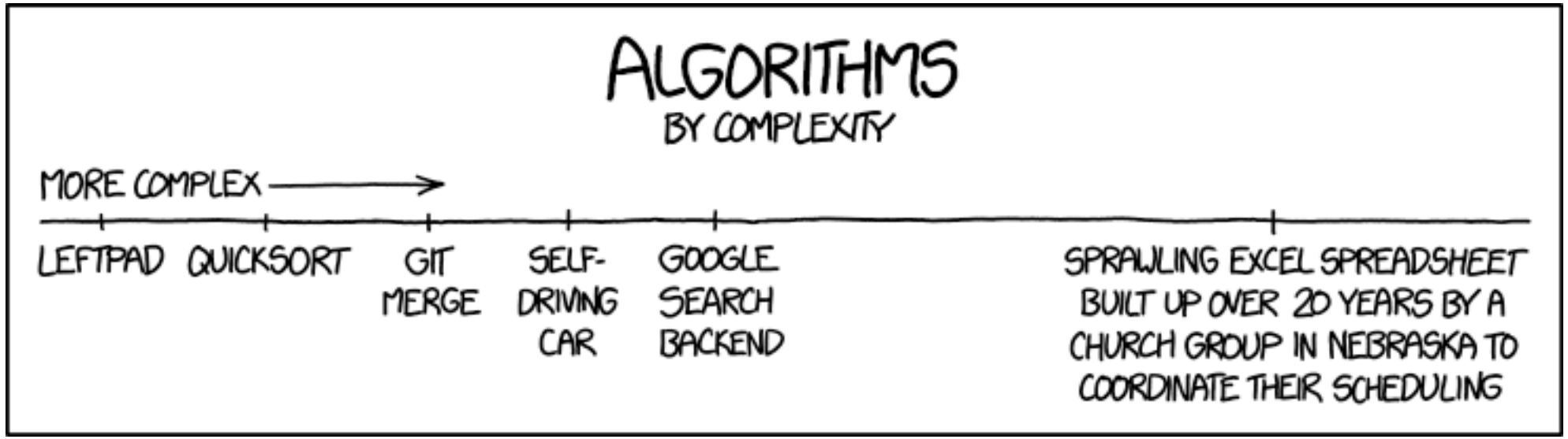
How hard is it to compute an atomic nucleus?



Credit: xkcd

Thomas Papenbrock
University of Tennessee & Oak Ridge National Laboratory

TRIUMF workshop on *Progress in Ab Initio Nuclear Theory*, 3/1/2023

SciDAC
Scientific Discovery through Advanced Computing

Work supported by the US Department of Energy

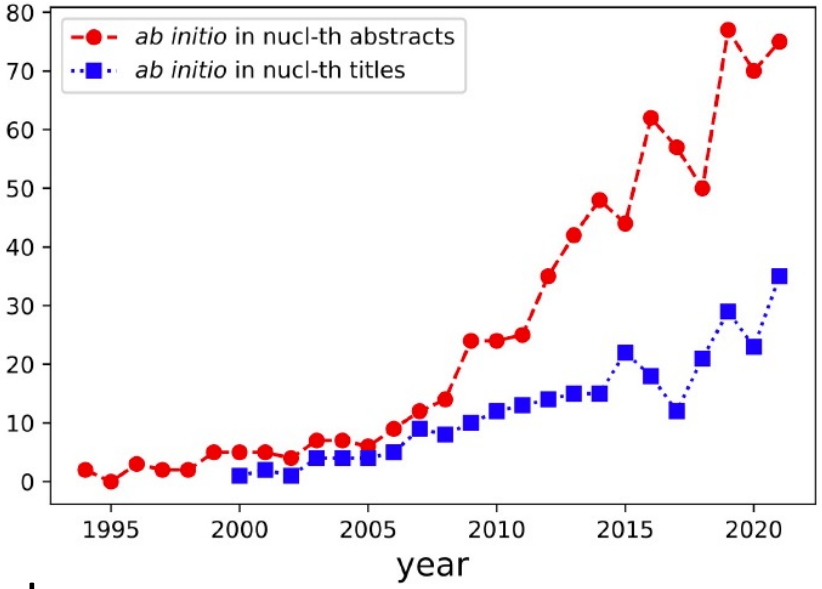
NUCLEI
Nuclear Computational Low-Energy Initiative
A SciDAC-5 collaboration

Collaborators

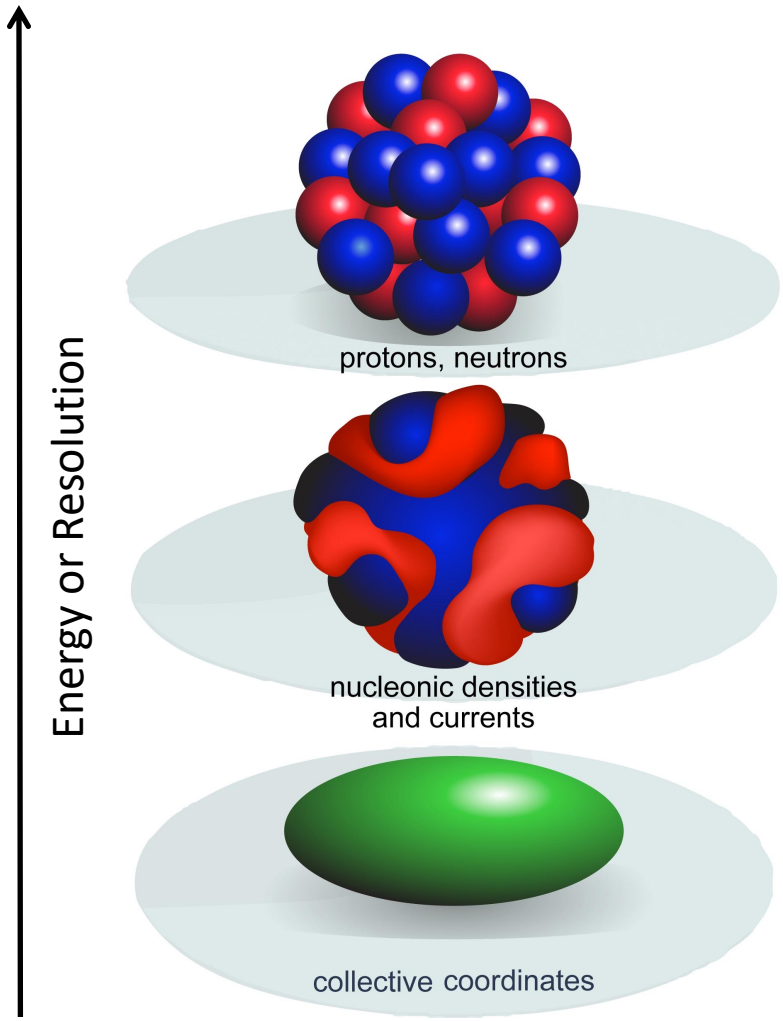
- ORNL: G. Hagen, G. Jansen, J. Lietz, **Zhonghao Sun**
- U of Tennessee: **Charles Bell**
- LANL: **Sam Novario**
- Saclay: T. Duguet
- TU Darmstadt: **Alex Tichai**

Incomplete and personal list: What's hard in ab initio

- Constructing accurate interactions
  - "Magic" 1.8/2.0, $NNLO_{sat}$, NLEFT, $\Delta NNLO_{GO}$, local-nonlocal, LENPIC, Norfolk, …
    - Evergreen
    - Been there, done that, check
- Convincing folks that ab initio does not end at mass 16
  - Coupled cluster, Green's functions, IMSRG, NLEFT, …
    - Google "ab initio" and "gruyere" for recent thoughts on this
- Deformed nuclei
  - NCSM, sym adap NCSM, IMSRG, Green's functions, coupled cluster
    - Ongoing



How hard should it be to compute rotational bands in chiral EFT?



Energy (MeV)

8 proton separation energy in lead

1.12 vibrational state in tin

0.043 rotational state in uranium

Ab initio methods: Clusters … supercomputers

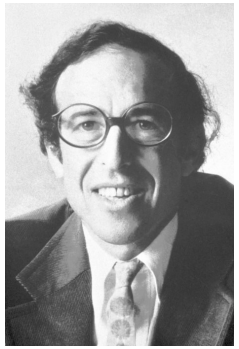
Density functional theory / GCM: Single CPU

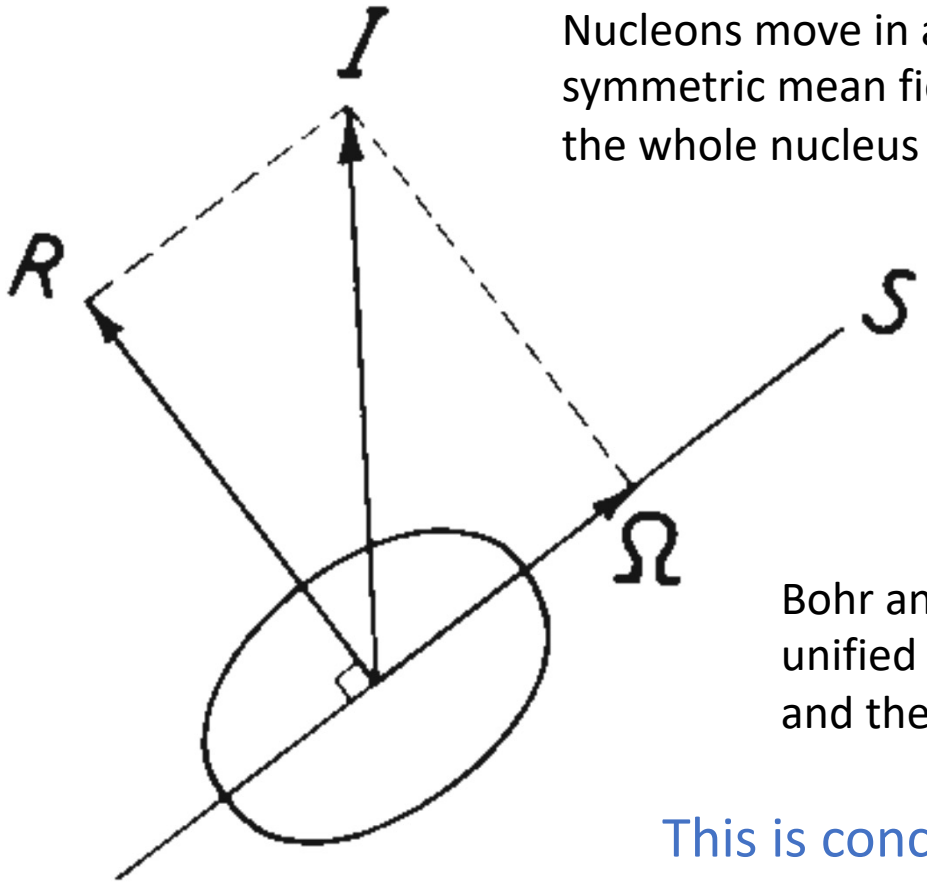
Collective models / EFTs: Pencil and paper

Ab initio computations of rotational bands within the NCSM / sym-adapt NCSM: Caprio, Draayer, Dytrych, Fasano, Launey, Maris, McCoy, Mersenne; Vary …

Fig.: Bertsch, Dean, Nazarewicz (2007)

1975 Nobel Prize for 1950s work: Aage Bohr, Ben Mottelson, Leo Rainwater



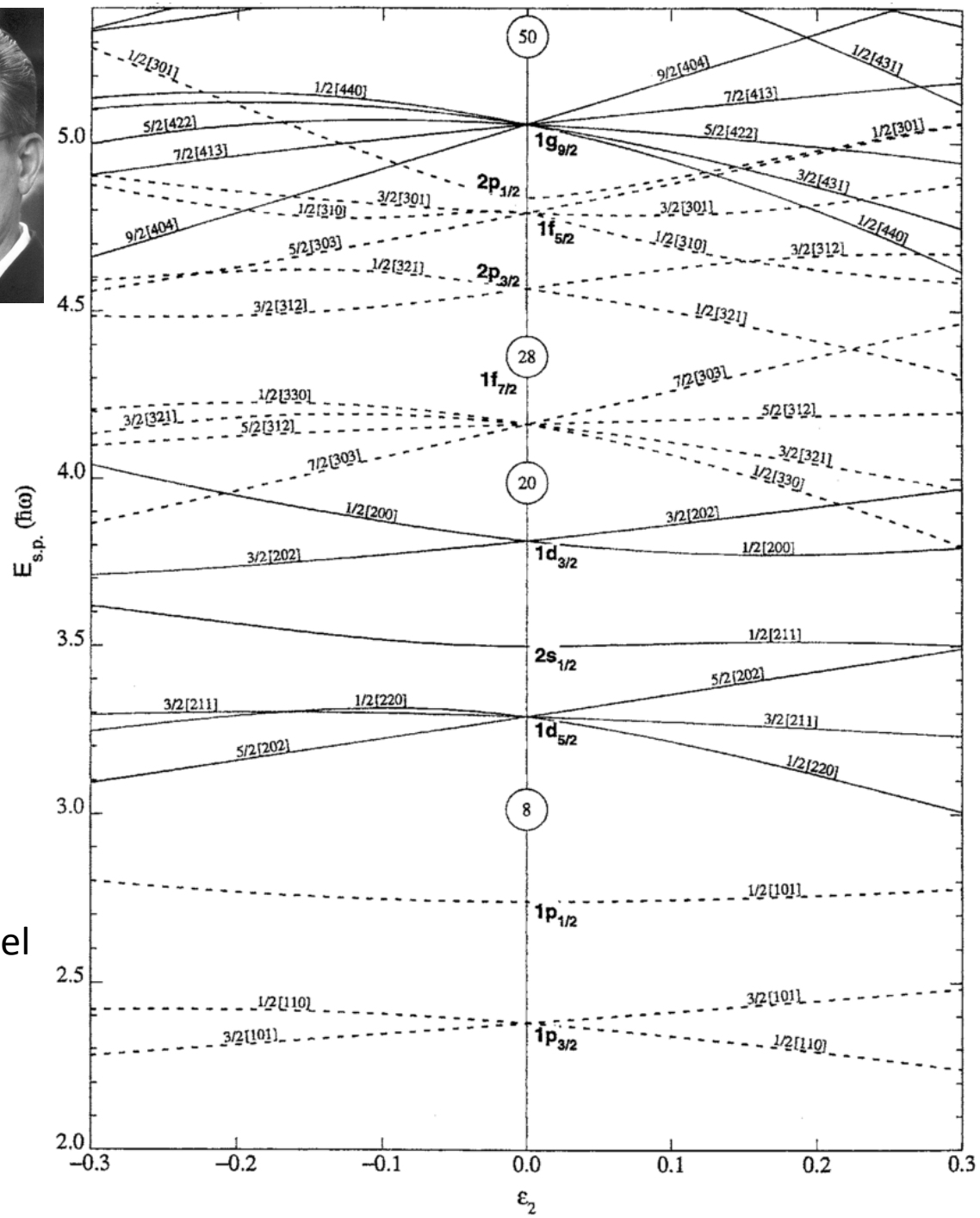


A. Bohr (1950s)

Nucleons move in an axially symmetric mean field and the whole nucleus rotates

Bohr and Mottelson's model unified the spherical shell model and the liquid drop model

This is conceptually simple!

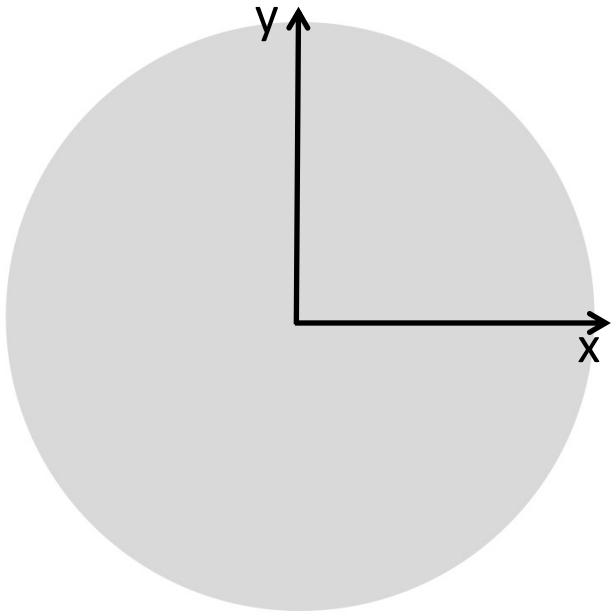


70 years later: Chiral EFT confirms Bohr and Mottelson's unified model

[Bally, Barbieri, Duguet, Ebran, Frosini, Hagen, Hergert, Jansen, Novario, TP, Ripoche, Roth, Soma, Sun, Tichai, …]

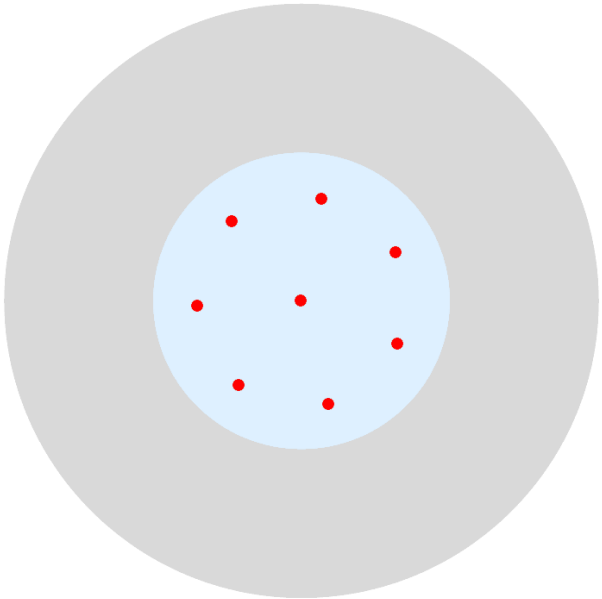
1. Take Hamiltonians from chiral effective field theory
2. Perform Hartree-Fock or Hartree-Fock-Bogoliubov computation
   a. Yields non-trivial vacuum state $|\Phi\rangle$
   b. Informs us about nuclear deformation and superfluidity
   c. Introduces Fermi momentum k_F as the dividing scale between IR and UV
   d. Allows us to normal-order Hamiltonian w.r.t. $|\Phi\rangle$
3. Include correlations / entanglement via your favorite method (Coupled-cluster theory, Green's function method, IMSRG, MBPT …)
   a. 2-particle–2-hole (2p-2h) excitations and 3p-3h excitations (UV physics) dominate size-extensive contributions to the binding energy
   b. Symmetry restoration and collective modes yield smaller (not size extensive) contributions

Hartree-Fock computation

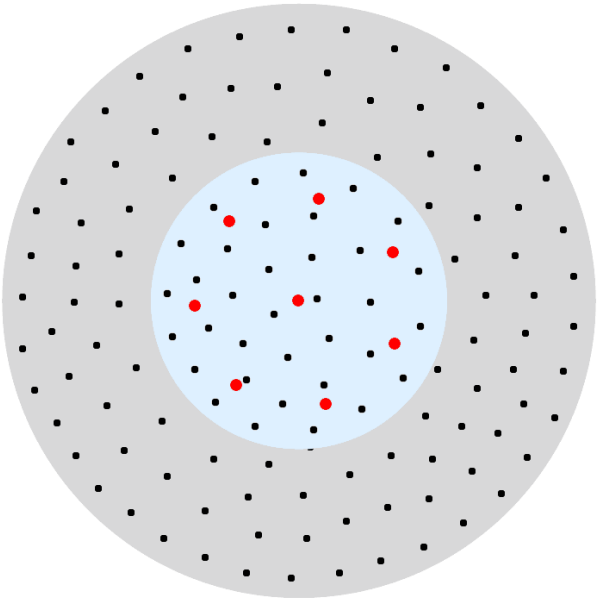


Hilbert space: Single particle states fill part of position space.

HF calculation: Divides Hilbert space into hole space (blue area with nuclear radius R) and particle space (grey remainder)

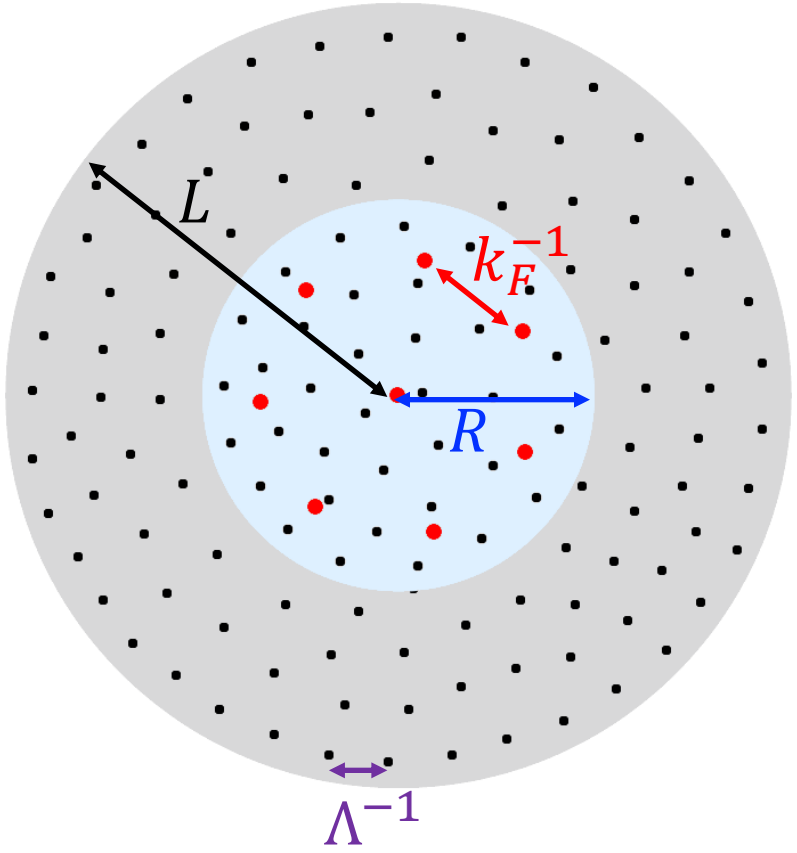


Hole space: Introduce localized basis functions (centered at red points) via unitary transformation; distance of points $\sim k_F^{-1}$.
Edmiston & Ruedenberg, RMP 1963; Høyvik et al, JCP 2012



Particle space: Introduce localized basis functions (centered at black points); distance of points $\sim \Lambda^{-1}$.

Efficient bases for post-HF methods



Localized bases scale efficiently

Hole space: A, particle space: n_u
Relevant particle space: $A(\Lambda/k_F)^3 \ll n_u$, or $(R/L)^3 n_u \ll n_u$

1. Natural orbitals probably are localized states [Tichai et al, Phys. Rev. C 99, 034321 (2019)]
2. Entanglement entropy between particle and hole space fulfills a volume law [Chenyi Gu et al in preparation (2023)]
3. Localized basis essential for quantum computing

Coupled-cluster computations

$$\overline{H} \equiv \mathrm{e}^{-T} H_N \mathrm{e}^{T}$$

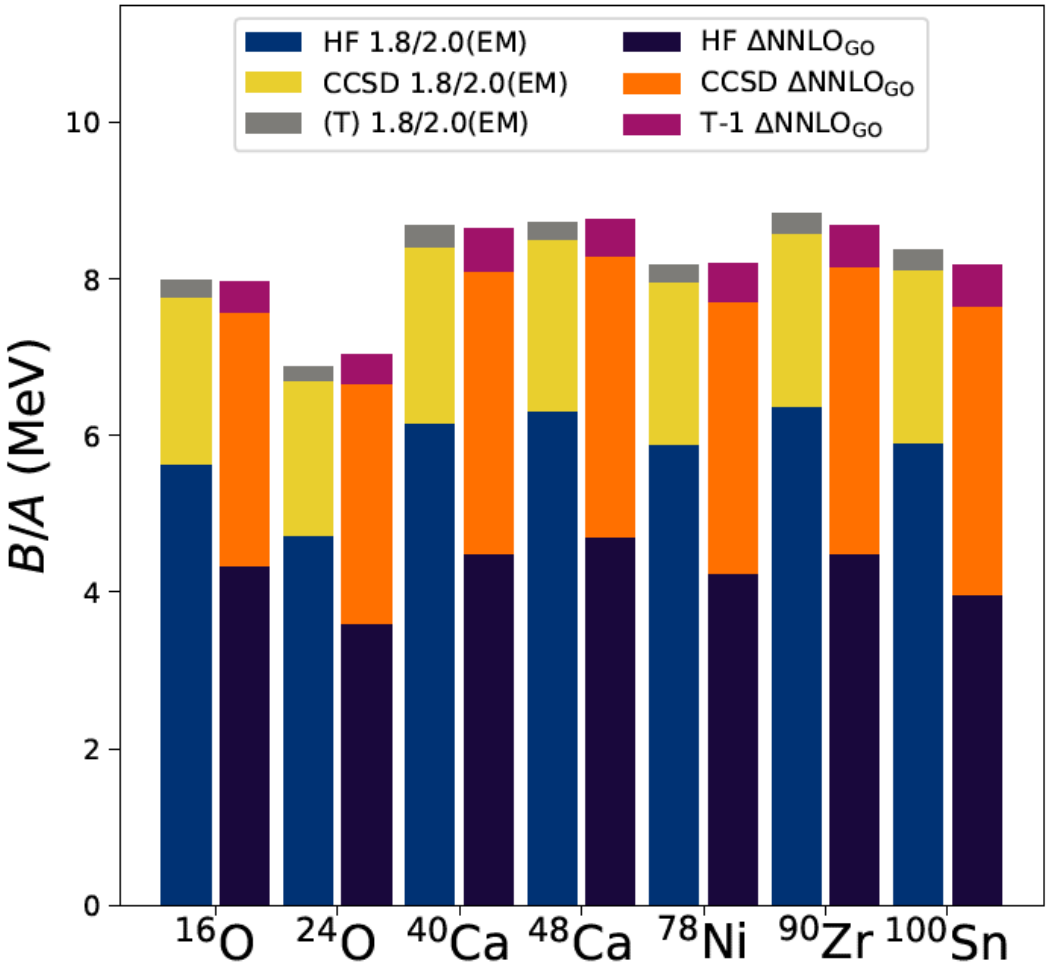
$$T = T_1 + T_2 + \cdots + T_A$$

$$T_1 = \sum_{ia} t_i^a a_a^\dagger a_i \ ,$$

$$T_2 = \frac{1}{4} \sum_{ijab} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i$$

Correlation energy in HF basis $E_{corr} = \frac{1}{4}\sum_{ijab} t_{ij}^{ab} H_{ab}^{ij}$

- Scaling: $E_{corr} \sim A$ though $1 \leq i, j \leq A$
- $H_{ab}^{ij} \neq 0$ only for $\langle i, j \rangle$ being neighbors
- $\sum_{ijab} \rightarrow \sum_{\langle i,j \rangle ab} \sim A$
- Only short-range correlations yield size-extensive contributions to the energy



Adapted from, Z.H. Sun, C. Bell, G. Hagen, TP (2022)

Projection onto good angular momentum

Projected energies

$$E^{(J)} = \frac{\int_0^\pi \mathrm{d}\beta \sin\beta d^J_{00}(\beta)\mathcal{H}(\beta)}{\int_0^\pi \mathrm{d}\beta \sin\beta d^J_{00}(\beta)\mathcal{N}(\beta)}$$

We follow:

- Qiu, Henderson, Scuseria, …
- Tsuchimochi & Ten'no
- Duguet, …

Approach 1: Coupled cluster kernels

$$\mathcal{N}(\beta) = \langle\Phi|R(\beta)|\Phi\rangle\langle\Phi|e^V e^T|\Phi\rangle\,,$$
$$\mathcal{H}(\beta) = \langle\Phi|R(\beta)|\Phi\rangle\langle\Phi|e^V H e^T|\Phi\rangle$$

Disentangled formalism

$$e^V e^T|\Phi\rangle \equiv e^{W_0+W_1+W_2+\cdots}|\Phi\rangle$$

Approach 2: Hermitian kernels

$$\mathcal{N}_H(\beta) \equiv \langle\Psi|R(\beta)|\Psi\rangle\,,$$
$$\mathcal{H}_H(\beta) \equiv \langle\Psi|R(\beta)H|\Psi\rangle$$

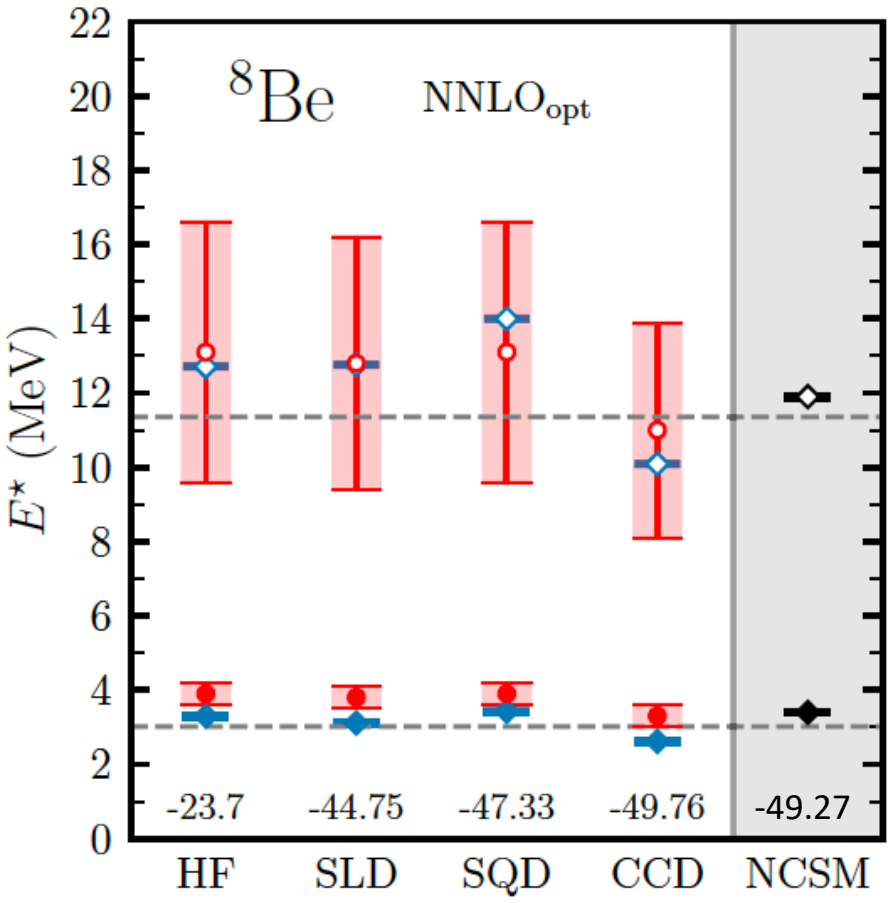
$$|\Psi_{\mathrm{SQD}}\rangle \equiv e^{T_1}\left(1+T_2+\frac{1}{2}T_2^2\right)|\Phi\rangle$$

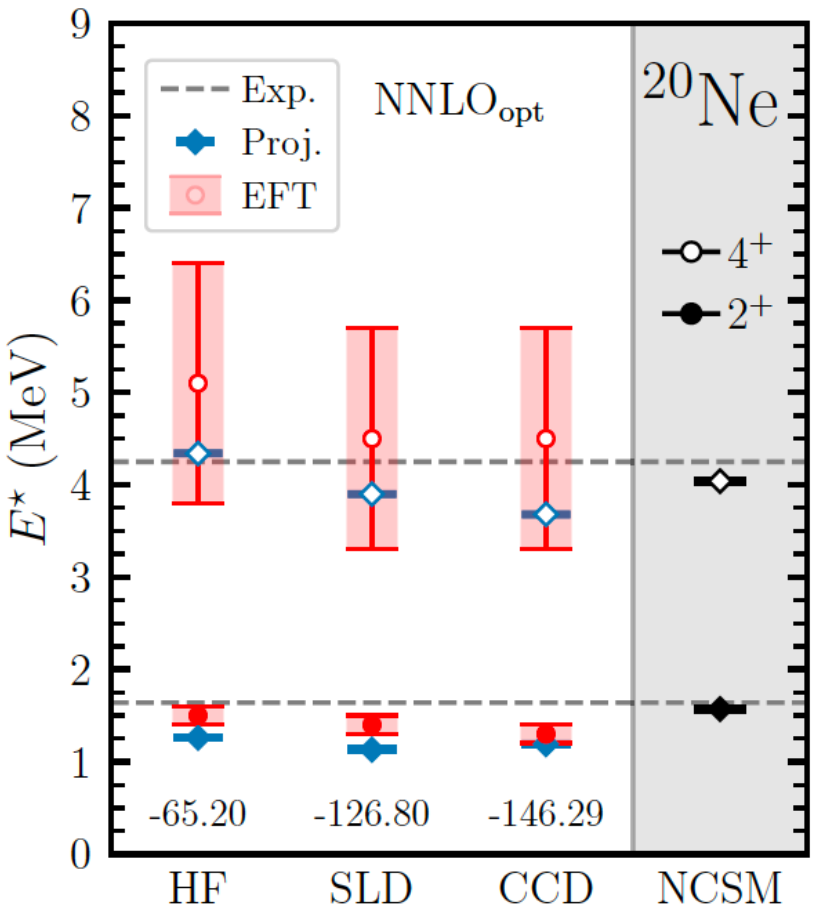
$$|\Psi_{\mathrm{SLD}}\rangle \equiv e^{T_1}\left(1+T_2\right)|\Phi\rangle$$

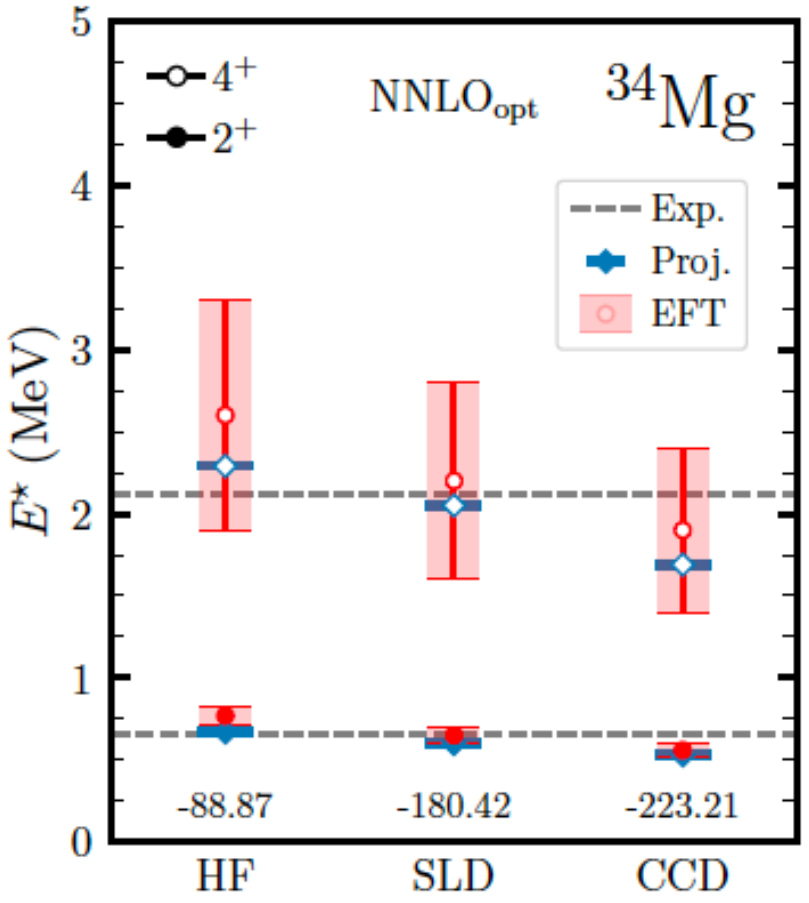
Computation ($NNLO_{opt}$) for ^{8}Be, ^{20}Ne, and ^{34}Mg

Benchmarks from NCSM
Caprio, Maris, Vary & Smith (2015)

Benchmarks from sym-adap NCSM
Dytrych, Launey et al. (2020)



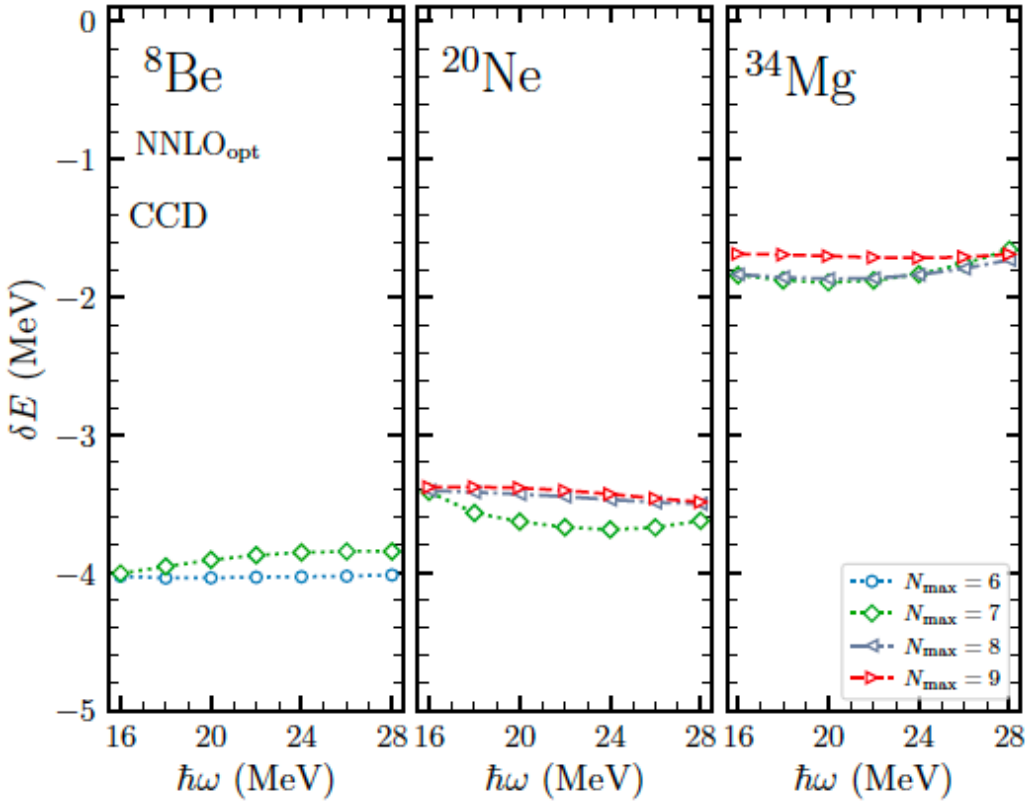




CCD spectra a bit too compressed, but we are getting there … . Note accuracy of projected HF

Hagen, Novario, Sun, TP, Jansen, Lietz, Duguet, Tichai, Phys Rev C 105, 064311 (2022)

Energy gain from projection decreases with increasing mass number



Rotation of the nucleus contains Ap-Ah excitations

The energy gain is not extensive (i.e. not proportional to mass number A)

The angular momentum expectation value decreases from Hartree-Fock (ref) to coupled cluster singles & doubles (SD) to triples (SDT-1)

	E_{ref}	$\langle J^2\rangle_{\text{ref}}$	$\langle Q_2\rangle_{\text{ref}}$	ΔE_{SD}	$\langle J^2\rangle_{\text{SD}}$	$\langle Q_2\rangle_{\text{SD}}$	$\Delta E_{\text{SDT}-1}$	$\langle J^2\rangle_{\text{SDT}-1}$	$\langle Q_2\rangle_{\text{SDT}-1}$	δE_{est}	E	E_{Exp}
^{8}Be	−16.74	11.17	19.46	−30.26	6.69	19.64	−3.24	5.82	18.86	−3.33	−53.58	−56.50
^{20}Ne	−59.62	21.26	35.84	−91.06	14.71	36.34	−11.27	12.09	35.71	−2.26	−164.21	−160.64
^{34}Mg	−90.21	22.62	38.56	−153.57	18.40	38.38	−20.56	15.03	36.97	−1.50	−265.84	−256.71

Matching to EFTs of rotations or pairing rotations

EFTs can be used for uncertainty estimates on ab initio computations without symmetry restoration

Energy gain from projection of angular momentum [Peierls & Yoccoz 1957; Novario et al 2022]

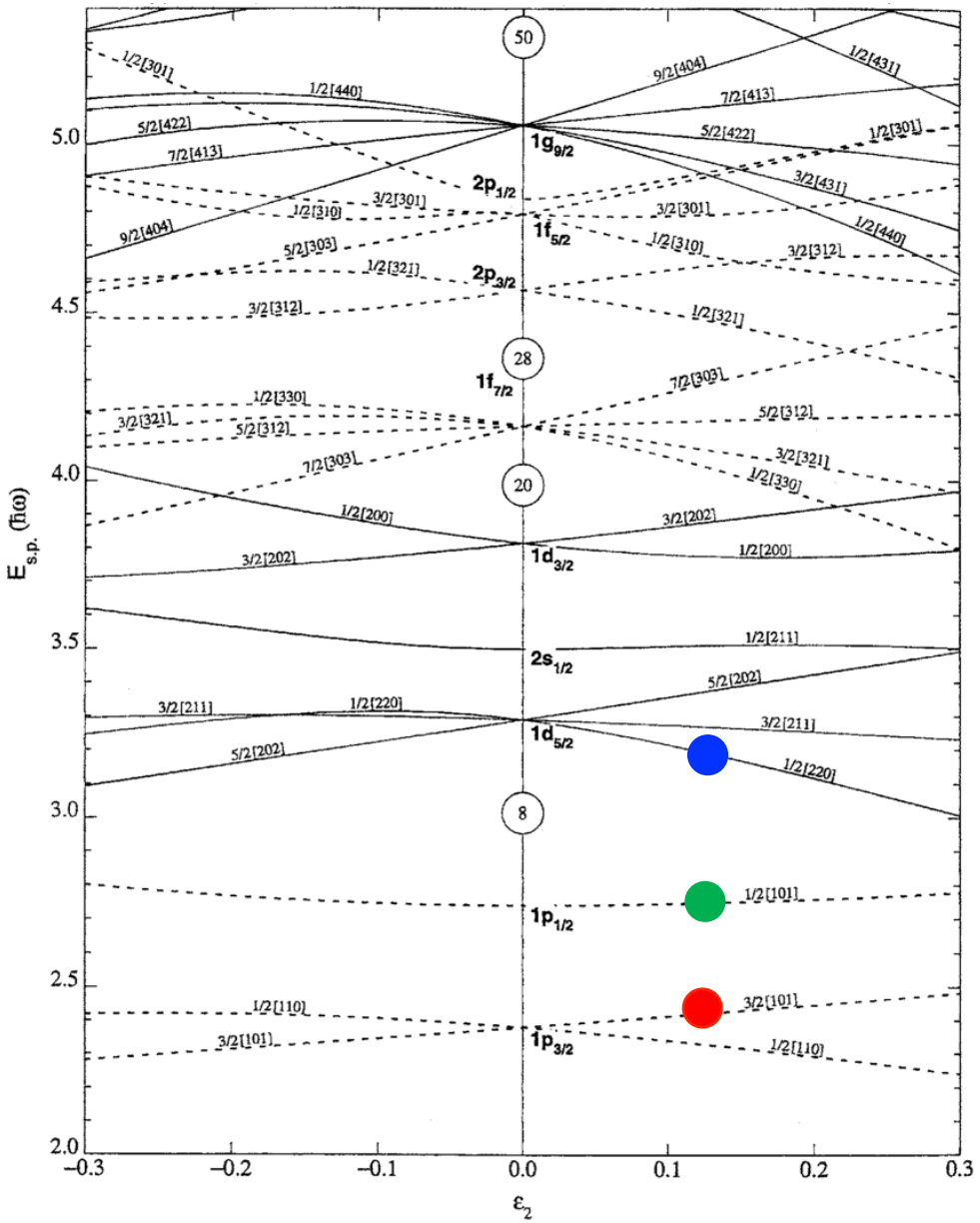
$$\delta E \approx (E_0 - E_2)\frac{\langle J^2 \rangle}{6}$$

Energy gain from projection of particle number [TP 2022]

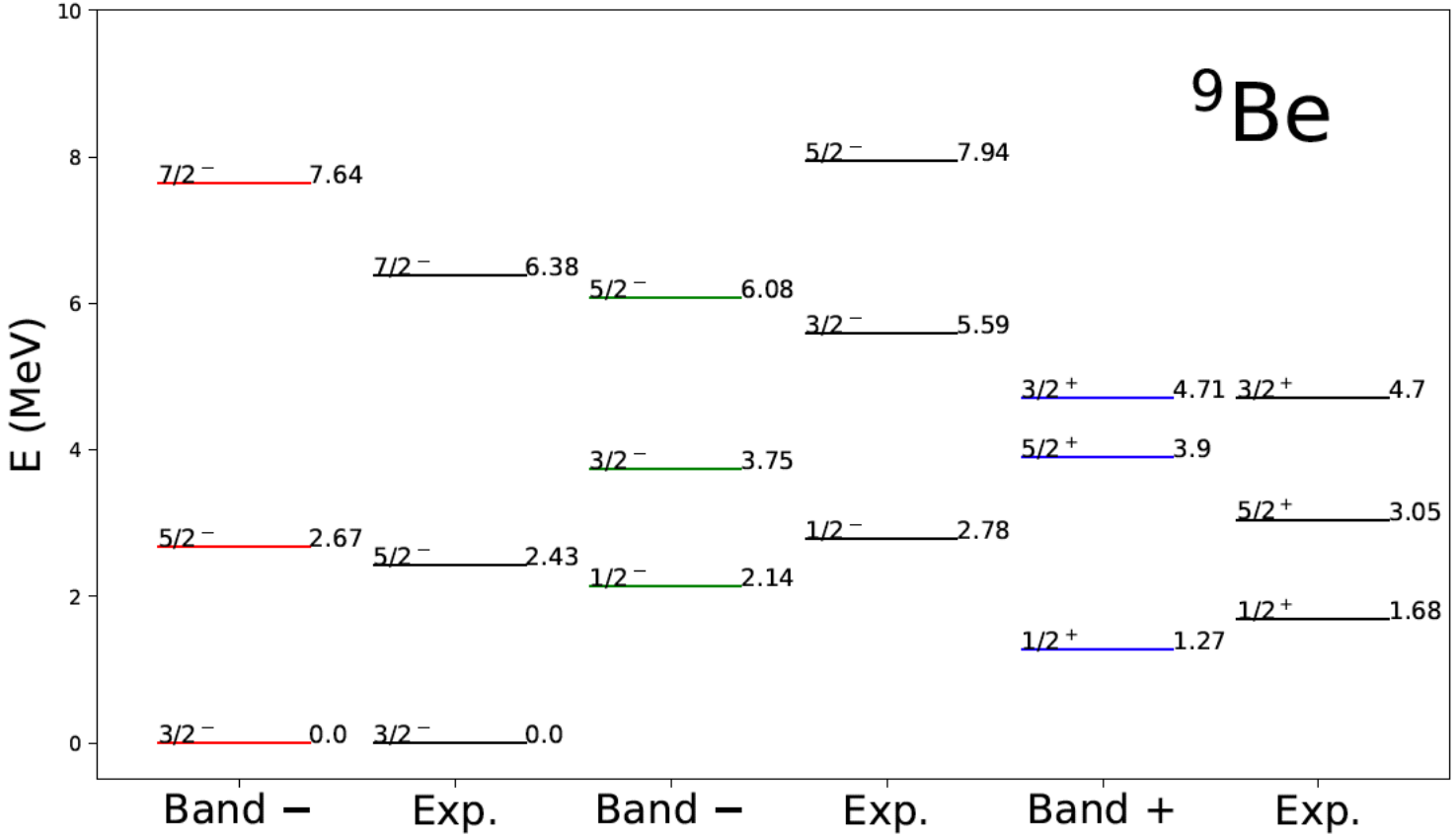
$$\delta E \approx (E_{N+2} - 2E_N + E_{N-2})\frac{\langle \Delta N^2 \rangle}{8}$$

Energy gained from projections vanishes for $A \to \infty$ (because symmetry is then spontaneously broken)

^{9}Be

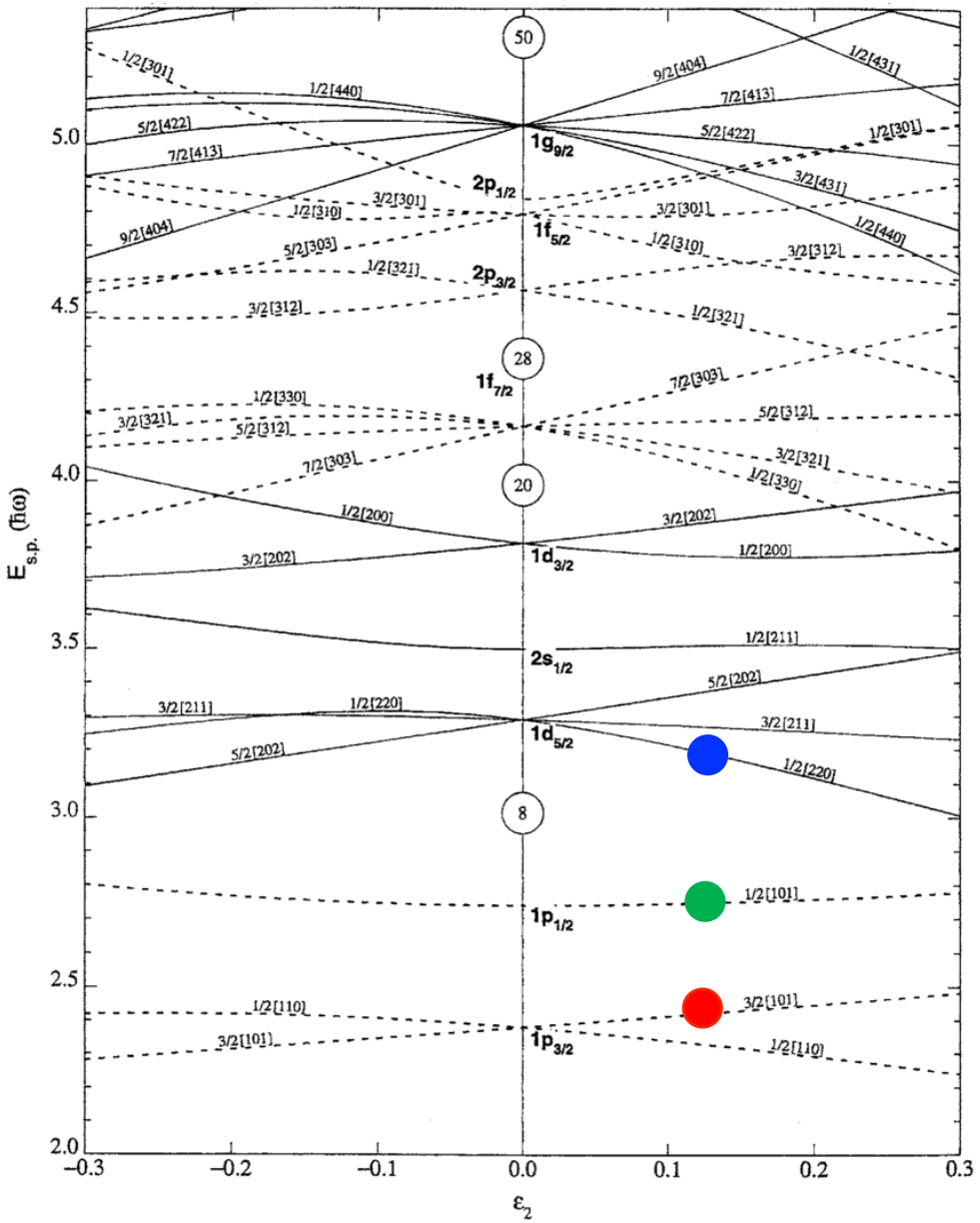


Bands computed by different fillings of the odd neutron
(NNLO$_{\text{opt}}$, projected HF, $N_{max} = 12$)

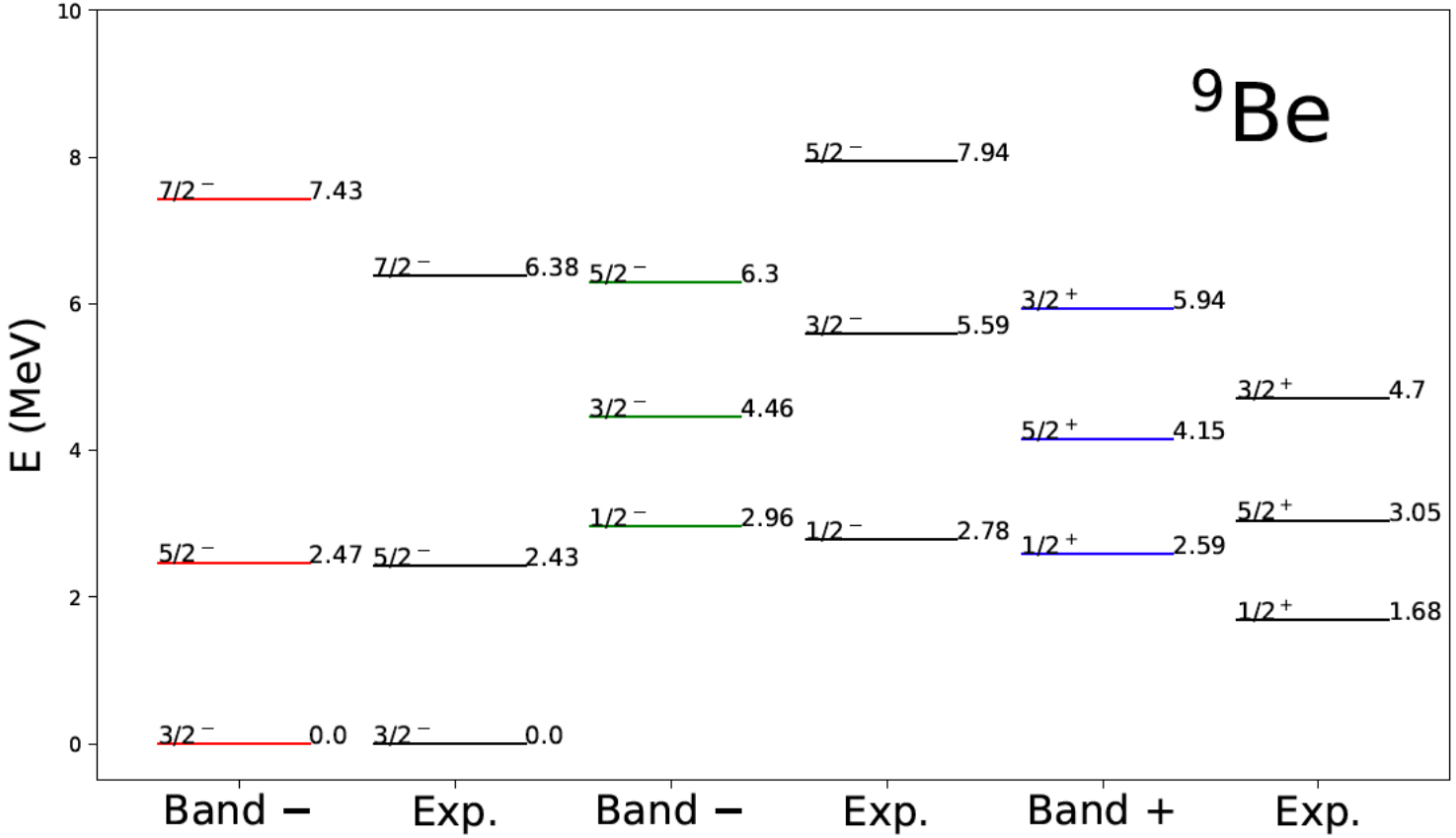


Zhonghao Sun, Hagen, TP, in preparation

^{9}Be

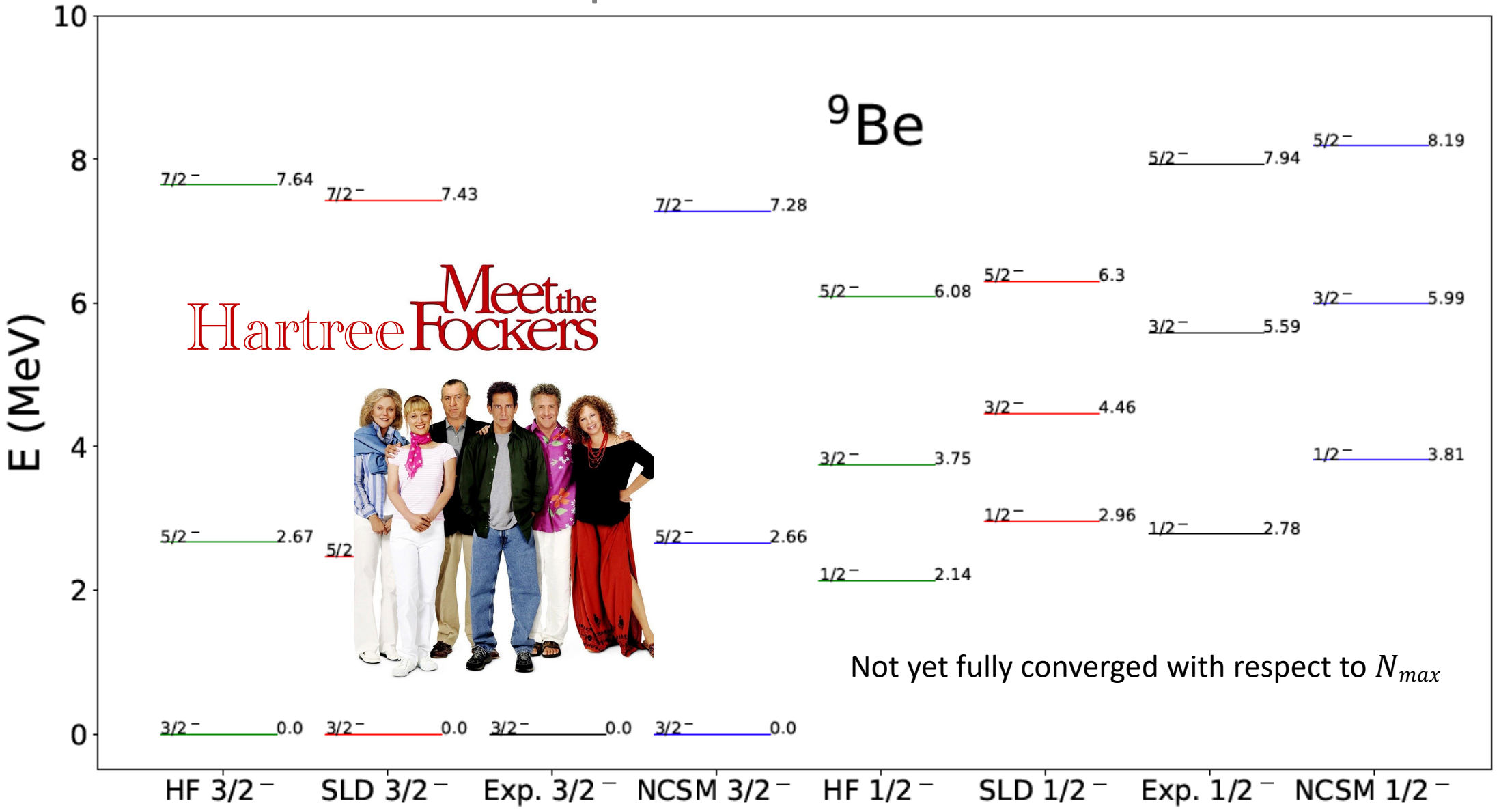


Bands computed by different fillings of the odd neutron
(NNLO$_{opt}$, projected coupled cluster SLD approximation, $N_{max} = 8$)



Zhonghao Sun, Hagen, TP, in preparation

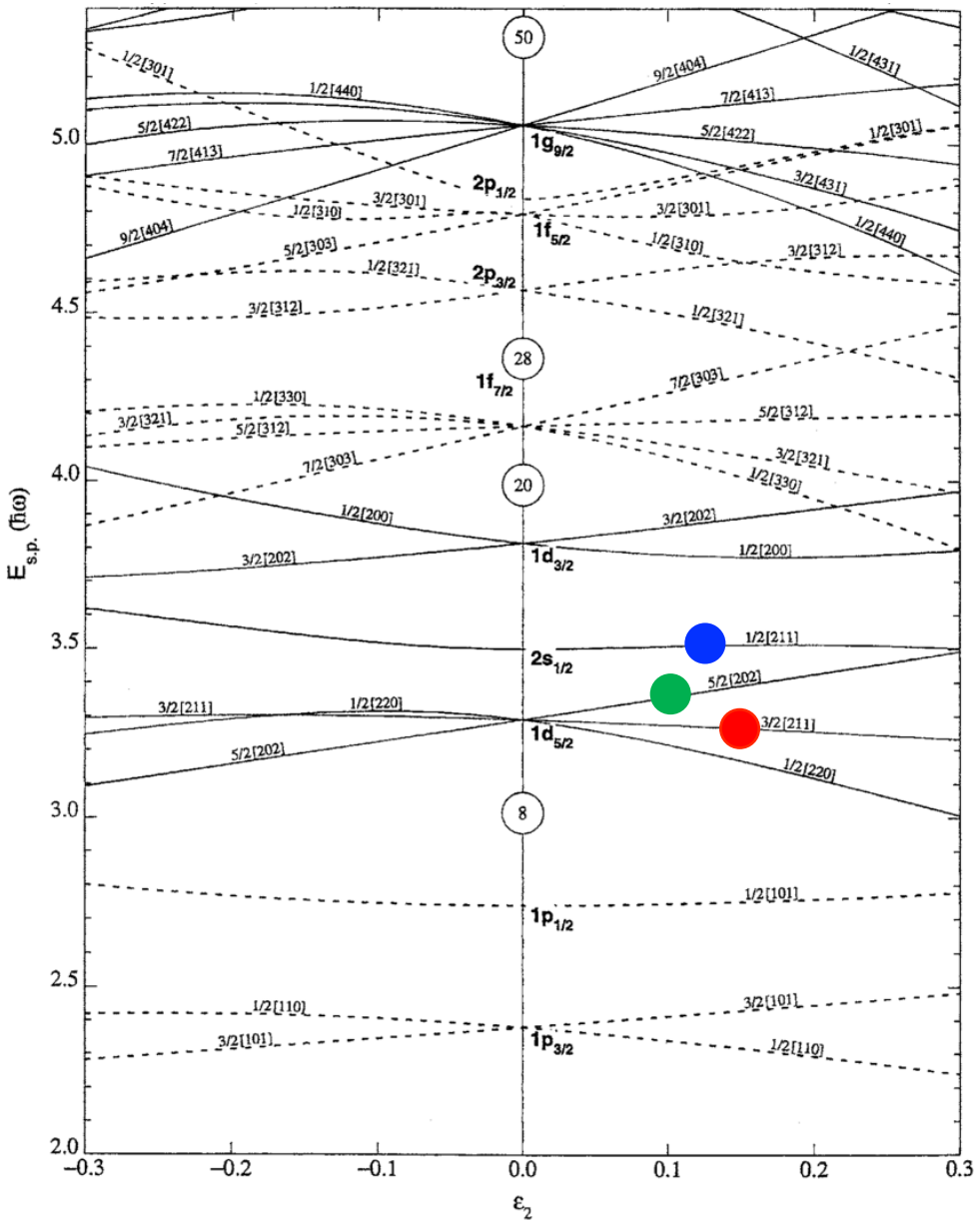
^{9}Be comparison with NCSM



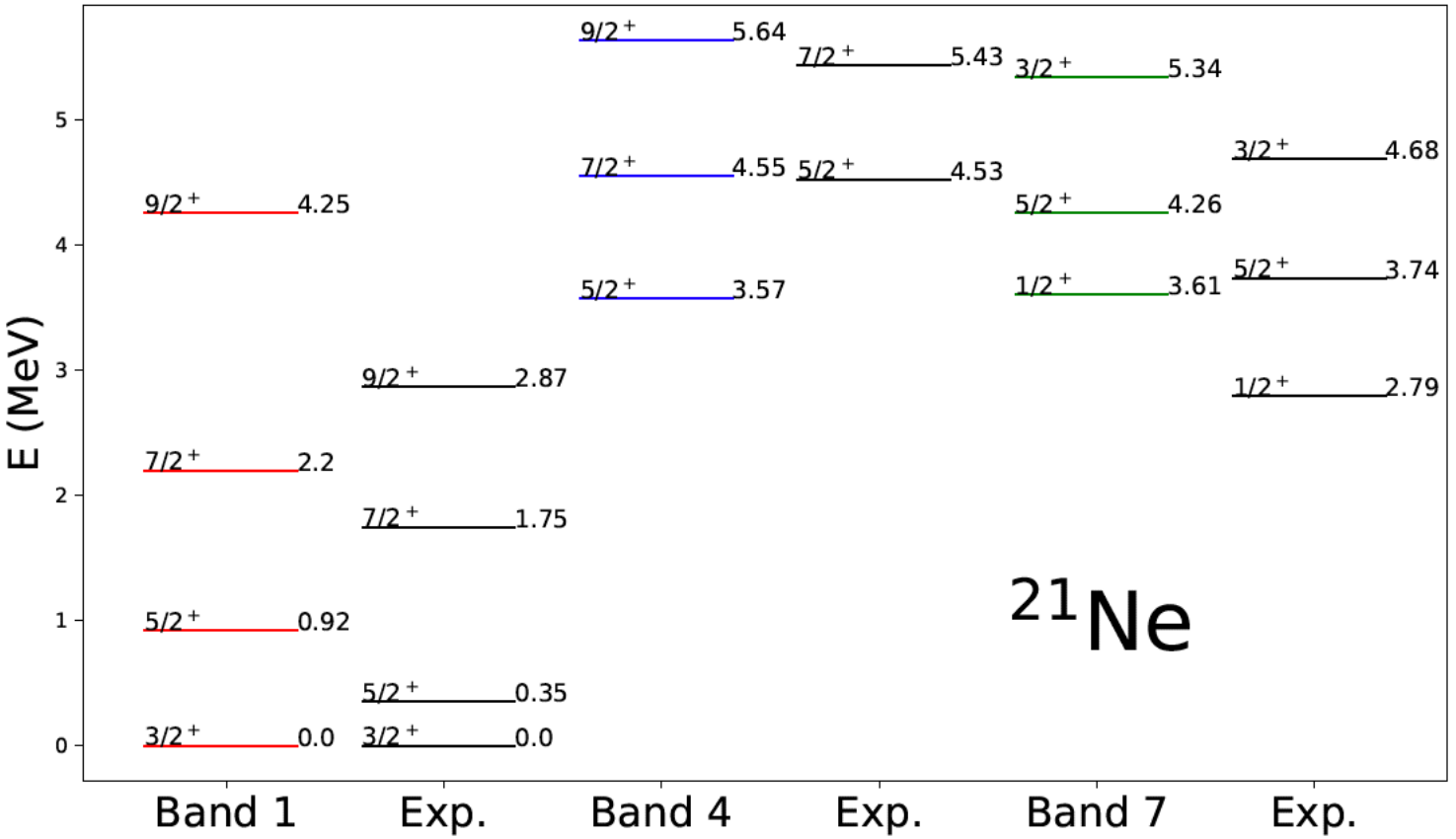
Not yet fully converged with respect to N_{max}

NCSM: Caprio, Maris, Vary & Smith (2015)

^{21}Ne



Bands computed by different filling of the odd neutron
($NNLO_{opt}$, projected Hartree-Fock)



Zhonghao Sun, Hagen, TP, forthcoming

Renormalizing CCSD computations

Proposal: Apply Lepage's insights to many-body computations

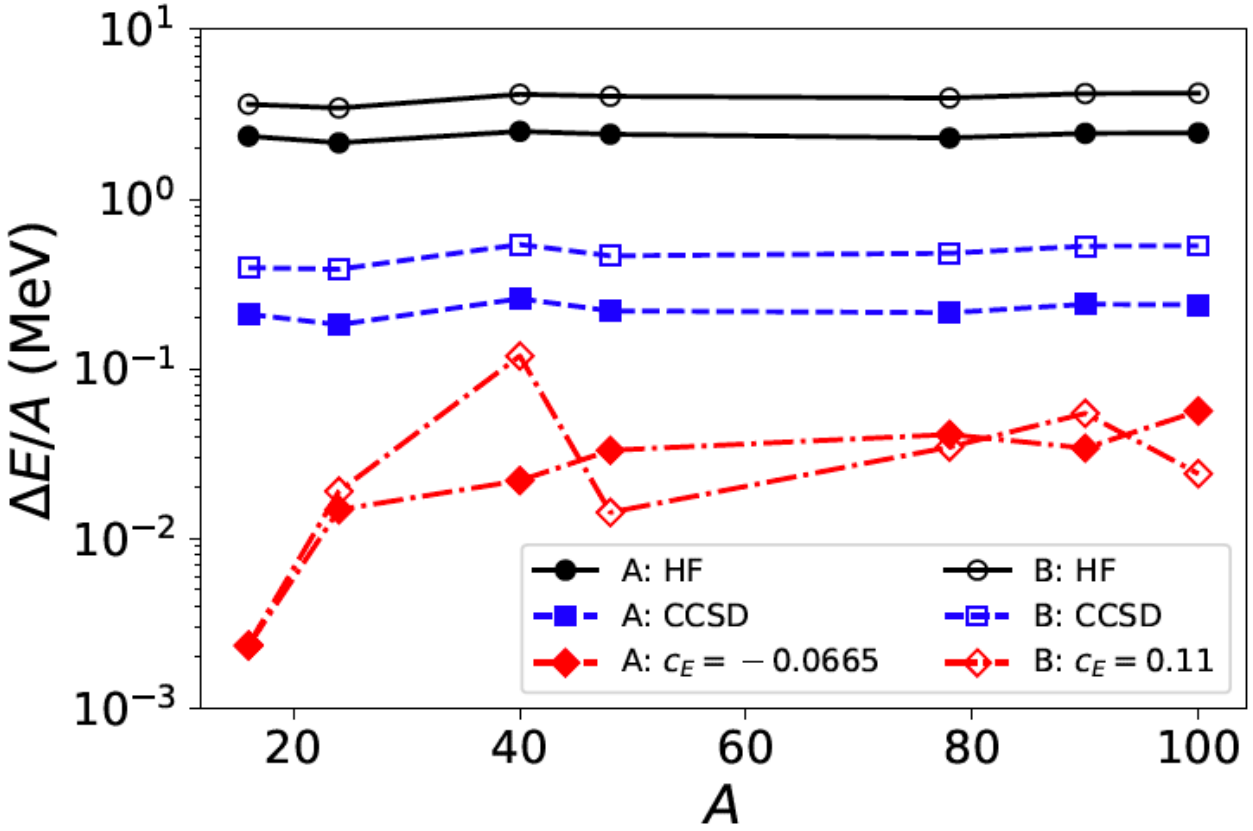
- CCSD lacks 3p-3h excitations, i.e. it has a very small cutoff in the three-body sector
- Hypothesis: Energy gain from 3p-3h dominated by short-range correlations; renormalize via three-body contact
- Follow Lepage (1997); Bedaque, Hammer, van Kolck (1999); Bogner & Roscher (2012)

Interaction	Name	c_E
A	1.8/2.0(EM)	−0.12 [52]
A renorm.		−0.0665
B	ΔNNLO$_{\rm GO}$(394)	−0.002 [67]
B renorm.		0.11

	Interaction and method				
	A renorm. CCSD	A Λ-CCSD(T)	B renorm. CCSD	B CCSDT-1	Exp.
^{16}O	127.8	127.8	127.5	127.5	127.62
^{24}O	166	165	169	169	168.96
^{40}Ca	346	347	341	346	342.05
^{48}Ca	420	419	419	420	416.00
^{78}Ni	642	638	636	639	641.55
^{90}Zr	798	795	777	782	783.90
^{100}Sn	842	836	816	818	825.30

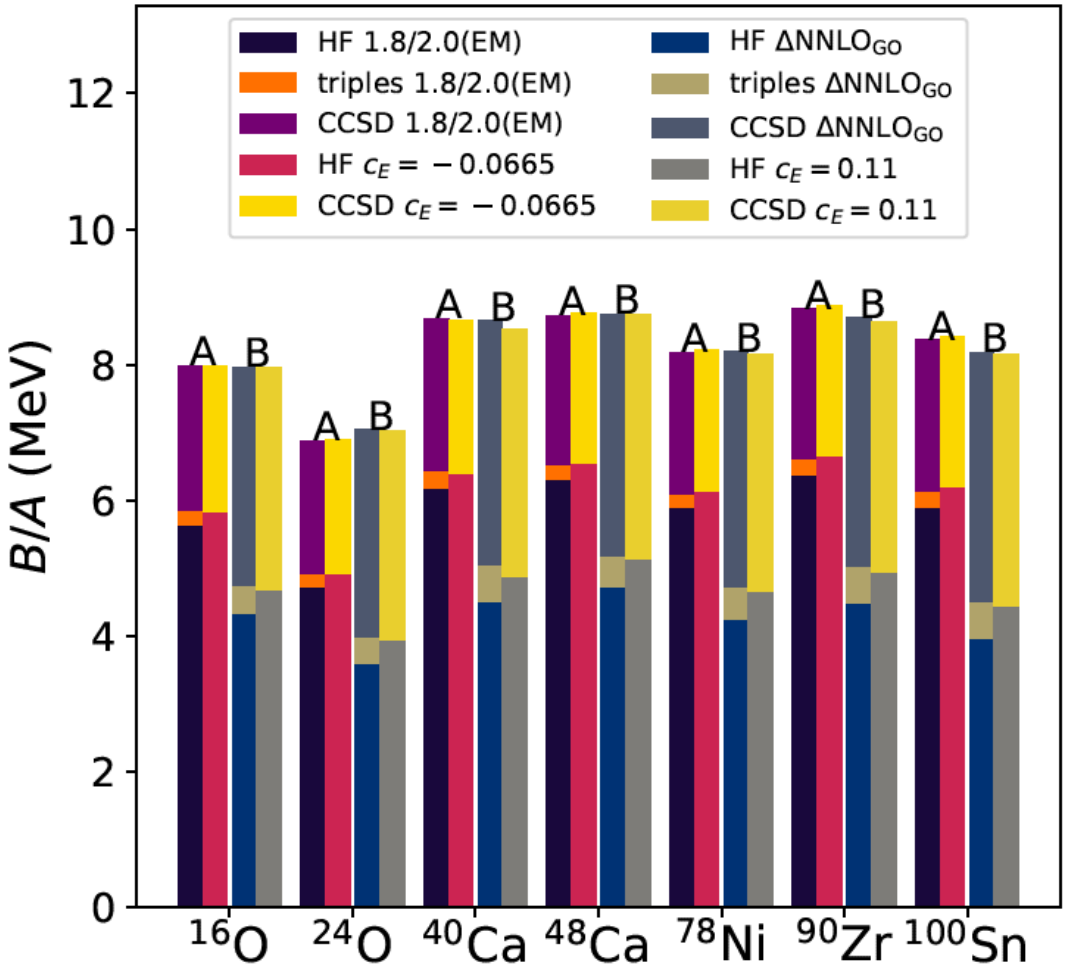
Zhonghao Sun, Charles Bell, G. Hagen, TP, Phys. Rev. 106, L061302 (2022)

Renormalizing CCSD computations



ΔE = differences to full triples

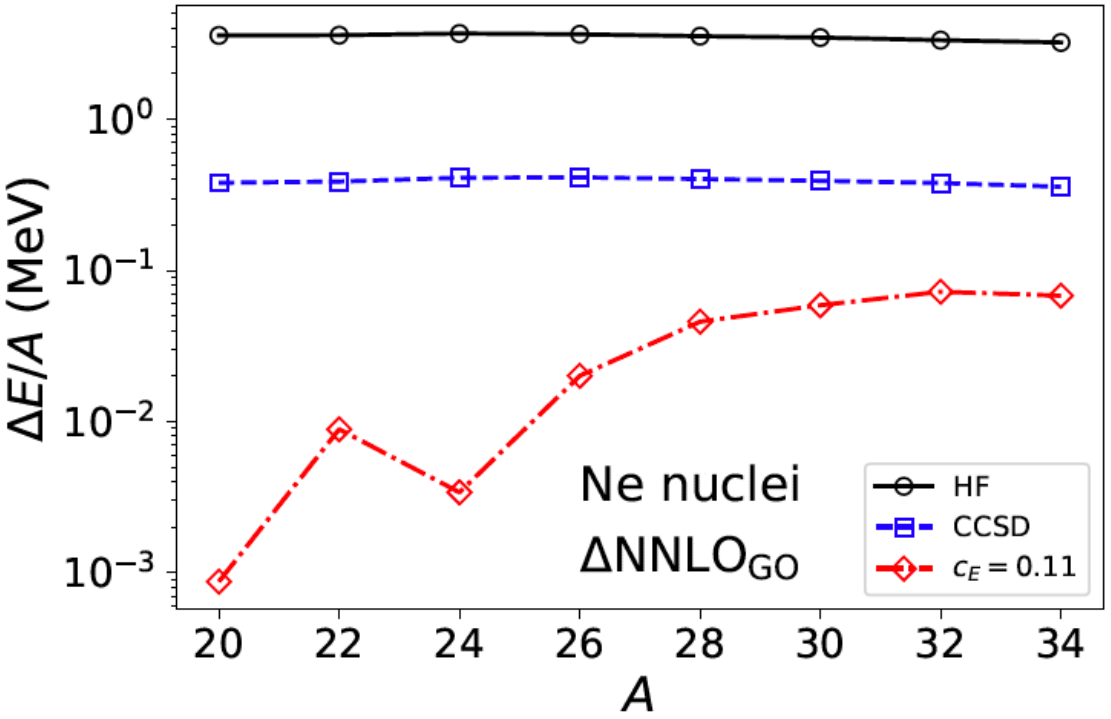
Systematic improvement from renormalization



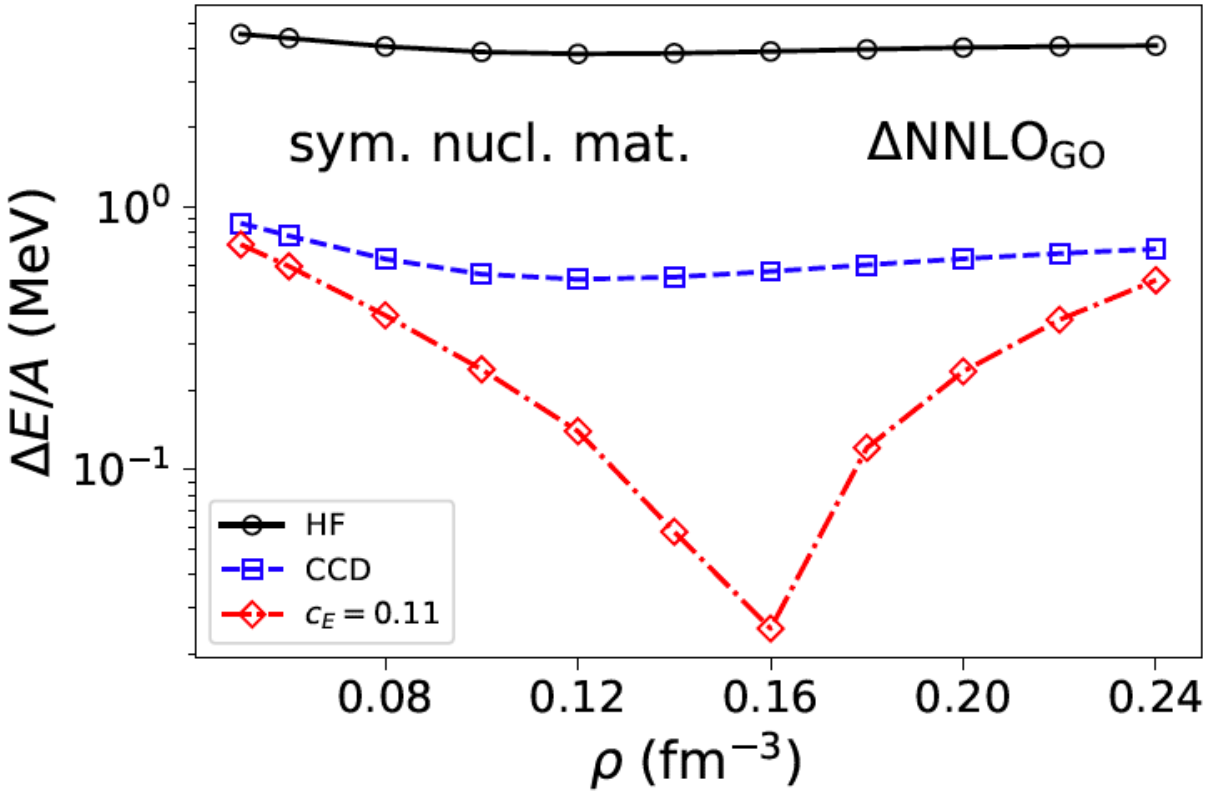
Energy from renormalization essentially goes to HF

Zhonghao Sun, Charles Bell, G. Hagen, TP, Phys. Rev. 106, L061302 (2022)

Renormalizing CCSD computations



Renormalization less accurate as the dripline is approached: dilute neutron densities



Nuclear matter only accurate around saturation as $\Delta E \propto c_E\, \rho^3$ in HF

Possible improvement via higher-order (derivative) 3NF contacts → Girlanda, Kievsky, Viviani (2011)

Zhonghao Sun, Charles Bell, G. Hagen, TP, Phys. Rev. 106, L061302 (2022)

Summary

- High-resolution chiral Hamiltonian confirms Bohr & Mottelson's unified model
  - Conceptual and computational simplicity
  - Symmetry breaking mean-field state is key
  - Separation of IR and UV physics via the mean field
  - Angular momentum projection yields rotational bands in even-even and odd nuclei
- Renormalize 3p-3h excitations via 3-body contact
  - Based on EFT/RG ideas
  - Works
  - Links wave function complexity to the renormalization group

Thank you!