Collectivity in nuclei from abinitio methods

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Fundamental Physics with Radioactive Molecules

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Ab-initio description of Schiff moments in heavy deformed nuclei?

Computation of Schiff moment in ²²⁵Ra relevant for EDM searches in atoms and molecules. Schiff moment is particularly sensitive to octupole deformation







J. Dobaczewski and J. Engel, PRL 2005

½+ and ½- parity doublet in ²²⁵Ra differ by only 50keV

Trend in realistic ab-initio calculations

- Tremendous progress in recent years because of ideas from EFT and the renormalization group
- Computational methods with polynomial cost (coupled clusters equantum computing e)
- Ever-increasing computer power?



Development with time (top500.org)



Multiscale physics of nuclei from ab-initio methods



What is ab initio in nuclear theory? A. Ekström et al, Frontiers (2023)

"we interpret the ab initio method to be a systematically improvable approach for quantitatively describing nuclei using the finest resolution scale possible while maximizing its predictive capabilities"

- Nuclei exhibit multiple energy scales ranging from hundreds of MeV in binding energies to fractions of an MeV for low-lying collective excitations.
- Describing these different energy scales within a unified ab-initio framework from chiral interactions is a long-standing challenge

Solving the quantum many-nucleon problem

An exponentially hard problem to solve!

1.1 exaflops



 $H|\Psi\rangle = E|\Psi\rangle$ Polynomial scaling

Systematically improvable approaches with controlled approximations: Coupled-cluster, IMSRG, Gorkov, SCGF,...



Emulators?



IBM Q Experience

Fault tolerant quantum computing??

Coupled-cluster computations of deformed nuclei

The key lies in choosing the correct starting point



Coupled-cluster method



Coupled-cluster computations of deformed nuclei

- 1. Compute Hartree-Fock reference state
 - Nontrivial vacuum state informs us about emergent breaking of symmetries
 - Yields normal-ordered two-body Hamiltonian
- 2. Include dynamical (extensive) correlations via coupled-cluster theory
 - (or via IMSRG, or Gorkov methods, or Green's functions)
 - Cost increases polynomial with mass number
- 3. Perform symmetry projections
 - Non-extensive contributions to the energy
 - Often relevant for transition matrix elements



What's going with the charge radius at N = 20?

Interaction/method deficiency or something else?



S. J. Novario, G. Hagen, G. R. Jansen, T. Papenbrock, Phys. Rev. C 102, 051303 (2020)

Onset of deformation and shape coexistence in nuclei



Onset of deformation and shape coexistence along N = 20



Shape co-existence in ³²Mg







K. Wimmer et al, PRL (2010)

Collectivity in neutron-rich neon and magnesium isotopes from coupled-cluster methods



G. Hagen, S. J. Novario, Z. H. Sun, T. Papenbrock, G. R. Jansen, J. G. Lietz, T. Duguet, A. Tichai Phys. Rev. C 105, 064311 (2022)
 S. J. Novario, G. Hagen, G. R. Jansen, T. Papenbrock, Phys. Rev. C 102, 051303 (2020)

Symmetry restored coupled-cluster theory

Projection after
$$E^{(J)}=rac{\langle\Psi|P_JH|\Psi
angle}{\langle\widetilde{\Psi}|P_J|\Psi
angle}$$
 variation (PAV):

Right coupled-cluster state: $|\Psi
angle=e^{T}|\Phi_{0}
angle$

Left state is parametrized differently:

$$\langle \widetilde{\Psi} | = \langle \Phi_0 | (1 + \Lambda) e^{-T}$$

Bi-variational

$$P_J = \frac{1}{2} \int_0^{\pi} d\beta \sin(\beta) d_{00}^J(\beta) R(\beta)$$



Image credit: Wikimedia Commons

For axial symmetry around the zaxis the rotation operator is:

$$R(\beta) \equiv e^{i\beta J_y}$$

Symmetry restored coupled-cluster theory

The kernels can be evaluated by using Thouless theorem:

 $\langle \Phi_0 | R(\beta) = \langle \Phi_0 | R(\beta) | \Phi_0 \rangle \langle \Phi_0 | e^{V_1(\beta)}$

$$\mathcal{H}(\beta) = \langle \Phi | \overline{R}(\beta) | \Phi \rangle \langle \Phi | Z(\beta) \widetilde{H}(\beta) e^{V(\beta)} e^{T_2} | \Phi \rangle$$
$$\mathcal{N}(\beta) = \langle \Phi | \overline{R}(\beta) | \Phi \rangle \langle \Phi | Z(\beta) e^{V(\beta)} e^{T_2} | \Phi \rangle$$

Similarity transformed rotation operator and Hamiltonian:

 $\overline{R}(\beta) = e^{-T_1} R(\beta) e^{T_1}$ $\widetilde{H}(\beta) = e^{V_1(\beta)} \overline{H} e^{-V_1(\beta)}$

$$e^{V(\beta)}e^{T_2}|\Phi\rangle = e^{W_0(\beta) + W_1(\beta) + W_2(\beta) + \dots}|\Phi\rangle$$

- Does not truncate
- How to evaluate the disentangled amplitudes?
 [Qiu et al, J. Chem. Phys. 147, 064111 (2017)]

Solving for the disentangled amplitudes [Qiu et al]

Approximate:
$$e^{V(\beta)}e^{T_2}|\Phi\rangle \approx e^{W_0(\beta)+W_1(\beta)+W_2(\beta)}|\Phi\rangle$$

Taking the derivative with respect to β leads to a set of ODEs with initial conditions: $W_0(\beta = 0) = W_1(\beta = 0) = 0, W_2(\beta = 0) = T_2$ [Qiu et al, J. Chem. Phys. 147, 064111 (2017)]

- Approximate restoration of symmetries
- Can lead to stiffness as $dV(\beta)/d(\beta)$ might be large for $\langle \Phi | R(\beta) | \Phi \rangle \approx 0$.
- The truncation at W_2 might lead to loss of accuracy at larger angles
- Kernels are not symmetric around $\beta = \frac{\pi}{2}$



New approach to solve for disentangled amplitudes

We write: $e^{\lambda V} e^{T_2} |\Phi\rangle \approx e^{W_0(\lambda) + W_1(\lambda) + W_2(\lambda)} |\Phi\rangle$

Taking the derivative with respect to λ for fixed β leads to a new set of ODEs with initial conditions: $W_n(\lambda = 0) = T_n$

- Approximate restoration of symmetries
- Significantly improves stability of ODEs
- Kernels are fully symmetric around $\beta = \frac{\pi}{2}$

Zhonghao Sun, A. Ekstrom, C. Forssen, G. Hagen. G. R. Jansen, T. Papenbrock (2024)



Electromagnetic transitions

$$B(E2,\downarrow) \equiv |\langle 0^+ ||Q_2||2^+ \rangle|^2$$
$$B(E2,\downarrow) = \frac{\langle \widetilde{\Psi} | P_0 Q_{20} P_2 | \Psi \rangle \langle \widetilde{\Psi} | P_2 Q_{20} P_0 | \Psi \rangle}{\langle \widetilde{\Psi} | P_0 | \Psi \rangle \langle \widetilde{\Psi} | P_2 | \Psi \rangle}$$

Recall the left and right coupled-cluster states:

$$\langle \widetilde{\Psi} | \equiv \langle \Phi_0 | (1 + \Lambda) e^{-T} \qquad |\Psi\rangle \equiv e^T |\Phi_0\rangle$$

Zhonghao Sun, A. Ekstrom, C. Forssen, G. Hagen. G. R. Jansen, T. Papenbrock (2024)

Benchmarking projected coupled-cluster in ²⁰Ne



Inclusion of three-body forces

- The normal ordered 2-body approximation breaks rotational symmetry when normal-ordered with respect to a broken symmetry reference state
- Perform spherical HF with fractional filling to normal-order three-nucleon force
- Use normal-ordered Hamiltonian in the 2-body approximation in a second HF calculation of deformed nuclei
 Ω^π l_j Ω^π



Ground-state energies of neon isotopes



- Use natural orbitals for better convergence of triples excitations
- Computed binding energies overall in good agreement
- Triples excitations yield ~10% of CCSD correlation energy

Zhonghao Sun, A. Ekstrom, C. Forssen, G. Hagen. G. R. Jansen, T. Papenbrock (2024)

Collectivity in neon isotopes



Rotational structure of neutron-rich neon isotopes in good agreement with data Spectra of ³⁰⁻³⁴Ne follow

that of a rigid rotor E(J) \propto J(J + 1)

Small energies reflect a large moment of inertia and a strong deformation

Zhonghao Sun, A. Ekstrom, C. Forssen, G. Hagen. G. R. Jansen, T. Papenbrock (2024)

Shape co-existence in ³⁰Ne



Zhonghao Sun, A. Ekstrom, C. Forssen, G. Hagen. G. R. Jansen, T. Papenbrock (2024)

Shape co-existence in ³²Mg



Zhonghao Sun, A. Ekstrom, C. Forssen, G. Hagen. G. R. Jansen, T. Papenbrock (2024)

Deformation in neutron-rich magnesium



Ikuko Hamamoto, Phys. Rev. C 93, 054328 (2016)

Making sense of spectra in odd-mass nuclei



Rotational bands in odd-mass nuclei

Protons are paired Neutron occupy (j = d5/2, j_z=1/2, 3/2 and 5/2) Proton occupy (j = d5/2, j_z=3/2) Neutrons are paired.



Zhonghao Sun et al., in preparation (2024)

Onset of deformation around ⁷⁸Ni





T Otsuka and Y Tsunoda J. Phys. G 43 024009 (2016)



Deformed band? Where is the band head?



Onset of deformation around ⁷⁸Ni



Coupled-cluster computations of strongly deformed nuclei around ⁸⁰Zr



Coupled-cluster computations of strongly deformed nuclei around ⁸⁰Zr



Baishan Hu, Zhonghao Sun, G. Hagen, T. Papenbrock. in preparation (2024)

Coupled-cluster computations of strongly deformed nuclei around ⁸⁰Zr



Ab-initio description of Schiff moments in heavy deformed nuclei?



Ab-initio description of Schiff moments in heavy deformed nuclei?



What drives deformation in nuclei?

- 50's: surface vibrations of a liquid drop (Bohr/Mottelson)
- 60's: competition between pairing and quadrupole interactions from HFB calculations in two shells (Baranger/Kumar)
- 70's: isoscalar neutron-proton interactions dominate over isovector pairing from shell model (Federman/Pittel, Dufour/Zuker)



Nuclear deformation viewed at different resolution scales



Global sensitivity analysis

<u>Sensitivity analysis</u> addresses the question 'How much does each model parameter contribute to the uncertainty in the prediction?'

<u>Global</u> methods deal with the uncertainties of the outputs due to input variations over the whole domain.

Computational bottleneck

A global sensitivity analyses of properties of atomic nuclei typically would require more than one million model evaluations





- Eigenvector continuation method [Frame D. et al., Phys. Rev. Lett. 121, 032501 (2018), S. König et al Phys. Lett. B 810 (2020) 135814]
- Write the Hamiltonian in a linearized form

$$H(\vec{\alpha}) = h_0 + \sum_{i=1}^{N_{\rm LECs}=17} \alpha_i h_i$$

- Select "training points" (snap-shots) where we solve the exact problem
- Project a target Hamiltonian onto subspace of training vectors and diagonalize the generalized eigenvalue problem

$$\mathbf{H}(\vec{\alpha}_{\odot}) \ \vec{c} = E(\vec{\alpha}_{\odot}) \ \mathbf{N} \ \vec{c}_{\odot}$$











Reduced order model for projected Hartree-Fock

Deformation is long-wave length physics and accurately described at projected Hartree-Fock level Goal: Construct accurate emulator of projected Hartree-Fock

$$ig|\phi_{\odot}
angle = \sum_{i}^{n_{t}} c_{i} |\phi_{i}
angle$$
 $\sum_{ij} \langle \phi_{i} | H_{\mathrm{HF}}(\vec{\alpha}_{\odot}) | \phi_{j}
angle c_{j} = E_{\odot} \sum_{ij} \langle \phi_{i} | \phi_{j}
angle c_{j}$

Using Thouless theorem we can evaluate the norm and Hamiltonian kernels between nonorthogonal Hartree-Fock states

The target rotational states:
$$E_{\odot}^{(J)} = \frac{\langle \phi_{\odot} | P_J H(\vec{\alpha}_{\odot}) | \phi_{\odot} \rangle}{\langle \phi_{\odot} | P_J | \phi_{\odot} \rangle}$$

Linking deformation to nuclear forces





- Constructed accurate and efficient emulator of projected HF using 68 training vectors
- Training points obtained by using Latin Hypercube sampling within
 20% of original low-energy constants

Linking deformation to nuclear forces



- Deformation is mainly driven by the pion-nucleon coupling LEC c3 and short range contact C1S0
- Adding short-range repulsion increase deformation presumably by reducing pairing
- Increasing the pion-nucleon coupling strength also increases deformation, presumably by adding attraction in higher partial waves



M1 transition in ⁴⁸Ca

- Large $B(M1: 0^+ \rightarrow 1^+)$ due to strong $\nu 1f_{7/2} \rightarrow \nu 1f_{5/2}$ excitation
- Darmstadt results are consistent with strong quenching factor (0.75) for the isovector strength
- Similarity of 1B operators in spinflip M1 and GT transitions has been used as explanation for strong quenching. We test this by explicitly including 2B operators.



Figure adapted from PRC 93, 041302(R) (2016)



Bijaya Acharya et al., arXiv:2311.11438

The resonant 1⁺ state in ⁴⁸Ca at 10.224 MeV



Scattering / reactions that probe the 1^+ state: (e, e'), (p, p'), (p, n), or (γ, n)

Simple picture of the 1⁺ state: neutron 1p-1h excitation; extreme single-particle model: $B(M1) = 12 \mu_N^2$



The resonant 1⁺ state in ⁴⁸Ca at 10.224 MeV



	S_n	ΔE	Γ	1p-1h
Interaction	(MeV)	$({ m MeV})$	(keV)	
$\Delta NNLO_{GO}(394)$	9.74	-0.44	0	91%
$\Delta NNLO_{GO}(450)$	9.38	-1.26	0	91%
NNLO _{sat}	9.34	-0.23	0	91%
1.8/2.0(EM)	10.00	0.55	4	92%
Experiment	9.95	0.28	≤ 17	

Bijaya Acharya et al., arXiv:2311.11438

The l = 3 orbital angular-momentum barrier permits a neutron resonant state

The magnetic dipole transition in ⁴⁸Ca



Two-body currents do not quench M1 transitions in light nuclei

$(J_i^\pi o J_f^\pi)$	$M1$ and Γ	IA	MEC	Total	Expt.
${}^{6}\text{Li}(0^{+} \rightarrow 1^{+})$	M1	3.63(1)	0.38	4.01(1)	
	Γ(eV)	6.90(2)		8.41(3)	8.19(17)
$^{7}\mathrm{Li}(\frac{1}{2}^{-} \rightarrow \frac{3}{2}^{-})$	M1	2.66(1)	0.47(1)	3.13(2)	
	$\Gamma(10^{-3} \text{ eV})$	4.47(5)		6.19(8)	6.30(31)
$^{7}\text{Be}(\frac{1}{2}^{-} \rightarrow \frac{3}{2}^{-})$	M1	2.31(2)	0.41(1)	2.72(2)	
	$\Gamma(10^{-3} \text{ eV})$	2.44(4)		3.39(6)	3.43(45)
$^{8}\text{Li}(1^{+} \rightarrow 2^{+})$	M1	3.47(4)	0.74(2)	4.21(5)	
	$\Gamma(10^{-2} \text{ eV})$	4.4(1)		6.5(2)	5.5(1.8)
$^{8}\mathrm{B}(1^{+}\rightarrow2^{+})$	M1	3.17(5)	0.67(2)	3.84(6)	
	$\Gamma(10^{-2} \text{ eV})$	1.8(1)		2.6(1)	2.52(11)
$^{8}\text{Li}(3^{+} \rightarrow 2^{+})$	M1	0.98(6)	0.20(5)	1.17(8)	
	$\Gamma(10^{-2} \text{ eV})$	1.8(2)		2.6(3)	7.0(3.0)
$^{8}\mathrm{B}(3^{+}\rightarrow2^{+})$	M1	1.31(6)	0.23(5)	1.56(8)	
	$\Gamma(10^{-2} \text{ eV})$	3.5(3)		4.9(5)	10(5)
${}^{9}\mathrm{Li}(\frac{1}{2}^{-} \rightarrow \frac{3}{2}^{-})$	M1	2.28(3)	0.36(4)	2.64(5)	
	$\Gamma(10^{-1} \text{ eV})$	5.9(2)		7.9(3)	n.a.
${}^{9}\text{Be}(\frac{5}{2}^{-} \rightarrow \frac{3}{2}^{-})$	M1	1.42(3)	0.20(2)	1.62(4)	
	$\Gamma(10^{-2} \text{ eV})$	5.6(3)		7.2(4)	8.9(1.0)

Pastore, Pieper, Schiavilla, Wiringa, Phys Rev C 87, 035503 (2013)

Magnetic dipole transition in ⁴⁸Ca



Summary

- Neutron-rich neon isotopes are strongly deformed: ³⁴Ne as rotational as ³²Ne and ³⁴Mg
- Electromagnetic transitions follow experimental trends
- Signatures of shape co-existence along N = 20 towards ²⁸O
- Nuclei around ⁸⁰Zr are strongly deformed with rich prolate and oblate structure
- Predict low-lying rotational states in ⁷⁸Ni consistent with data and shell-model predictions
- Towards Schiff moment calculations in ²²⁵Ra

Summary

- The discrepancy between (e, e') and (γ, n) experiments regarding B(M1) in ⁴⁸Ca is puzzling
- Our ab initio computations based on chiral effective field theory, including treatment of the state as a resonance, yield $7\mu_N^2 < B(M1) < 10 \ \mu_N^2$
 - Two-body currents do not yield a quenching
- Resolution of this situation will impact ab initio computations and/or theory of neutrino-nucleus reactions relevant for supernova signals and dynamics

Thank you for your attention!