

Role of neutron-proton pairing in the exact description of the deuteron at mean-field cost

Benjamin Bally

A. Scalesi, V. Somà, L. Zurek, T. Duguet

[arXiv:2410.03356](https://arxiv.org/abs/2410.03356)

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- Design efficient *ab initio* many-body method
 - ◊ Extension to heavy nuclei
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- “Boosted mean field” or “mean field on steroids”
 - ◊ Symmetry-breaking/restoration scheme
 - ◊ Low-dimensional linear superposition of product states à la PGCM
 - ◊ Inherently conserves a (naive) n_{dim}^4 scaling

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 - ◊ Inherently conserves a (naive) n_{dim}^4 scaling
- Specific questions regarding the deuteron:
 - ◊ Is the deuteron bound at the (boosted) mean-field level?
 - ◊ How accurately can the observables be described?
 - ◊ What are the key ingredients to include?

Intrinsic Hamiltonian

- Two-body Hamiltonian in the intrinsic frame

$$H_{\text{int}} \equiv T_{\text{tot}} - T_{\text{com}} + V$$

- $V \equiv \text{EM500 (chiral EFT at N3LO)} + \text{SRG(1.8)}$

Entem, PRC 68, 041001(R) (2003) ; Hebeler, PRC 83, 031301 (2011)

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- Reference calculations

- ◇ No-Core Shell Model (NCSM) → Takayuki Miyagi
- ◇ Coupled Cluster with singles and doubles (CCSD) → Gaute Hagen

Center of mass (COM): Gloeckner-Lawson method

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- Consider the modified Hamiltonian

$$\begin{aligned} H(\beta_L, \omega_L) &\equiv H_{\text{int}} + \beta_L H_{\text{com}}(\omega_L) \\ &\equiv H_{\text{int}} + \beta_L \left(T_{\text{com}} + \frac{1}{2} m A \omega_L^2 R_{\text{com}}^2 - \frac{3}{2} \hbar \omega_L \right) \end{aligned}$$

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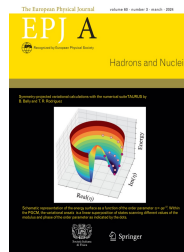
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- As in NCSM, we take $\omega_L = \omega$
- In the calculations:
 - ◊ $\beta_L = 0$ for the energy
 - ◊ $\beta_L = 1$ for the spectroscopic observables

- Numerical suite TAURUS

Bally, EPJA 57, 69 (2021) ; Bally, EPJA 60, 62 (2024)

- ◇ Spherical Harmonic Oscillator basis (m -scheme)
- ◇ Real general Bogoliubov reference states
- ◇ Variation after particle-number projection
- ◇ Projection after variation: Z , N , J , M , π
- ◇ Configuration mixing of projected states

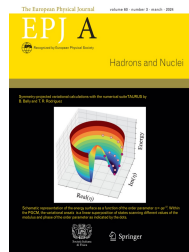
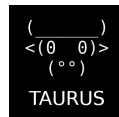


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Computational aspects

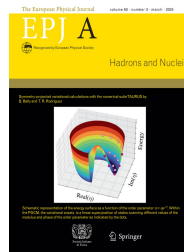
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- Topaze supercomputer (CEA/CCRT)



First attempt: deformed Hartree-Fock (dHF)

- Minimizes the energy exploring the variational space of Slater determinants

$$\delta \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = 0 \quad \text{with} \quad |\Phi\rangle = \prod_i a_i^\dagger |0\rangle$$

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- Very general HF: breaks all spatial symmetries! \rightarrow deformed HF

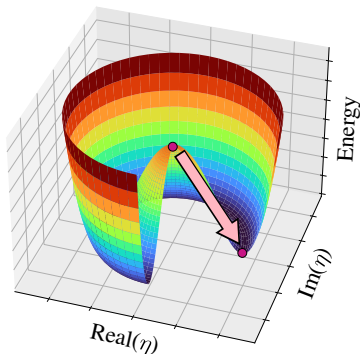
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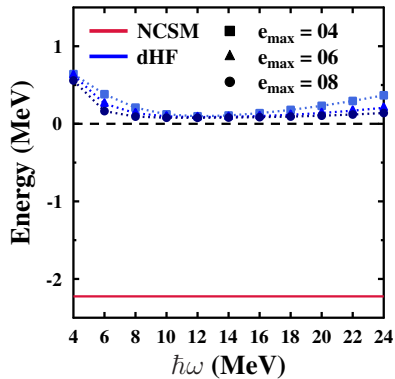
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Order parameter: $\eta \equiv qe^{i\Omega}$



Results for dHF



- Not bound at dHF level

Boost: projection after variation (PAV)

- Symmetry-broken states (rotational invariance, parity) do not have good quantum numbers

$$|\Phi\rangle = \sum_{JK\pi} \sum_{\epsilon} c_{\epsilon}^{JK\pi} |\Theta_{\epsilon}^{JK\pi}\rangle$$

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- Restore the symmetries through quantum-number projection

$$|\Theta_{\epsilon}^{JM\pi}\rangle \equiv \sum_{K=-J}^K f_{\epsilon K}^{J\pi} P_{MK}^J P^{\pi} |\Phi\rangle$$

with

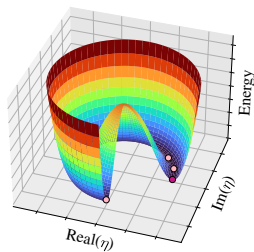
$$P_{MK}^J = \frac{2J+1}{16\pi^2} \int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin(\beta) \int_0^{4\pi} d\gamma D_{MK}^{J*}(\alpha, \beta, \gamma) R(\alpha, \beta, \gamma)$$

$$P^{\pi} = \frac{1}{2}(1 + \pi\Pi)$$

$$\text{diag}(\langle\Phi|HP_{KK'}^JP^{\pi}|\Phi\rangle) \longrightarrow f_{\epsilon K}^{J\pi}$$

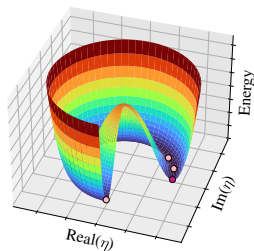
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- Explores the phase of the order parameter



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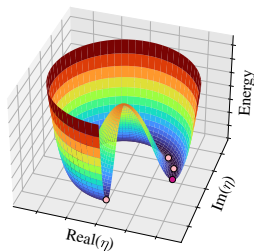
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 - ◇ Superposition of rotated states \rightarrow not a product state anymore!
 - ◇ Good quantum numbers
 - ◇ At least one of them has a lower energy than $\langle \Phi | H | \Phi \rangle$

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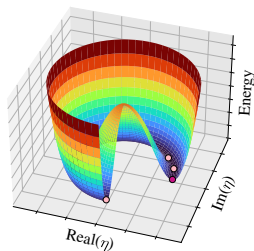
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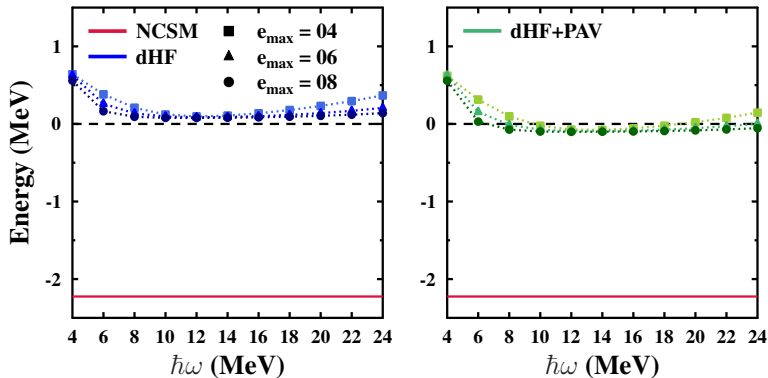
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 - ◇ At least one of them has a lower energy than $\langle \Phi | H | \Phi \rangle$
 - ◇ Depends inherently on reference state $|\Phi\rangle$
- PAV: determine $|\Phi\rangle$ and then project

Results for dHF+PAV



- Bound by ≈ 100 keV, but very far away from NCSM reference value

Boost: Hartree-Fock-Bogoliubov (pairing)

- Minimizes the energy exploring the variational space of Bogoliubov quasi-particle states

$$\delta \frac{\langle \Phi | H - \lambda_n N - \lambda_z Z | \Phi \rangle}{\langle \Phi | \Phi \rangle} = 0 \quad \text{with} \quad |\Phi\rangle = \prod_i \beta_i |0\rangle$$

$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix} \equiv \mathcal{W}^\dagger \begin{pmatrix} a \\ a^\dagger \end{pmatrix} \quad \mathcal{W}\mathcal{W}^\dagger = \mathcal{W}^\dagger\mathcal{W} = 1$$

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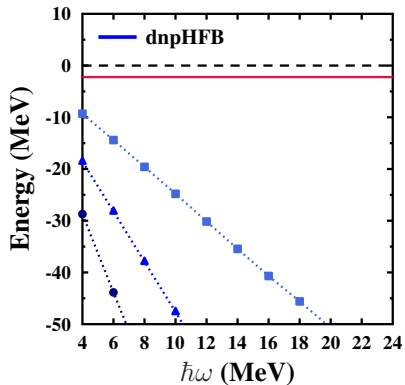
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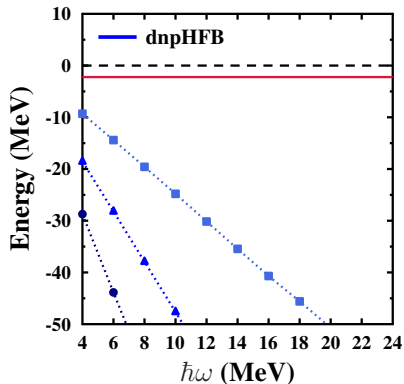
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- Very general HFB \rightarrow *dnp*HFB
 - neutron-proton pairing
 - odd-odd nuclei
 - breaks all spatial symmetries

Results for $dnpHFB$



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- Particle-number nonconserving theory with $\langle A \rangle \sim \langle (\Delta A)^2 \rangle$

In particular: missing 3N, wrong center of mass, E changes rapidly with A

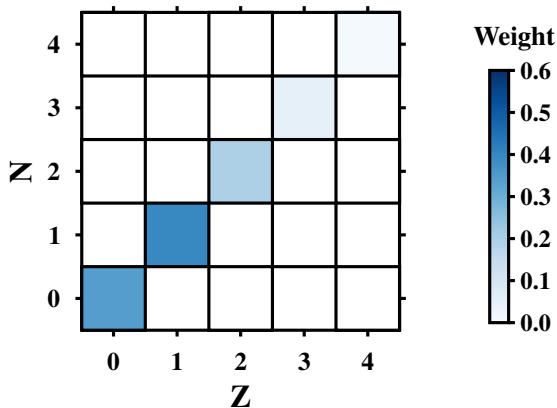
- Projected state now reads

$$|\Theta_{\epsilon}^{ZNJ\pi}\rangle \equiv \sum_{K=-J}^K f_{\epsilon K}^{ZNJ\pi} P^Z P^N P_{MK}^J P^{\pi} |\Phi\rangle$$

with

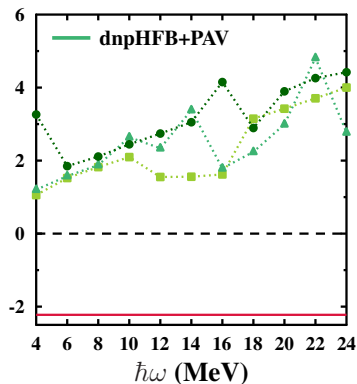
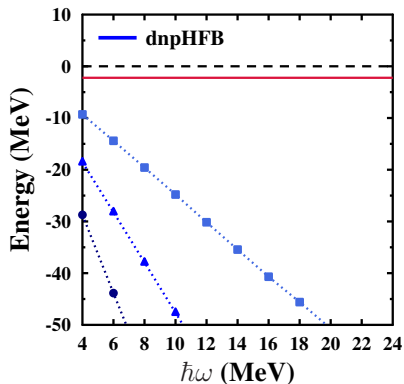
$$P^Z = \frac{1}{2\pi} \int_0^{2\pi} d\phi_Z e^{i\phi_Z(Z-Z)}$$
$$P^N = \frac{1}{2\pi} \int_0^{2\pi} d\phi_N e^{i\phi_N(N-N)}$$
$$\text{diag}(\langle \Phi | H P^Z P^N P_{KK'}^J P^{\pi} | \Phi \rangle) \longrightarrow f_{\epsilon K}^{ZNJ\pi}$$

Decomposition (Z, N) of the $dn\bar{p}$ HFB states



- $dn\bar{p}$ HFB favors $N = Z$ components \rightarrow consistent with $2N$ interaction

Boost: $dnpHFB+PAV$



- Not bound anymore and even worse than dHF

Boost: variation after projection (VAP)

- Minimizes the particle-number projected energy exploring the variational space of Bogoliubov quasi-particle states

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- More computationally demanding

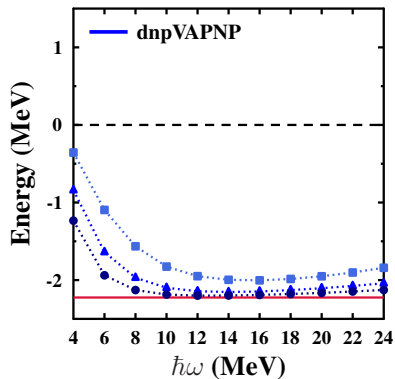
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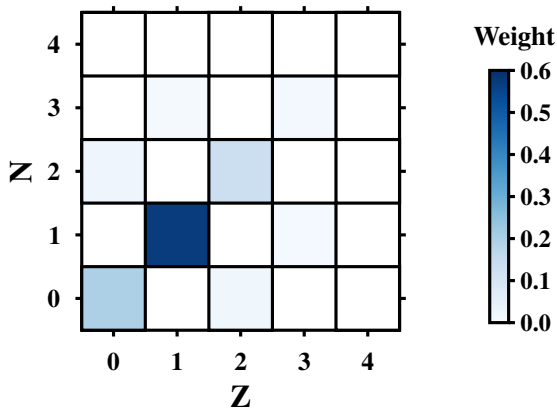
- Explores the correct subspace (Z, N) of the Hilbert space
- More computationally demanding
- Combined with PAV: $dnpVAPNP + PAV \rightarrow$ “mean field on steroids (MFS)”

Results for $dnpVAPNP$



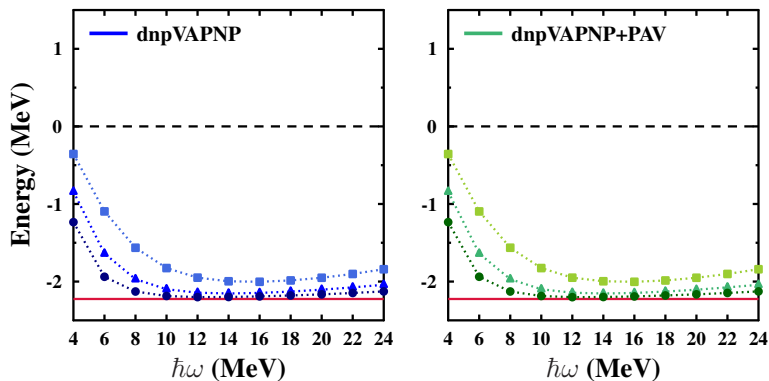
- Bound and very good agreement with NCSM reference value

Decomposition (Z, N) of the $dnpVAPNP$ states



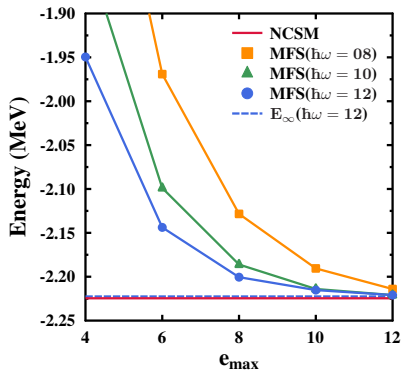
- Different decompositions for $dnpHFB$ and $dnpVAPNP$

Results for $dnpVAPNP+PAV$



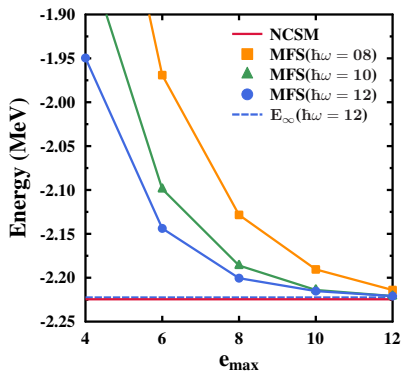
- Does not change much ($dnpVAPNP$ states are almost pure $J^\pi = 1^+$)

Convergence and extrapolation



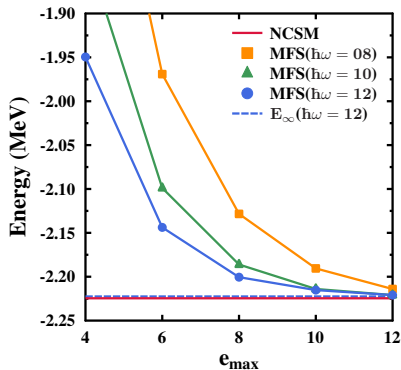
- For $e_{\max} = 12$, $\hbar\omega = 12$ MeV, we have $E = -2.2209$ MeV

Convergence and extrapolation



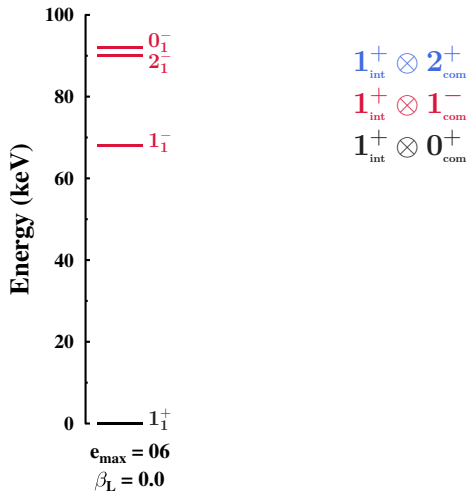
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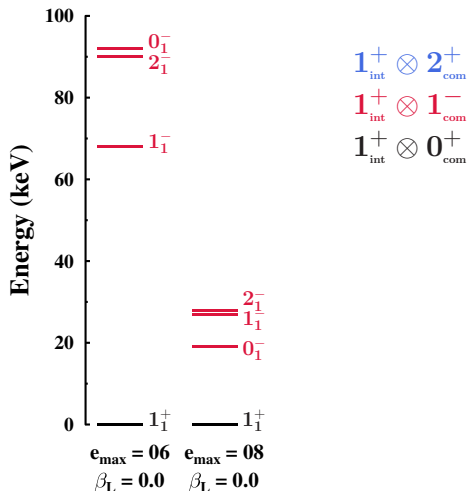


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- CCSD reference value: $E = -2.2211$ MeV
- Extrapolation to infinite basis ($\hbar\omega = 12$): $E_{\infty} = -2.2225(12)$ MeV
- NCSM reference value: $E = -2.2246$ MeV \rightarrow relative accuracy: +0.09 %

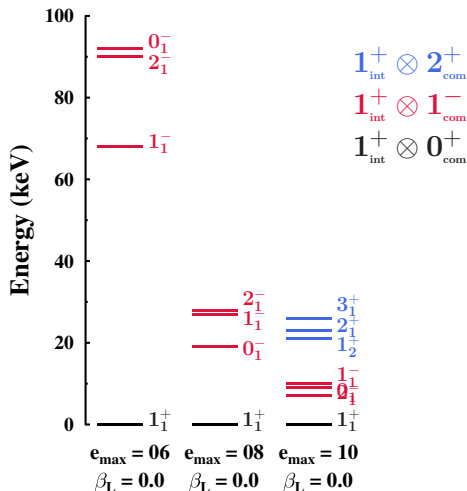
Center-of-mass contamination



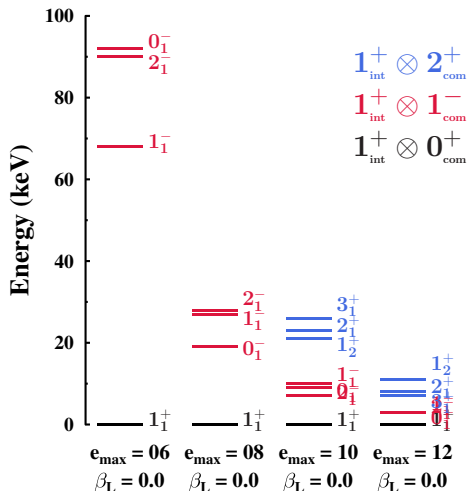
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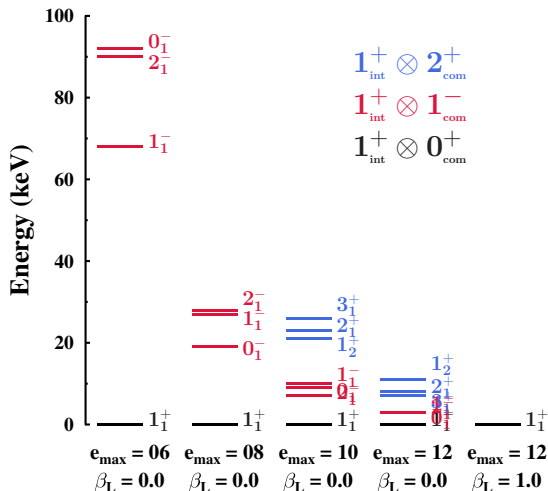
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COM: Gloeckner-Lawson method

- Using Gloeckner-Lawson method \rightarrow clean factorization with only 0_{com}^+
- For $e_{\text{max}} = 12$ and $\hbar\omega = 12$ MeV

β_L	$\langle \Phi(\beta_L) H_{\text{com}}(\omega) \Phi(\beta_L) \rangle$
0.0	1.227 MeV
1.0	0.001 MeV

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- But impacts energy in calculations not converged w.r.t. model space

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- Not necessary for $E \dots$ but **necessary for the spectroscopic observables**

Spectroscopic observables

- Other observables associated with the deuteron ground state

$$\mu = \langle \Psi_1^{1111+} | g_l l + g_s s | \Psi_1^{1111+} \rangle ,$$

$$Q_s = \sqrt{\frac{16\pi}{5}} \langle \Psi_1^{1111+} | r_p^2 Y_{20} | \Psi_1^{1111+} \rangle ,$$

$$r_{\text{rms},p} = \sqrt{\langle \Psi_1^{1111+} | r_{p+\text{com}}^2 | \Psi_1^{1111+} \rangle} .$$

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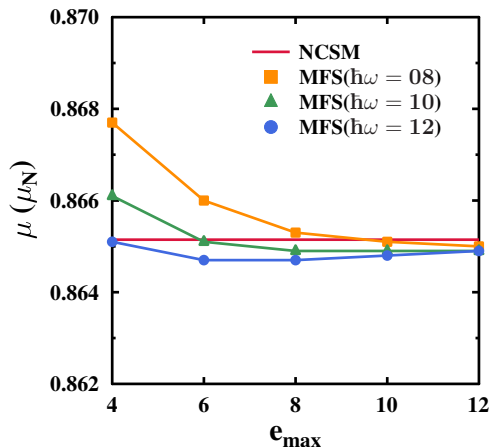
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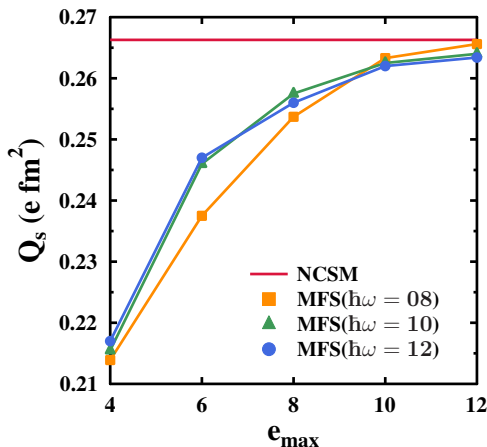
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 - ◊ Q_s and μ are pure one-body operators
 - ◊ $r_{\text{rms},p}$ also includes the center-of-mass correction (one- and two-body)
- Higher-order corrections would be needed to compare with experimental results
 - ◊ SRG evolution Miyagi, PRC 100, 034310 (2019)
 - ◊ Two-body currents Miyagi, PRL 132, 232503 (2024)
 - ◊ Relativistic corrections Reinhard, PRC 103, 054310 (2021)

Magnetic dipole moment



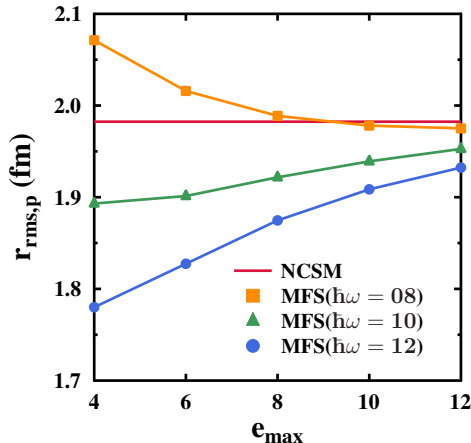
- Average at $e_{\max} = 12$: $\mu = +0.8649 \mu_N$
- NCSM reference value: $\mu = +0.8651 \mu_N \rightarrow$ relative accuracy: -0.02%

Electric quadrupole moment



- Average at $e_{\text{max}} = 12$: $Q_s = +0.2643 \text{ efm}^2$
- NCSM reference value: $Q_s = +0.2663 \text{ efm}^2 \rightarrow$ relative accuracy: -0.75%

Root-mean-square point-proton radius



- Taking $e_{\text{max}} = 12$, $\hbar\omega = 8$ MeV: $r_{\text{rms},p} = 1.975$ fm
- NCSM reference value: $r_{\text{rms},p} = 1.982$ fm → relative accuracy: -0.35 %
- CCSD reference value at $e_{\text{max}} = 12$: $r_{\text{rms},p} = 1.973$ fm

np scattering in the 3S_1 channel

- Deuteron is the bound state solution in the 3S_1 channel
- Harmonic trap: $H_t = H + \frac{1}{2}m\omega_t^2 r^2$

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Stetcu, Ann. Phys. 325, 1644 (2010)

$$-2 \frac{\sqrt{(\mu_m c^2) \hbar \omega_t}}{\hbar c} \frac{\Gamma(\frac{3}{4} - \frac{E_t}{2\hbar\omega_t})}{\Gamma(\frac{1}{4} - \frac{E_t}{2\hbar\omega_t})} = k \cot(\delta_0[k]) = \underbrace{-\frac{1}{a_2} + \frac{1}{2}r_2 k^2 + \frac{1}{4}P_2 k^4 + \dots}_{\text{Effective Range Expansion (ERE)}}$$

with $\mu_m = \frac{m}{2}$ and $k = \frac{\sqrt{(\mu_m c^2) E_t}}{\hbar c}$

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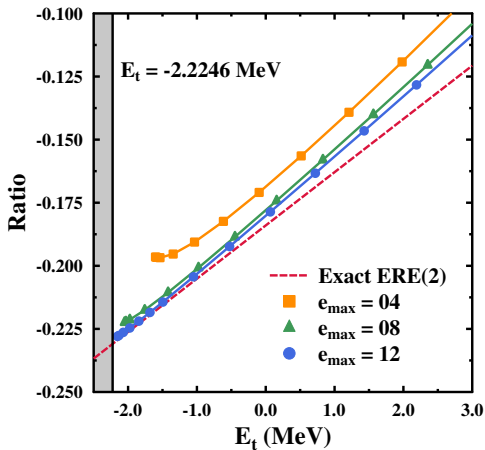
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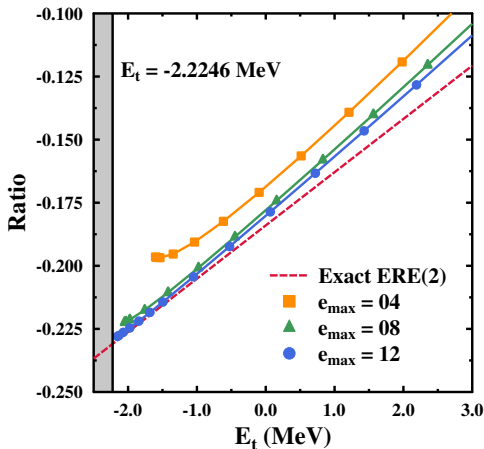
- We can stop at ERE(2) at low energies

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- For $e_{\max} = 12$, $\hbar\omega_t \lesssim \frac{(hc)^2}{(\mu_m c^2)a_2^2} \approx 3 \text{ MeV}$, a fit gives: $a_2 = 5.44(3)$, $r_2 = 1.71(5)$

Summary

Quantity	Unit	Reference	MFS	Relative error
J^π		1^+	1^+	
E	MeV	-2.2246	-2.2225(12)	+0.09 %
Q_s	efm ²	+0.2663	+0.2643	-0.75 %
μ	μ_N	+0.8651	+0.8649	-0.02 %
$r_{\text{rms},p}$	fm	1.982	1.975	-0.35 %
a_2	fm	5.417	5.44(3)	+0.42 %
r_2	fm	1.752	1.71(5)	-2.40 %

- Sub-percent accuracy description of spectroscopic observables
- Important to remove center-of-mass contaminations to get precise results (Q_s and $r_{\text{rms},p}$)

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- For a finite deuteron \Rightarrow projection on Z, N *before* variation

Conclusions

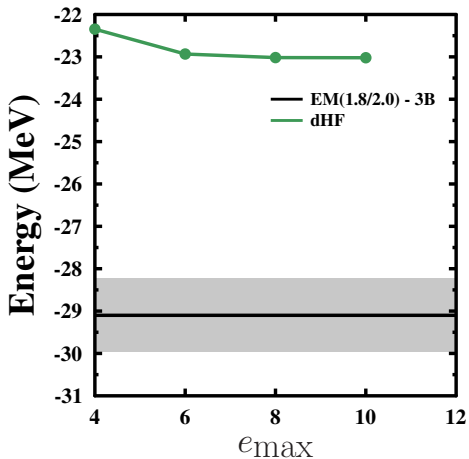
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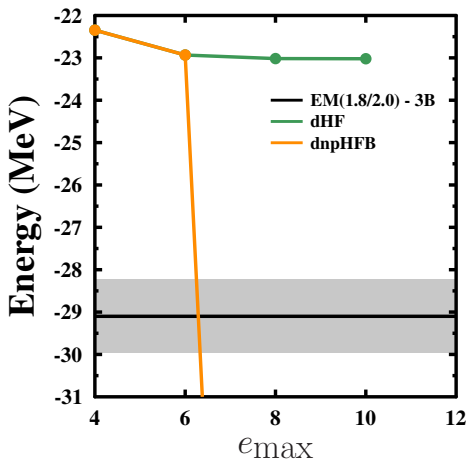
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- Study the growing importance of dynamical correlations with A
Next: ^3H and $^3,4\text{He}$

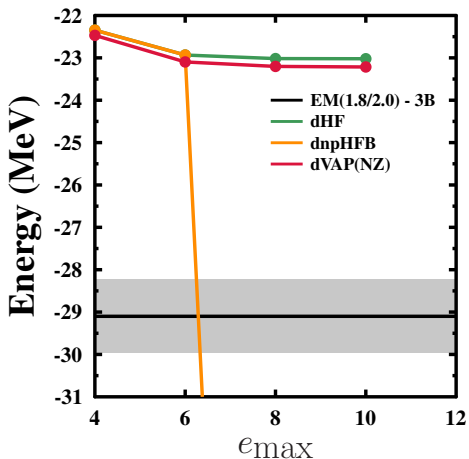
Preliminary results on ${}^4\text{He}$ ($\hbar\omega = 12$)



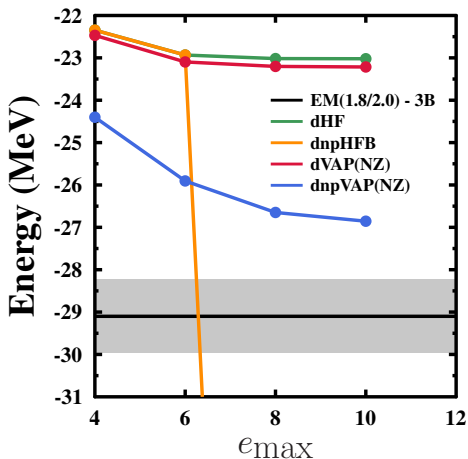
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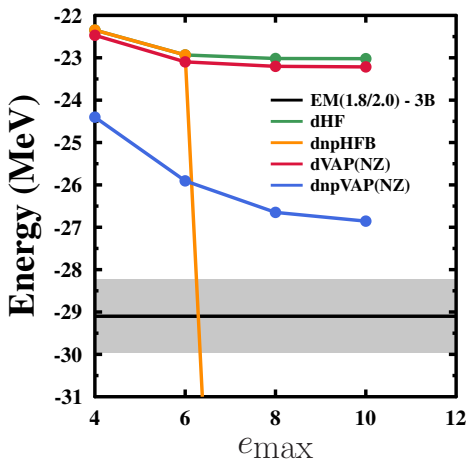
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- Possible improvements:
 - ◇ VAP also on π and/or J
 - ◇ Multi-reference calculation (PGCM)

Occupations in sHO basis of 1^+ state ($e_{\max} = 12$)

