Mean-field approximation on steroids: description of the deuteron

Benjamin Bally

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

ESNT workshop - 21/05/2024

cea irfu

Motivations

- Can we describe the deuteron with a mean-field-like picture?
  - Is the mean-field approximation justified for light systems?

Motivations

- Can we describe the deuteron with a mean-field-like picture?
  - Is the mean-field approximation justified for light systems?
  - Is deuteron even bound?

Motivations

- Can we describe the deuteron with a mean-field-like picture?
  - ◇ Is the mean-field approximation justified for light systems?
  - ◇ Is deuteron even bound?
  - ◇ If yes, how good a description can we get?

Motivations

- Can we describe the deuteron with a mean-field-like picture?
  - Is the mean-field approximation justified for light systems?
  - Is deuteron even bound?
  - If yes, how good a description can we get?

- Spectroscopy of an odd-odd nucleus!

Motivations

- Can we describe the deuteron with a mean-field-like picture?
  - Is the mean-field approximation justified for light systems?
  - Is deuteron even bound?
  - If yes, how good a description can we get?

- Spectroscopy of an odd-odd nucleus!

- Playground to study the impact of many-body approximations on renormalization

  Drissi *et al.*, EPJA 56, 119 (2020)

Motivations

- Can we describe the deuteron with a mean-field-like picture?
  - Is the mean-field approximation justified for light systems?
  - Is deuteron even bound?
  - If yes, how good a description can we get?

- Spectroscopy of an odd-odd nucleus!

- Playground to study the impact of many-body approximations on renormalization

  Drissi *et al.*, EPJA 56, 119 (2020)

- Introduce many concepts that will be discussed this week

  $\Rightarrow$ **talks by Andrea, Mikael, Alberto, Jiangming, Thomas, ...**

Chiral Hamiltonian

- Two-body Hamiltonian: EM500 at N3LO + SRG(1.8)

  Entem *et al.*, PRC 68, 041001(R) (2003) ; Hebeler *et al.*, PRC 83, 031301 (2011)

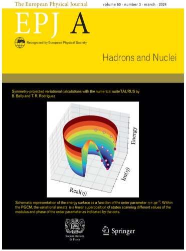
Quantity	Experiment	EM500
J^π	1^+	1^+
E (MeV)	-2.2246	-2.2246
Q_s (efm^2)	+0.286	+0.285*
μ (μ_N)	+0.857	?
a_2 (fm)	5.419(7)	5.417
r_2 (fm)	1.753(8)	1.752

* "Including MEC and RC in the amount of 0.010 fm^2" $\rightarrow \approx +0.275$ at one-body level

- Numerical suite TAURUS

  Bally *et al.*, EPJA 57, 69 (2021) ; Bally *et al.*, 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, π

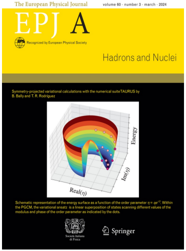


- Numerical suite TAURUS

  Bally *et al.*, EPJA 57, 69 (2021) ; Bally *et al.*, EPJA 60, 62 (2024)

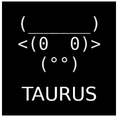
  - ◇ Spherical Harmonic Oscillator basis (*m*-scheme)
  - ◇ Real general Bogoliubov reference states
  - ◇ Variation after particle-number projection
  - ◇ Projection after variation: Z, N, J, π

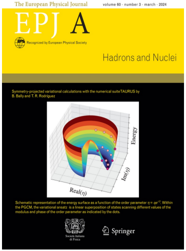
- GitHub: `https://github.com/project-taurus`



Computational aspects

- Numerical suite TAURUS
  Bally *et al.*, EPJA 57, 69 (2021) ; Bally *et al.*, 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, π





- GitHub: `https://github.com/project-taurus`

- Topaze supercomputer (CEA/CCRT)

Natural attempt: Hartree-Fock (HF)

- Minimizes the energy exploring the variational space of Slater determinants

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

Natural attempt: Hartree-Fock (HF)

- Minimizes the energy exploring the variational space of Slater determinants

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

- Very general HF: breaks all spatial symmetries! → deformed HF (dHF)

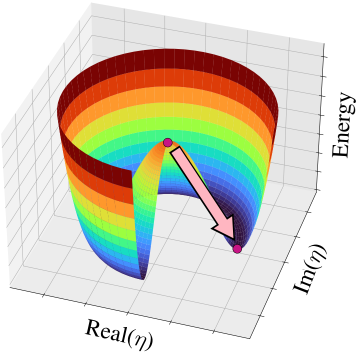
Natural attempt: Hartree-Fock (HF)

- Minimizes the energy exploring the variational space of Slater determinants

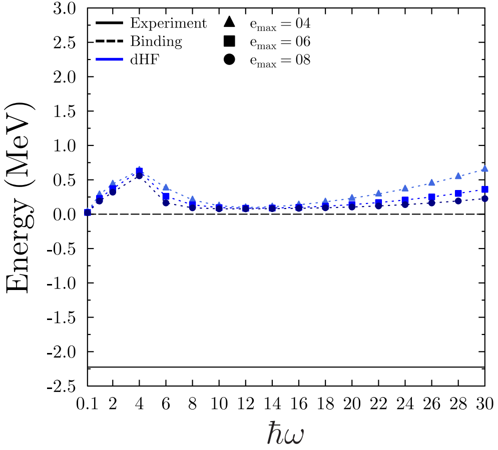
$$\delta \frac{\langle \Phi | H | \Phi \rangle}{\langle \Phi | \Phi \rangle} = 0 \quad \text{with} \quad |\Phi\rangle = \prod_i a_i^\dagger |0\rangle$$

- Very general HF: breaks all spatial symmetries! → deformed HF (dHF)

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



Natural attempt: Hartree-Fock



- Not bound at dHF level

Some juice: projection after variation (PAV)

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

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

Some juice: projection after variation (PAV)

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

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

- Restore the symmetries through quantum-number projection

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

with

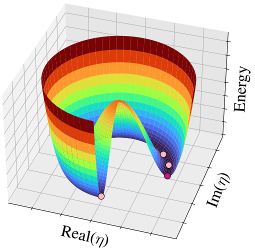
$$P_{MK}^{J} = \frac{2J+1}{16\pi^2} \int_0^{2\pi} d\alpha \int_0^{\pi} d\beta \sin(\beta) \int_0^{4\pi} d\gamma \; D_{MK}^{J*}(\alpha,\beta,\gamma)\, R(\alpha,\beta,\gamma)$$

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

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

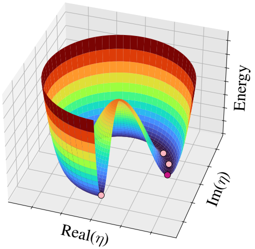
Some juice: projection after variation (PAV)

- Explores the phase of the order parameter



Some juice: projection after variation (PAV)

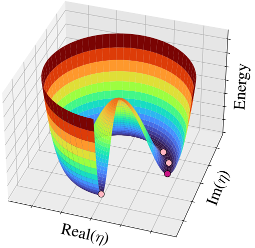
- Explores the phase of the order parameter



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

Some juice: projection after variation (PAV)

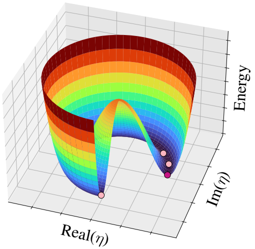
- Explores the phase of the order parameter



- Projected states:
  - Superposition of rotated states → not a product state anymore!
  - Good quantum numbers
  - At least one of them has a lower energy than $\langle \Phi | H | \Phi \rangle$
  - Depends inherently on reference state $|\Phi\rangle$

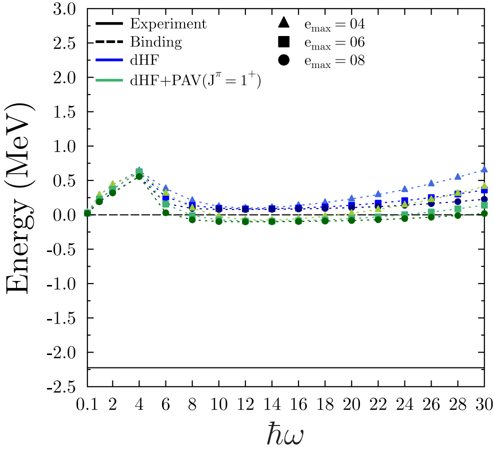
Some juice: projection after variation (PAV)

- Explores the phase of the order parameter



- Projected states:
  - Superposition of rotated states → not a product state anymore!
  - Good quantum numbers
  - 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

Some juice: dHF + PAV



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

Different juice: Hartree-Fock-Bogoliubov (pairing)

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

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

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

Different juice: Hartree-Fock-Bogoliubov (pairing)

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

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

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

- Includes pairing correlations but breaks particle-number conservation

$$|\Phi\rangle = \sum_{ZNJK\pi} \sum_{\epsilon} c_\epsilon^{ZNJK\pi} |\Psi_\epsilon^{ZNJK\pi}\rangle$$

Different juice: Hartree-Fock-Bogoliubov (pairing)

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

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

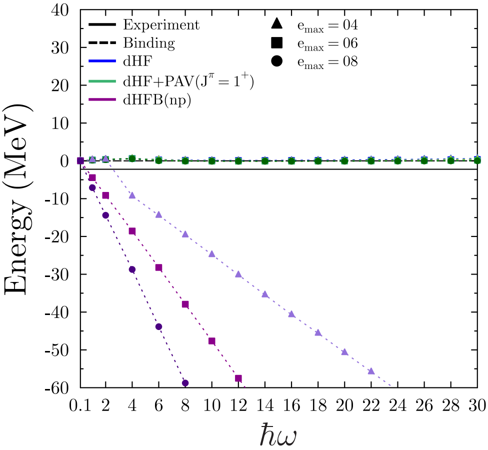
$$\begin{pmatrix} \beta \\ \beta^\dagger \end{pmatrix} = \begin{pmatrix} U^\dagger & V^\dagger \\ V^T & U^T \end{pmatrix} \begin{pmatrix} a \\ a^\dagger \end{pmatrix} \equiv \mathcal{W}^\dagger \begin{pmatrix} a \\ a^\dagger \end{pmatrix} \qquad \mathcal{W}\mathcal{W}^\dagger = \mathcal{W}^\dagger \mathcal{W}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

- Includes pairing correlations but breaks particle-number conservation

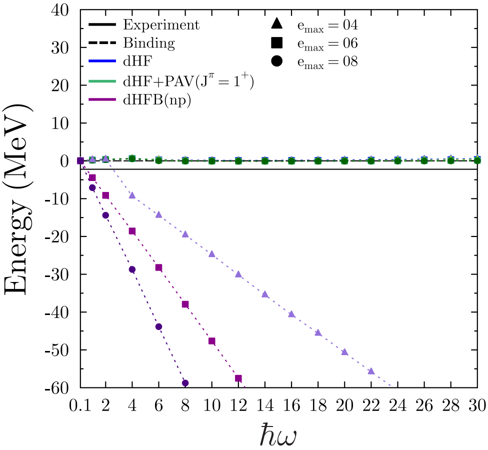
$$|\Phi\rangle = \sum_{ZNJK\pi} \sum_{\epsilon} c_\epsilon^{ZNJK\pi} |\Psi_\epsilon^{ZNJK\pi}\rangle$$

- Very general HFB → dHFB(np)
  - ◇ neutron-proton pairing
  - ◇ odd-odd nuclei
  - ◇ breaks all spatial symmetries

Different juice: dHFB(np)



Different juice: dHFB(np)



- Particle-number nonconserving theory: missing 3N and wrong center of mass

  Hergert *et al.*, PLB 682, 27 (2009)

- Projected state now reads

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

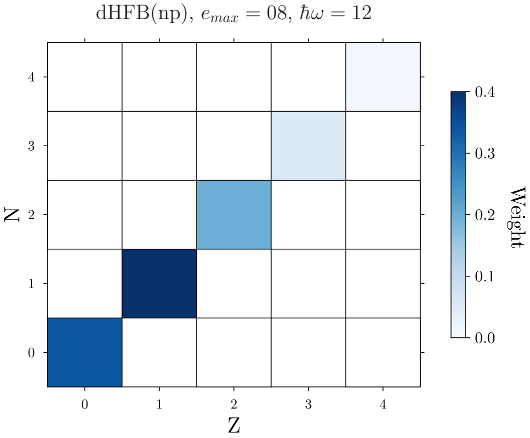
with

$$P^{Z} = \frac{1}{2\pi} \int_{0}^{2\pi} d\phi_{Z}\, e^{i\phi_{Z}(\mathrm{Z}-Z)}$$

$$P^{N} = \frac{1}{2\pi} \int_{0}^{2\pi} d\phi_{N}\, e^{i\phi_{N}(\mathrm{N}-N)}$$

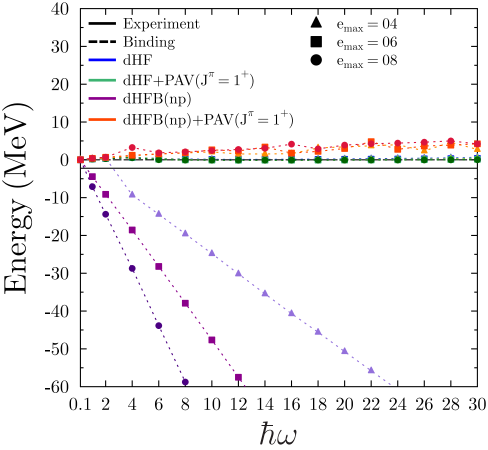
$$\mathrm{diag}(\langle\Phi| H P^{Z} P^{N} P^{J}_{KK'} P^{\pi} |\Phi\rangle) \longrightarrow f_{\epsilon K}^{ZNJ\pi}$$

Decomposition (Z,N) of the reference states



- dHFB(np) favors $N = Z$ components → consistent with 2N interaction

Cocktail of juices: dHFB(np) + PAV



- Not bound anymore and even worse than dHF

Much stronger juice: variation after projection (VAP)

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

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

Much stronger juice: variation after projection (VAP)

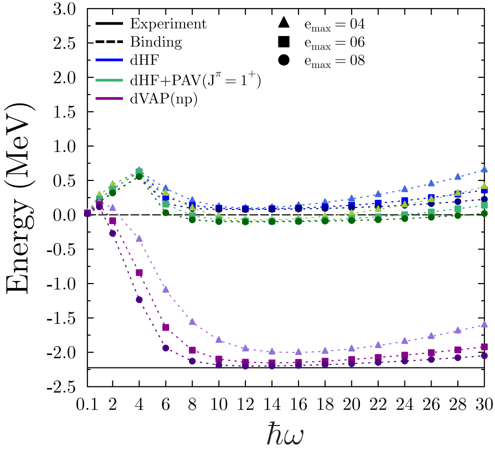
- Minimizes the particle-number projected energy exploring the variational space of Bogoliubov quasi-particle states

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

- Explores the correct subspace (Z, N) of the Hilbert space

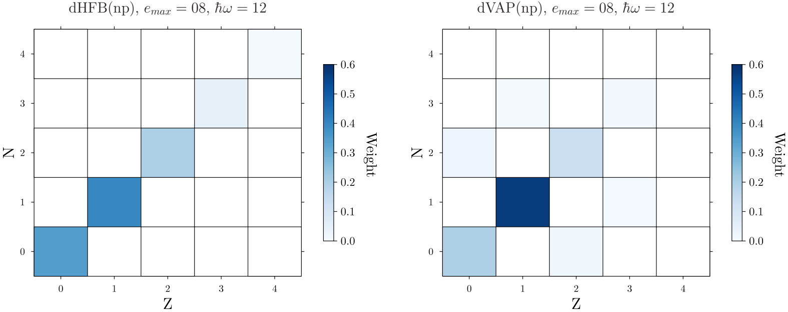
- Much more computationally demanding

Much stronger juice: dVAP



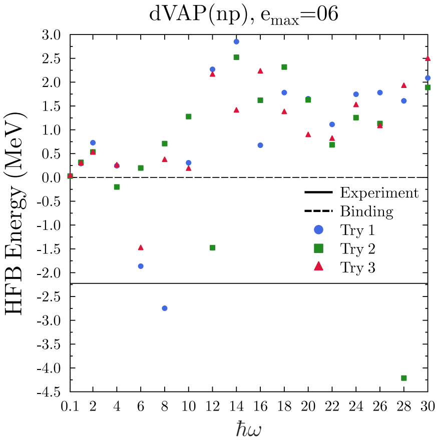
- Bound and very good agreement with experimental data

Decomposition (Z, N) of the reference states



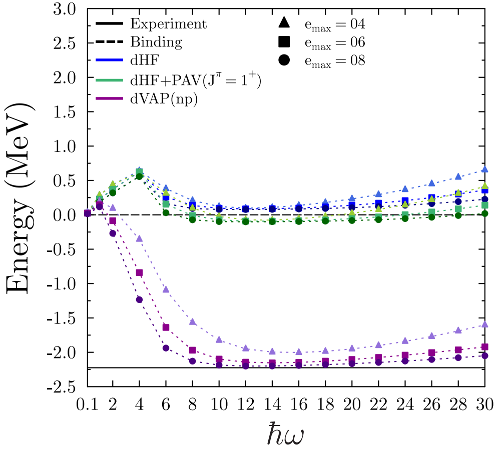
- Different decompositions for dHFB(np) and dVAP(np)

Variability of reference states



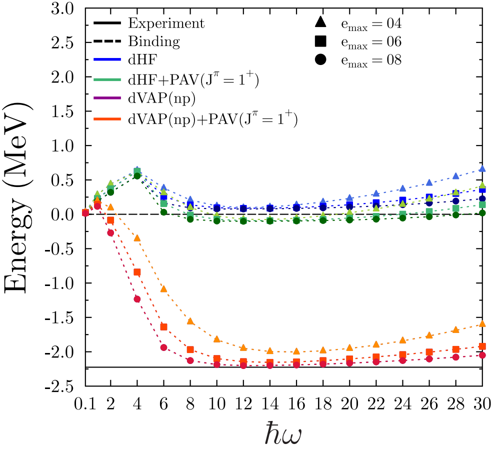
- Different Bogoliubov states can give same projected energy at dVAP(np) level

Much stronger juice: dVAP



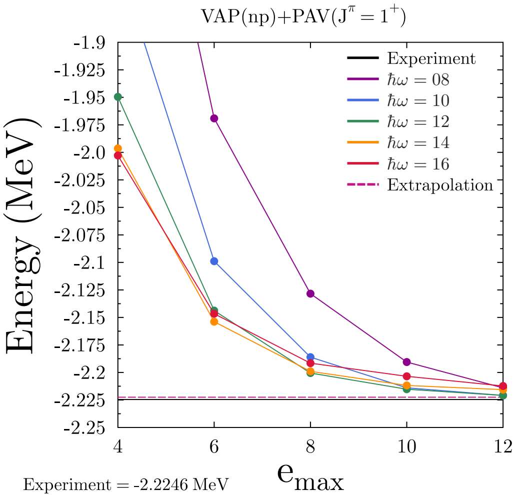
- Bound and very good agreement with experimental data

Cocktail of juices: dVAP + PAV



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

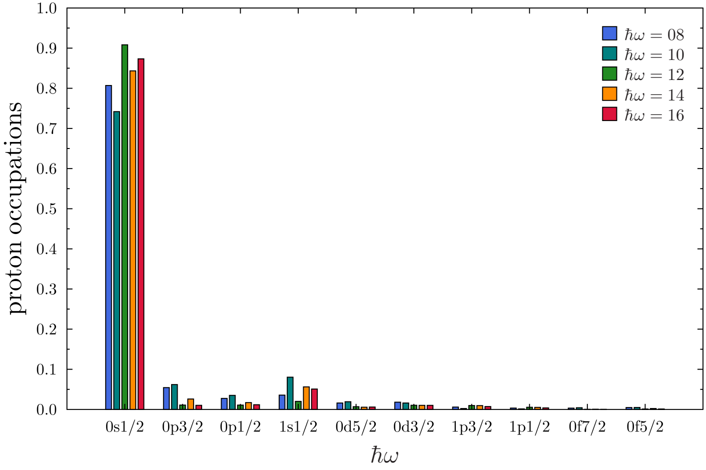
Convergence of the energy



Experiment = -2.2246 MeV

Extrapolation = -2.222 MeV

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



- We use textbook one-body operators

$$\mu(J^\pi_\epsilon) = \langle \Psi_\epsilon^{ZNJM=J\pi} | g_l l + g_s s | \Psi_\epsilon^{ZNJM=J\pi} \rangle$$

$$Q_s(J^\pi_\epsilon) = \sqrt{\frac{16\pi}{5}} \langle \Psi_\epsilon^{ZNJM=J\pi} | e r^2 Y_{20} | \Psi_\epsilon^{ZNJM=J\pi} \rangle$$

$$r^2_{ch}(J^\pi_\epsilon) = \langle \Psi_\epsilon^{ZNJM\pi} | r_p^2 | \Psi_\epsilon^{ZNJM\pi} \rangle + \langle r^2 \rangle_{(p)} + \frac{N}{Z} \langle r^2 \rangle_{(n)} + \langle r^2 \rangle_{(so)} + \frac{3(\hbar c)^2}{4(mc^2)^2}$$

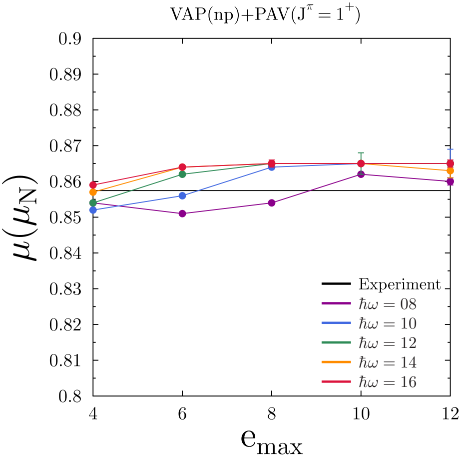
(includes center of mass correction)

- Higher-order corrections would be needed to get exact results

Miyagi *et al.*, arXiv:2311.14383 (2023)

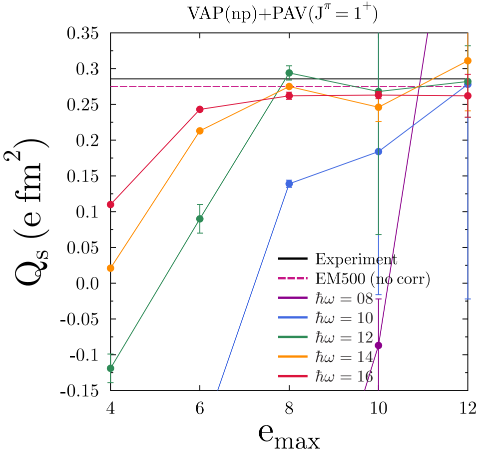
Epelbaum, talk at TRIUMF *ab initio* workshop (2024)

Magnetic moment



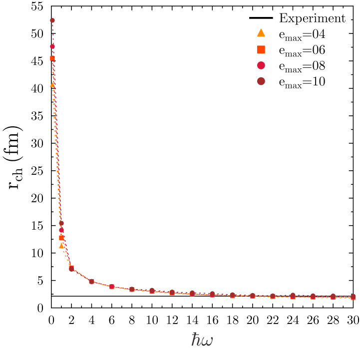
- Good convergence and close to experimental value

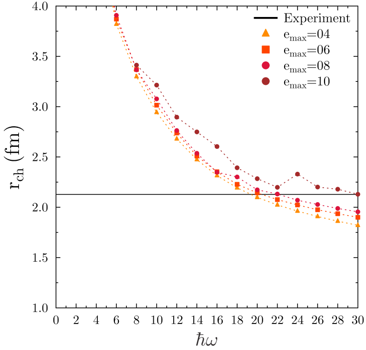
Quadrupole moment



- At $e_{max} = 10, 12$, large variations depending on K-mixing
- Still, seems to converge towards the correct (EM500) value

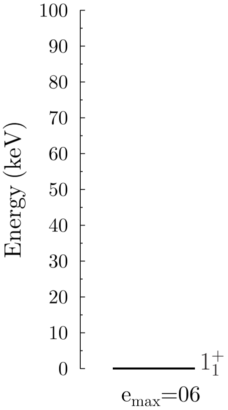
Charge radius





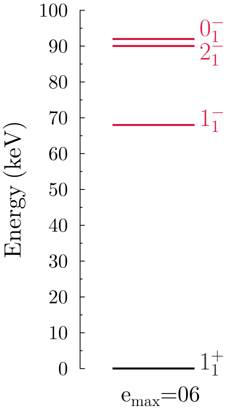
- Charge radius not converged in terms of $\hbar\omega$ and e_{max}
- Importance of higher-order corrections?

Energy "spectrum" ($\hbar\omega$ = 12)

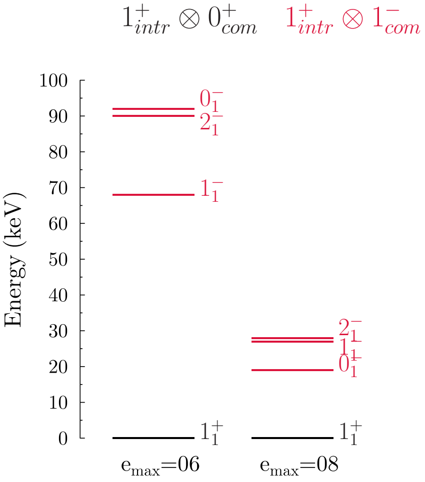


Energy "spectrum" ($\hbar\omega$ = 12)

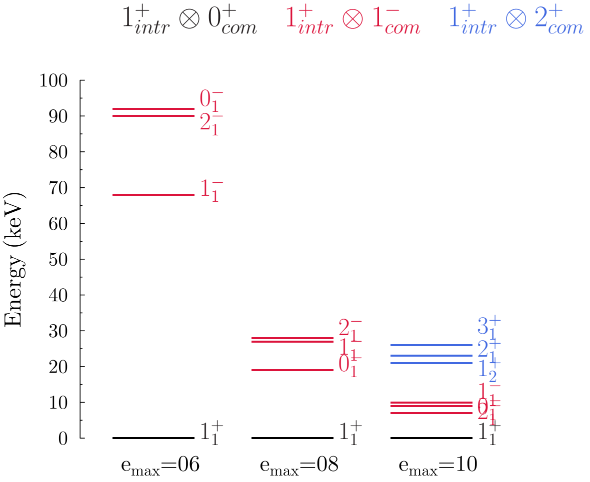
$1^+_{intr} \otimes 0^+_{com}$ $\quad$ $1^+_{intr} \otimes 1^-_{com}$



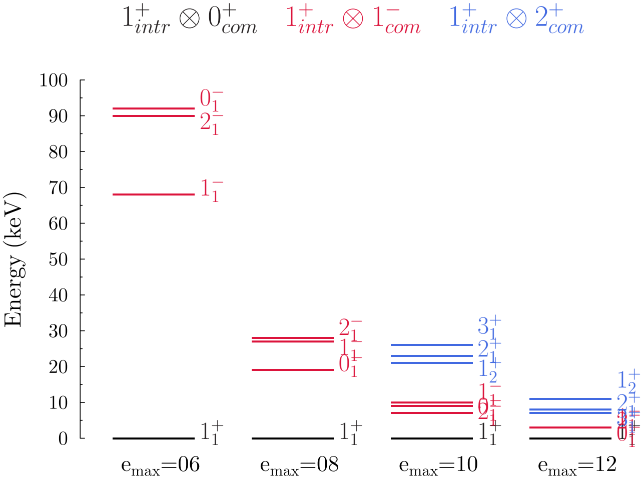
Energy "spectrum" ($\hbar\omega$ = 12)

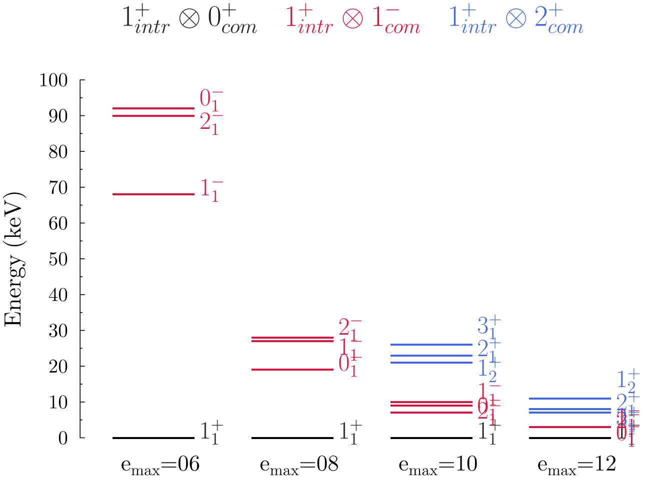


Energy "spectrum" ($\hbar\omega$ = 12)



Energy "spectrum" ($\hbar\omega$ = 12)

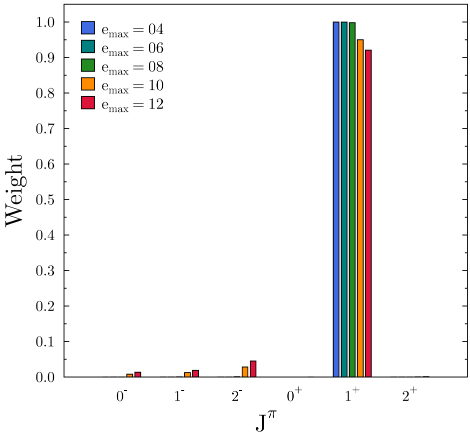




- Factorization of the center of mass

  Hagen *et al.*, PRL 103, 062503 (2009)

Decomposition (J^π) of the reference states ($\hbar\omega = 12$)



- Components from center of mass excitations become larger with increasing e_{max}

Scattering properties

- Harmonic trap: $H_t = H + \frac{1}{2} m\omega_t^2 r^2 = H + \frac{1}{2} \frac{(mc^2)(\hbar\omega_t)^2}{(\hbar c)^2} r^2$

Scattering properties

- Harmonic trap: $H_t = H + \frac{1}{2} m\omega_t^2 r^2 = H + \frac{1}{2} \frac{(mc^2)(\hbar\omega_t)^2}{(\hbar c)^2} r^2$

- Busch (or BERW) formula for $l = 0$

  Stetcu *et al.*, Ann. Phys. 325, 1644 (2010)

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

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

Scattering properties

- Harmonic trap: $H_t = H + \frac{1}{2} m\omega_t^2 r^2 = H + \frac{1}{2} \frac{(mc^2)(\hbar\omega_t)^2}{(\hbar c)^2} r^2$

- Busch (or BERW) formula for $l = 0$

Stetcu *et al.* , Ann. Phys. 325, 1644 (2010)

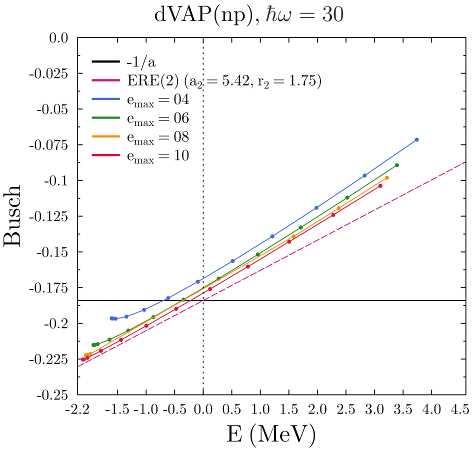
$$-2\frac{\sqrt{(\mu c^2)\hbar\omega_t}}{\hbar c}\frac{\Gamma(\frac{3}{4} - \frac{E_t}{2\hbar\omega_t})}{\Gamma(\frac{1}{4} - \frac{E_t}{2\hbar\omega_t})} = k\cot(\delta_0[k]) = \underbrace{-\frac{1}{a_2} + \frac{1}{2} r_2 k^2 + \frac{1}{4} P_2 k^4 + \dots}_{\text{Effective Range Expansion (ERE)}}$$

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

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

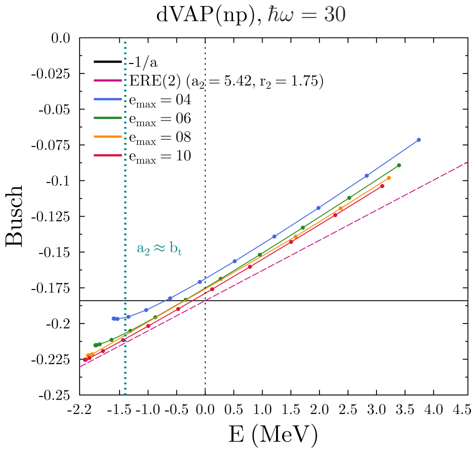
$$-2\frac{\sqrt{(\mu c^2)\hbar\omega_t}}{\hbar c}\frac{\Gamma(\frac{3}{4} - \frac{E_t}{2\hbar\omega_t})}{\Gamma(\frac{1}{4} - \frac{E_t}{2\hbar\omega_t})} = -\frac{1}{a_2} + \frac{1}{2}\frac{(\mu c^2) r_2}{(\hbar c)^2} E_t$$

Scattering properties



- Correct behavior but would need large values of e_{max} to fully converge

Scattering properties



- At $e_{max} = 10$, for $\hbar\omega_t \lesssim \frac{(\hbar c)^2}{(\mu c^2) a_2^2}$, a fit gives: $a_{2t} = 5.49$, $r_{2t} = 1.71$

Summary

Quantity	Experiment	EM500	dVAP(pn)+PAV
J^π	1^+	1^+	1^+
E (MeV)	-2.2246	-2.2246	-2.222
Q_s (efm^2)	+0.286	+0.275*	[+0.25,+0.31]
μ (μ_N)	+0.857	?	[+0.860,+0.865]
a_2 (fm)	5.419(7)	5.417	5.49 (e_{max} = 10)
r_2 (fm)	1.753(8)	1.752	1.71 (e_{max} = 10)

- Need to remove the center of mass (Q_s)
- Very good description of observables

Summary

Quantity	Experiment	EM500	dVAP(pn)+PAV
J^π	1^+	1^+	1^+
E (MeV)	-2.2246	-2.2246	-2.222
Q_s (efm^2)	+0.286	+0.275*	[+0.25,+0.31]
μ (μ_N)	+0.857	?	[+0.860,+0.865]
a_2 (fm)	5.419(7)	5.417	5.49 (e_{max} = 10)
r_2 (fm)	1.753(8)	1.752	1.71 (e_{max} = 10)

- Need to remove the center of mass (Q_s)
- Very good description of observables

  → reminder: BCS(np) exact in low-density symmetric nuclear matter

  Baldo *et al.*, PRC 52, 975 (1995) ; Lombardo *et al.*, PRC 64, 064314 (2001)

Conclusions

- Mean-field approximation on steroids perfectly describes the deuteron!

Conclusions

- Mean-field approximation on steroids perfectly describes the deuteron!

- Illustrates the usefulness of symmetry-breaking/restoration schemes

Conclusions

- Mean-field approximation on steroids perfectly describes the deuteron!
- Illustrates the usefulness of symmetry-breaking/restoration schemes
- Study the growing importance of dynamical correlations with A

Conclusions

- Mean-field approximation on steroids perfectly describes the deuteron!
- Illustrates the usefulness of symmetry-breaking/restoration schemes
- Study the growing importance of dynamical correlations with A
- Analyze renormalization in pionless EFT