Funded by
the European Union

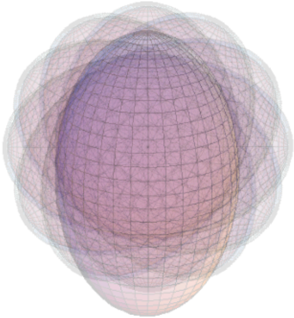
European Research Council
Established by the European Commission

DeformedNuclei

TECHNISCHE
UNIVERSITÄT
DARMSTADT

SYMMETRY-PROJECTED COUPLED-CLUSTER THEORY FOR STRONGLY CORRELATED NUCLEI

Many-Body Theory: Nuclear Physics Meets Quantum Chemistry



Mualla Aytekin
with Benjamin Bally, Thomas Duguet, Alexander Tichai

MOTIVATION

Challenge:

- Nuclei exhibit emergent collective phenomena
- Standard CC
  - → good at dynamic correlations/few ph excitations
  - → at low-orders fails to capture collectivity

Strategy:

- **Symmetry breaking** → static correlations
- **Coupled Cluster** → dynamic correlations
- **Symmetry restoration** → physical quantum numbers (J^π)

Ab initio framework: *see talk by H. Hergert*

- Describe phenomenology via systematically improvable interactions and many-body methods with quantified uncertainties

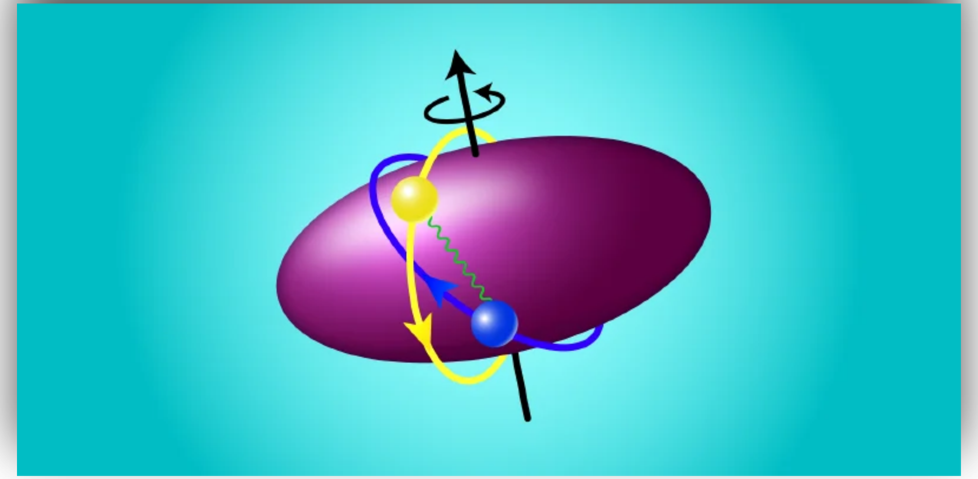


Figure by C. Cain, adapted from Stroberg, Physics 18, 28 (2025)

Study the emergence of nuclear collectivity from microscopic nuclear interactions

AB INITIO CALCULATIONS FOR DEFORMED NUCLEI

TECHNISCHE UNIVERSITÄT DARMSTADT

- **Deformed Hartree-Fock (HF) Reference** $|\Phi\rangle$

  Determine the deformed minimum from the energy surface

  Breaks rotational invariance → not good J

- **Coupled Cluster (CC) Expansion**

  Captures dynamic correlations via few particle-hole excitations

  Key Feature: **Size-extensive.**

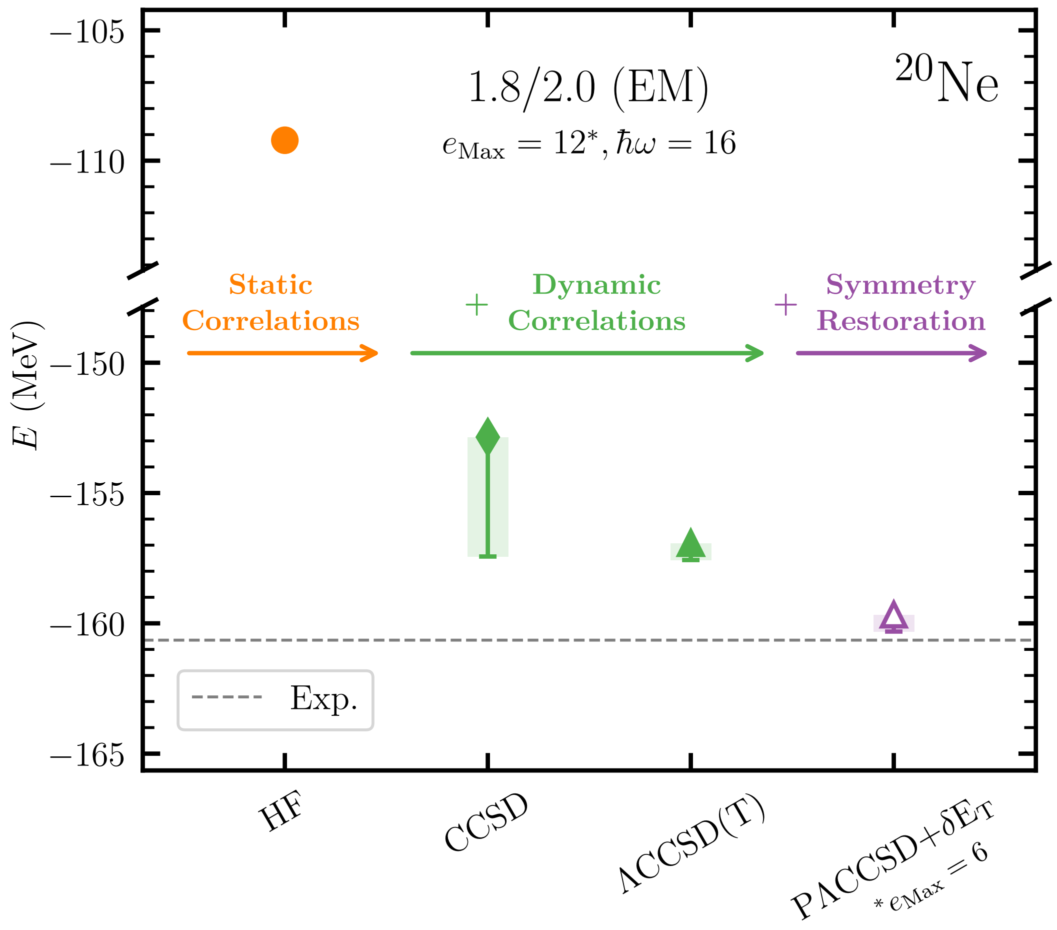
- **Angular Momentum Projection**

  Restores symmetry → good J

  Energy gain from projection **is not size-extensive!**

Static correlations
Dynamic correlations
Symmetry restoration

(Deformed) Coupled Cluster Theory



STATIC CORRELATIONS

Closed-shell nuclei:

- Global minimum is spherical → rotationally invariant
- Adding ph correlations on top is sufficient
- J-scheme (↔ spin adapted) implementation

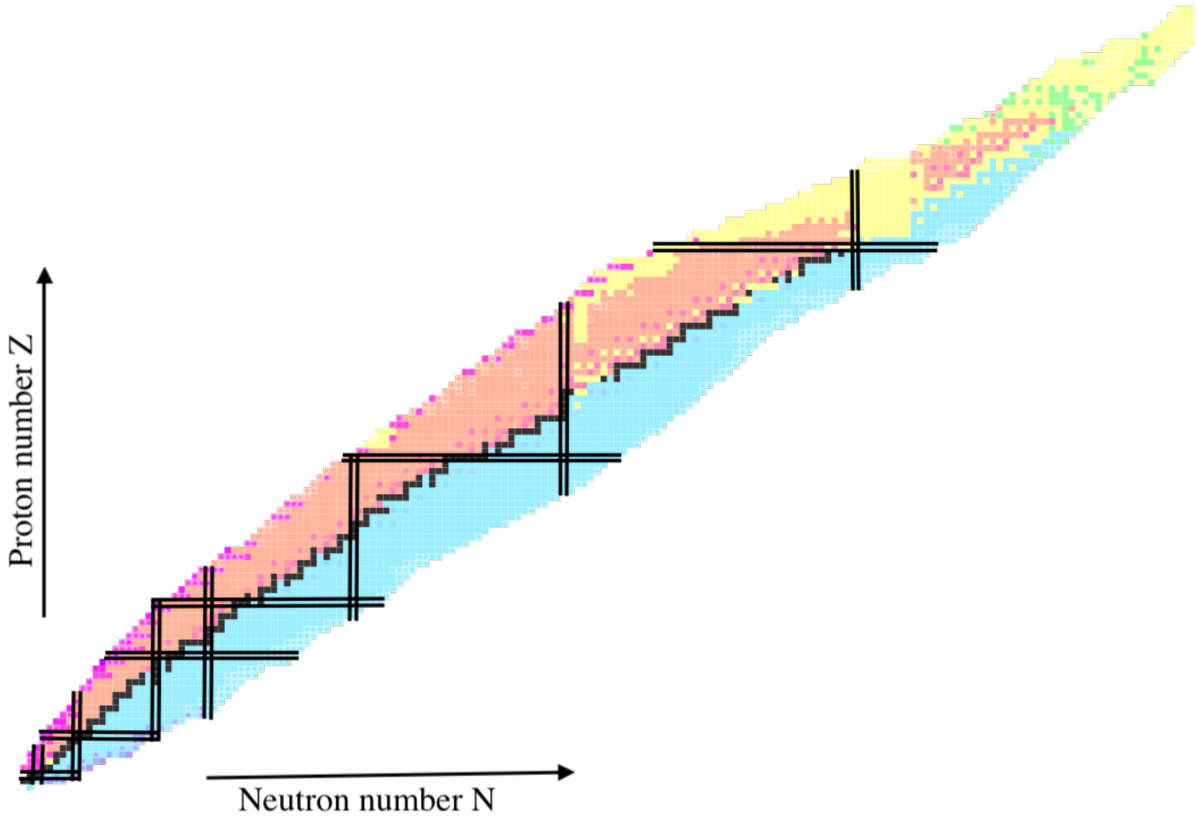


Figure adapted from 'The colorful nuclide chart'. https://people.physics.anu.edu.au/~ecs103/chart/, Version 2.157. Accessed: 2026-08-24, 2026.

STATIC CORRELATIONS

TECHNISCHE UNIVERSITÄT DARMSTADT

Closed-shell nuclei:

- Global minimum is spherical → rotationally invariant
- Adding ph correlations on top is sufficient
- J-scheme (↔ spin adapted) implementation

Open-shell nuclei:

- Global minimum is deformed → breaks rot. invariance
- Deformation (axial) is parametrized by

$$\beta \equiv \frac{4\pi}{3AR_0^2}\langle \Phi | \hat{Q}_{20} | \Phi \rangle$$

⇒ existence of prolate/oblate minima

⇒ energy gain

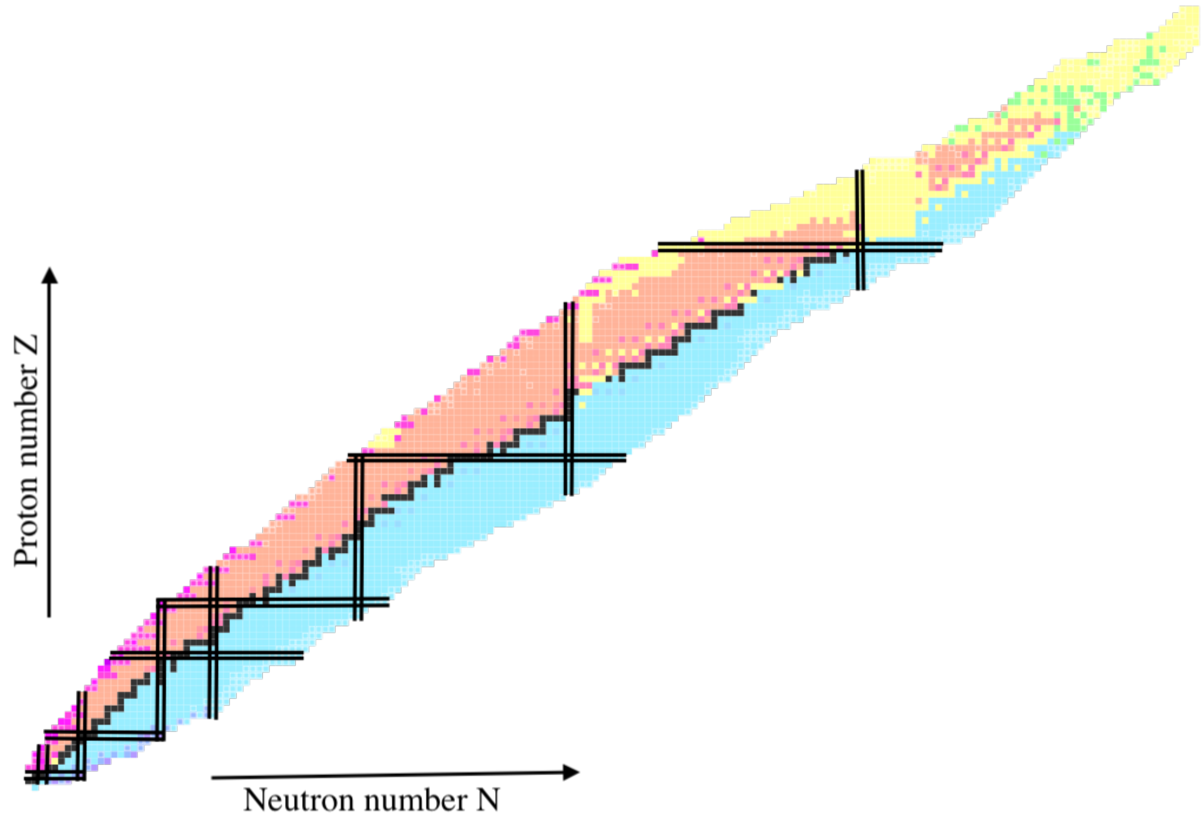


Figure adapted from 'The colorful nuclide chart'. https://people.physics.anu.edu.au/~ecs103/chart/, Version 2.157. Accessed: 2026-08-24, 2026.

STATIC CORRELATIONS

Closed-shell nuclei:

- Global minimum is spherical → rotationally invariant
- Adding ph correlations on top is sufficient
- J-scheme (↔ spin adapted) implementation

Open-shell nuclei:

- Global minimum is deformed → breaks rot. invariance
- Deformation (axial) is parametrized by

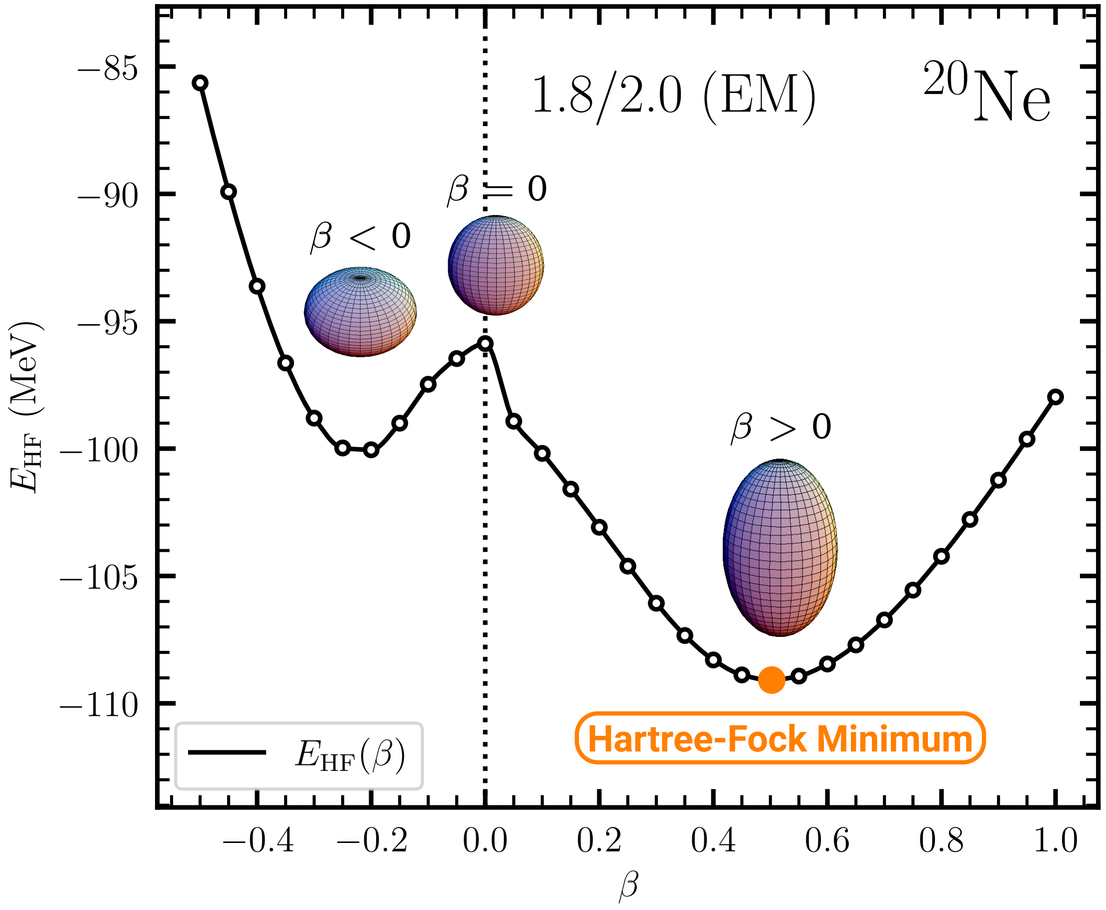
$$\beta \equiv \frac{4\pi}{3AR_0^2}\langle\Phi\,|\,\hat{Q}_{20}\,|\,\Phi\rangle$$

⇒ existence of prolate/oblate minima

⇒ energy gain

Mean field: Rotational symmetry breaking

Interaction: 1.8/2.0 (EM) Hebeler et al., PRC (2011)



DYNAMIC CORRELATIONS

Coupled Cluster Theory: *see talk by R. Bartlett*

- Exponential ansatz: $|\Psi\rangle = e^{\hat{T}}|\Phi\rangle$
- Cluster operator: $\hat{T} = \hat{T}_1 + \hat{T}_2 + \dots$
- Amplitude equations: $\langle\Phi_{i\dots}^{a\dots}|\hat{H}_N e^{\hat{T}}|\Phi\rangle_C = 0$

DYNAMIC CORRELATIONS

Hagen et al., RPP (2014)
Bartlett and Musiał, RMP (2007)

TECHNISCHE UNIVERSITÄT DARMSTADT

Coupled Cluster Theory: *see talk by R. Bartlett*

- Exponential ansatz: $|\Psi\rangle = e^{\hat{T}}|\Phi\rangle$
- Cluster operator: $\hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots$
- Amplitude equations: $\langle \Phi_{i\ldots}^{a\ldots} | \hat{H}_N e^{\hat{T}} | \Phi \rangle_C = 0$

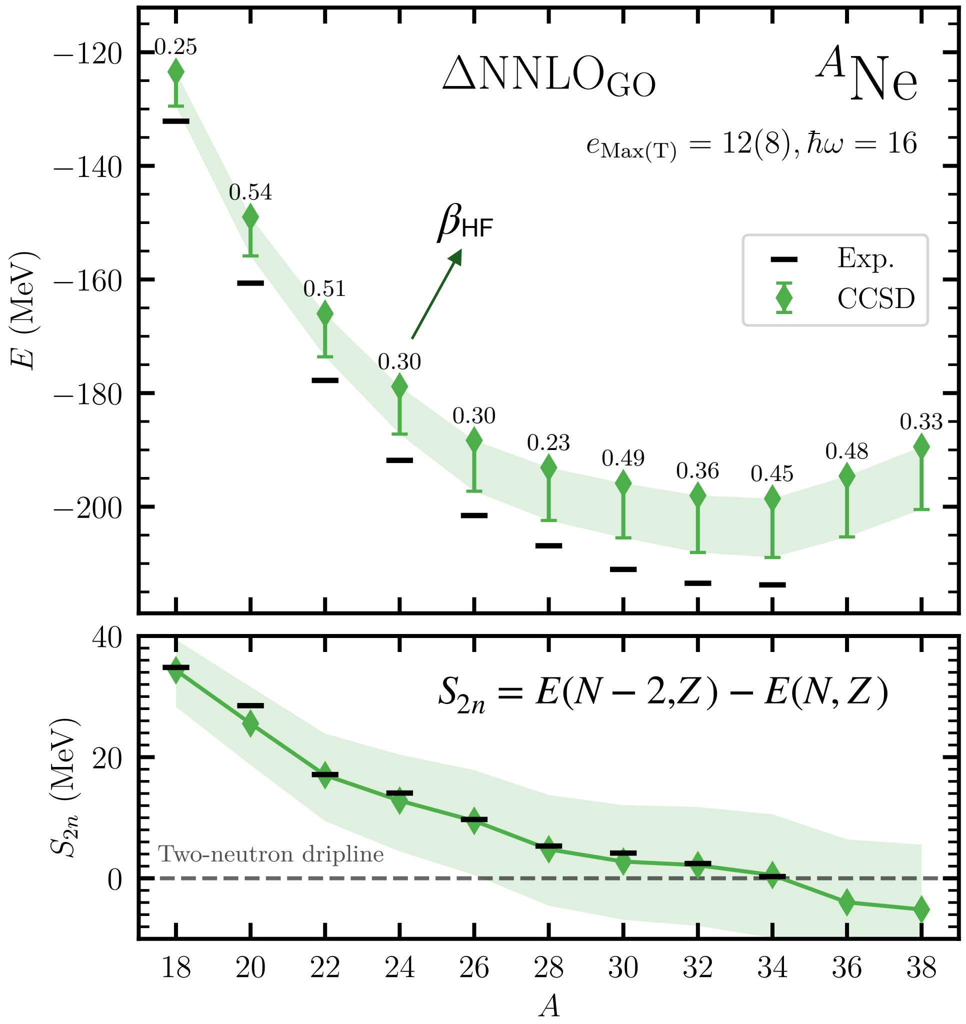
Realistic calculations:

- CCSD - e_{Max} = 12 *(1820 basis states)*

Source	Uncertainties
Finite basis size	$0.5\,\%\,\Delta E_{CCSD}$
Truncation error	$10\,\%\,\Delta E_{CCSD}$

(Deformed) Coupled Cluster

Interaction: ΔNNLO$_{GO}$(394) Jiang et al., PRC (2020).



see also Novario *et al.*, PRC (2020)

DYNAMIC CORRELATIONS

Coupled Cluster Theory: *see talk by R. Bartlett*

- Exponential ansatz: $|\Psi\rangle = e^{\hat{T}}|\Phi\rangle$
- Cluster operator: $\hat{T} = \hat{T}_1 + \hat{T}_2 + \dots$
- Amplitude equations: $\langle \Phi_{i\dots}^{a\dots} | \hat{H}_N e^{\hat{T}} | \Phi \rangle_C = 0$

Realistic calculations:

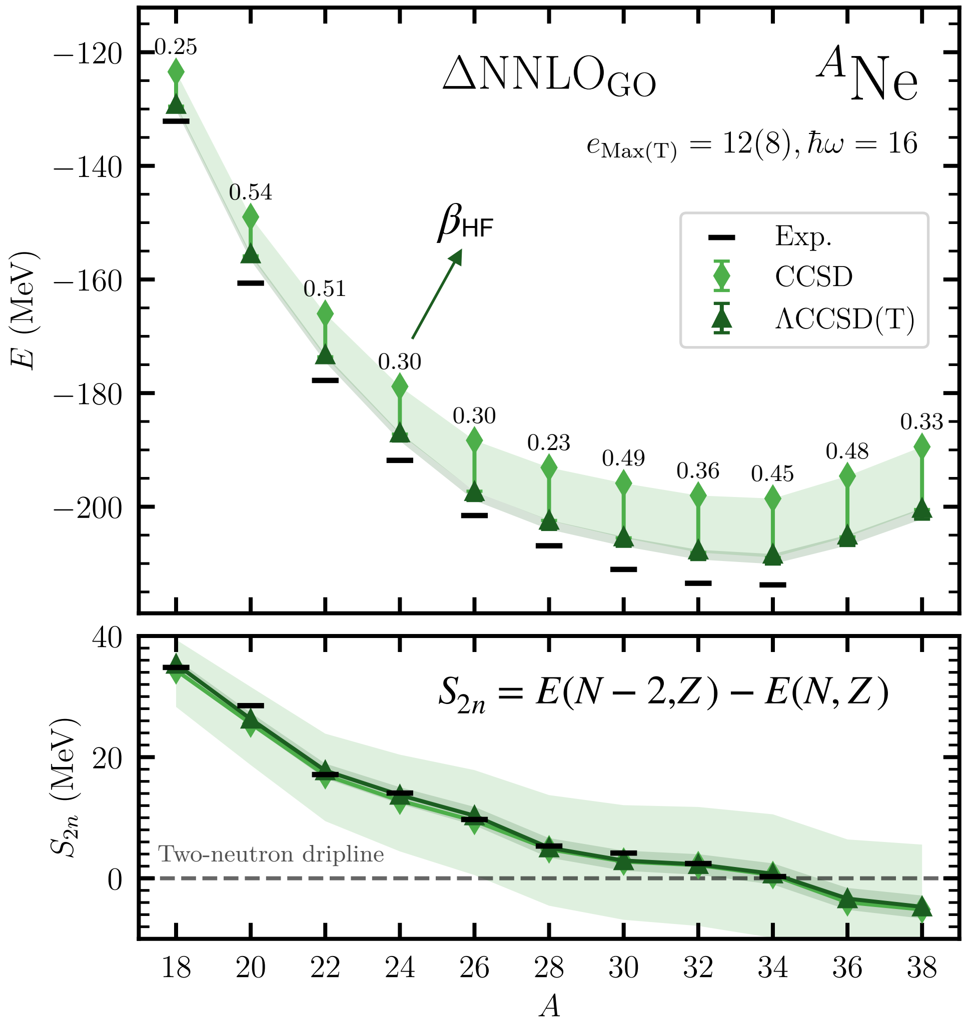
- CCSD - e$_{\text{Max}}$ = 12 *(1820 basis states)*
- Approximate triples correction: $\delta E_{(T)} = \langle \Phi | \hat{\Lambda} \big[\hat{H}_N \hat{T}_3^{[2]}\big]_C | \Phi \rangle$

  ΛCCSD(T) - e$_{\text{Max}}$ = 8 *(660 basis states)*

Source	Uncertainties
Finite basis size	$0.5\,\%\,\Delta E_{CCSD} + 3\,\%\,\delta E_T$
Truncation error	$10\,\%\,\delta E_T$

(Deformed) Coupled Cluster

Interaction: ΔNNLO$_{\text{GO}}$(394) Jiang et al., PRC (2020).



see also Novario *et al.*, PRC (2020)

Hagen et al., RPP (2014)
Bartlett and Musiał, RMP (2007)

TECHNISCHE UNIVERSITÄT DARMSTADT

DYNAMIC CORRELATIONS

Coupled Cluster Theory: *see talk by R. Bartlett*

- Exponential ansatz: $|\Psi\rangle = e^{\hat{T}}|\Phi\rangle$
- Cluster operator: $\hat{T} = \hat{T}_1 + \hat{T}_2 + \ldots$
- Amplitude equations: $\langle\Phi_{i\ldots}^{a\ldots}|\hat{H}_N e^{\hat{T}}|\Phi\rangle_C = 0$

Realistic calculations:

- CCSD - e_{Max} = 12 *(1820 basis states)*
- Approximate triples correction: $\delta E_{(T)} = \langle\Phi|\hat{\Lambda}\big[\hat{H}_N\hat{T}_3^{[2]}\big]_C|\Phi\rangle$

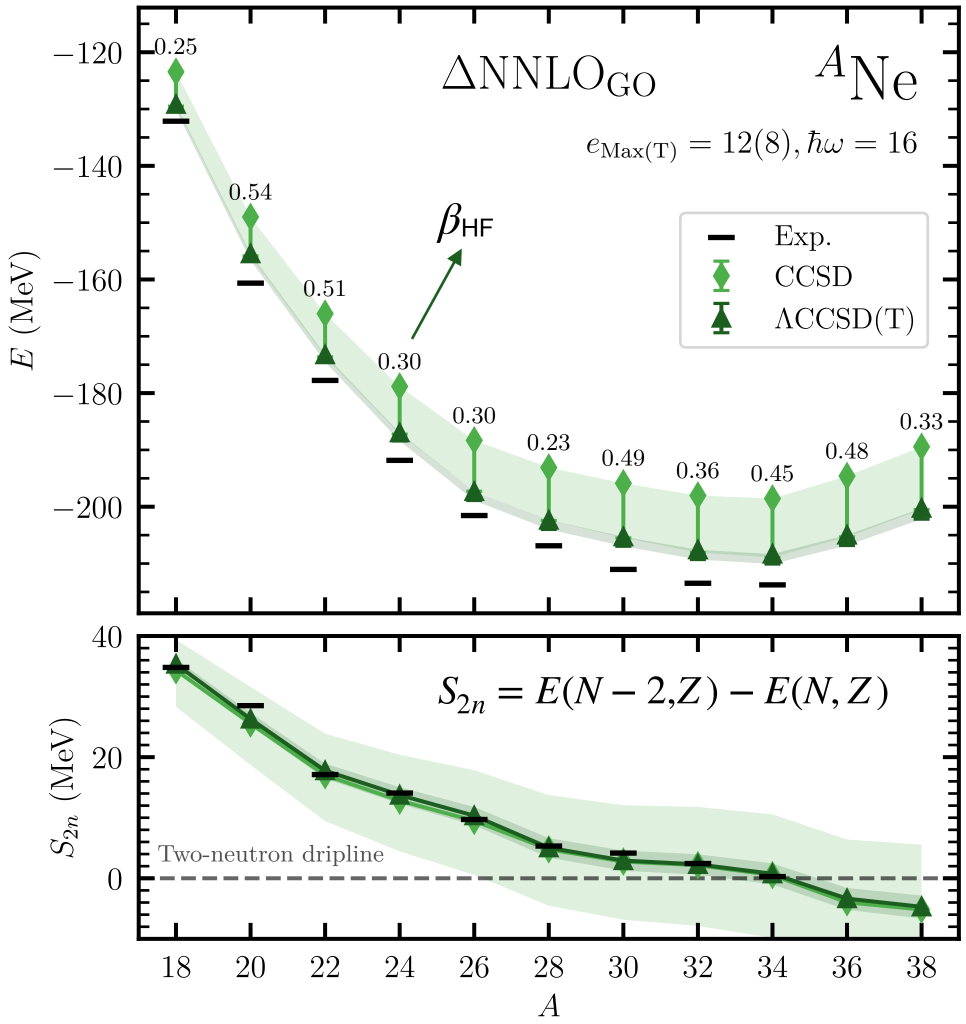
  ΛCCSD(T) - e_{Max} = 8 *(660 basis states)*

Source	Uncertainties
Finite basis size	$0.5\,\%\,\Delta E_{CCSD} + 3\,\%\,\delta E_T$
Truncation error	$10\,\%\,\delta E_T$

ΛCCSD(T) is systematically off by $\sim 5\ MeV$
Which correlations are missing?

(Deformed) Coupled Cluster

Interaction: ΔNNLO$_{GO}$(394) Jiang et al., PRC (2020).



see also Novario *et al.*, PRC (2020)

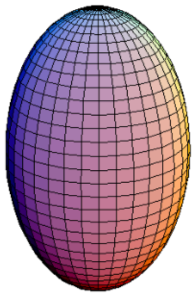
SYMMETRY RESTORATION

Bally & Bender, PRC (2021)

Projection operator
(axial case)

$$\hat{P}^J = \frac{2J+1}{2}\int_0^{\pi} d\beta\, \sin\beta\, d^J_{00}(\beta)\hat{R}(\beta)$$

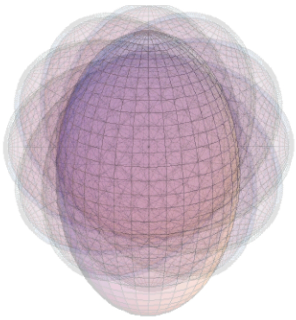
Initial state: $|\,\Phi\,\rangle$, $|\,\Psi\rangle_{CC}$



The ‘**intrinsic**’ **state** breaks SU(2) symmetry to capture static correlations.

$\hat{P}^J$

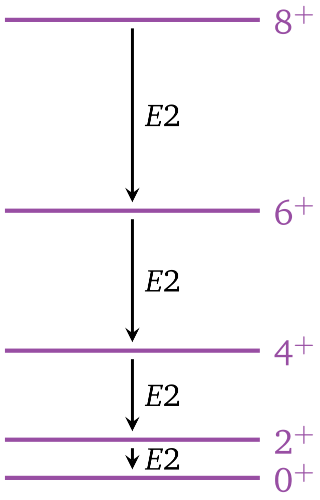
Projected state: $|\,\Psi^J_M\rangle$



Projection restores this symmetry by "averaging" over orientations

$$O^J = \frac{\langle\Psi\,|\,\hat{P}^J\,\hat{O}\,\hat{P}^J\,|\,\Psi\rangle}{\langle\Psi\,|\,\hat{P}^J\,|\,\Psi\rangle}$$

Observable evaluation



SYMMETRY RESTORATION

- Projection grants access to different J states

$$E^J = \frac{\langle \Psi | \hat{P}^J \hat{H} | \Psi \rangle}{\langle \Psi | \hat{P}^J | \Psi \rangle} \qquad R_{42} = \frac{E(4^+)}{E(2^+)} \approx 3.3$$

which display $\sim J(J+1)$ trend (rigid-rotor picture)

SYMMETRY RESTORATION

- Projection grants access to different J states

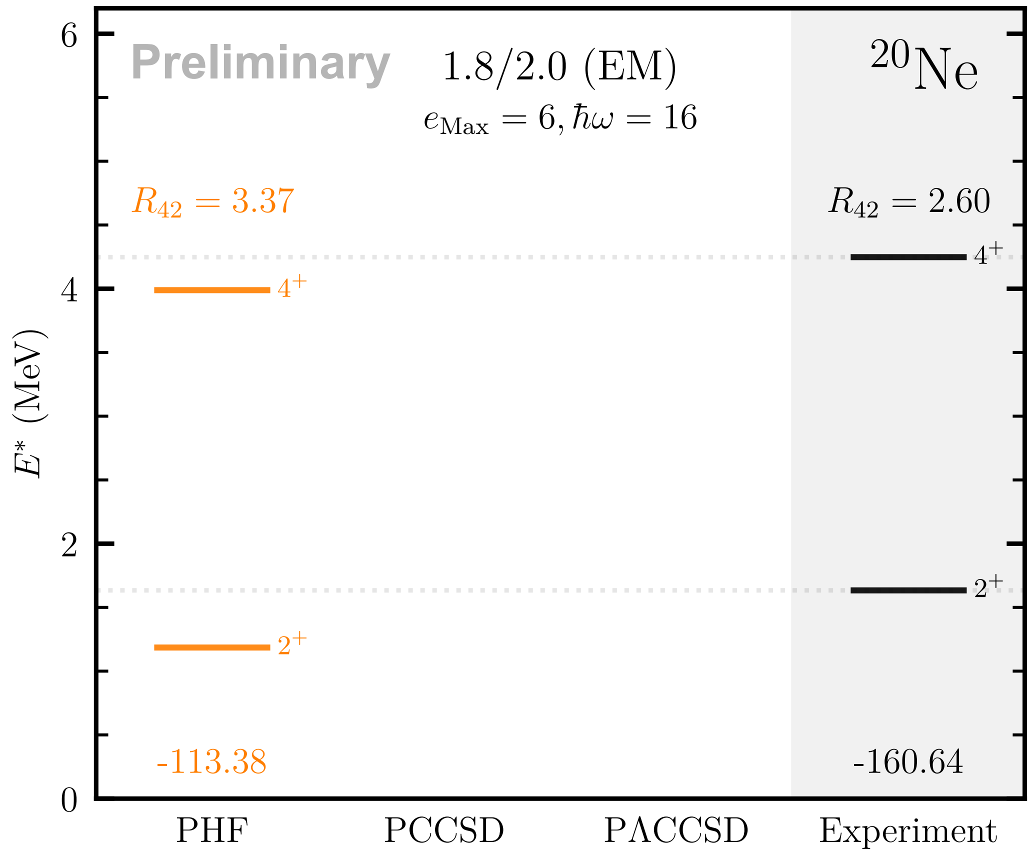
$$E^J = \frac{\langle \Psi | \hat{P}^J \hat{H} | \Psi \rangle}{\langle \Psi | \hat{P}^J | \Psi \rangle} \qquad R_{42} = \frac{E(4^+)}{E(2^+)} \approx 3.3$$

which display $\sim J(J+1)$ trend (rigid-rotor picture)

- Projected mean field: good spectrum but far in total energy

Rotational bands of ^{20}Ne

Interaction: 1.8/2.0 (EM) Hebeler et al., PRC (2011)



Duguet, JPG (2015)
Qiu et al., J. Chem. Phys. (2017)
Hagen et al., PRC (2022)
Sun et al., PRX (2025)

SYMMETRY RESTORATION

- Projection grants access to different J states

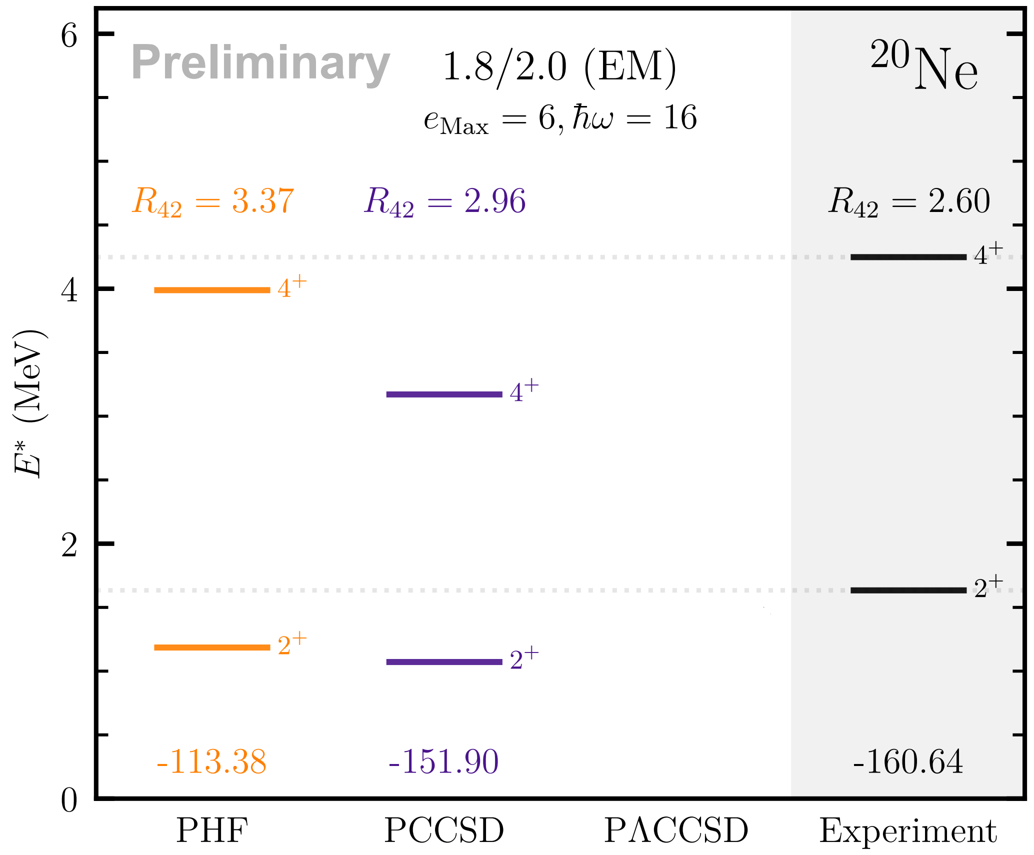
$$E^J = \frac{\langle \Psi | \hat{P}^J \hat{H} | \Psi \rangle}{\langle \Psi | \hat{P}^J | \Psi \rangle} \qquad R_{42} = \frac{E(4^+)}{E(2^+)} \approx 3.3$$

which display $\sim J(J+1)$ trend (rigid-rotor picture)

- Projected mean field: good spectrum but far in total energy
- Projected coupled cluster: captures bulk but bad spectrum

Rotational bands of ^{20}Ne

Interaction: 1.8/2.0 (EM) Hebeler et al., PRC (2011)



Duguet, JPG (2015)
Qiu et al., J. Chem. Phys. (2017)
Hagen et al., PRC (2022)
Sun et al., PRX (2025)

SYMMETRY RESTORATION

- Projection grants access to different J states

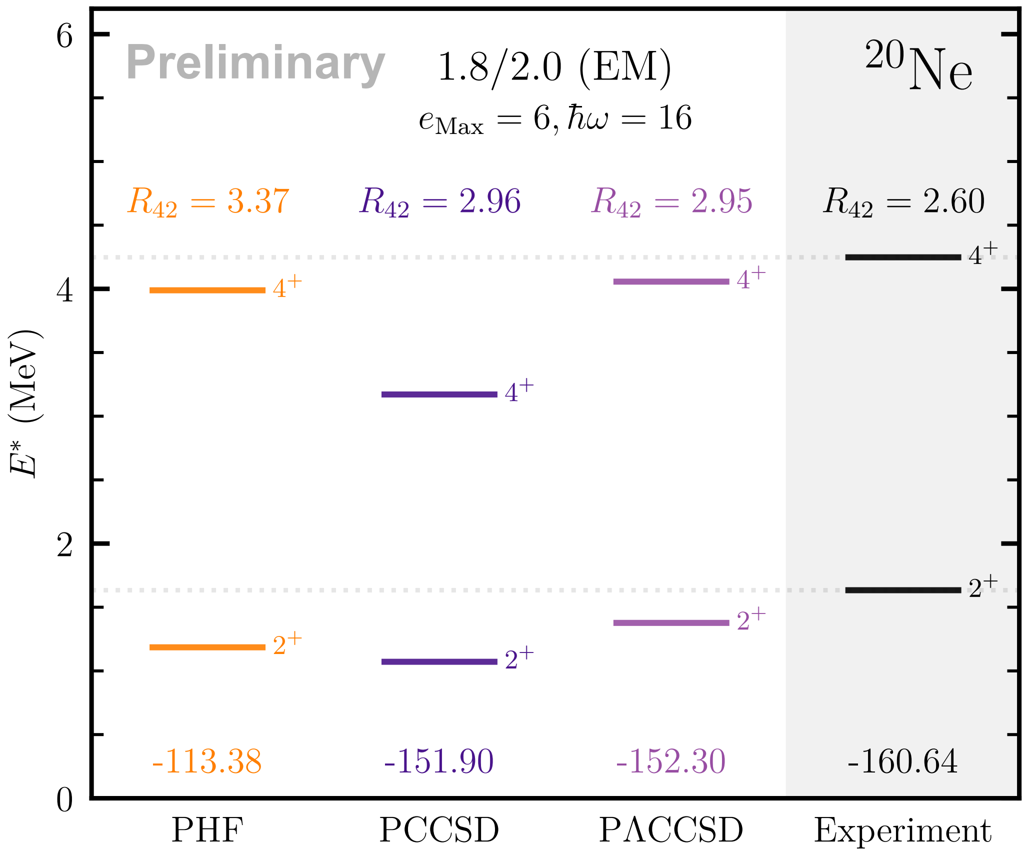
$$E^J = \frac{\langle \Psi | \hat{P}^J \, \hat{H} | \Psi \rangle}{\langle \Psi | \hat{P}^J | \Psi \rangle} \qquad R_{42} = \frac{E(4^+)}{E(2^+)} \approx 3.3$$

which display $\sim J(J+1)$ trend (rigid-rotor picture)

- Projected mean field: good spectrum but far in total energy
- Projected coupled cluster: captures bulk but bad spectrum
- Bivariational treatment is needed reproduce absolute and relative properties simultaneously.

Rotational bands of ^{20}Ne

Interaction: 1.8/2.0 (EM) Hebeler et al., PRC (2011)



Duguet, JPG (2015)
Qiu et al., J. Chem. Phys. (2017)
Hagen et al., PRC (2022)
Sun et al., PRX (2025)

SYMMETRY RESTORATION

- Projection grants access to different J states

$$E^J = \frac{\langle \Psi | \hat{P}^J \hat{H} | \Psi \rangle}{\langle \Psi | \hat{P}^J | \Psi \rangle} \qquad R_{42} = \frac{E(4^+)}{E(2^+)} \approx 3.3$$

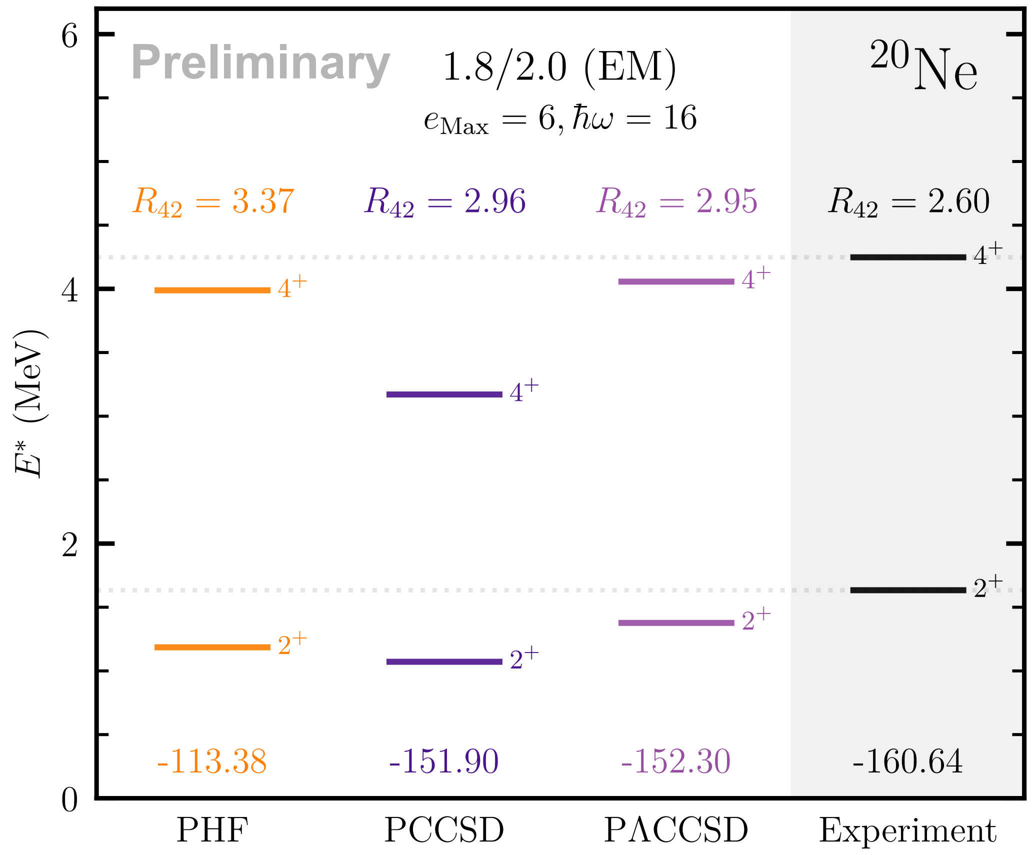
which display $\sim J(J+1)$ trend (rigid-rotor picture)

- Projected mean field: good spectrum but far in total energy
- Projected coupled cluster: captures bulk but bad spectrum
- Bivariational treatment is needed reproduce absolute and relative properties simultaneously.

Unified framework for dynamic (particle-hole) and static (collective) correlations.

Rotational bands of ^{20}Ne

Interaction: 1.8/2.0 (EM) Hebeler et al., PRC (2011)

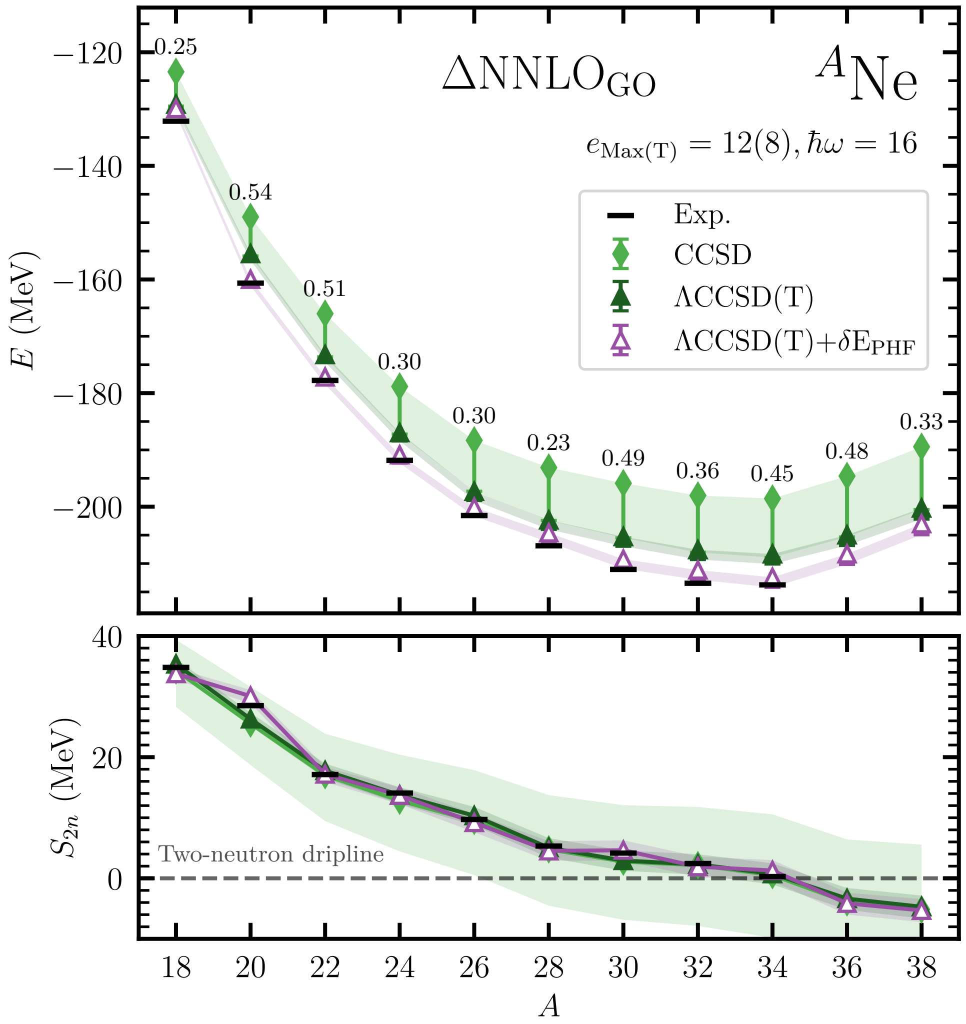


Duguet, JPG (2015)
Qiu et al., J. Chem. Phys. (2017)
Hagen et al., PRC (2022)
Sun et al., PRX (2025)

UNIFIED TREATMENT OF STATIC AND COLLECTIVE CORRELATIONS

(Deformed) Coupled Cluster

Interaction: ΔNNLO$_{GO}$(394) Jiang et al., PRC (2020).



Neon chain systematics:

- Missing correlations are accounted by projection
- δE_{PHF} is used as a proxy for δE_{PCC}

See also Novario et al., PRC (2020)

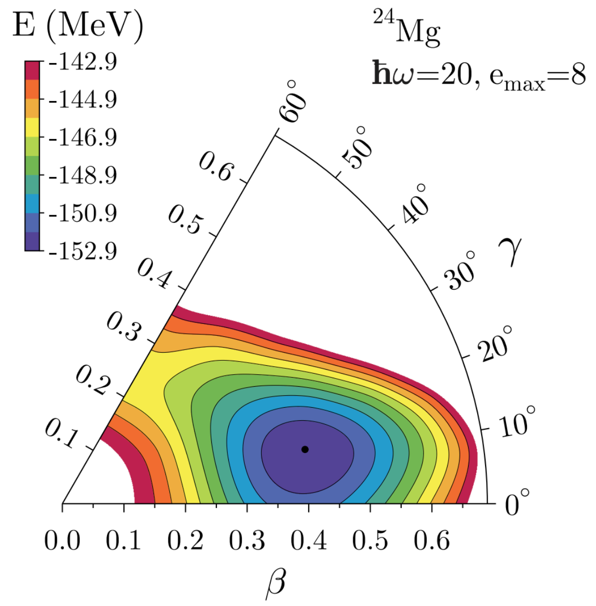
- Overall good agreement and good prediction of the dripline

OUTLOOK

- Potential overestimation by δE_{PHF}
- Full P(Λ)CC calculation is the next step.
- Observables: Charge radii and electromagnetic transitions strengths, B(E2).

OUTLOOK: TRIAXIAL DEFORMATION IN NUCLEI

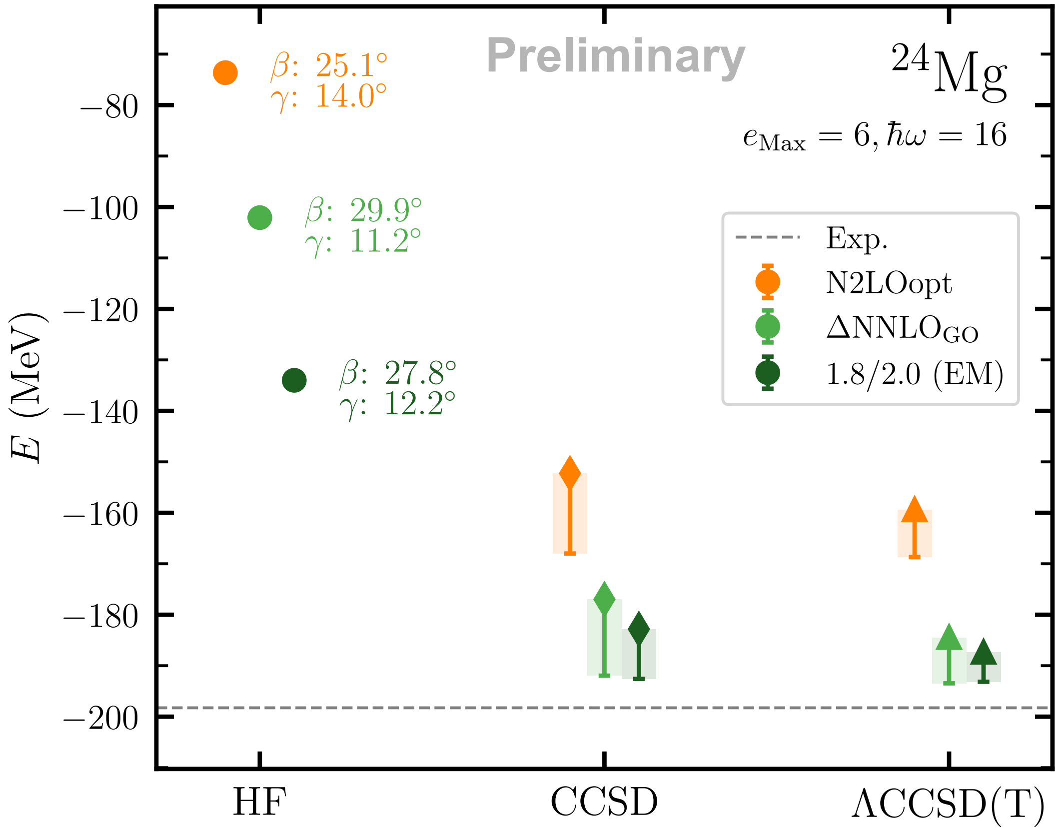
Triaxial ^{24}Mg



Bally et al., EPJA (2020)

Coupled-cluster solver can fully adapt to spatial symmetries

Coupled cluster for triaxial reference states



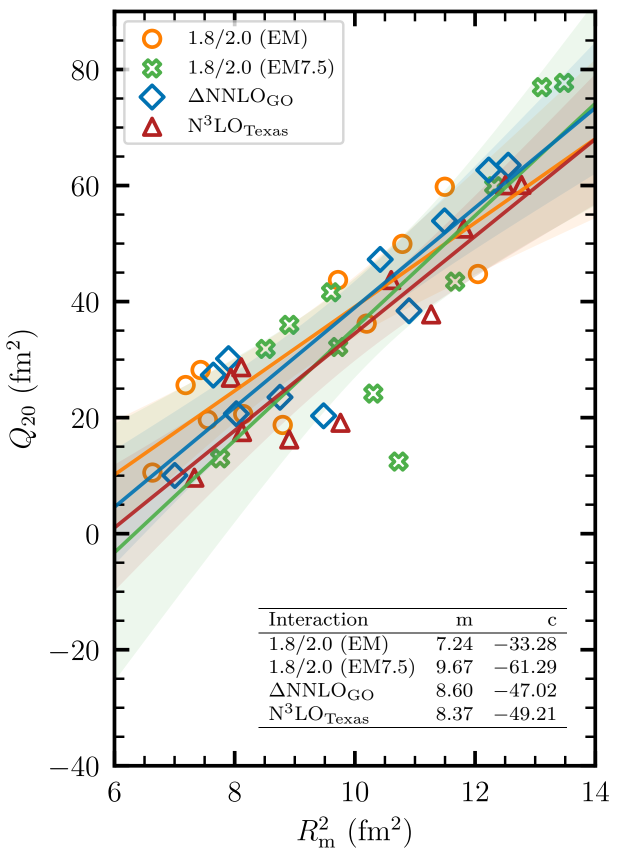
Ekström et al., PRL (2013)
Jiang et al., PRC (2020)
Hebeler et al., PRC (2011)

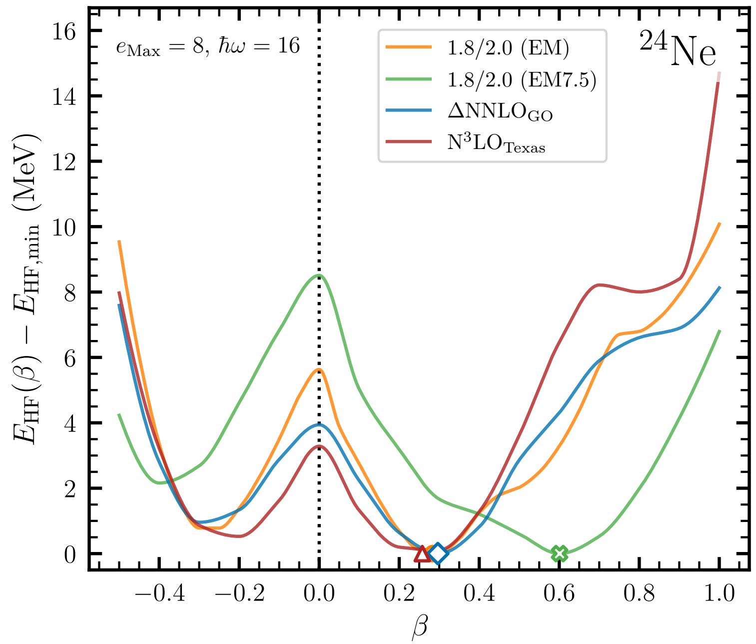
OUTLOOK

- Pave the way for ab initio nuclear matrix elements in BSM searches
- Example: strong triaxiality in $0\nu2\beta$ candidate nucleus ^{76}Ge

OUTLOOK: FROM CHIRAL INTERACTIONS TO DEFORMATION

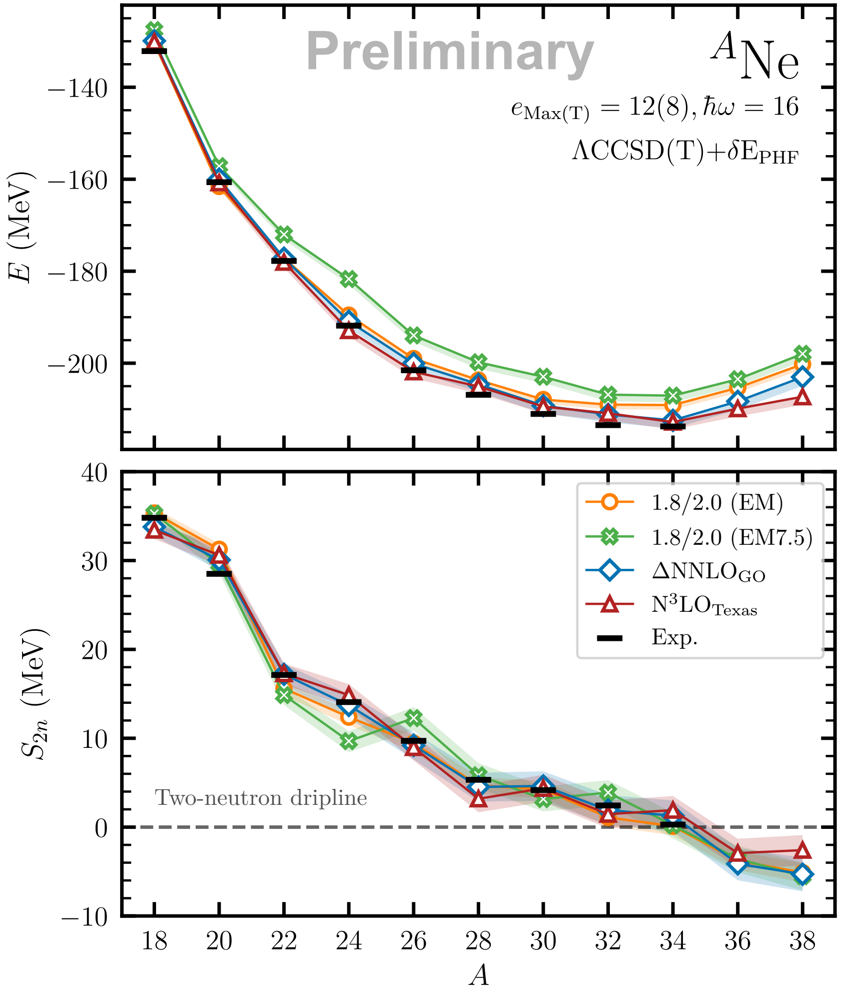
Correlation between R^2 and collective observables





Which **Low-Energy Constants (LECs)** drive nuclear **quadrupole collectivity**?

Interaction sensitivity of neon isotopes



Hebeler et al., PRC (2011)
Arthuis et al., EPJA (2026)
Jiang et al., PRC (2020).
Hu et al., arXiv (2025),

OUTLOOK

- Analyze how B(E2) transition strengths and radii depend on specific Chiral EFT interaction LECs.

Funded by the European Union

European Research Council
Established by the European Commission

DeformedNuclei

TECHNISCHE UNIVERSITÄT DARMSTADT

Thank you for your attention!

Collaborators:
TU Darmstadt: Benjamin Bally, Alexander Tichai
CEA Saclay: Thomas Duguet

PROJECTION THEORY

TECHNISCHE UNIVERSITÄT DARMSTADT

Projection operator (triaxial case)

$$\hat{P}^J_{MK} = \frac{2J+1}{16\pi^2}\int_0^{2\pi} d\alpha \int_0^{\pi} d\beta\ \sin\beta \int_0^{4\pi} d\gamma\, D^{J*}_{MK}(\alpha,\beta,\gamma)\,\hat{R}(\alpha,\beta,\gamma)$$

Observable evaluation

$$\langle O\rangle^J \equiv \frac{\langle\Psi_\mathrm{L}|P^J O|\Psi_\mathrm{R}\rangle}{\langle\Psi_\mathrm{L}|P^J|\Psi_\mathrm{R}\rangle} = \frac{\int_0^\pi d\beta\ \sin\beta\, d^J_{00}(\beta)\mathcal{O}(\beta)}{\int_0^\pi d\beta\ \sin\beta\, d^J_{00}(\beta)\mathcal{N}(\beta)}$$

$$B(E2) = \frac{\langle\Psi|\hat{P}^0 Q_{20}|\Psi\rangle\langle\Psi|Q_{20}\hat{P}^2|\Psi\rangle}{\langle\Psi|\hat{P}^0|\Psi\rangle\langle\Psi|\hat{P}^2|\Psi\rangle}$$

Operator kernels

$$\mathcal{O}(\beta) \equiv \langle\Psi_\mathrm{L}|R(\beta)O|\Psi_\mathrm{R}\rangle = \langle\Phi|R(\beta)|\Phi\rangle\langle\Phi|\breve{\underline{\tilde{L}}}(\beta)\breve{O}(\beta)e^{W(\beta)}|\Phi\rangle$$

Where we make use the Thouless operator $Z(\beta)$: $\langle\Phi|R(\beta) = \langle\Phi|R(\beta)|\Phi\rangle\langle\Phi|e^{Z(\beta)}$

Rotated operator and left amplitudes: $\breve{O}(\beta) \equiv e^{Z(\beta)}Oe^{-Z(\beta)}$ $\quad\breve{\underline{\tilde{L}}}(\beta) \equiv e^{Z(\beta)}R^{-1}(\beta)\,e^{\hat{T}}(1+\hat{\Lambda})e^{-\hat{T}}\,R(\beta)e^{-Z(\beta)}$

Disentangled cluster operator

$$e^{W(\beta)}|\Phi\rangle \equiv e^{Z(\beta)}\,e^{T}|\Phi\rangle \quad \text{where} \quad W(\beta) \equiv W_0(\beta)+W_1(\beta)+W_2(\beta)+\ldots+W_A(\beta)$$

Duguet, JPG (2015)
Qiu et al., J. Chem. Phys. (2017)
Hagen et al., PRC (2022)
Sun et al., PRX (2025)

SEMI-EMPIRICAL CONVERGENCE ESTIMATION