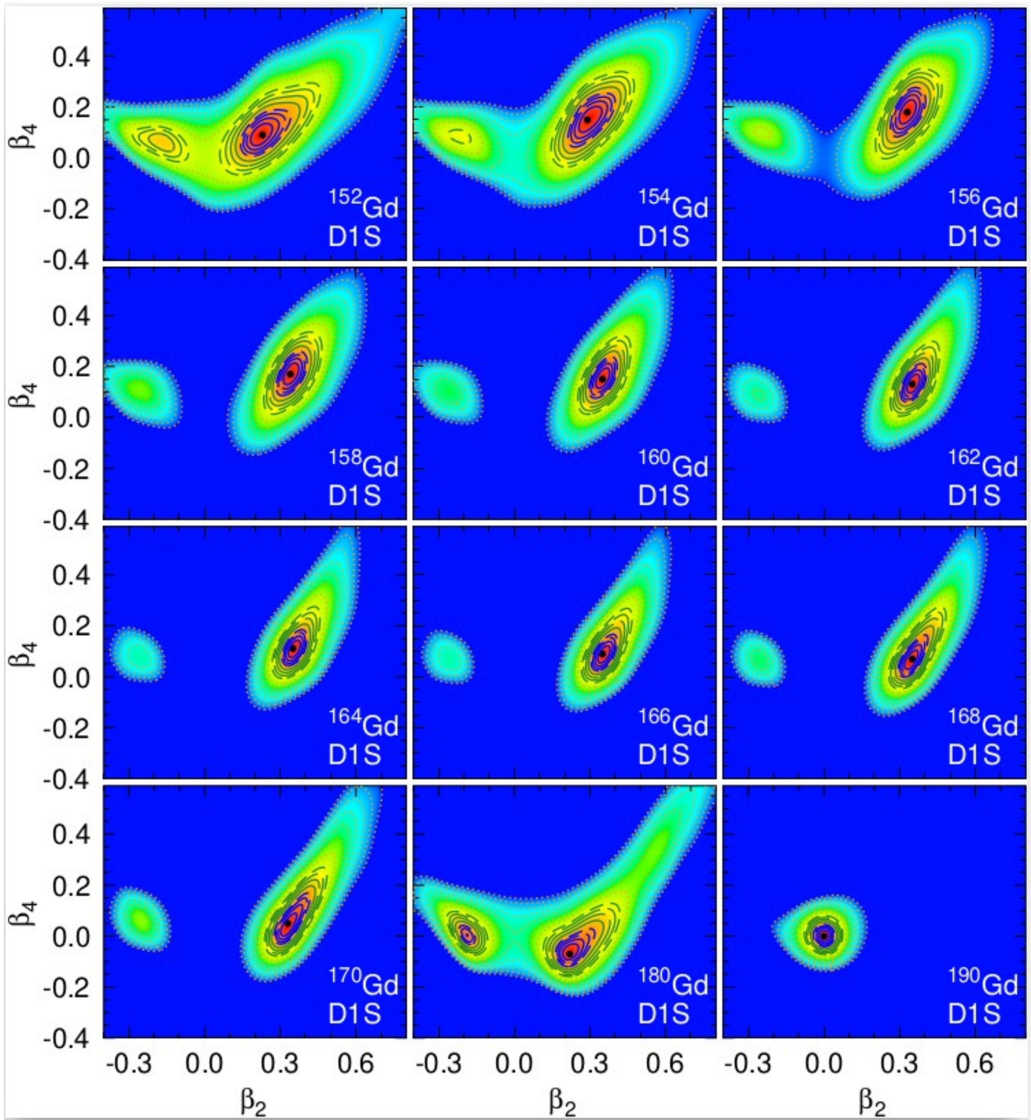


- Extended **triaxial projected shell model** approach for odd-neutron nuclei
  Phys. Rev. C 105, 054310
- Nuclear states **projected** from a pair condensate, Phys. Rev. C 105, 034317
- Variational **approximations to exact solutions in shell-model valence spaces**: Systematic calculations in the sd shell, Phys. Rev. C 104, 054306
- Restoring broken symmetries for nuclei and **reaction fragments**
  Phys. Rev. C 104, 054601

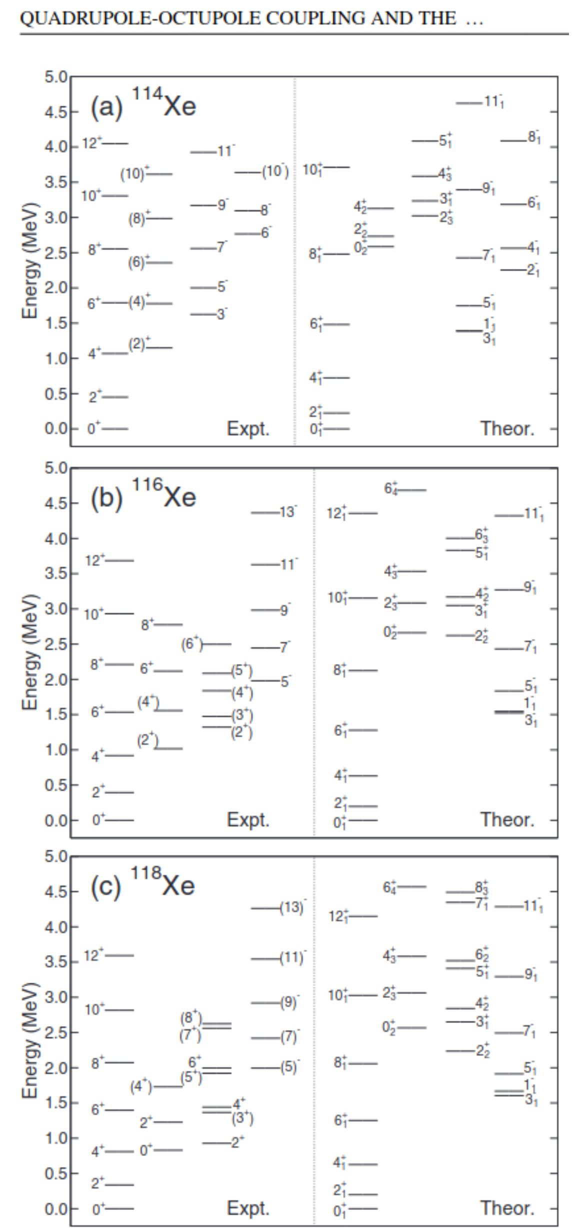
TAURUS

Collective excitations

Combined with symmetry restoration or alone, fluctuations in collective degrees of freedom provide a convenient framework to study **collective excitations:** shape vibrations, octupole states, etc

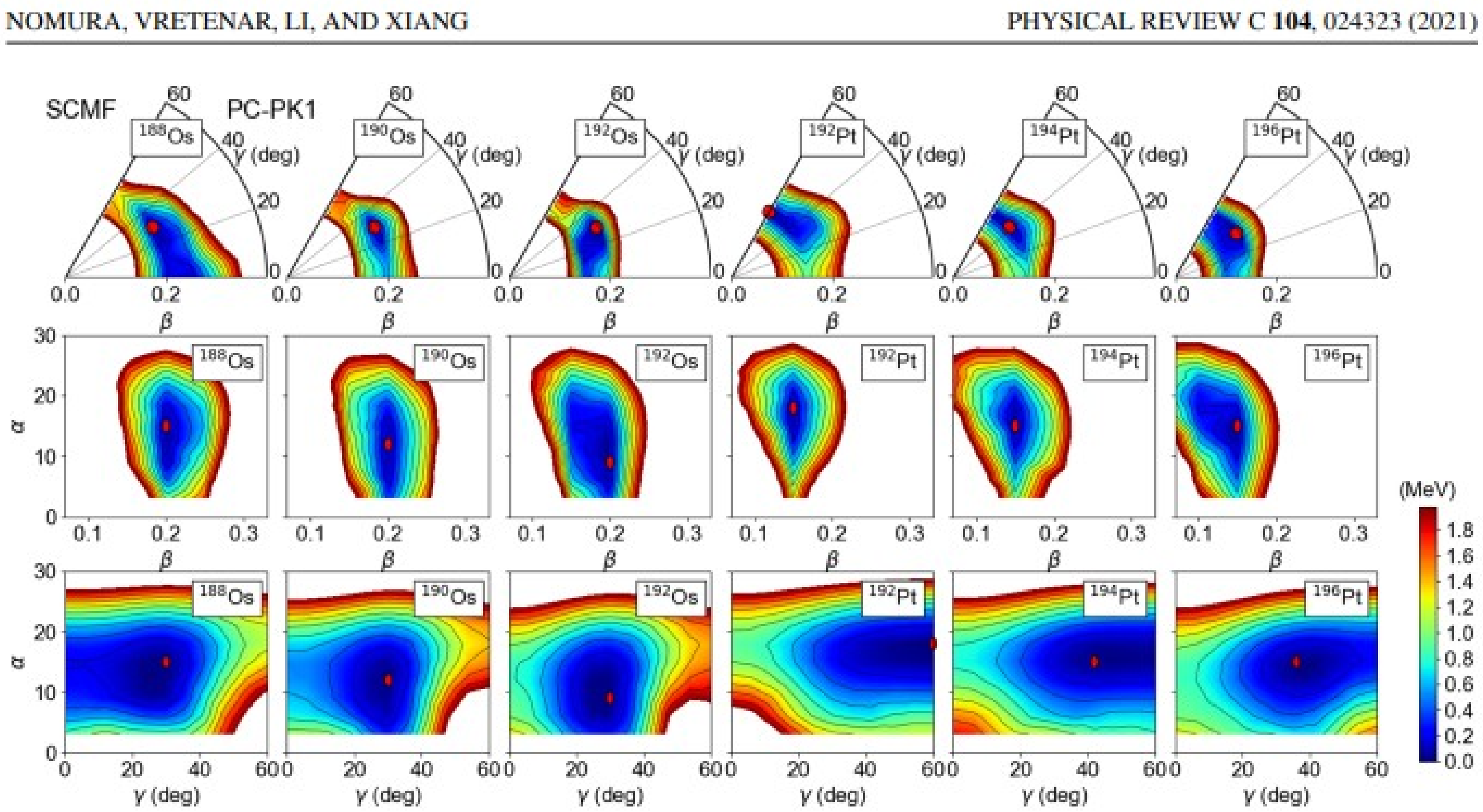


Work in progress



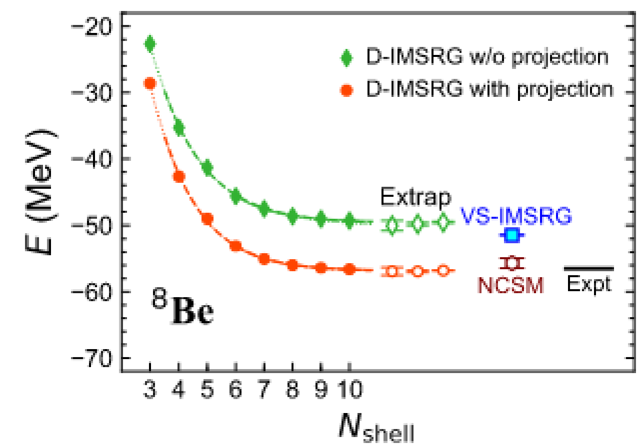
PHYSICAL REVIEW C 104, 054320 (2021)

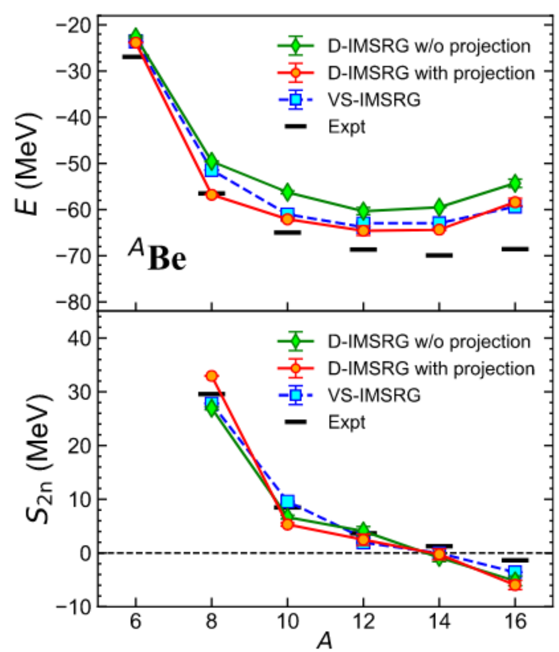
Collective excitations



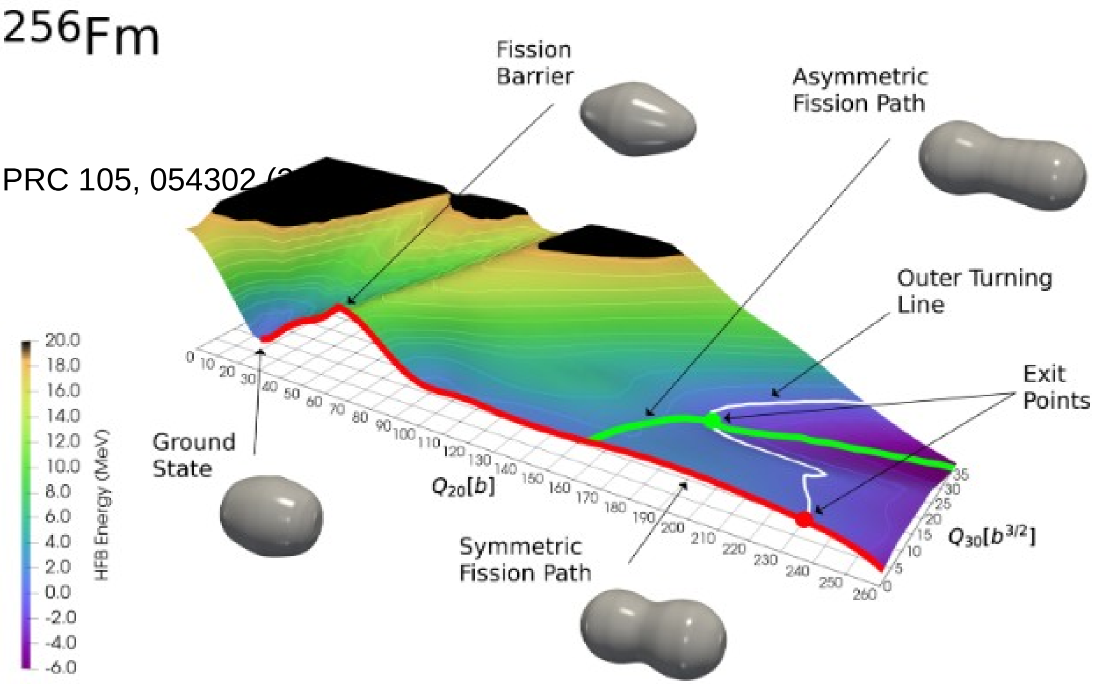
Bohr Hamiltonian including **pairing as a relevant ingredient**: Pairing strongly influence dynamics through the collective inertia

- Deformed **in-medium similarity renormalization group**
  Phys. Rev. C 105, L061303
- Angular-momentum projection in **coupled-cluster theory**
  Phys. Rev. C 105, 064311
- **Natural orbitals** for the ab initio no-core configuration interaction approach, Phys. Rev. C 105, 054301
- Ab initio calculation of the **β decay** from 11Be to a 10Be +p resonance, Phys. Rev. C 105, 054316
- **Ab initio coupled-cluster** calculations of ground and dipole excited states in 8 He, Phys. Rev. C 105, 034313
- **Importance truncation for the in-medium similarity renormalization group**, Phys. Rev. C 105, 034324
- **Converged ab initio calculations of heavy nuclei**
  Phys. Rev. C 105, 014302
- Overview of symmetric nuclear matter properties from **chiral interactions up to fourth order of the chiral expansion**
  Phys. Rev. C 104, 064312



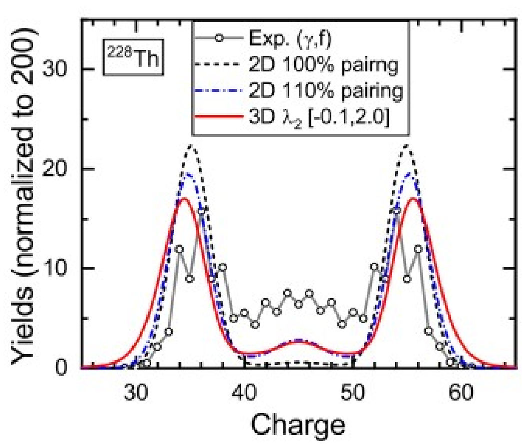


Fission has traditionally been studied using old Bohr’s idea of a deformation coordinate and a potential energy driving the dynamics. The starting point: mean field with constraints



PRC 105, 054302 (2

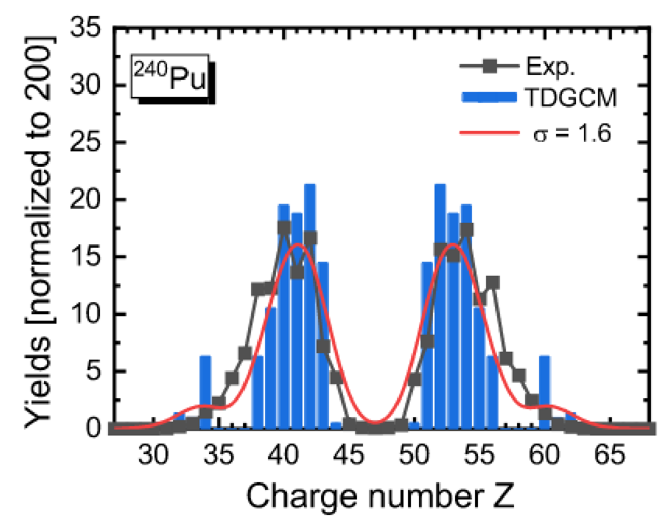
- Shift from least energy to least action path
- Inertias and pairing
- Approximate TDHFB for fragment’s properties
- Implementation of TDGCM
- Statistical modeling based on potential energies surfaces



PHYSICAL REVIEW C 104, 044612 (2021)

Microscopic analysis of induced nuclear fission dynamics,
Phys. Rev. C 105, 044313

PHYSICAL REVIEW C **105**, 044313 (2022)



Beta decay

Single Beta decay has been traditionally studied with pn-QRPA models assuming the same structure in parent and daughter.

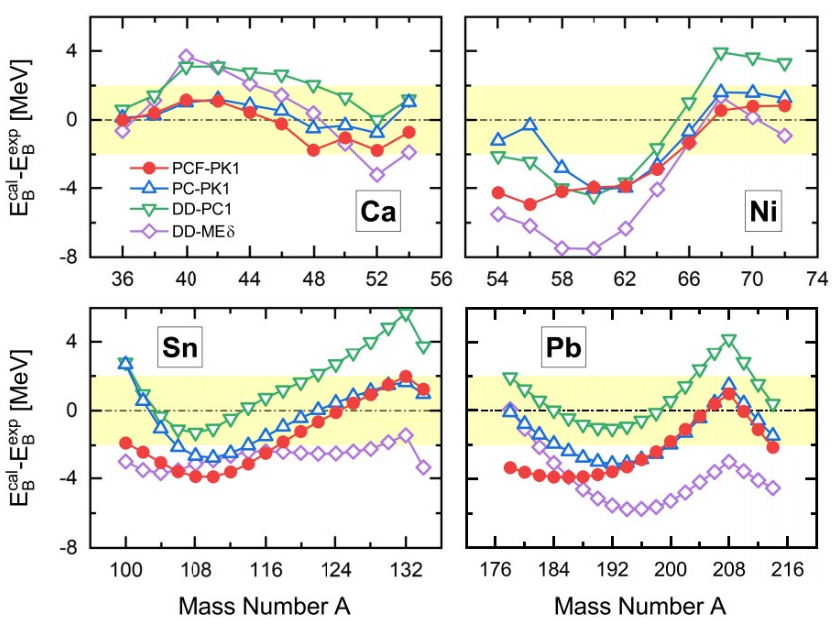
- **Neutrinoless double beta** studied with **ab-initio** approaches to introduce more involved transition operators, Phys. Rev. C 106, 014315, Phys. Rev. C 106, 034309
- Standard **beta decay studied with pn-QRPA** with schematic interactions, Phys. Rev. C 105, 044314, Phys. Rev. C 106, 024306, Phys. Rev. C 105, 064315
- **Fermion-boson** models are gaining ground as an **alternative to pn-QRPA**, Phys. Rev. C 105, 044306
- **GCM** with beta-gamma degrees of freedom +Angular momentum projection to overcome limitations with **parent and daughter having different structure**, see Tomas Rodriguez talk on tuesday
- Two-neutrino double-β decay in the mapped **interacting boson model** Phys. Rev. C 105, 04430

- **Covariant density functional theory with localized exchange terms**, PRC 106, 034315

- **Tensor interaction**
  - Finite-range simple effective interaction including tensor terms, Phys. Rev. C 106, 024313
  - Role of tensor interaction as salvation of cluster structure in 44Ti Phys. Rev. C 105, 064314

- **Skyrme pseudopotentials** at next-to-next-to-leading order: Construction of local densities and first symmetry-breaking calculations, Phys. Rev. C 104, 044308

ZHAO, REN, ZHAO, AND MENG PHYSICAL REVIEW C **106**, 034315 (2022)



These are regular nuclei with one or several strange (charmed) barions, like Λ, Ξ, etc added in a deep 1s orbit

Studied mostly at the mean field level, the NΛ interaction needs to be characterized

- Phys. Rev. C 106, L012802: Hyper-heavy nuclei in a **neutron-star** environment

- ΛΛ pairing effects in spherical and deformed **multi-Λ hyperisotopes**
  Phys. Rev. C 105, 034322

- Skyrme force for all known **Ξ− hypernuclei**
  Phys. Rev. C 104, L061307

- Ground state properties of **charmed hypernuclei** within a mean field approach
  Phys. Rev. C 104, 064306

- **New effective interactions for hypernuclei** in a density-dependent relativistic mean field model
  Phys. Rev. C 104, 05432

Machine learning techniques are essentially “super-interpolators” and / or “super-extrapolators” The method defines a model based on neural networks is and the parameters are “taught” by trying to reproduce some given data (experimental, theoretical, etc)

- **β-delayed one-neutron emission** probabilities within a neural network model, Phys. Rev. C 104, 054303
- **Nuclear energy density functionals** from machine learning
  Phys. Rev. C 105, L031303
- Learning correlations in **nuclear masses** using neural networks
  Phys. Rev. C 105, L031306
- Machine learning approach to **pattern recognition** in nuclear dynamics from the ab initio symmetry-adapted no-core shell model
  Phys. Rev. C 105, 034306

PHYSICAL REVIEW C **106**, L021301 (2022)

Physically interpretable machine learning for nuclear masses

PHYSICAL REVIEW C **105**, 064306 (2022)

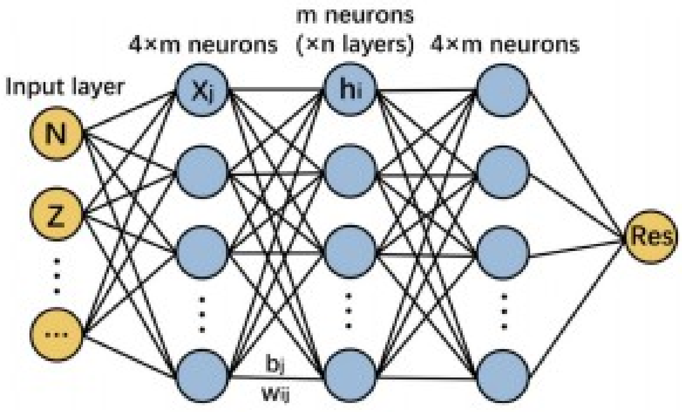


FIG. 1. The adjustable neural network structure with the number of hidden layers changed by *n* and the width of hidden layers changed by *m*. The output layer is the residual defined in Eq. (2).

Applications of reduced-basis methods to the nuclear single-particle spectrum

PHYSICAL REVIEW C 106, L031302 (2022)

Machine learning (2)

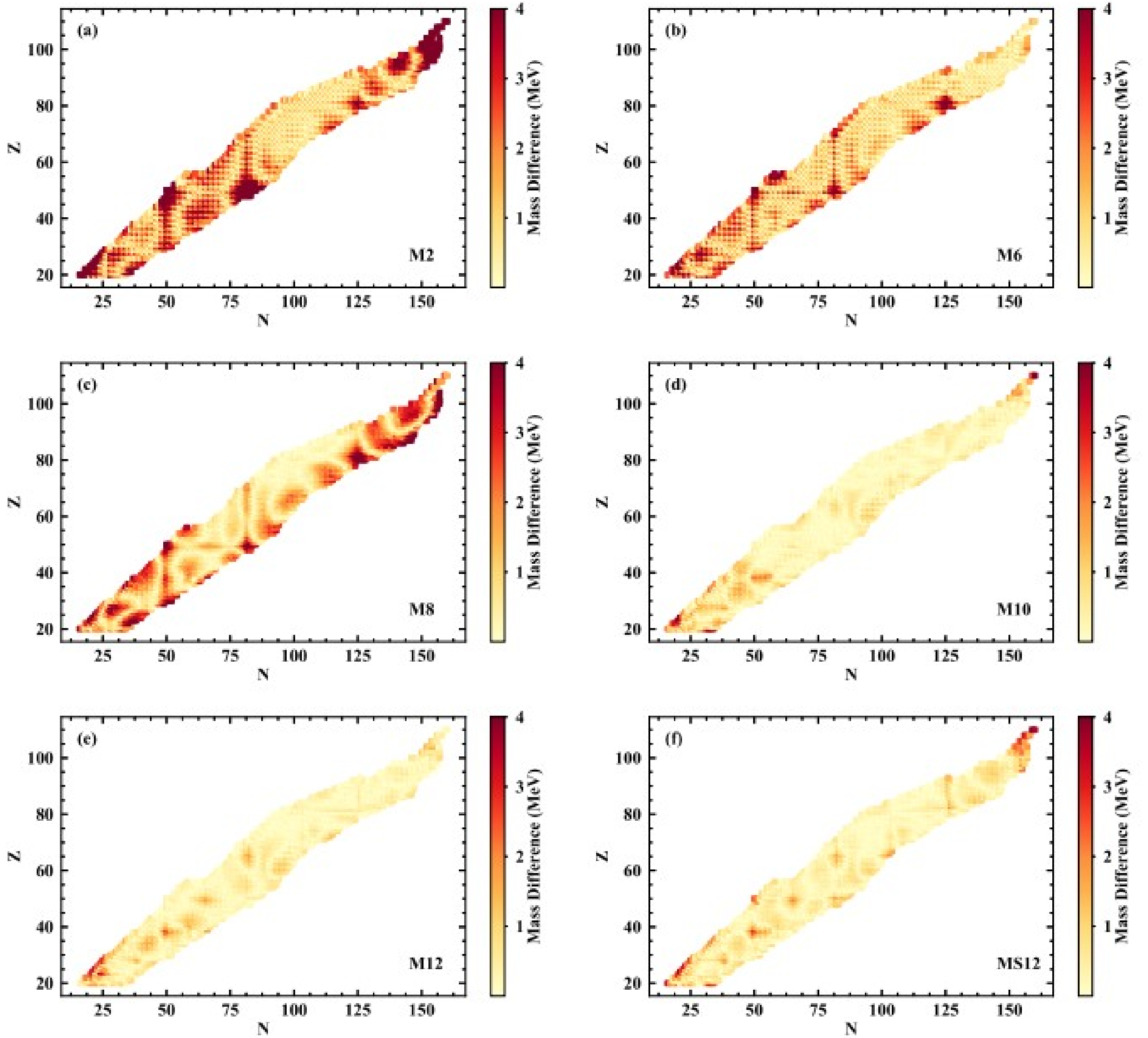


FIG. 1. Mass difference between the MDN predictions and the AME2016 (in MeV) across the nuclear chart for the six models studied in this work: (a) M2, (b) MS2, (c) MS6, (d) MS8, (e) MS10, and (f) MS12. Darker colors indicate regions of larger differences between the AME and the MDN predictions.

Quantum computers and quantum inforamtion

PHYSICAL REVIEW C **106**, 034325 (2022)

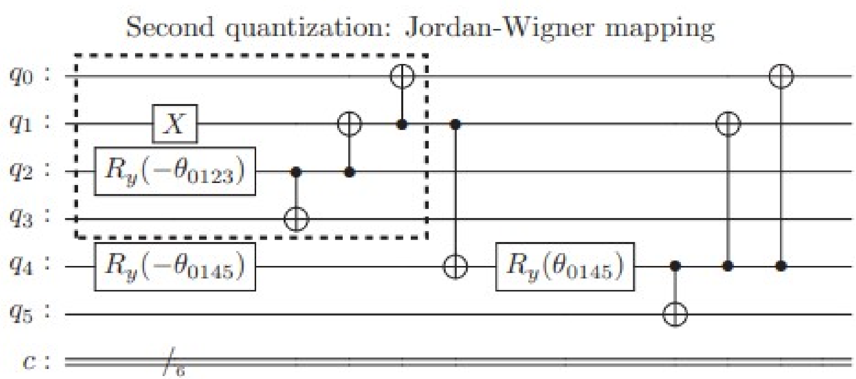
Quantum computing of the [6]Li nucleus via ordered unitary coupled clusters

PHYSICAL REVIEW C **106**, 024303 (2022)

Entanglement and seniority

- Simulating excited states of the Lipkin model on a quantum computer Phys. Rev. C 106, 024319

VARIATIONAL APPROACHES TO CONSTRUCTING THE … PHYSICAL REVIEW C **105**, 064308 (2022)



Accessing ground-state and excited-state energies in a many-body system after **symmetry restoration using quantum computers**
Phys. Rev. C 105, 024324

POOJA SIWACH AND P. ARUMUGAM PHYSICAL REVIEW C **105**, 064318 (2022)

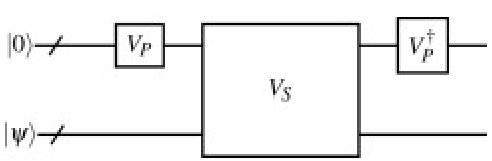


FIG. 1. The quantum circuit to calculate $\mathcal{O}|\psi\rangle$, where $\mathcal{O}$ is represented as a linear combination of unitaries (LCU) through V_P and V_S.

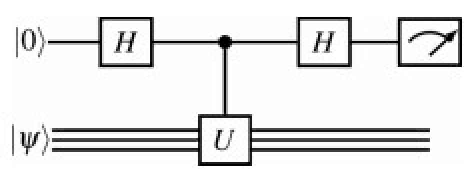
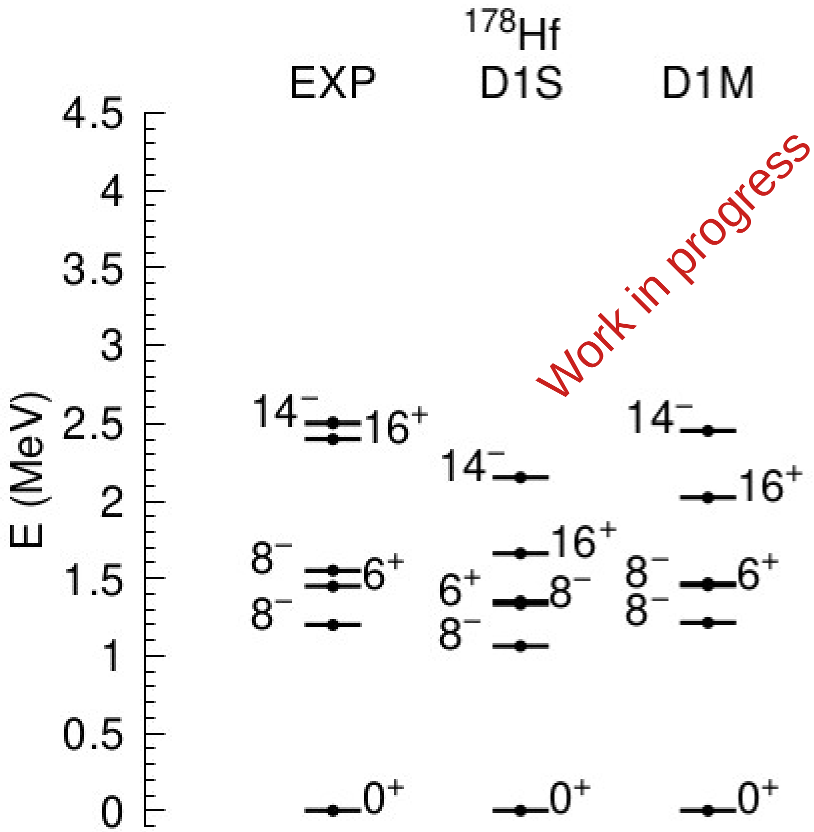


FIG. 3. The quantum circuit corresponding to Hadamard test (H-test) for calculating $\mathrm{Re}(\langle\psi|U|\psi\rangle)$.

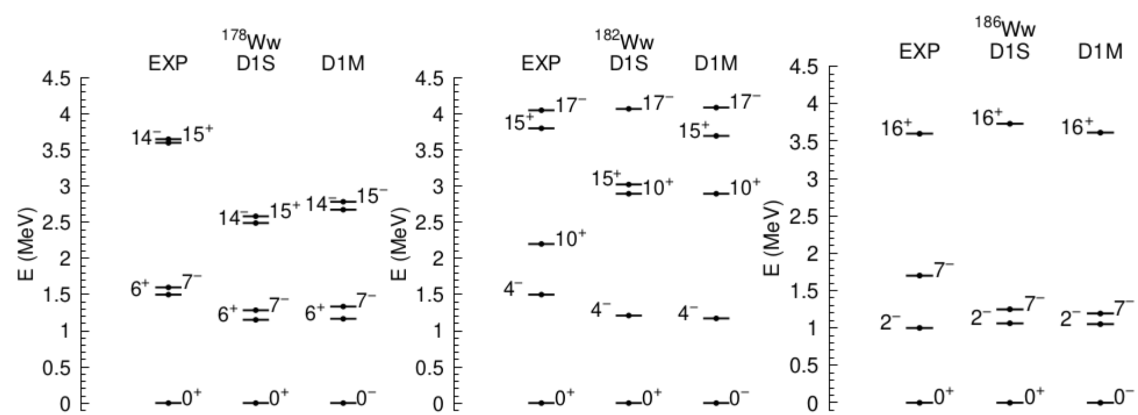
- Solving nuclear structure problems with the adaptive variational quantum algorithm, **Phys. Rev. C 105, 064317**

Described as **two, four, etc quasiparticle excitations** using **selfconsistent blocking** and taking into account all time-odd fields. The "universal" Gogny force is used.



- Preliminary results (LMR)
- Good agreement for excitation energies

- "Universal" Gogny gives predictive power
- As cranking and triaxial states can be treated on the same footing, opens up the door to understand the decay out of high-K isomeric states



Same technique can be extended to study 0+ states

Thank you for your attention !

Motivation