New Frontiers in Nuclear Structure Theory

From Realistic Interactions to the Nuclear Chart

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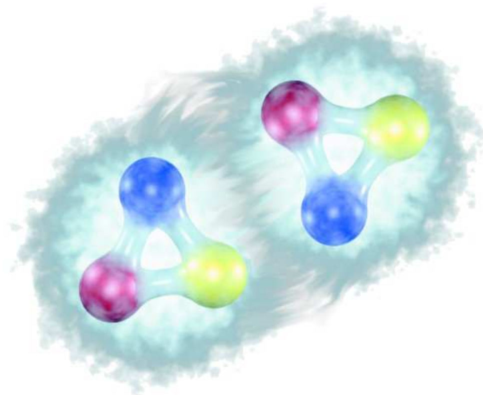


Overview

- Motivation
- Nucleon-Nucleon Interactions
- Solving the Many-Body Problem
- Correlations & Unitary Correlation Operator Method
- Applications

Nuclear Structure in the 21st Century

new frontiers in nuclear structure physics

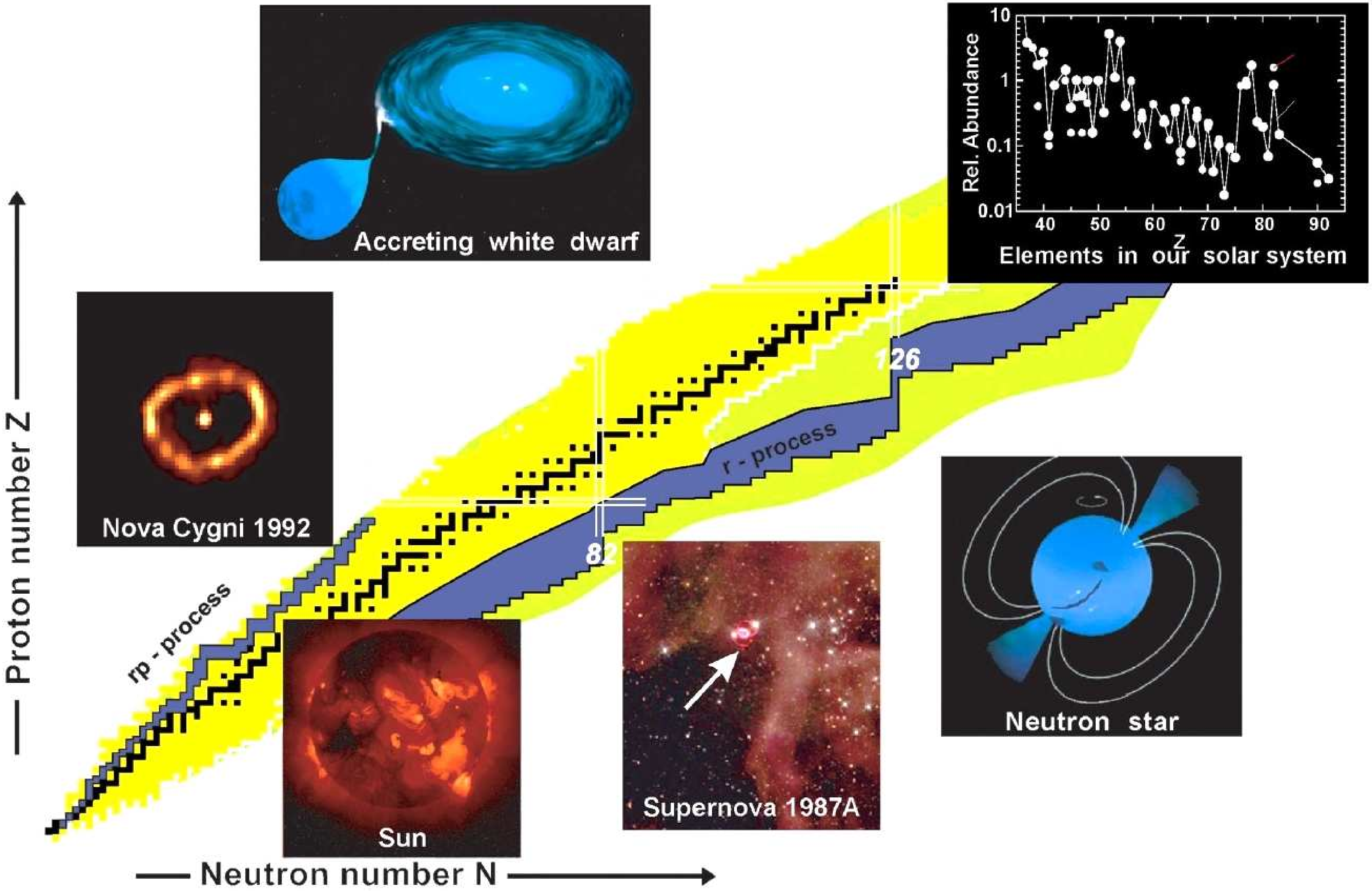
Experiment

- fundamental astrophysical questions need nuclear input
- possibilities to investigate nuclei far off stability
- new nuclear structure facilities: FAIR@GSI, RIA,...

Theory

- improved understanding of fundamental degrees of freedom / QCD
- high-precision realistic nucleon-nucleon potentials
- *ab initio* treatment of the many-body problem

Astrophysical Challenges

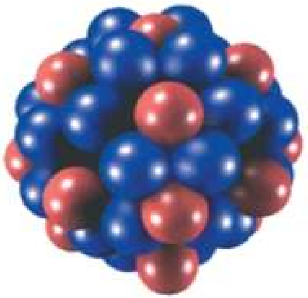


Theoretical Context

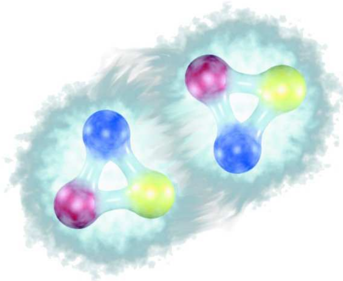
better resolution / more fundamental

Nuclear Structure

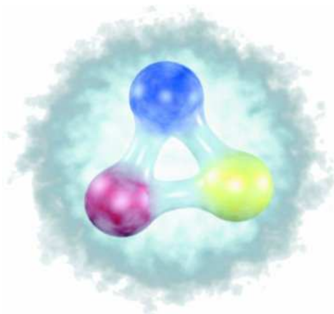
Quantum Chromo Dynamics



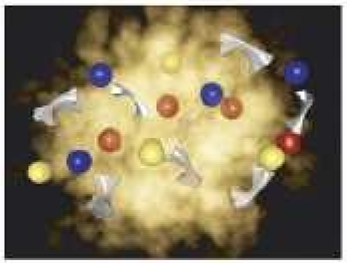
- finite nuclei



- few-nucleon systems
- nucleon-nucleon interaction

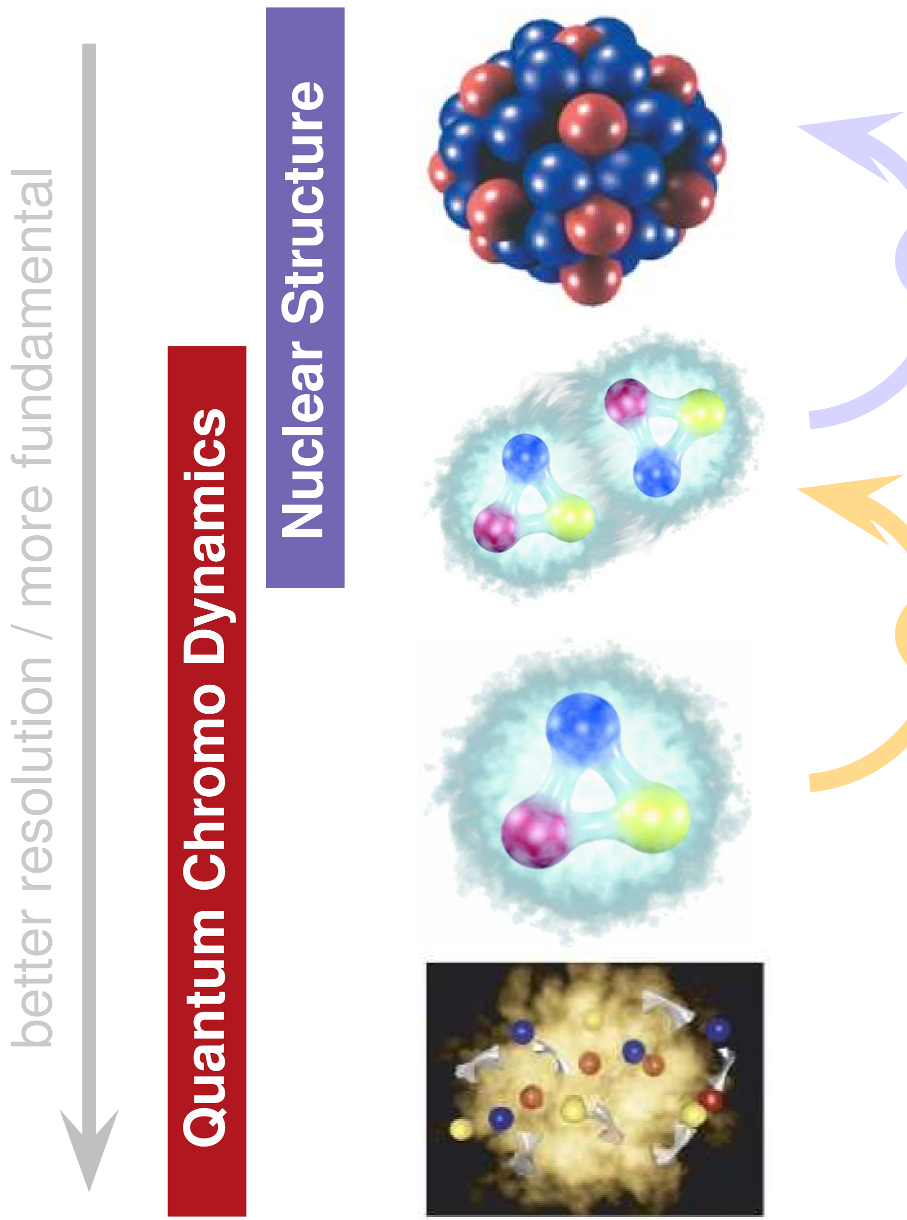


- hadron structure



- quarks & gluons
- deconfinement

Theoretical Context

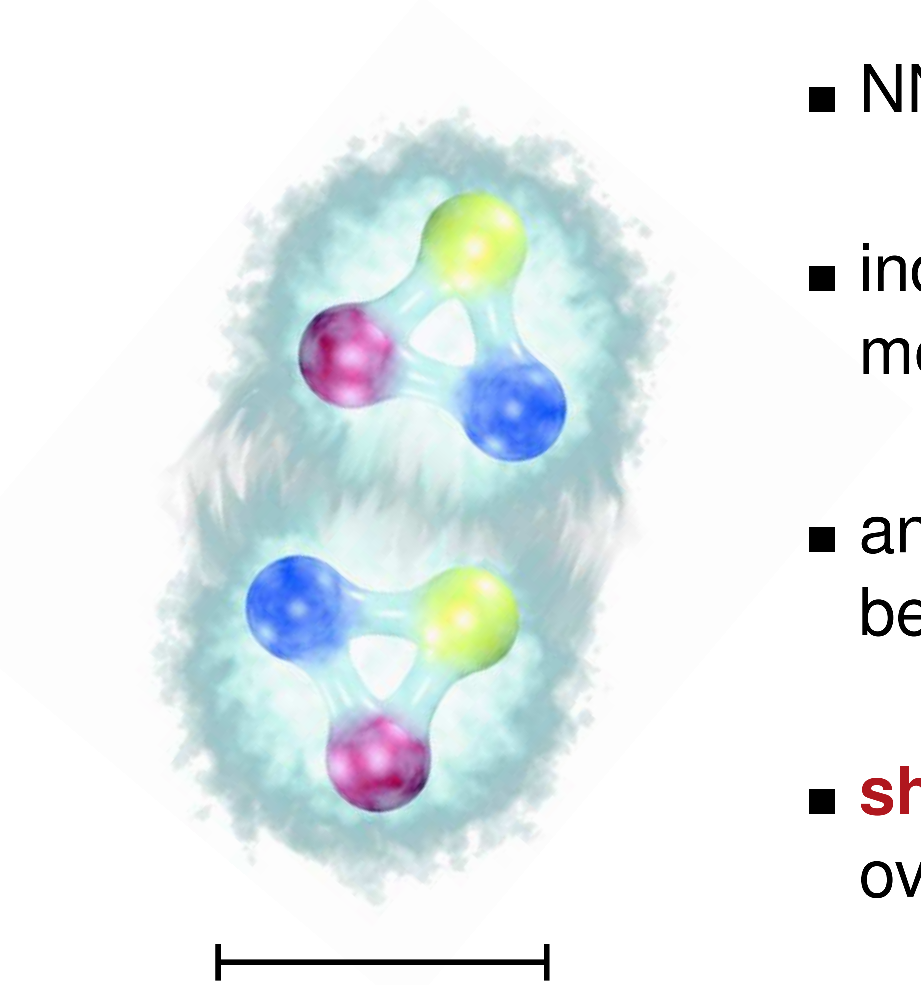


“solve”
the interacting nuclear
many-body problem

“construct”
a realistic nucleon-nucleon
interaction from QCD

Realistic
Nucleon-Nucleon Potentials

Nature of the NN-Interaction



$\sim 1.6\text{fm}$

$\rho_0^{-1/3} = 1.8\text{fm}$

- NN-interaction is **not fundamental**
- induced via mutual **polarisation** of virtual meson cloud (simple picture)
- analogous to **van der Waals** interaction between neutral atoms
- **short-ranged**: acts only if the nucleons overlap
- genuine **NNN-interaction** is important

How to Construct the NN-Potential?

- **QCD input**
  - symmetries
  - meson-exchange picture
  - chiral perturbation theory
- **short-range phenomenology**
  - ansatz for short-range behaviour
- **experimental two-body data**
  - scattering phase-shifts & deuteron properties
  - reproduced with $\chi^2/\mathrm{datum} \approx 1$

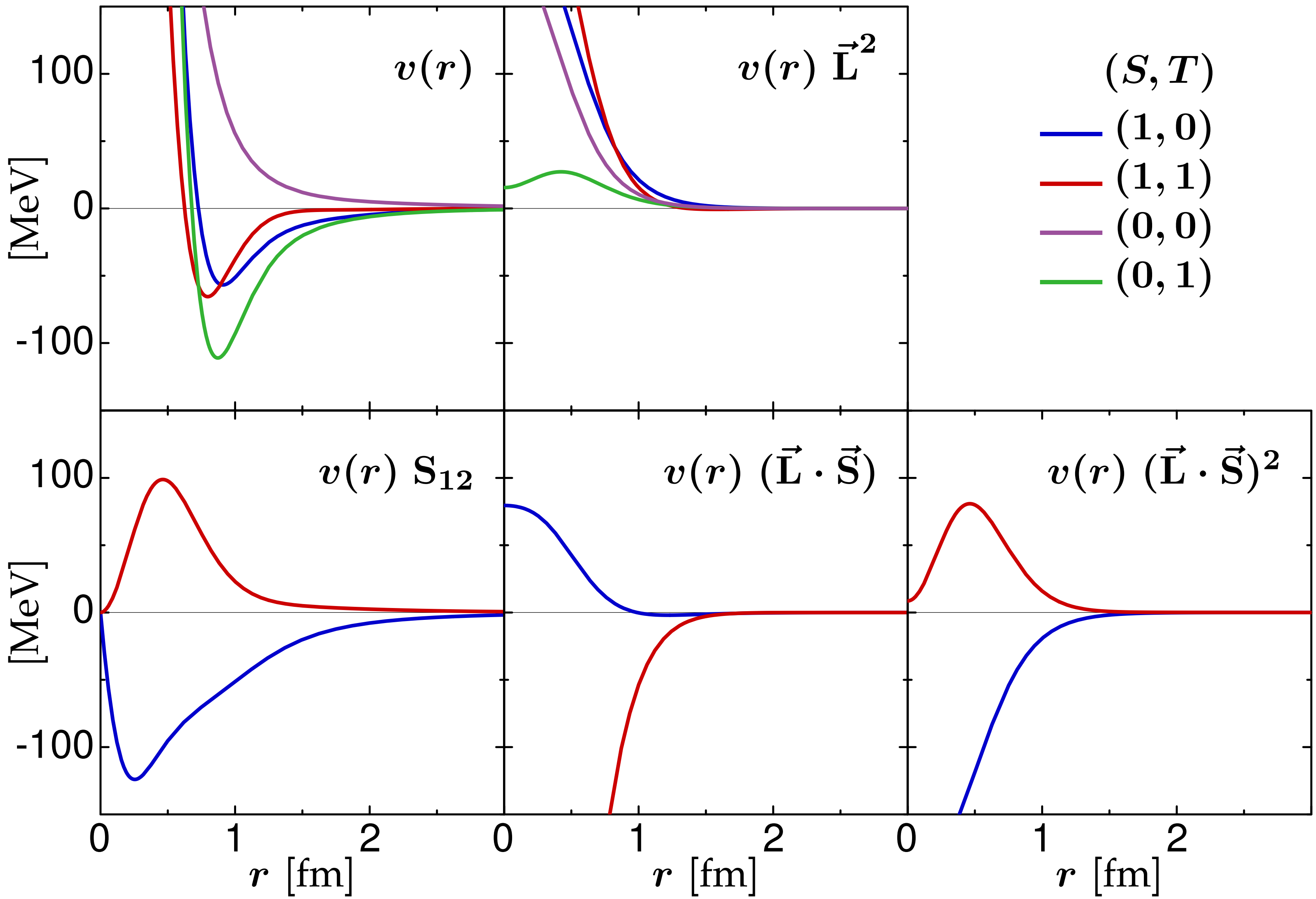
Argonne V18

CD Bonn

Nijmegen I/II

Chiral...

Argonne V18 Potential



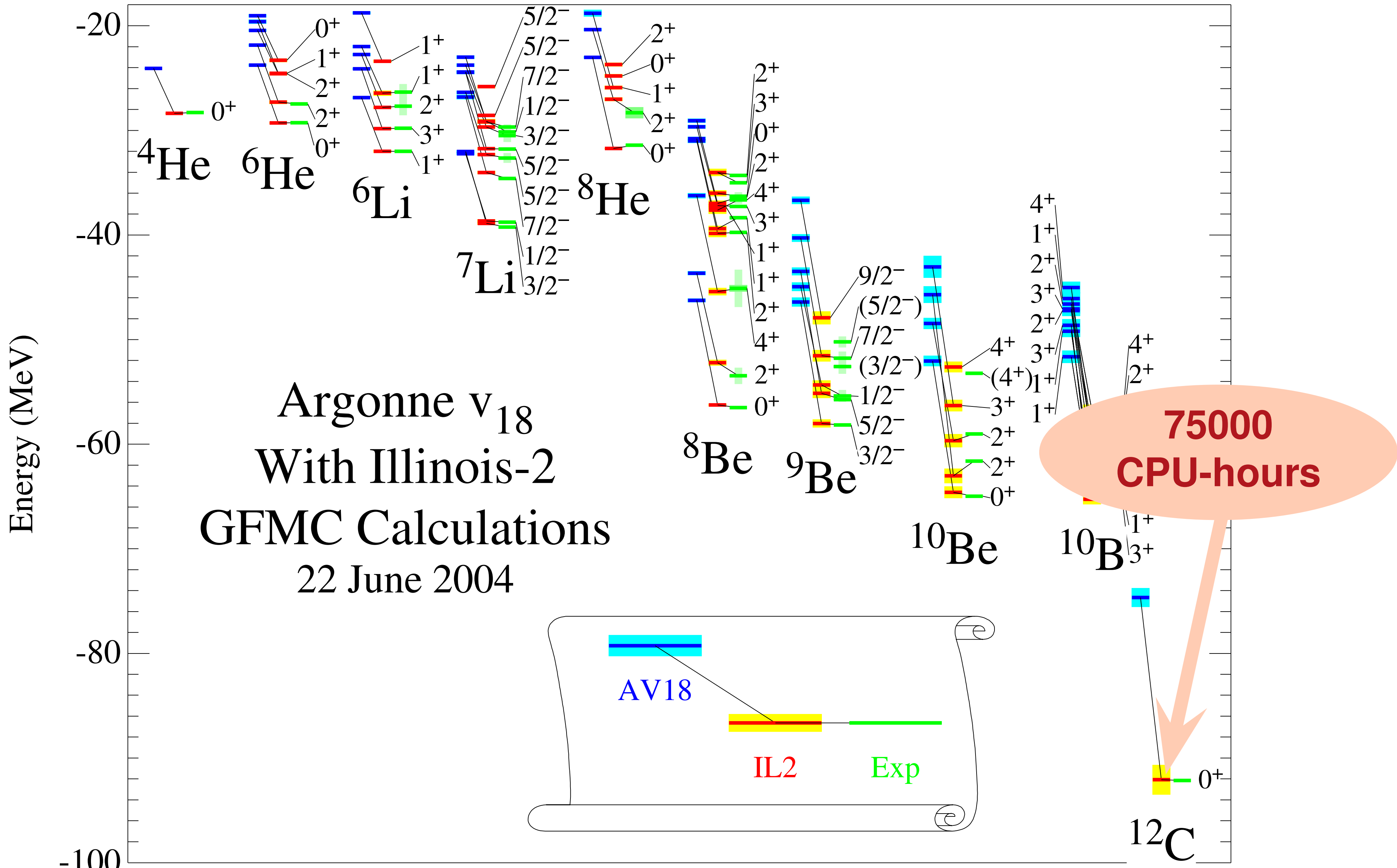
Nuclear
Many-Body Problem

Ab initio Calculations

solve the quantum many-body problem for A nucleons interacting via a realistic NN-potential

- exact numerical solution possible for small systems at an enormous computational cost
- **Green's Function Monte Carlo**: Monte Carlo sampling of the A-body wave function in coordinate space; imaginary time cooling
- **No-Core Shell Model**: large-scale diagonalisation of the Hamiltonian in a harmonic oscillator basis

Green's Function Monte Carlo



[S. Pieper, private comm.]

^{12}C results are preliminary.

Our Goal

nuclear structure calculations
across the **whole nuclear chart**
based on **realistic NN-potentials**
and as close as possible to
an **ab initio** treatment

bound to **simple Hilbert spaces** for large particle numbers

need to deal with strong **interaction-induced correlations**

What are Correlations?

correlations:

everything beyond the independent particle picture

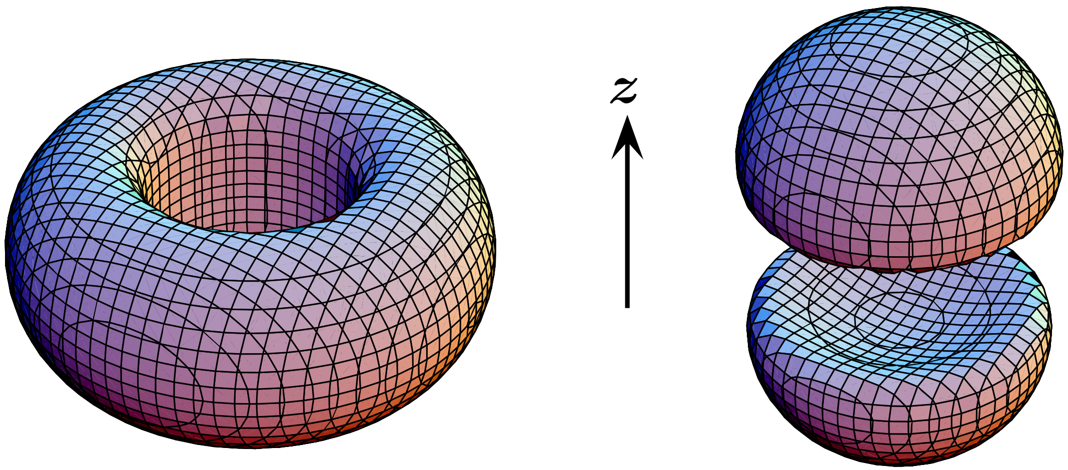
- the quantum state of A independent (non-interacting) fermions is a **Slater determinant**

$$|\psi\rangle = \mathcal{A}\left(|\phi_1\rangle \otimes |\phi_2\rangle \otimes \cdots \otimes |\phi_A\rangle\right)$$

- Slater determinants **cannot describe correlations** by definition

Deuteron: Manifestation of Correlations

$\boldsymbol{M_S = 0}$ | $\boldsymbol{M_S = \pm 1}$
$\frac{1}{\sqrt{2}}(\,|\!\uparrow\downarrow\rangle + |\!\downarrow\uparrow\rangle)$ | $|\!\uparrow\uparrow\rangle,\ |\!\downarrow\downarrow\rangle$



- spin-projected two-body density $\rho^{(2)}_{1,M_S}(\vec{r})$
- **exact deuteron solution** for Argonne V18 potential

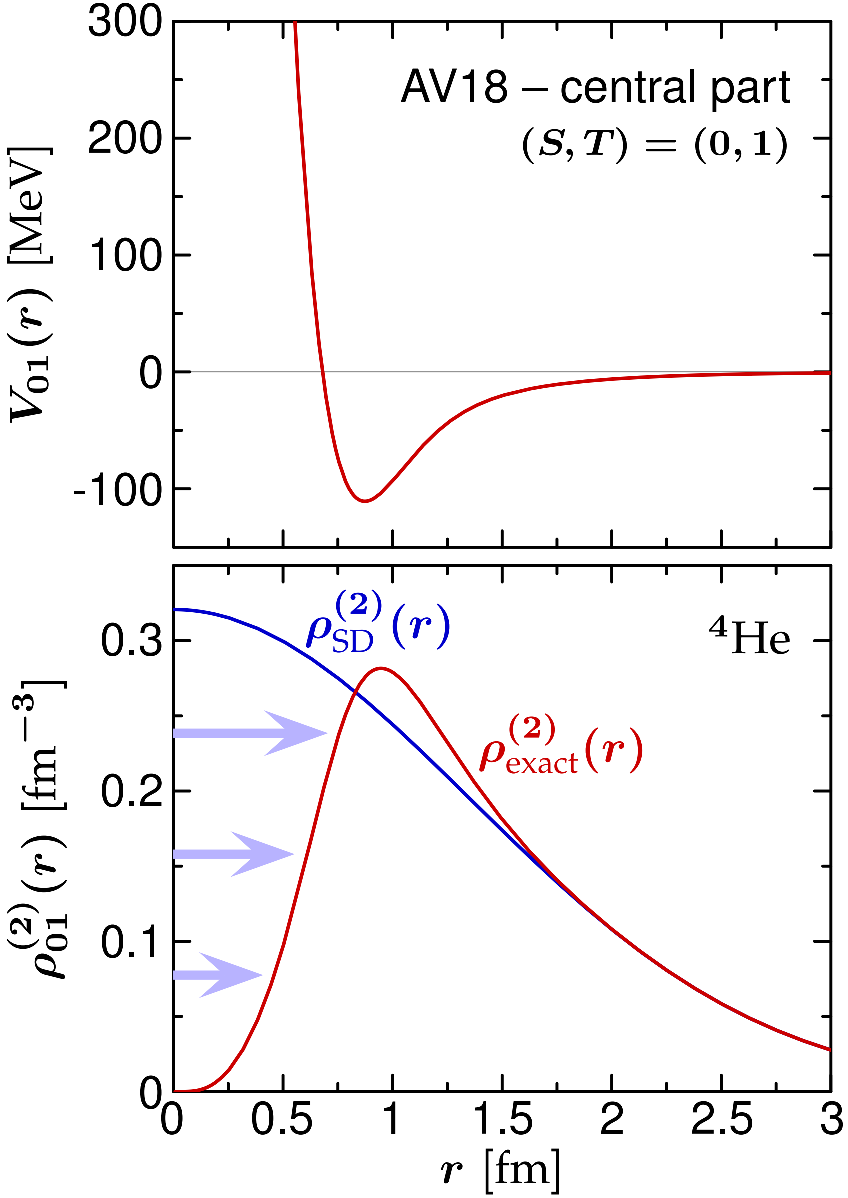
two-body density fully suppressed at small particle distances $|\vec{r}|$

central correlations

angular distribution depends strongly on relative spin orientation

tensor correlations

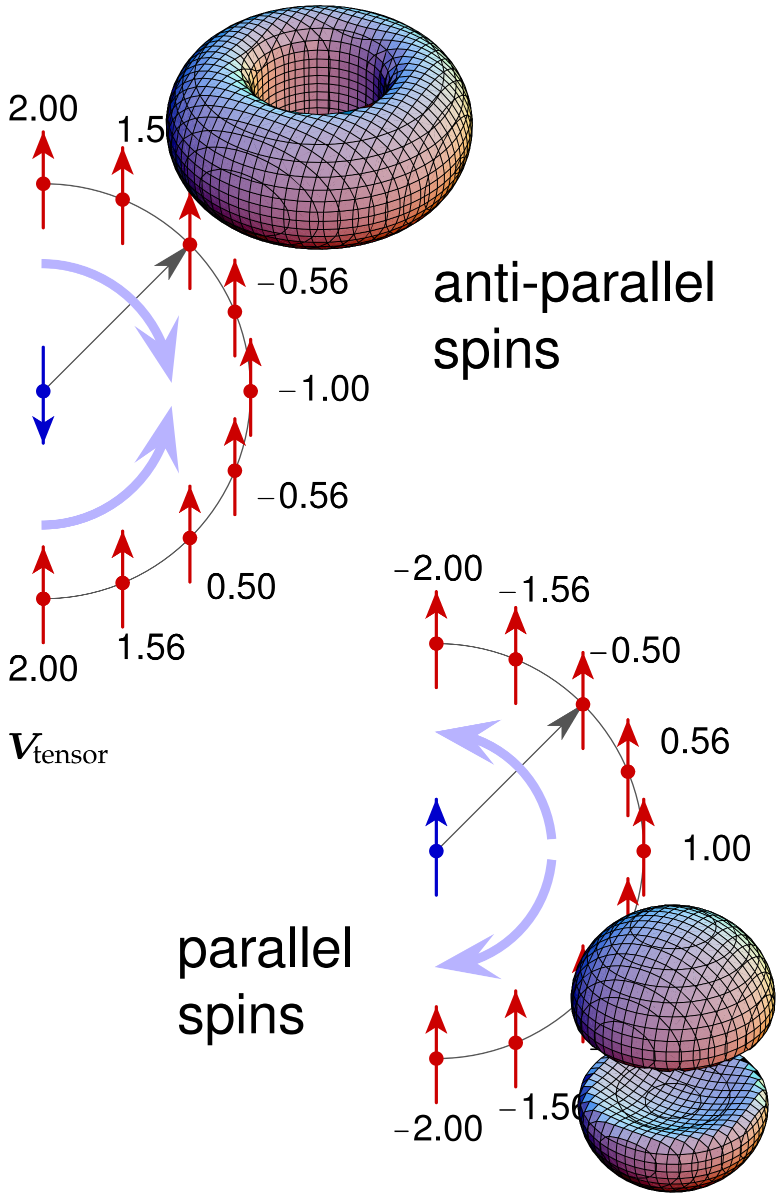
Central Correlations



- strong repulsive core in central part of realistic interactions
- suppression of the probability density for finding two nucleons within the core ➔ **central correlations**

"shift"
the nucleons out of the core region

Tensor Correlations



- analogy with dipole-dipole interaction

$$V_{\text{tensor}} \sim -\left(3\,\frac{(\vec{\sigma}_1\vec{r})(\vec{\sigma}_2\vec{r})}{r^2} - \vec{\sigma}_1\vec{\sigma}_2\right)$$

- couples the relative spatial orientation of two nucleons with their spin orientation ➔ **tensor correlations**

“rotate” nucleons towards pole or equator depending on spin

Unitary Correlation Operator Method (UCOM)

Unitary Correlation Operator Method

Correlation Operator

introduce correlations by means of an unitary transformation with respect to the relative coordinates of all pairs

$$\mathrm{C} = \exp[-\mathrm{i}\,\mathrm{G}] = \exp\Big[-\,\mathrm{i}\sum_{i<j}\mathrm{g}_{ij}\Big]$$

$$\mathrm{g} = \mathrm{g}(\vec{\mathrm{r}}, \vec{\mathrm{q}}; \vec{\sigma}_1, \vec{\sigma}_2, \vec{\tau}_1, \vec{\tau}_2)$$

$$\mathrm{G}^\dagger = \mathrm{G}$$

$$\mathrm{C}^\dagger\mathrm{C} = 1$$

Correlated States

$$|\widetilde{\psi}\rangle = \mathrm{C}\;|\psi\rangle$$

Correlated Operators

$$\widetilde{\mathrm{O}} = \mathrm{C}^\dagger\;\mathrm{O}\;\mathrm{C}$$

$$\langle\widetilde{\psi}|\,\mathrm{O}\,|\widetilde{\psi}'\rangle = \langle\psi|\,\mathrm{C}^\dagger\;\mathrm{O}\;\mathrm{C}\,|\psi'\rangle = \langle\psi|\,\widetilde{\mathrm{O}}\,|\psi'\rangle$$

Central and Tensor Correlators

$$\mathbf{C} = \mathbf{C}_{\Omega}\mathbf{C}_r$$

Central Correlator C_r

- radial distance-dependent shift in the relative coordinate of a nucleon pair

$$\mathrm{g}_r = \frac{1}{2}\left[s(\mathrm{r})\ \mathrm{q}_r + \mathrm{q}_r\ s(\mathrm{r})\right]$$

$$\mathrm{q}_r = \tfrac{1}{2}\left[\tfrac{\vec{\mathrm{r}}}{\mathrm{r}} \cdot \vec{\mathrm{q}} + \vec{\mathrm{q}} \cdot \tfrac{\vec{\mathrm{r}}}{\mathrm{r}}\right]$$

Tensor Correlator C_{Ω}

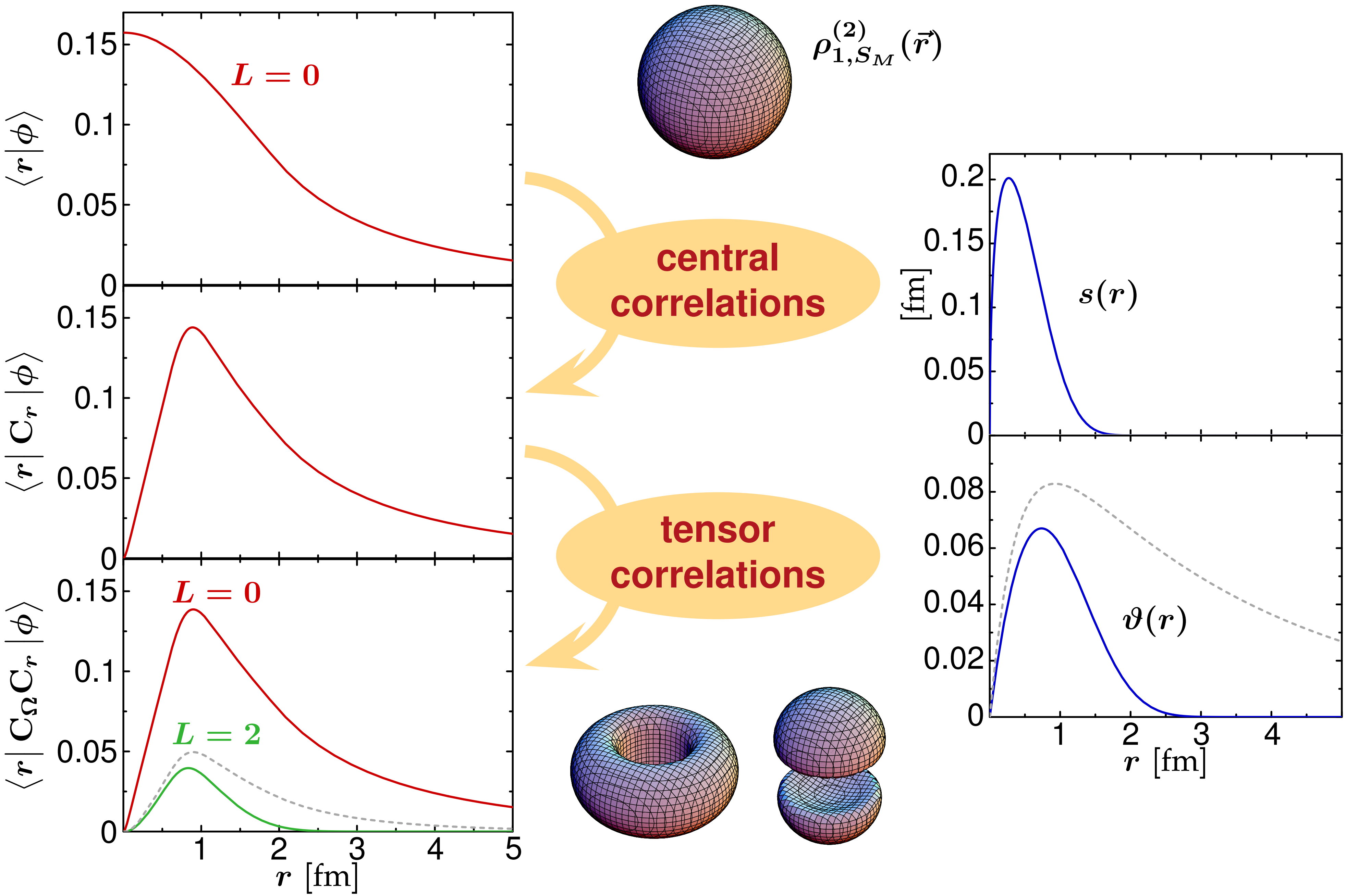
- angular shift depending on the orientation of spin and relative coordinate of a nucleon pair

$$\mathrm{g}_{\Omega} = \frac{3}{2}\vartheta(\mathrm{r})\left[(\vec{\sigma}_1 \cdot \vec{\mathrm{q}}_{\Omega})(\vec{\sigma}_2 \cdot \vec{\mathrm{r}}) + (\vec{\mathrm{r}} \leftrightarrow \vec{\mathrm{q}}_{\Omega})\right]$$

$$\vec{\mathrm{q}}_{\Omega} = \vec{\mathrm{q}} - \tfrac{\vec{\mathrm{r}}}{\mathrm{r}}\ \mathrm{q}_r$$

$s(r)$ and $\vartheta(r)$
encapsulate the physics of
short-range correlations

Correlated States



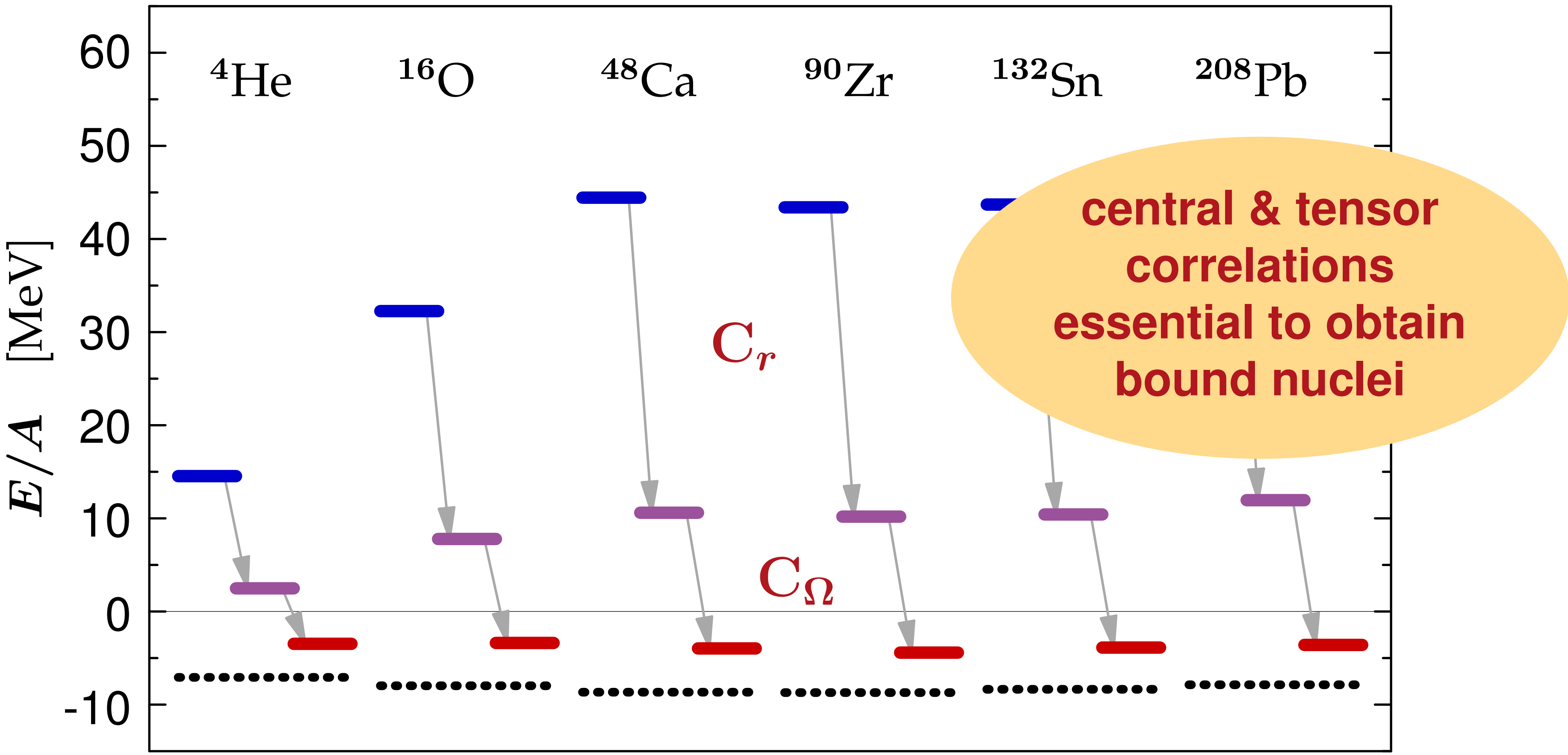
Correlated NN-Potential — V_{UCOM}

$$\widetilde{\mathrm{H}} = \mathrm{T} + \mathrm{V}_{\mathrm{UCOM}} + \mathrm{V}^{[3]}_{\mathrm{UCOM}} + \cdots$$

- **closed operator expression** for the correlated interaction $\mathrm{V}_{\mathrm{UCOM}}$ in two-body approximation
- correlated interaction and original NN-potential are **phase shift equivalent** by construction
- unitary transformation results in a **pre-diagonalisation** of Hamiltonian
- momentum-space matrix elements of correlated interaction are **similar to $V_{\text{low}-k}$**

Simplistic "Shell-Model" Calculation

- expectation value of Hamiltonian (with AV18) for Slater determinant of harmonic oscillator states



Application I

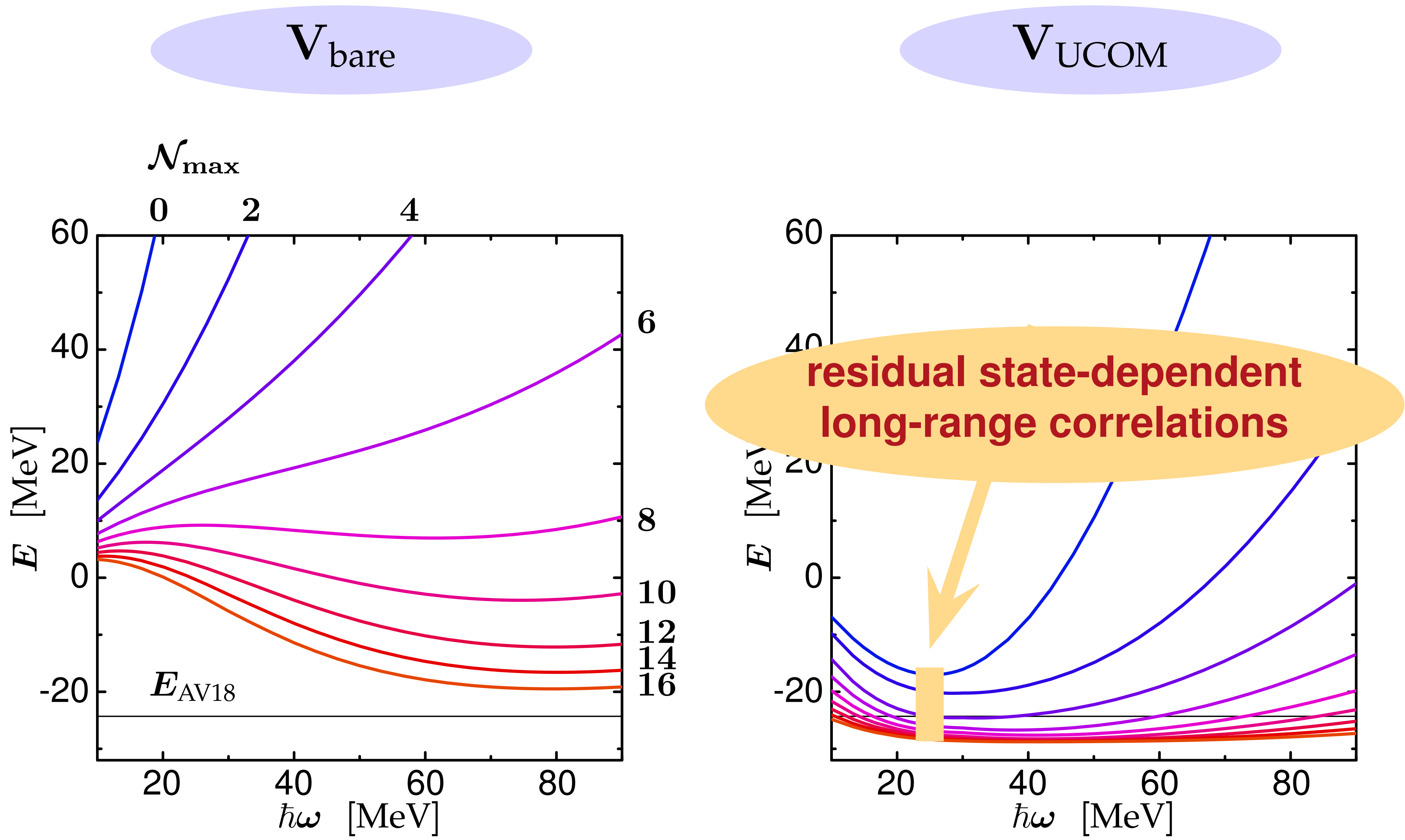
No-Core Shell Model

UCOM + NCSM

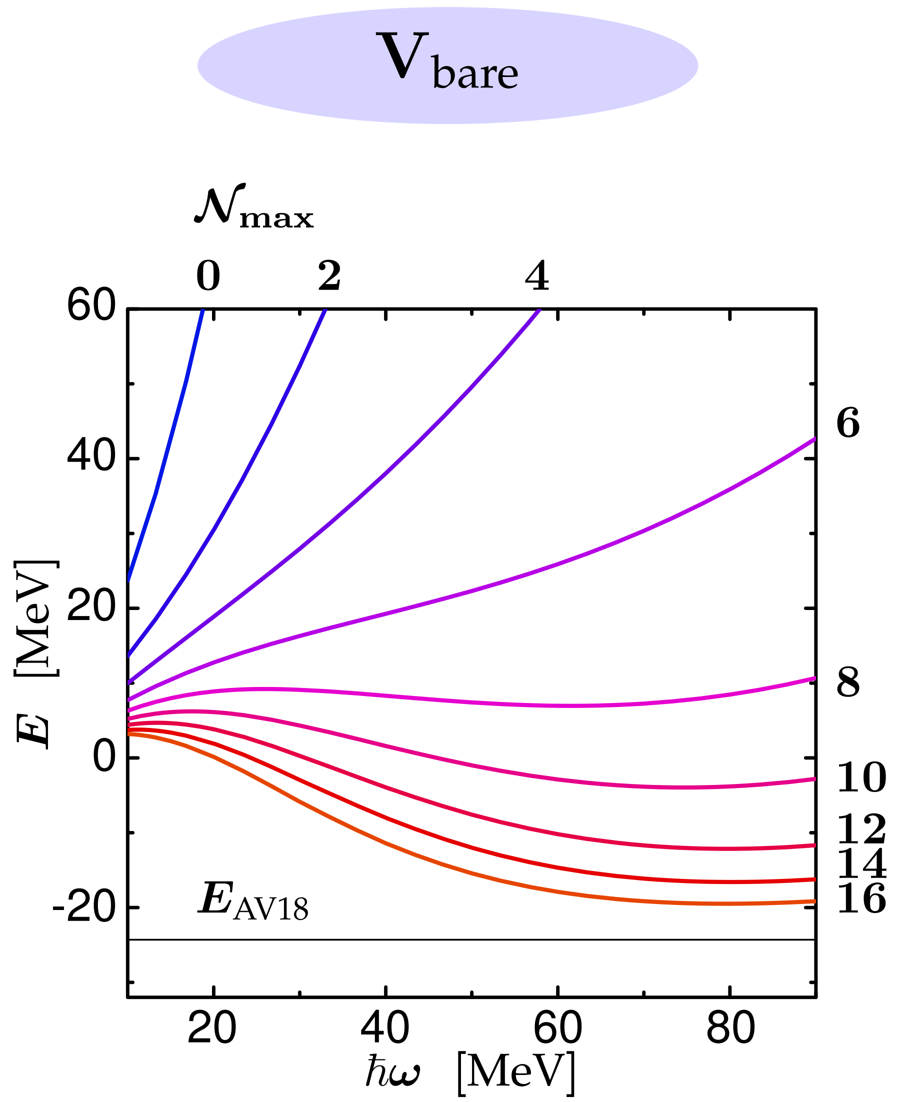
No-Core Shell Model
+
Matrix Elements of Correlated Realistic NN-Interaction $\mathrm{V}_{\mathrm{UCOM}}$

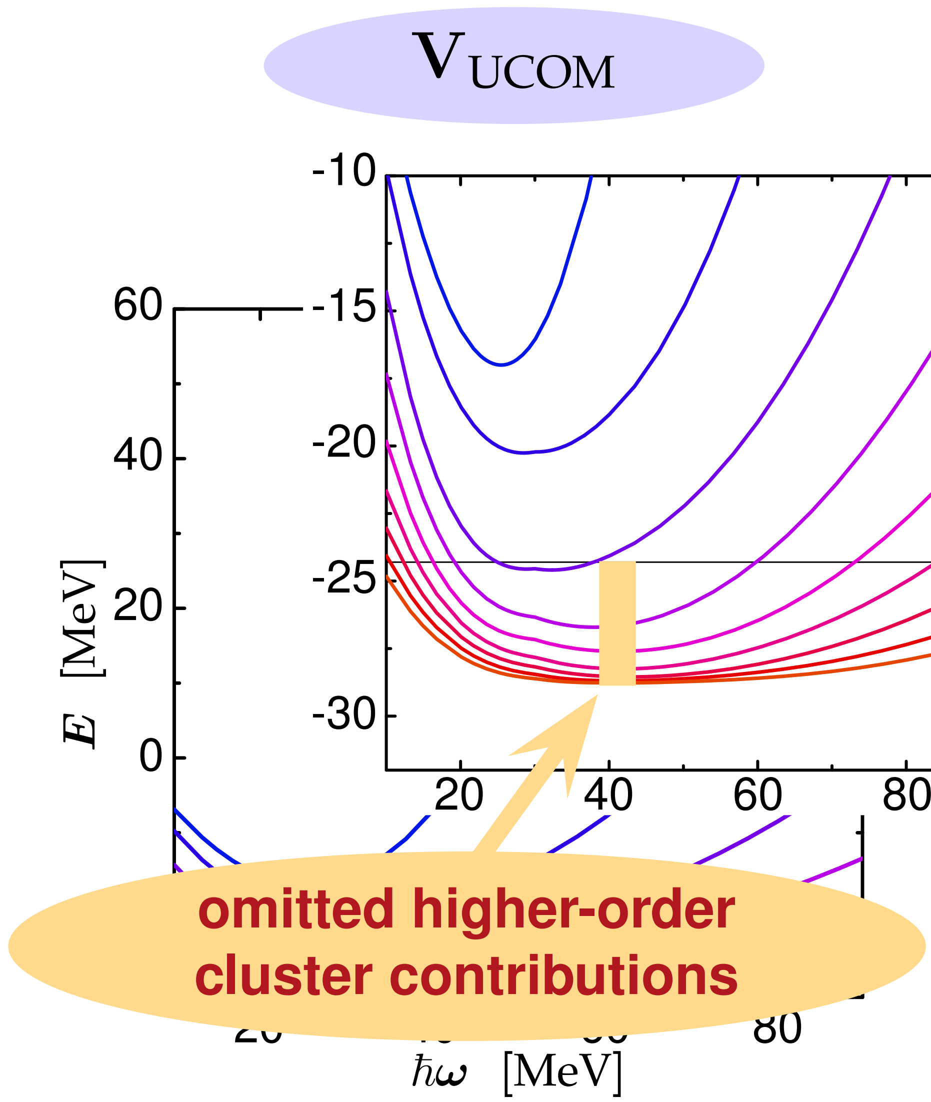
- many-body state is expanded in Slater determinants of harmonic oscillator single-particle states
- large scale diagonalisation of Hamiltonian within a truncated model space ($\mathcal{N}\hbar\omega$ truncation)
- assessment of short- and long-range correlations
- NCSM code by Petr Navrátil [PRC 61, 044001 (2000)]

^{4}He: Convergence

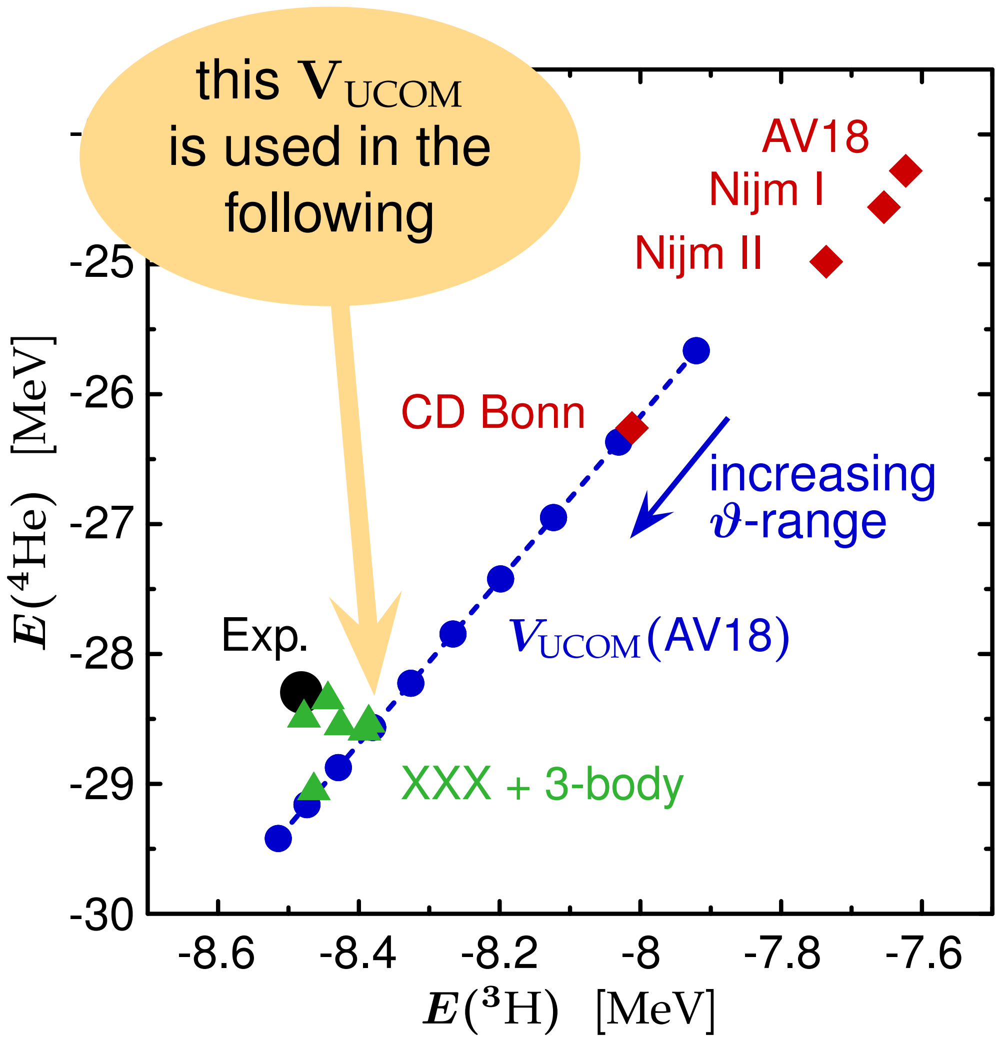


^{4}He: Convergence





Tjon-Line and Correlator Range



- **Tjon-line**: $E(^4\mathrm{He})$ vs. $E(^3\mathrm{H})$ for phase-shift equivalent NN-interactions

- change in correlator range results in shift along Tjon-line

choose correlator with energies close to experimental value, i.e., **minimise net three-body force**

Application II:

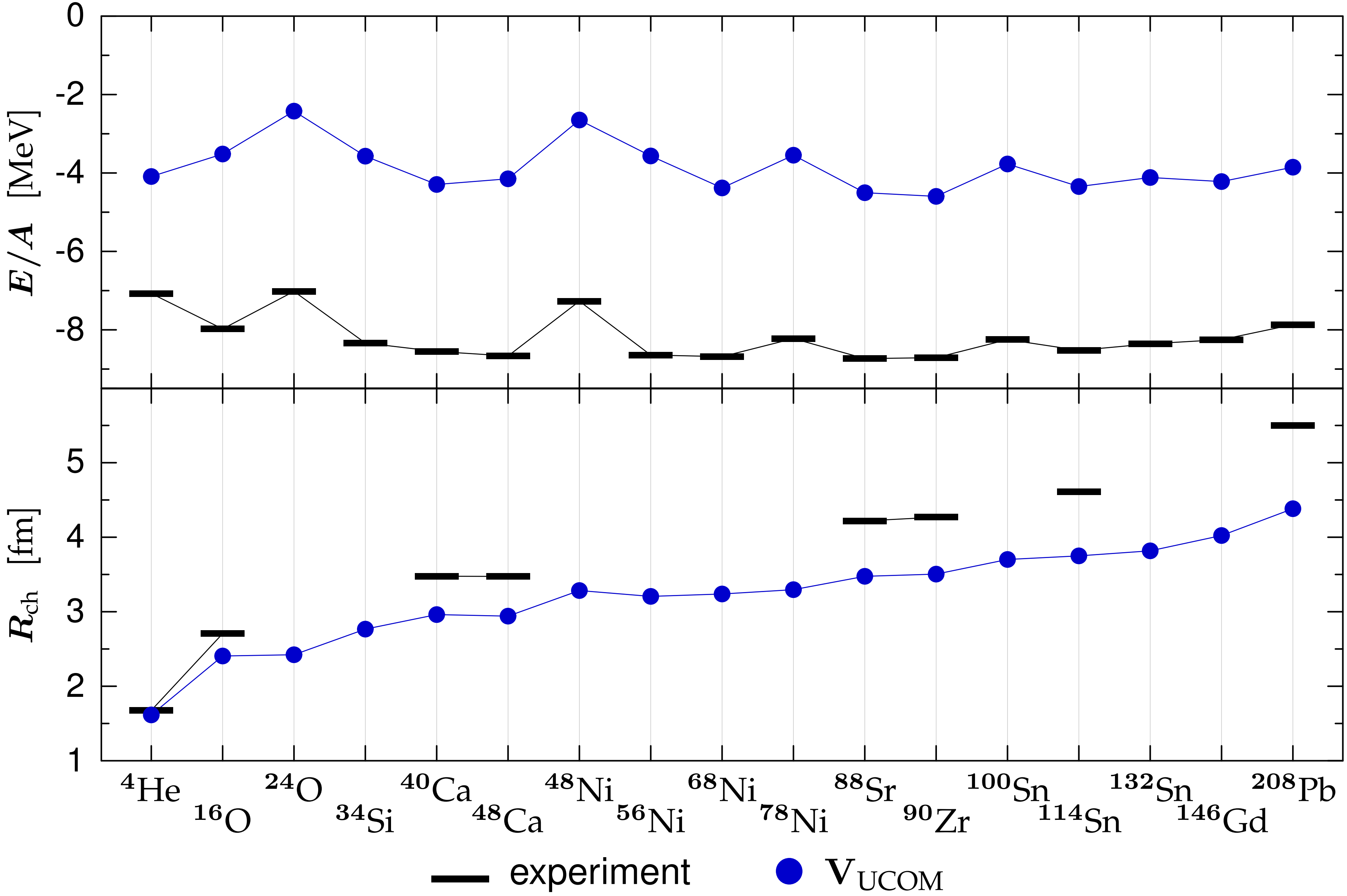
Hartree-Fock Calculations

UCOM-Hartree-Fock Approach

Standard Hartree-Fock
+
Matrix Elements of Correlated Realistic NN-Interaction V_{UCOM}

- many-body state is a **Slater determinant** of single-particle states obtained by energy minimisation
- **correlations cannot be described** by Hartree-Fock states
- bare realistic NN-potential leads to **unbound nuclei**

Correlated Argonne V18



Missing Pieces

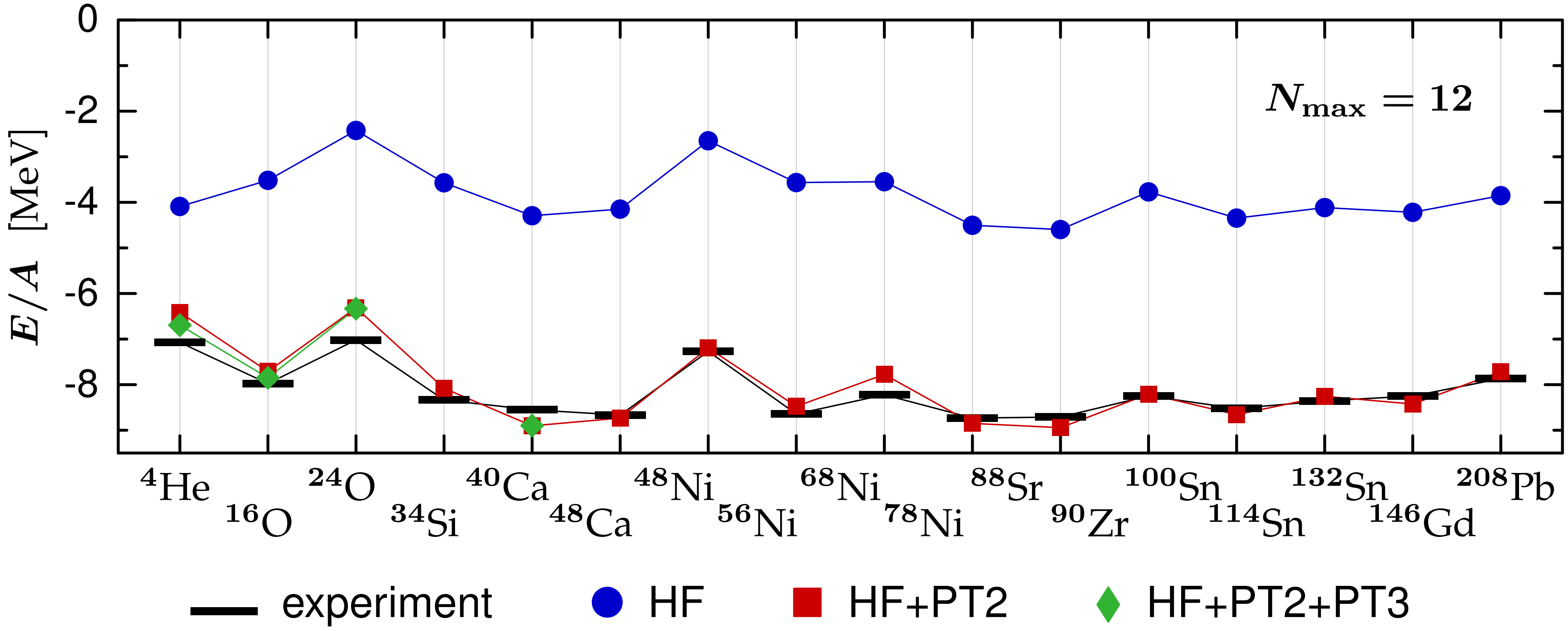
Beyond Hartree-Fock

- improve many-body states such that long-range correlations are included
- many-body perturbation theory (MBPT), configuration interaction (CI), coupled-cluster (CC),...

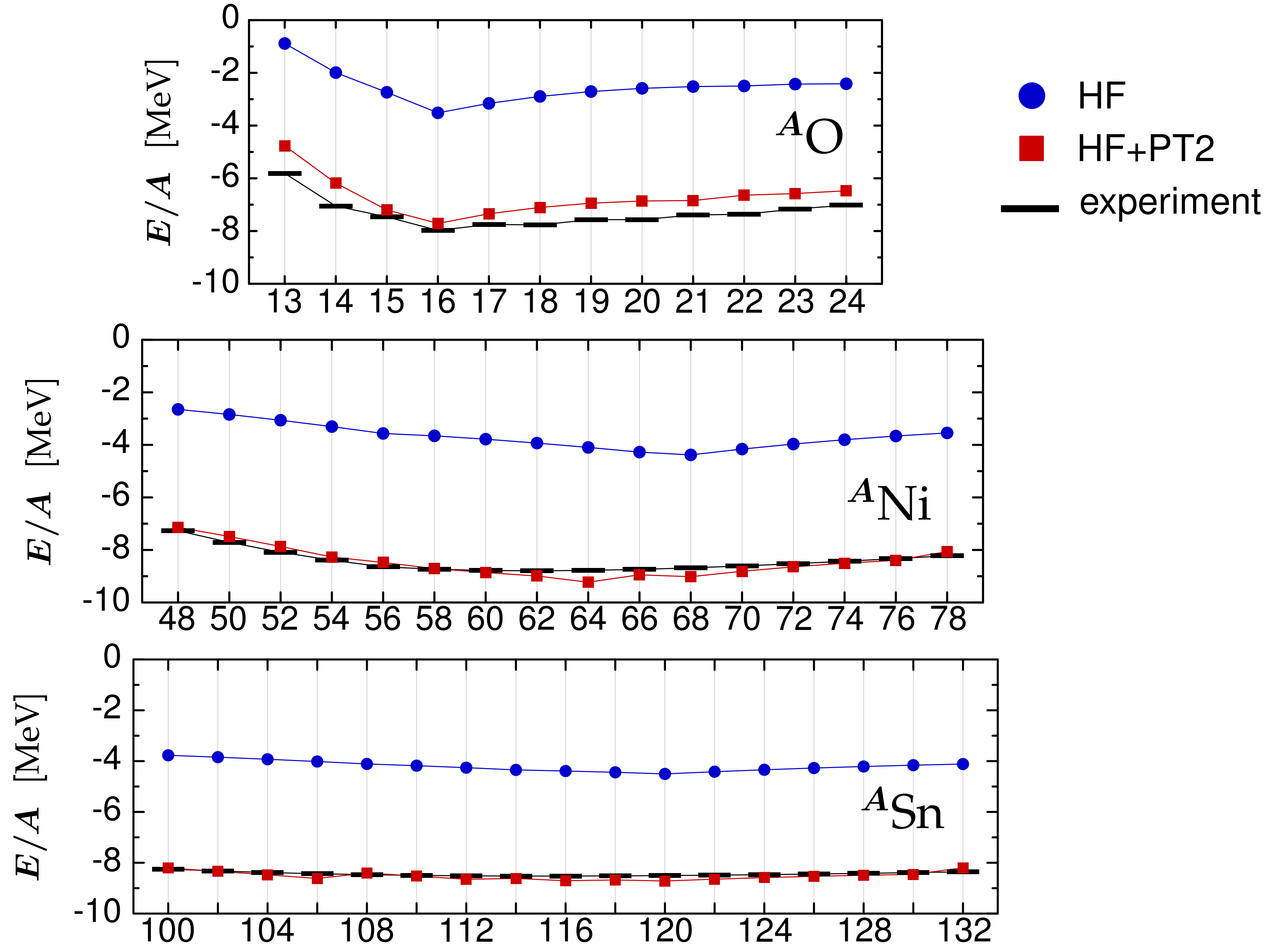
Long-Range Correlations: MBPT

- **many-body perturbation theory**: second-order energy shift gives estimate for influence of long-range correlations

$$\Delta E^{(2)} = -\frac{1}{4} \sum_{i,j}^{\text{occu.}} \sum_{a,b}^{\text{unoccu.}} \frac{\left|\left\langle \phi_a \phi_b \right| \mathrm{T}_{\text{int}} + \mathrm{V}_{\text{UCOM}} \left| \phi_i \phi_j \right\rangle\right|^2}{\epsilon_a + \epsilon_b - \epsilon_i - \epsilon_j}$$



Long-Range Correlations: MBPT



Missing Pieces

long-range correlations

genuine three-body forces

three-body cluster contributions

Beyond Hartree-Fock

- residual long-range correlations are **perturbative**
- mostly long-range **tensor correlations**
- easily tractable within MBPT, CI, CC,...

Net Three-Body Force

- small effect on binding energies for all masses
- cancellation does not work for all observables
- construct simple effective three-body force

Application III

Fermionic Molecular Dynamics (FMD)

UCOM-FMD Approach

Gaussian Single-Particle States

$$\left|q\right\rangle = \sum_{\nu=1}^{n} c_\nu \left|a_\nu, \vec{b}_\nu\right\rangle \otimes \left|\chi_\nu\right\rangle \otimes \left|m_t\right\rangle$$

$$\left\langle \vec{x} \middle| a_\nu, \vec{b}_\nu \right\rangle = \exp\left[-\frac{(\vec{x} - \vec{b}_\nu)^2}{2\, a_\nu} \right]$$

a_ν : complex width

$\vec{b}_\nu$: mean position & momentum

χ_ν : spin orientation

Slater Determinant

$$\left|Q\right\rangle = \mathcal{A}\left(\left|q_1\right\rangle \otimes \left|q_2\right\rangle \otimes \cdots \otimes \left|q_A\right\rangle \right)$$

Correlated Hamiltonian

$$\widetilde{\mathrm{H}} = \mathrm{T} + \mathrm{V}_{\mathrm{UCOM}} + \delta\mathrm{V}_{c+p+ls}$$

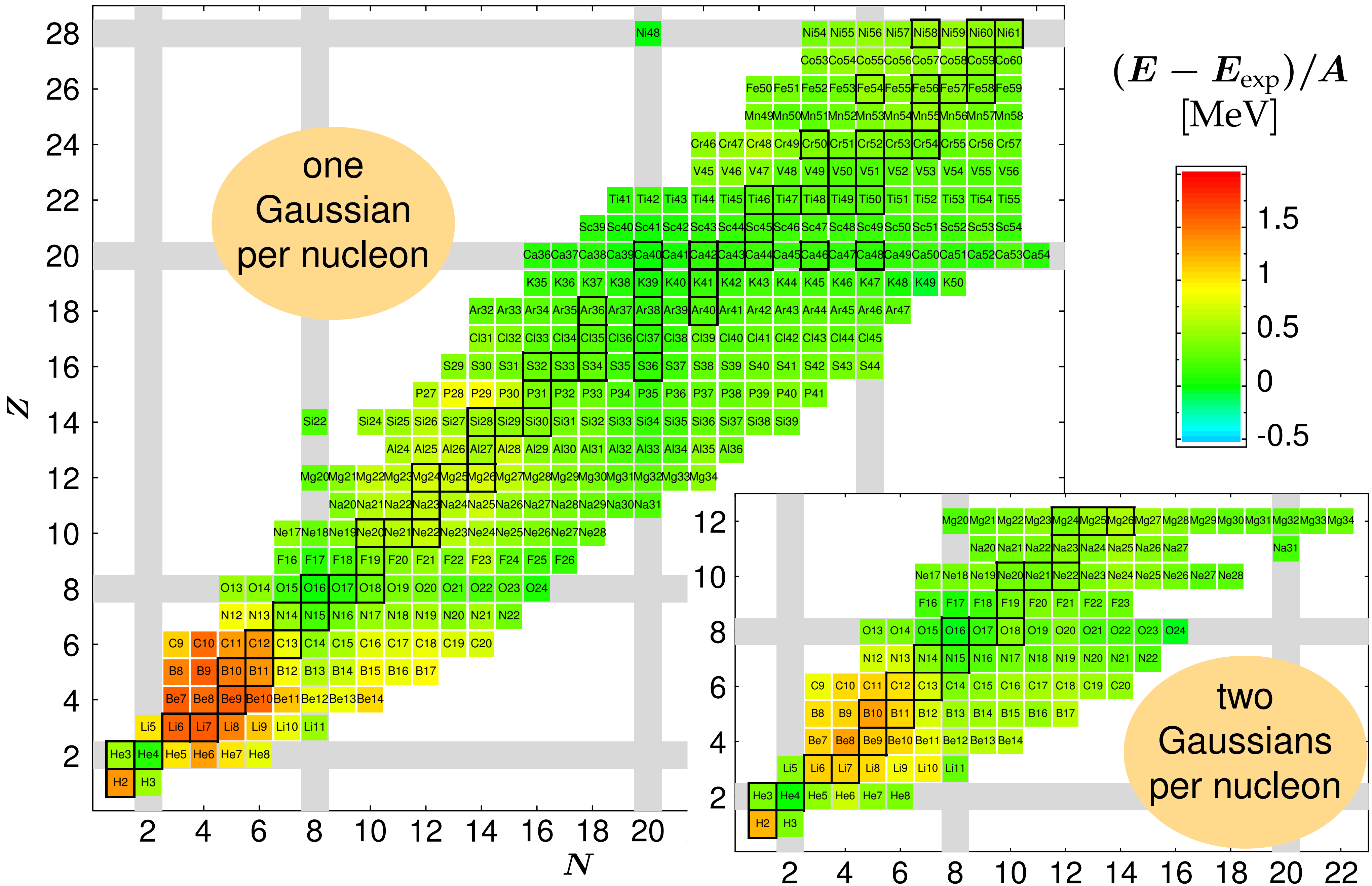
Variation

$$\frac{\left\langle Q \right| \widetilde{\mathrm{H}} - \mathrm{T}_{\mathrm{cm}} \left| Q \right\rangle}{\left\langle Q \middle| Q \right\rangle} \longrightarrow \min$$

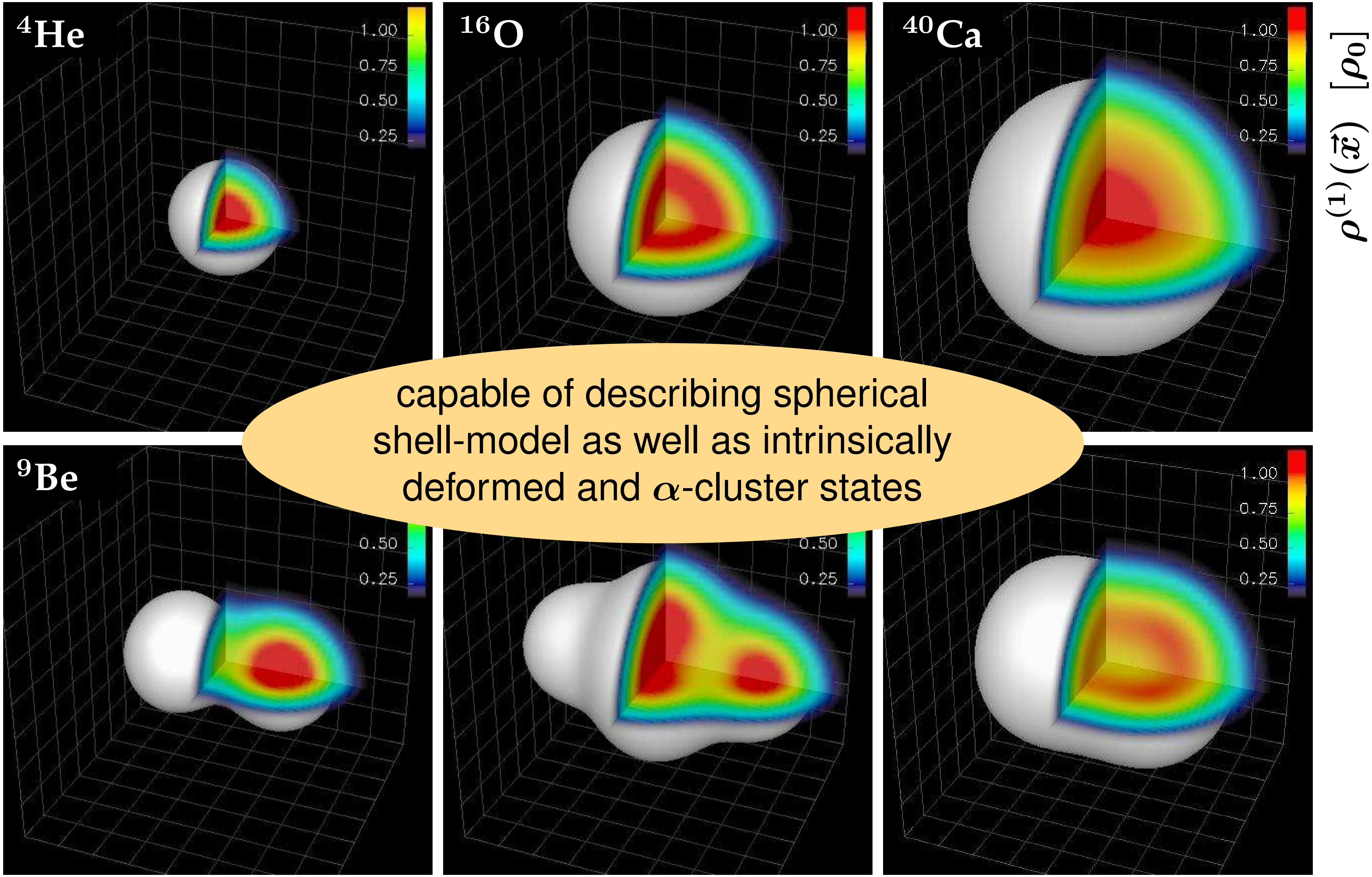
Diagonalisation

in sub-space spanned by several non-orthogonal Slater determinants $\left|Q_i\right\rangle$

Variation: Chart of Nuclei



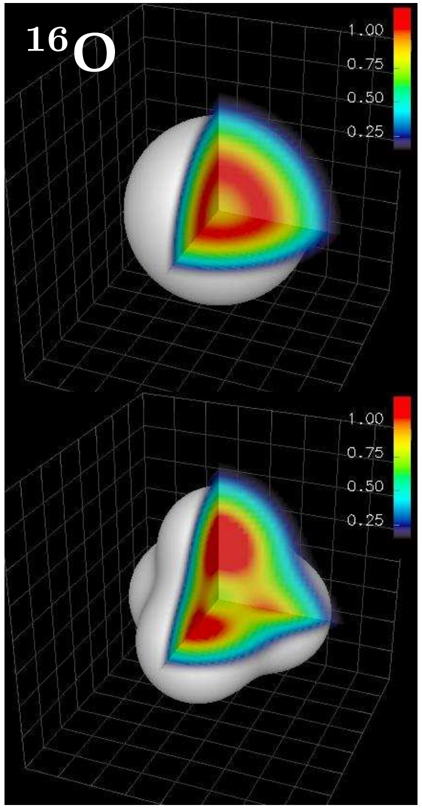
Intrinsic One-Body Density Distributions



capable of describing spherical shell-model as well as intrinsically deformed and α-cluster states

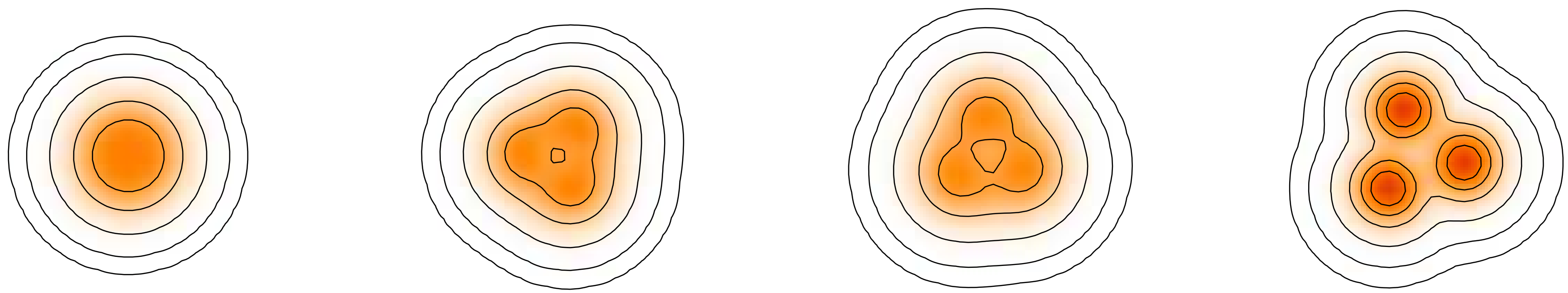
Beyond Simple Variation

- **Projection after Variation (PAV)**
  - restore inversion and rotational symmetry by angular momentum projection
- **Variation after Projection (VAP)**
  - find energy minimum within parameter space of parity and angular momentum projected states
  - implementation via generator coordinate method (constraints on multipole moments)



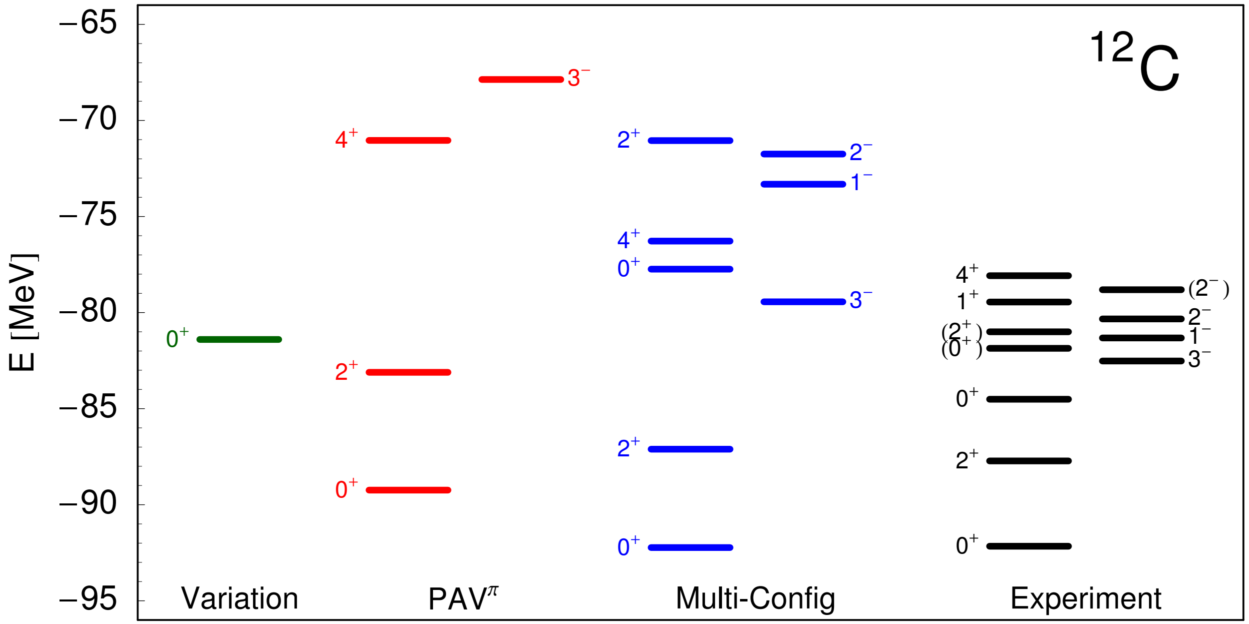
- **Multi-Configuration**
  - diagonalisation within a set of different Slater determinants

Intrinsic Shapes of ^{12}C



	intrinsic	projected	intrinsic	projected	intrinsic	projected	intrinsic	projected
$\langle \mathbf{H} \rangle$	-81.4	**-81.5**	-77.0	**-88.5**	-74.1	**-85.5**	-57.0	**-75.9**
$\langle \mathbf{T} \rangle$	212.1	212.1	189.2	186.1	182.8	179.0	213.9	201.4
$\langle \mathbf{V}_{ls} \rangle$	-39.8	-40.2	-12.0	-17.1	-5.8	-8.0	0.0	0.0
$\sqrt{\langle \mathbf{r}^2 \rangle}$	2.22	2.22	2.40	2.37	2.45	2.42	2.44	2.42

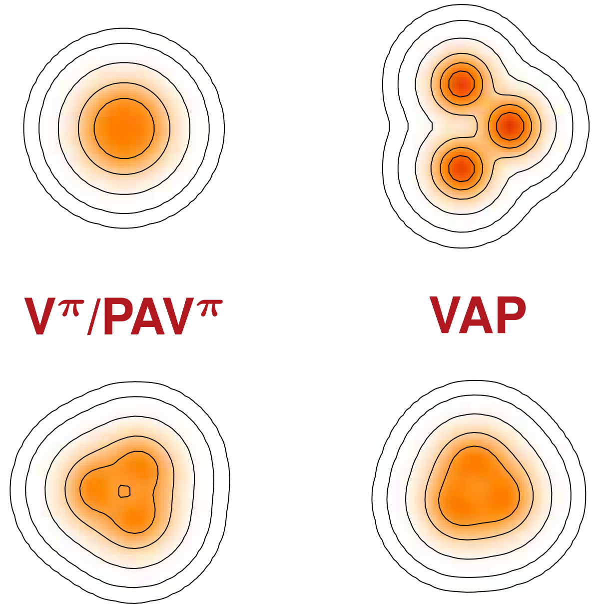
Structure of ^{12}C



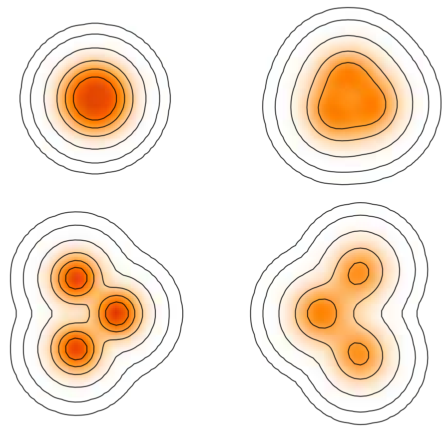
	E [MeV]	R_{ch} [fm]	$B(E2)$ $[e^2\ \mathrm{fm}^4]$
V/PAV	81.4	2.36	-
VAP α-cluster	79.1	2.70	76.9
PAV$^\pi$	88.5	2.51	36.3
VAP	89.2	2.42	26.8
Multi-Config	92.2	2.52	42.8
Experiment	92.2	2.47	39.7 ± 3.3

V/PAV **VAPα**

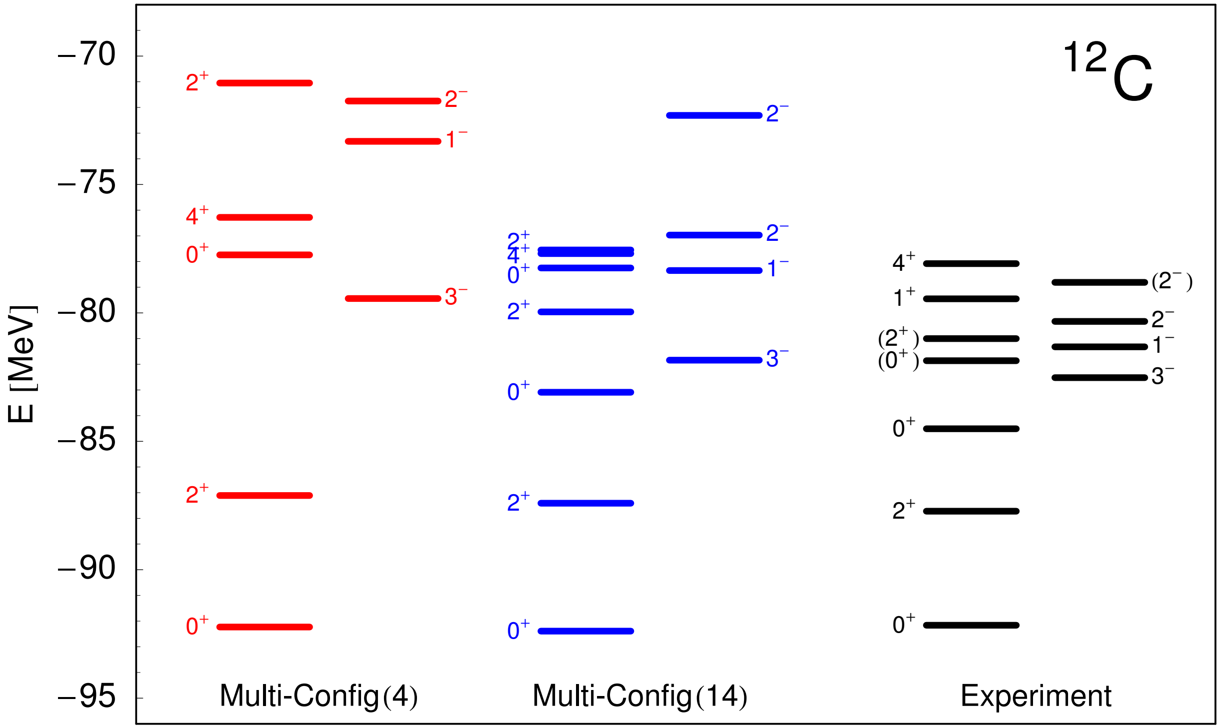
V$^\pi$/PAV$^\pi$ **VAP**

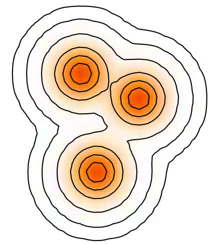


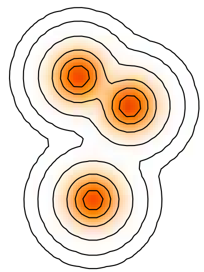
Multi-Config

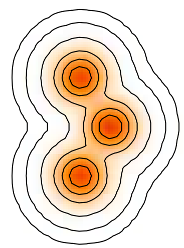


Structure of ^{12}C — Hoyle State



$\big|\big\langle$  $\big|0_2^+\big\rangle\big| = 0.76$

$\big|\big\langle$  $\big|0_2^+\big\rangle\big| = 0.71$

$\big|\big\langle$  $\big|0_2^+\big\rangle\big| = 0.50$

	Multi-Config	Experiment
$\boldsymbol{E}$ [MeV]	92.4	92.2
$\boldsymbol{R}_{\mathrm{ch}}$ [fm]	2.52	2.47
$\boldsymbol{B(E2, 0_1^+ \rightarrow 2_1^+)}$ $[e^2\,\mathrm{fm}^4]$	42.9	39.7 ± 3.3
$\boldsymbol{M(E0, 0_1^+ \rightarrow 0_2^+)}$ $[\mathrm{fm}^2]$	5.67	5.5 ± 0.2

Conclusions

- exciting times for nuclear structure physics!
- realistic NN-potentials & *ab initio* calculations
- systematic schemes to derive effective interactions
- innovative ways to treat the many-body problem

unified description of nuclear structure across the whole nuclear chart is within reach

Epilogue

- **thanks to my group & my collaborators**
  - H. Hergert, N. Paar, P. Papakonstantinou, A. Zapp
    Institut für Kernphysik, TU Darmstadt
  - T. Neff
    NSCL, Michigan State University
  - H. Feldmeier
    Gesellschaft für Schwerionenforschung (GSI)

supported by the DFG through SFB 634 “Nuclear Structure, Nuclear Astrophysics and Fundamental Experiments...”

Supplements

Correlated Operators

Cluster Expansion

$$\widetilde{\mathrm{O}} = \mathrm{C}^{\dagger}\,\mathrm{O}\,\mathrm{C} = \widetilde{\mathrm{O}}^{[1]} + \widetilde{\mathrm{O}}^{[2]} + \widetilde{\mathrm{O}}^{[3]} + \cdots$$

Cluster Decomposition Principle

if the correlation range is small compared to the mean particle distance, then higher orders are small

Two-Body Approx.

$$\widetilde{\mathrm{O}}^{C2} = \widetilde{\mathrm{O}}^{[1]} + \widetilde{\mathrm{O}}^{[2]}$$

operators of all observables can be and have to be correlated consistently

Correlated NN-Potential — $V_{\rm UCOM}$

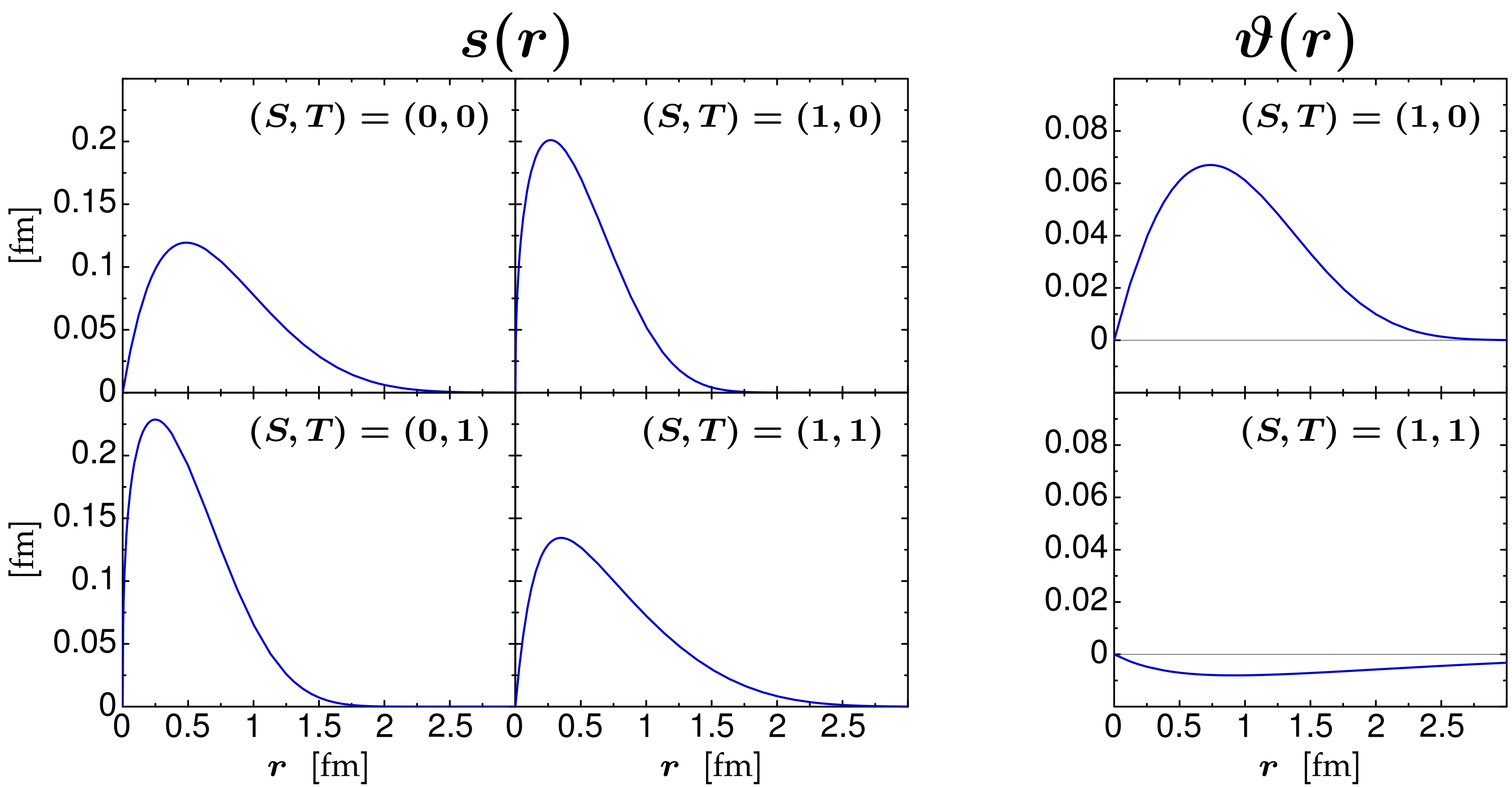
$$\mathbf{V}_{\rm UCOM} = \sum_p \tfrac{1}{2}\big[\widetilde{v}_p(\mathbf{r})\ \mathbf{O}_p + \mathbf{O}_p\ \widetilde{v}_p(\mathbf{r})\big]$$

$$\begin{aligned}\mathbf{O} = \{1,\ (\vec{\sigma}_1\cdot\vec{\sigma}_2),\ \vec{\mathbf{q}}^2,\ \vec{\mathbf{q}}^2(\vec{\sigma}_1\cdot\vec{\sigma}_2),\ \vec{\mathbf{L}}^2,\ \vec{\mathbf{L}}^2(\vec{\sigma}_1\cdot\vec{\sigma}_2),\\ (\vec{\mathbf{L}}\cdot\vec{\mathbf{S}}),\ \mathbf{S}_{12}(\vec{\mathbf{r}},\vec{\mathbf{r}}),\ \mathbf{S}_{12}(\vec{\mathbf{L}},\vec{\mathbf{L}}),\\ \bar{\mathbf{S}}_{12}(\vec{\mathbf{q}}_\Omega,\vec{\mathbf{q}}_\Omega),\ \mathbf{q}_r\,\mathbf{S}_{12}(\vec{\mathbf{r}},\vec{\mathbf{q}}_\Omega),\ \vec{\mathbf{L}}^2(\vec{\mathbf{L}}\cdot\vec{\mathbf{S}}),\\ \vec{\mathbf{L}}^2\bar{\mathbf{S}}_{12}(\vec{\mathbf{q}}_\Omega,\vec{\mathbf{q}}_\Omega),\ \dots\}\otimes\{1,\ (\vec{\tau}_1\cdot\vec{\tau}_2)\}\end{aligned}$$

- $\mathbf{C}_r$-transformation evaluated directly
- $\mathbf{C}_\Omega$-transformation through Baker-Campell-Hausdorff expansion
- $\widetilde{v}_p(r)$ uniquely determined by bare potential and correlation functions

Optimal Correlation Functions

- $s(r)$ and $\vartheta(r)$ determined by two-body **energy minimisation**
- constraint on range of the tensor correlators $\vartheta(r)$ to isolate state independent **short-range correlations**



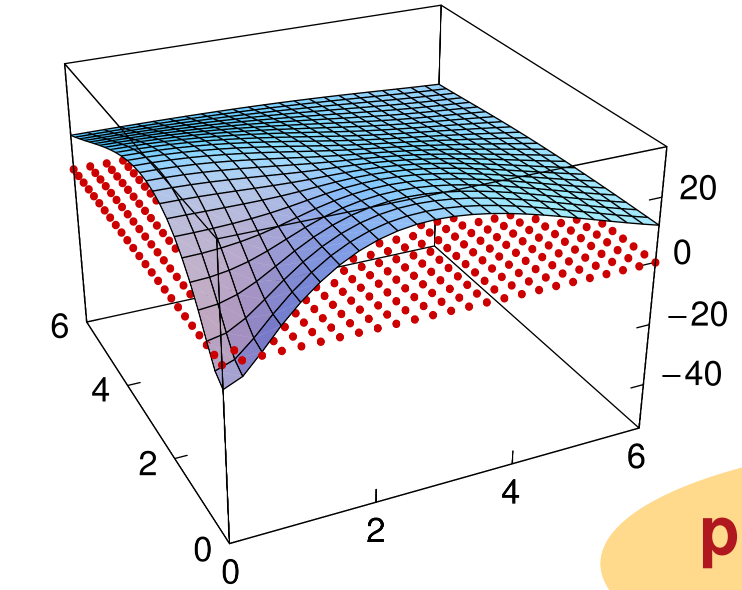
Correlated NN-Potential — V_{UCOM}

$$\widetilde{\mathbf{H}}^{C2} = \widetilde{\mathbf{T}}^{[1]} + \widetilde{\mathbf{T}}^{[2]} + \widetilde{\mathbf{V}}^{[2]} = \mathbf{T} + \mathbf{V}_{\mathrm{UCOM}}$$

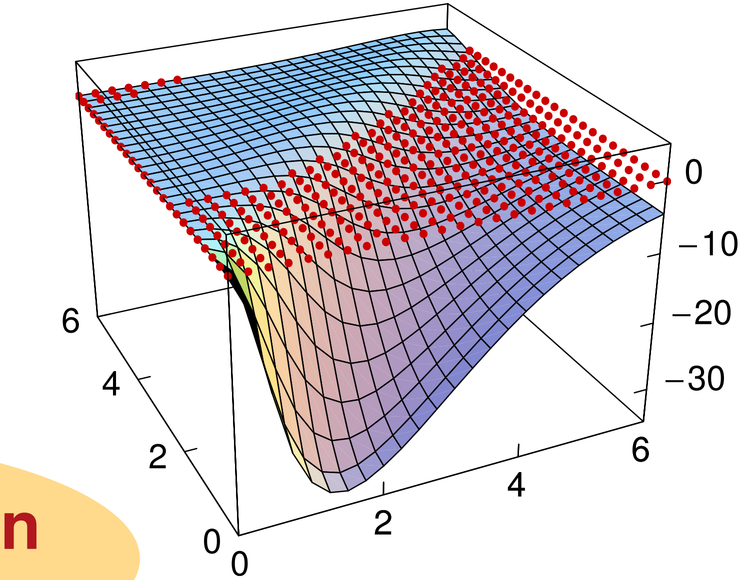
- **closed operator expression** for the correlated interaction $\mathbf{V}_{\mathrm{UCOM}}$ in two-body approximation
- correlated interaction and original NN-potential are **phase shift equivalent** by construction
- unitary transformation results in a **pre-diagonalisation** of Hamiltonian
- momentum-space matrix elements of correlated interaction are **similar to $V_{\mathrm{low}-k}$**

Momentum-Space Matrix Elements

$^3S_1$



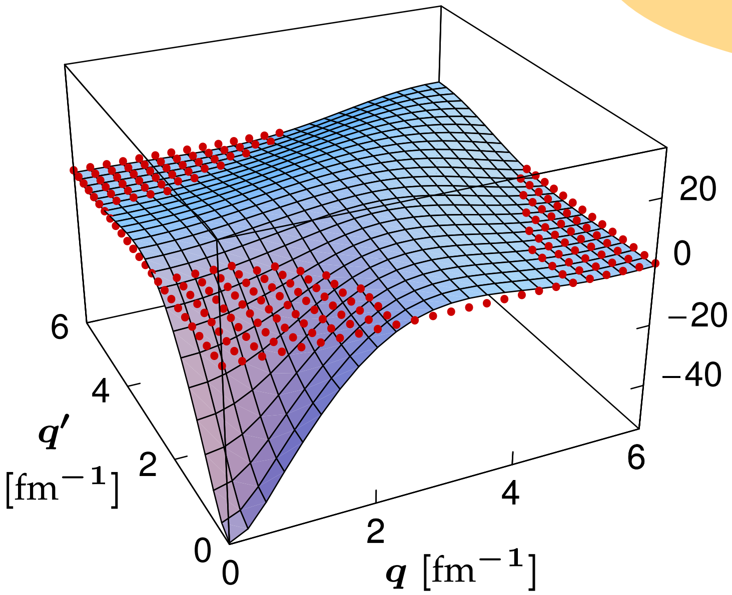
$^3S_1 - ^3D_1$

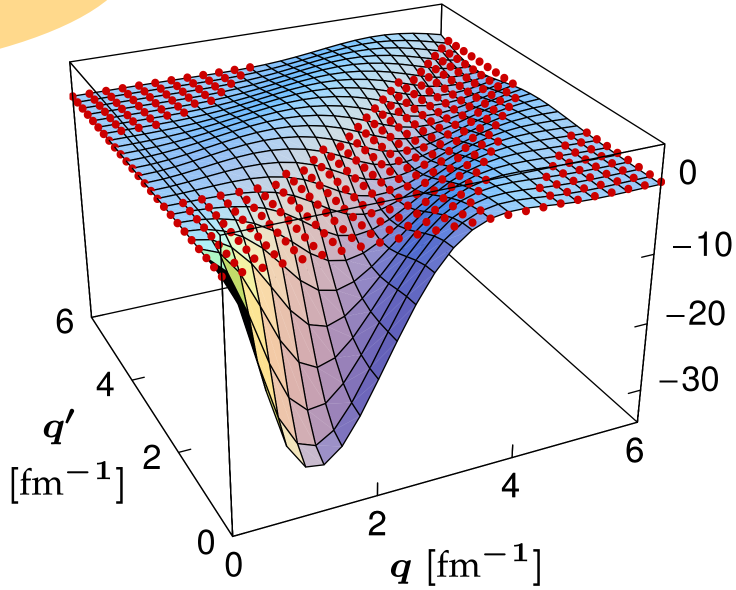


V_{bare}

pre-diagonalisation of Hamiltonian

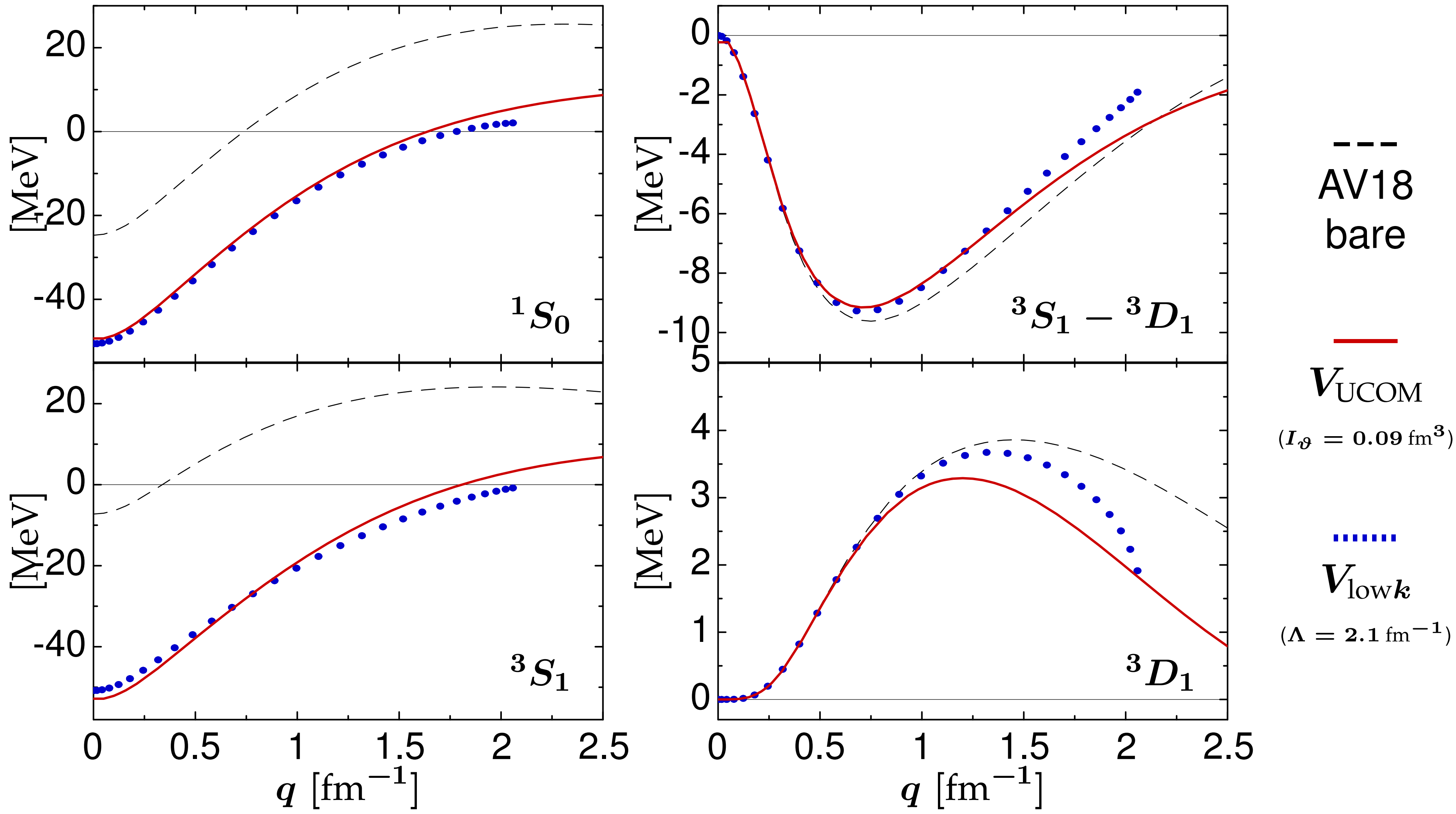
V_{UCOM}





AV18

Comparison with $V_{\text{low}\,k}$



UCOM / Lee-Suzuki / $V_{\mathrm{low}k}$

Lee-Suzuki

- decoupling of P and Q space by similarity transformation
- same representation as used in many-body method
- (state dependent)

$V_{\mathrm{low}k}$

- decimation to low-momentum P space; Q space discarded
- uses momentum representation
- state independent
- phase-shift equivalent

UCOM

- pre-diagonalisation with respect to short-range correlations
- no specific model-space or representation
- state independent
- phase-shift equivalent

Correlated Oscillator Matrix Elements

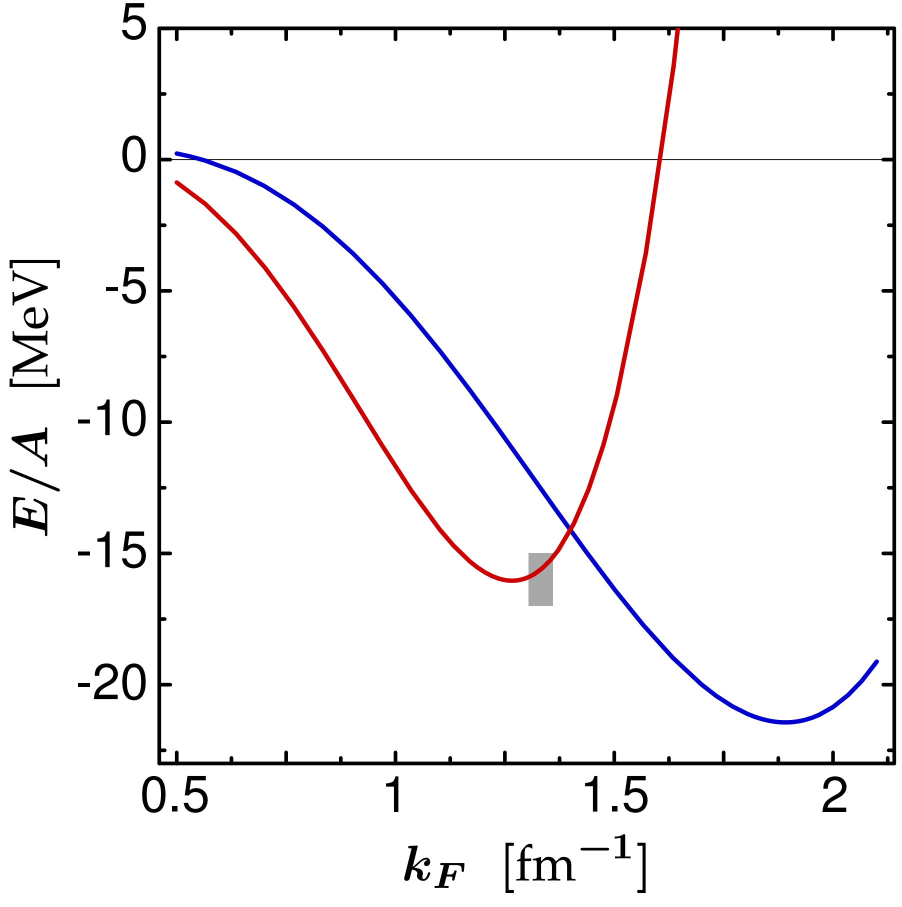
$$\langle n(LS)JT|\, \mathbf{C}_r^\dagger \mathbf{C}_\Omega^\dagger \,\mathrm{H}\, \mathbf{C}_\Omega \mathbf{C}_r \,|n'(L'S)JT\rangle$$
$$= \langle n(LS)JT|\, \mathrm{T} + \mathrm{V}_{\mathrm{UCOM}} \,|n'(L'S)JT\rangle$$

calculate using uncorrelated states and operator form of $\mathrm{V}_{\mathrm{UCOM}}$

map correlator onto states and use bare interaction (avoids BCH expansion)

- Talmi-Moshinsky transformation & recoupling to obtain jj-coupled matrix elements
- input for all kinds of many-body methods (HF, NCSM, CC,...)

Nuclear Matter: Equation of State



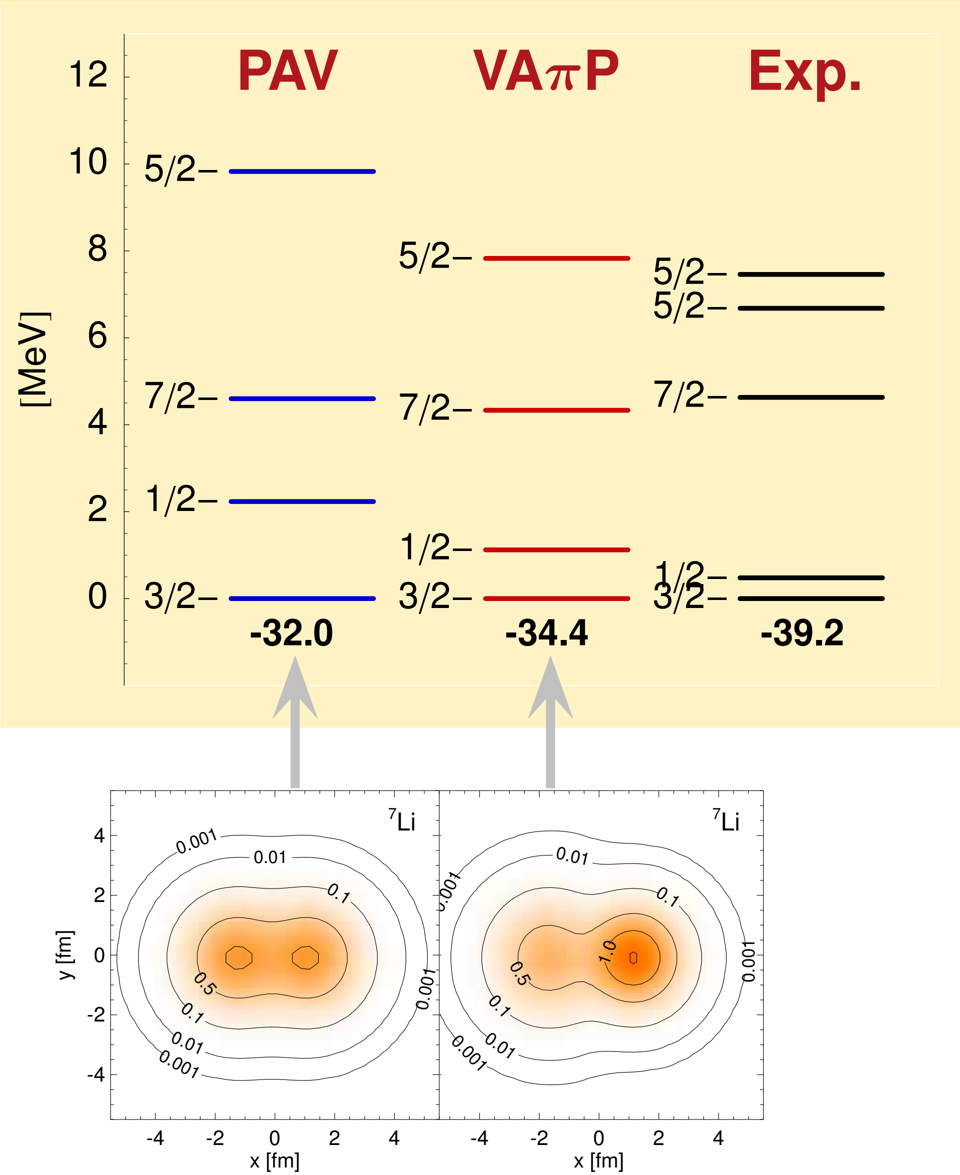
- symmetric nuclear matter
- Slater determinant of plane-wave states $|\vec{k}| \leq k_F$
- correlated momentum space matrix elements
- saturation point:

$$(E/A)_0 \approx -16.0\,\text{MeV}$$
$$\rho_0 \approx 0.14\,\text{fm}^{-3}$$
$$K_0 \approx 280\,\text{MeV}$$

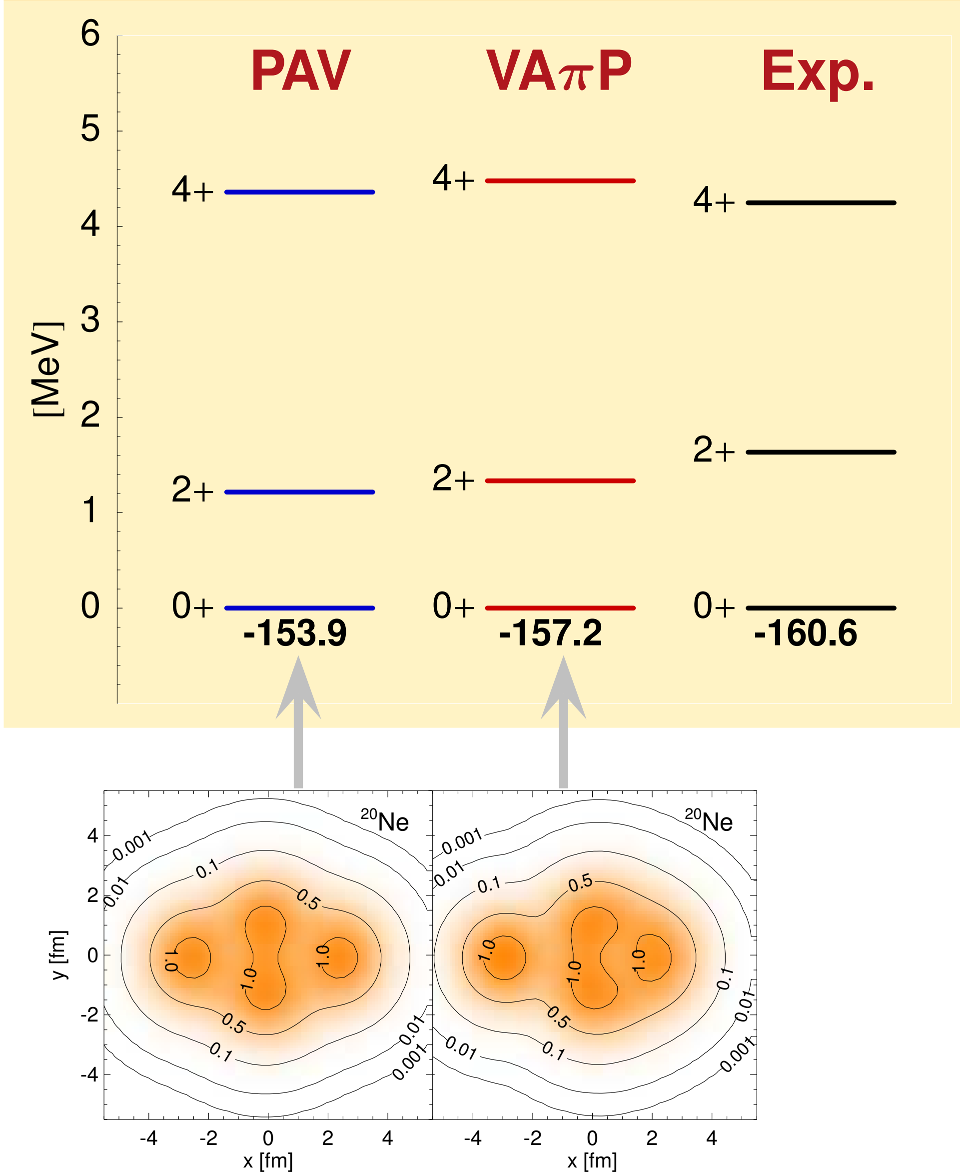
- HvH theorem fulfilled

Parity and Angular Momentum Projection

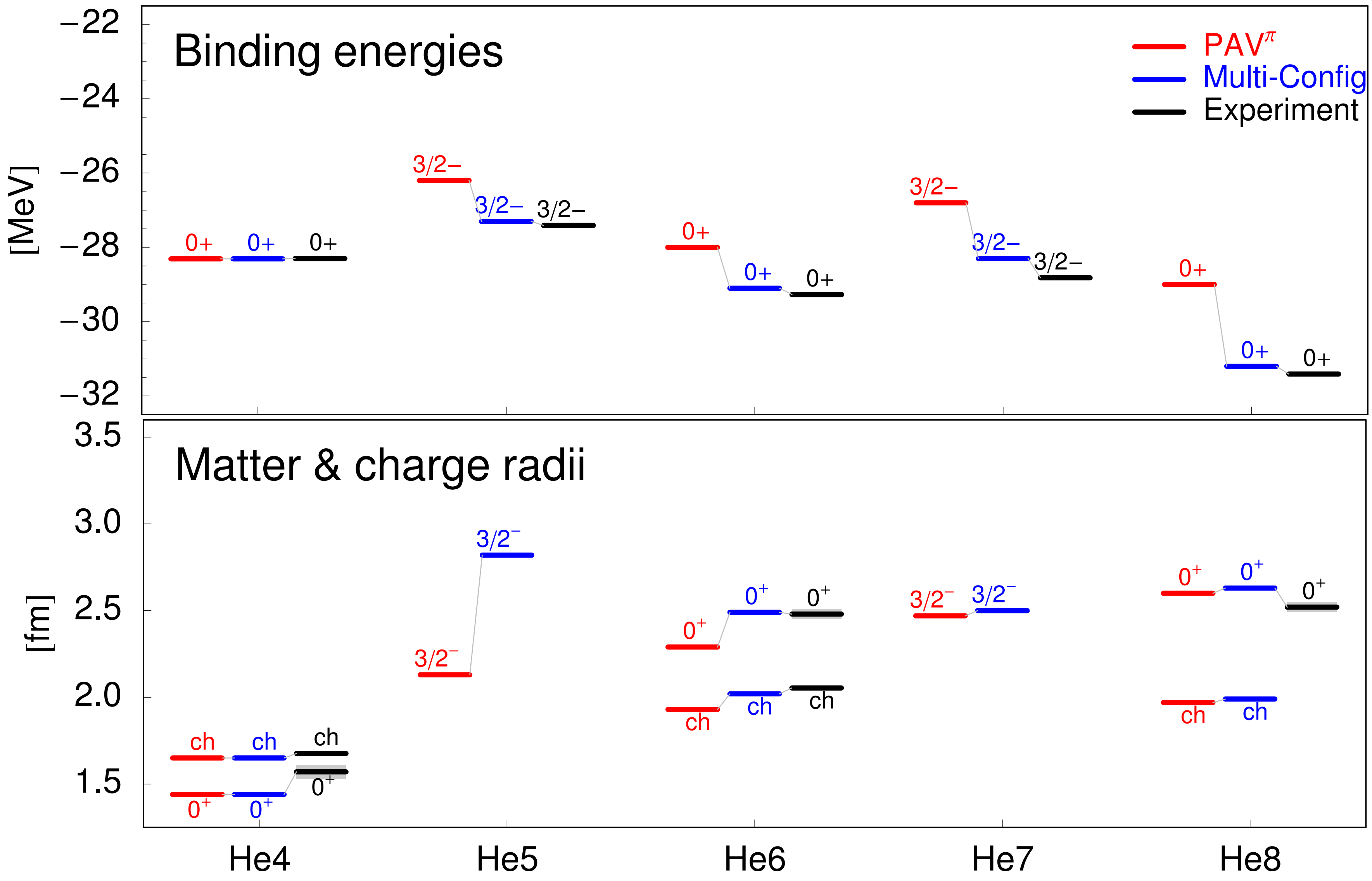
^{7}Li



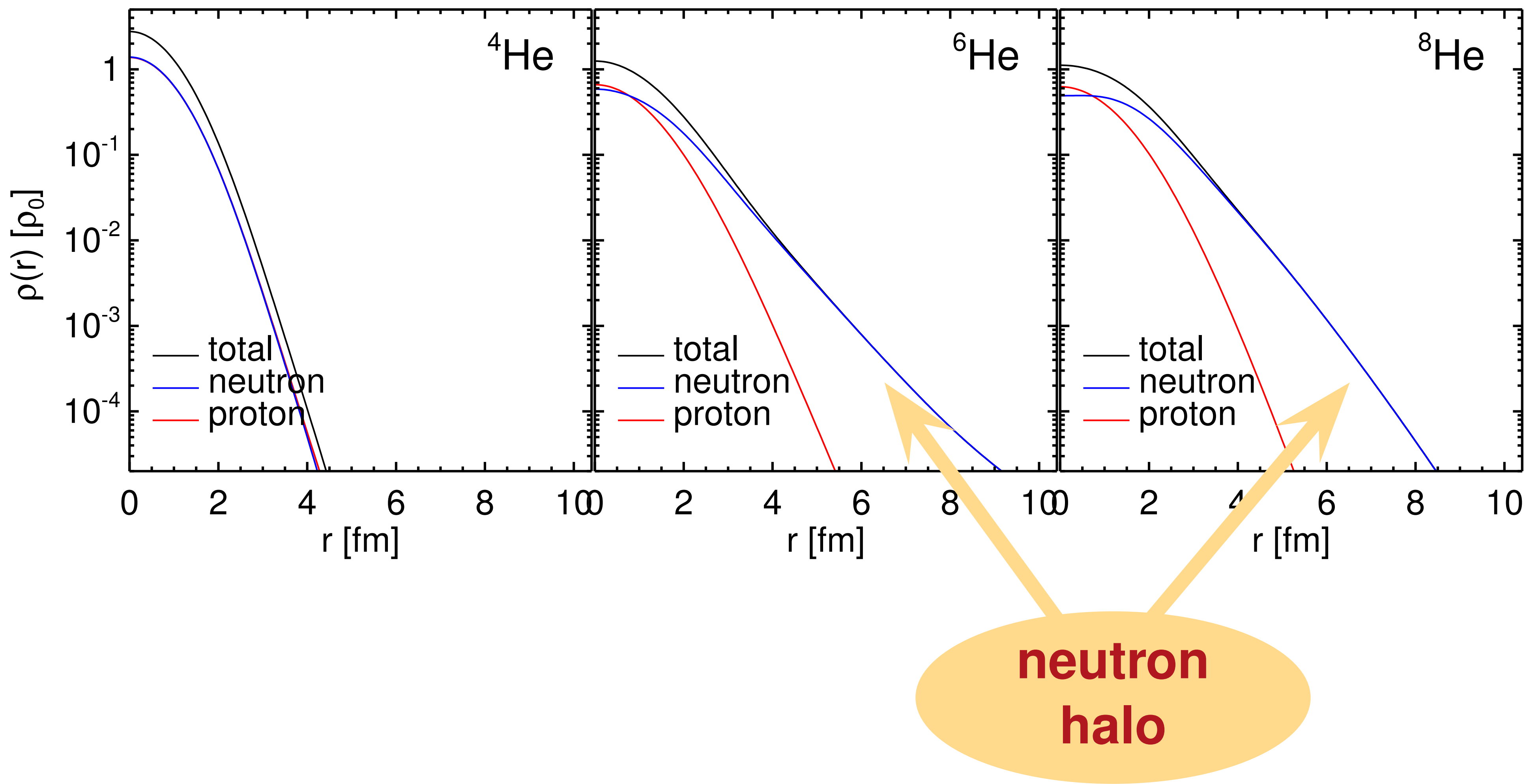
^{20}Ne



Helium Isotopes: Energies & Radii



Helium Isotopes: Density Profiles



Summary

- **Unitary Correlation Operator Method (UCOM)**
  - short-range central and tensor correlations treated explicitly
  - long-range correlations have to be accounted for by model space

- **Correlated Realistic NN-Potential V_{UCOM}**
  - low-momentum / phase-shift equivalent / operator representation
  - robust starting point for all kinds of many-body calculations

Summary

- **UCOM + No-Core Shell Model**
  - dramatically improved convergence
  - tool to assess long-range correlations & higher-order contributions
- **UCOM + Hartree-Fock**
  - closed shell nuclei across the whole nuclear chart
  - basis for improved many-body calculations
- **UCOM + Fermionic Molecular Dynamics**
  - clustering and intrinsic deformations in p- and sd-shell
  - projection / multi-config provide detailed structure information

Outlook

- **residual “long-range” correlations**
  - many-body perturbation theory
  - configuration interaction & coupled-cluster calculations
  - pairing correlations, Hartree-Fock-Bogoliubov
- **collective excitations**
  - random phase approximation (RPA, SRPA, QRPA)
- **make contact to experiment!!!**