Fermionic Molecular Dynamics for Nuclear Structure and Reactions

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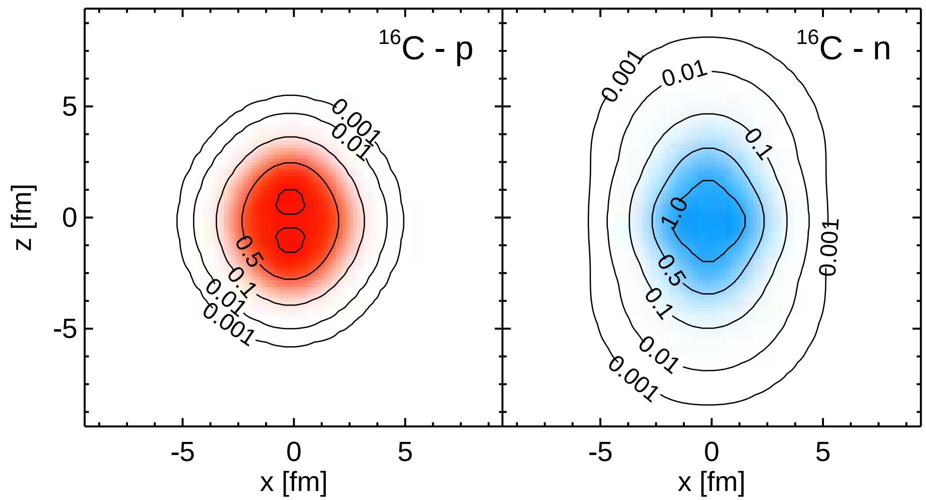


Overview

Introduction

Unitary Correlation Operator Method

Fermionic Molecular Dynamics

Cluster degrees of freedom, Reactions

Introduction

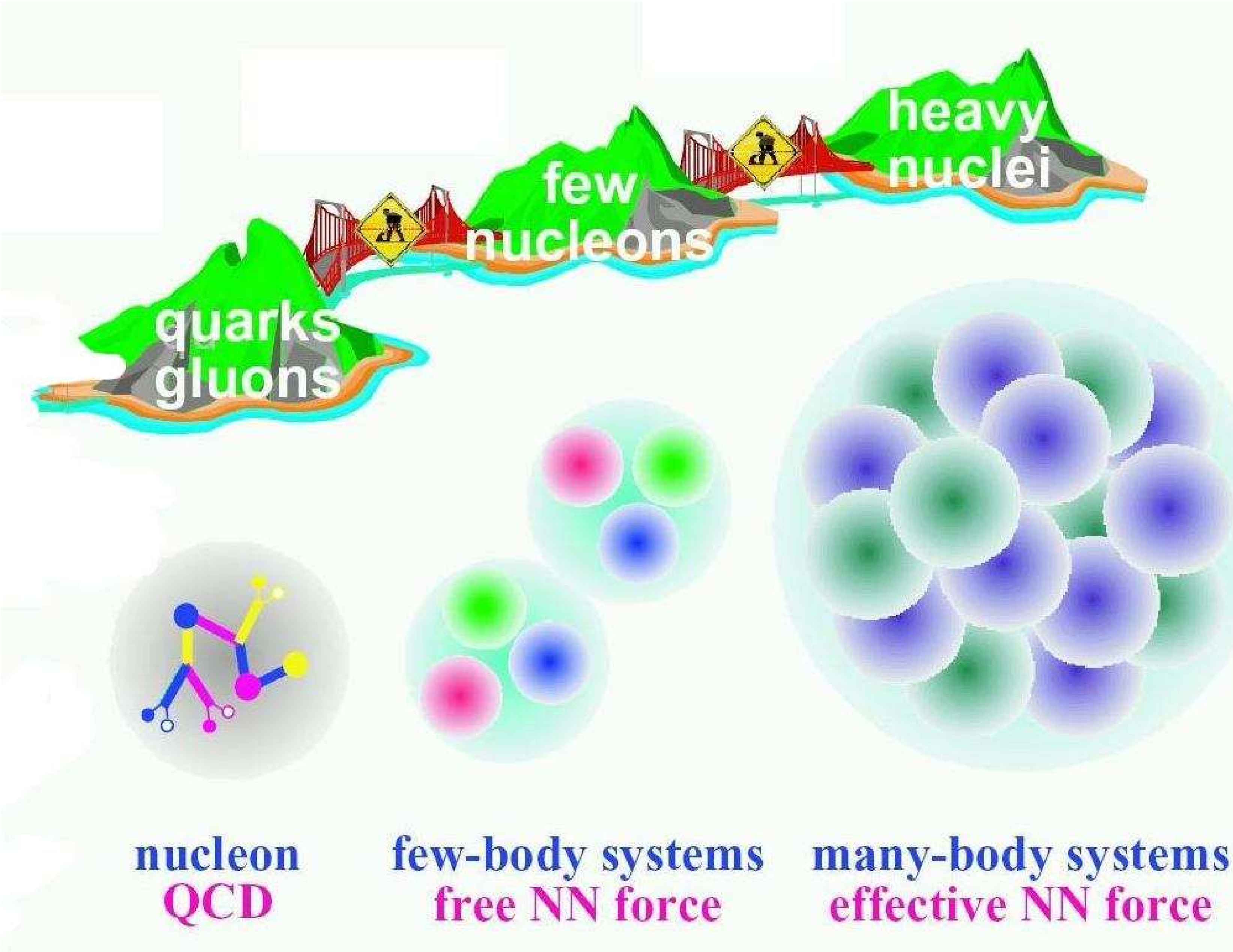
Nuclear Degrees of Freedom

Many-body Methods

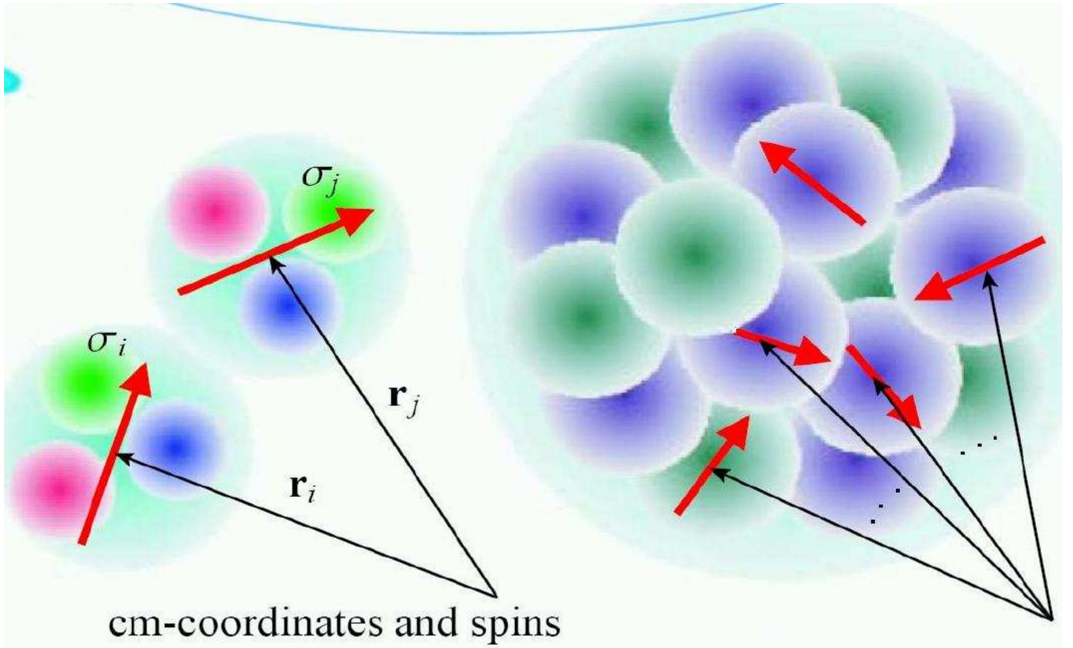
Two-Nucleon System

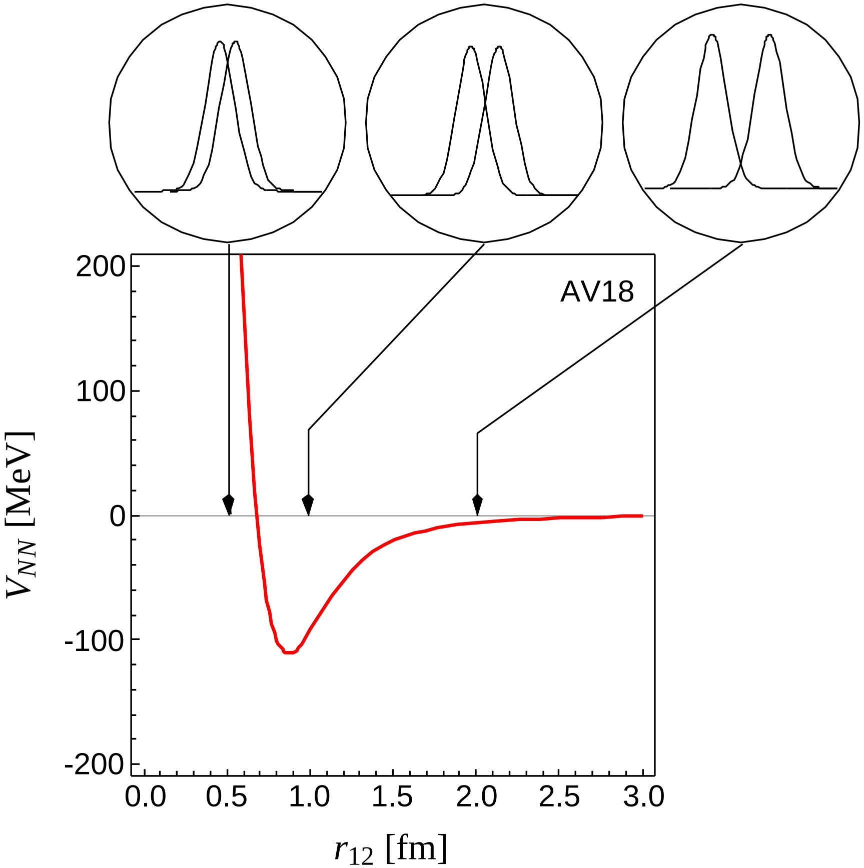
Nucleon-Nucleon Interaction

Nuclear Degrees of Freedom



Nucleons as effective Degrees of Freedom

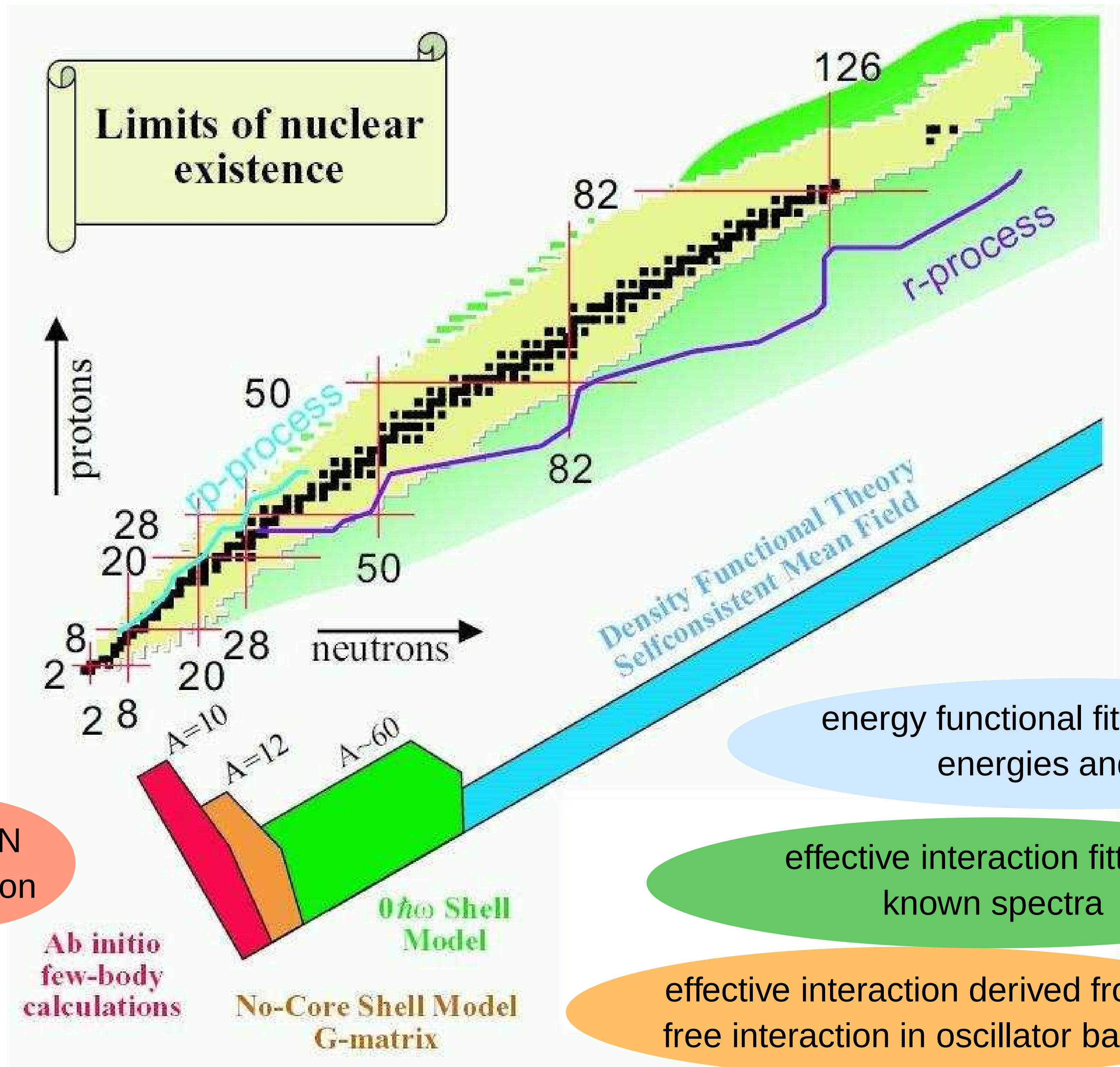




- at low energies nuclei can be described as a system of nucleons
- nucleons are not point-like particles, proton radius $\sqrt{r_p^2} \approx 0.89$ fm

➡ nucleon-nucleon force is something like the van-der-Waals force between atoms

Quest for a unified Description of Nuclei



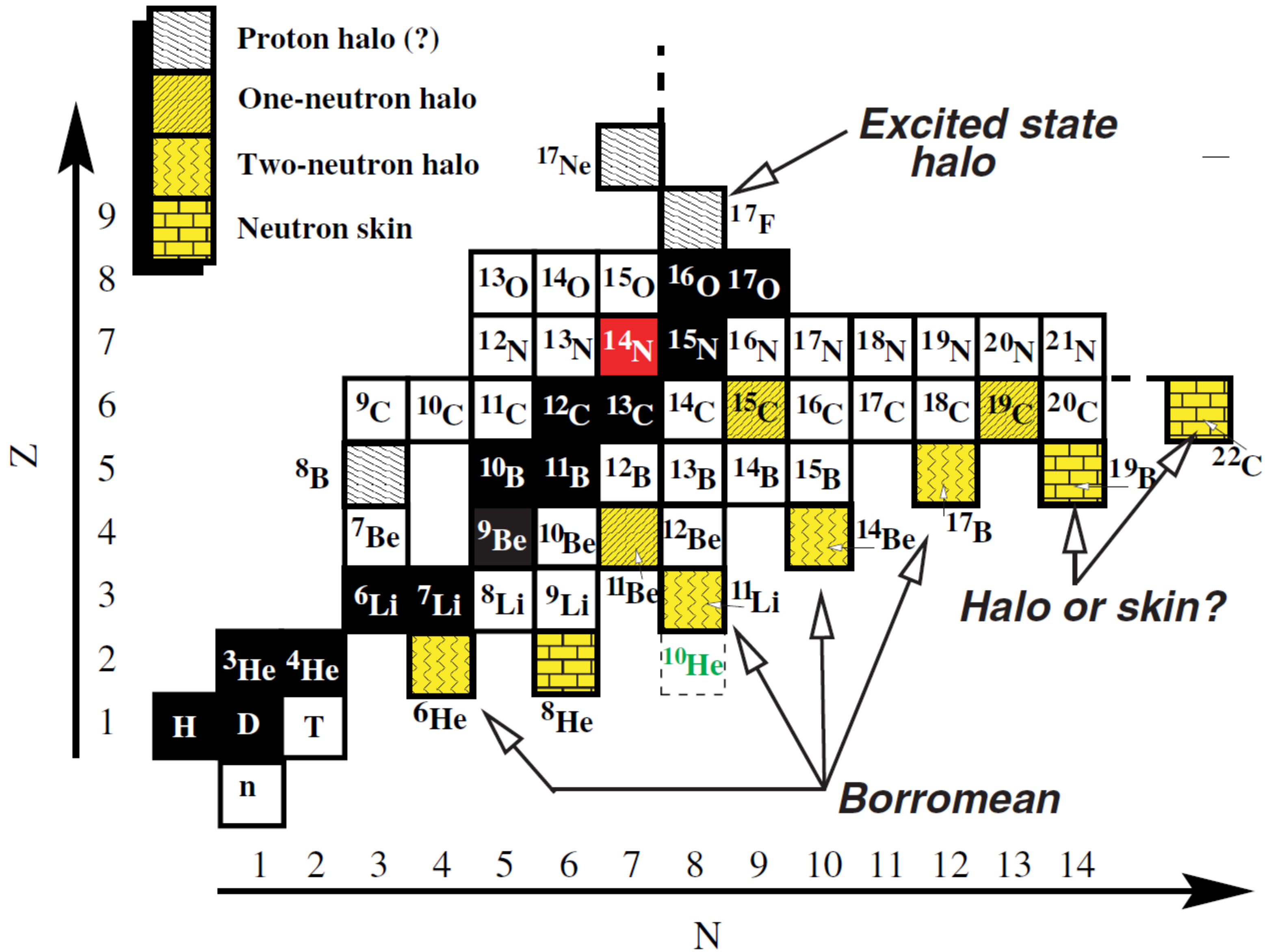
Free NN interaction

energy functional fitted to binding energies and radii

effective interaction fitted to known spectra

effective interaction derived from free interaction in oscillator basis

Exotica: Special Challenges



Two-Nucleon System (Relative Motion)

- Couple Spin and Isospin

$$\left|S, M_S\right\rangle = \sum_{m_{s1}, m_{s2}} C\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \bigg| & S \\ m_{s1} & m_{s2} & \bigg| & M_S \end{pmatrix} \left|\tfrac{1}{2}, m_{s1}\right\rangle \otimes \left|\tfrac{1}{2}, m_{s2}\right\rangle, \qquad S = 0, 1$$

$$\left|T, M_T\right\rangle = \sum_{m_{t1}, m_{t2}} C\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \bigg| & T \\ m_{t1} & m_{t2} & \bigg| & M_T \end{pmatrix} \left|\tfrac{1}{2}, m_{t1}\right\rangle \otimes \left|\tfrac{1}{2}, m_{t2}\right\rangle, \qquad T = 0, 1$$

Spin/Isospin
Singlet, Triplet

- Couple Orbital Angular Momentum with Spin

$$\left\langle \mathbf{r} \middle| \alpha, (LS)JM; TM_T \right\rangle = \sum_{M_L, M_S} C\begin{pmatrix} L & S & \bigg| & J \\ M_L & M_S & \bigg| & M \end{pmatrix} \phi_\alpha(r) Y_{LM_L}(\hat{\mathbf{r}}) \left|S, M_S\right\rangle \otimes \left|T, M_T\right\rangle$$

- Antisymmetry

$$(S, T) = (0, 1) \text{ or } (1, 0) \qquad \longrightarrow \qquad L = 0, 2, 4, \ldots$$

Even channels

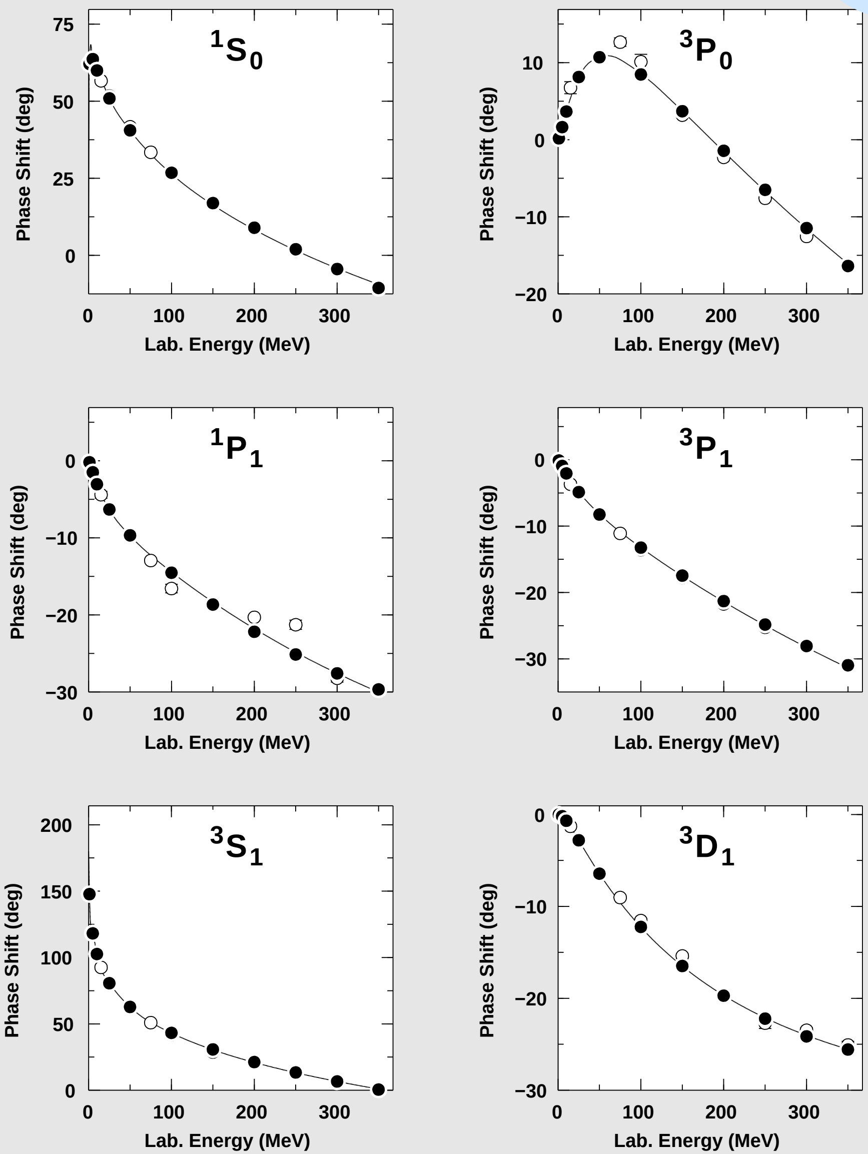
$$(S, T) = (0, 0) \text{ or } (1, 1) \qquad \longrightarrow \qquad L = 1, 3, 5, \ldots$$

Odd channels

Nucleon-Nucleon Force

NN scattering data

$^{2S+1}L_J$



Realistic Interactions

- describe NN phaseshifts (χ^2/datum ≈ 1)
- describe deuteron properties

- short-range (high-momentum) and off-shell behavior not constrained by data

➨ **nucleon-nucleon force not completely constrained**

Some Realistic Interactions

- **Bonn**-Potentials
  (based on meson-exchange)
- **Argonne V18**
  (local, phenomenological ansatz)
- Potentials based on
  Chiral Perturbation Theory

Argonne V18 Interaction

- (almost) local interaction in coordinate space

$$
\begin{aligned}
V(\mathbf{r}_1,\mathbf{r_2},\mathbf{p}_1,\mathbf{p_2},\boldsymbol{\sigma}_1,\boldsymbol{\sigma}_2,\boldsymbol{\tau}_1,\boldsymbol{\tau}_2) = \; & V(r) + V^{\sigma}(r)\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 + V^{\tau}(r)\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 + V^{\sigma\tau}(r)\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 + \\
& V_{l^2}(r)\mathbf{L}^2 + V^{\sigma}_{l^2}(r)\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\mathbf{L}^2 + V^{\tau}_{l^2}(r)\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2\mathbf{L}^2 + V^{\sigma\tau}_{l^2}(r)\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2\mathbf{L}^2 + \\
& V_{ls}(r)\mathbf{L}\cdot\mathbf{S} + V^{\tau}_{ls}(r)\mathbf{L}\cdot\mathbf{S} + \\
& V_{ls^2}(r)(\mathbf{L}\cdot\mathbf{S})^2 + V^{\tau}_{ls^2}(r)\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2(\mathbf{L}\cdot\mathbf{S})^2 + \\
& V_t(r)S_{12} + V^{\tau}_t(r)\boldsymbol{\tau}_1\cdot\boldsymbol{\tau}_2 S_{12} +
\end{aligned}
$$

Central

Spin-Orbit

Tensor

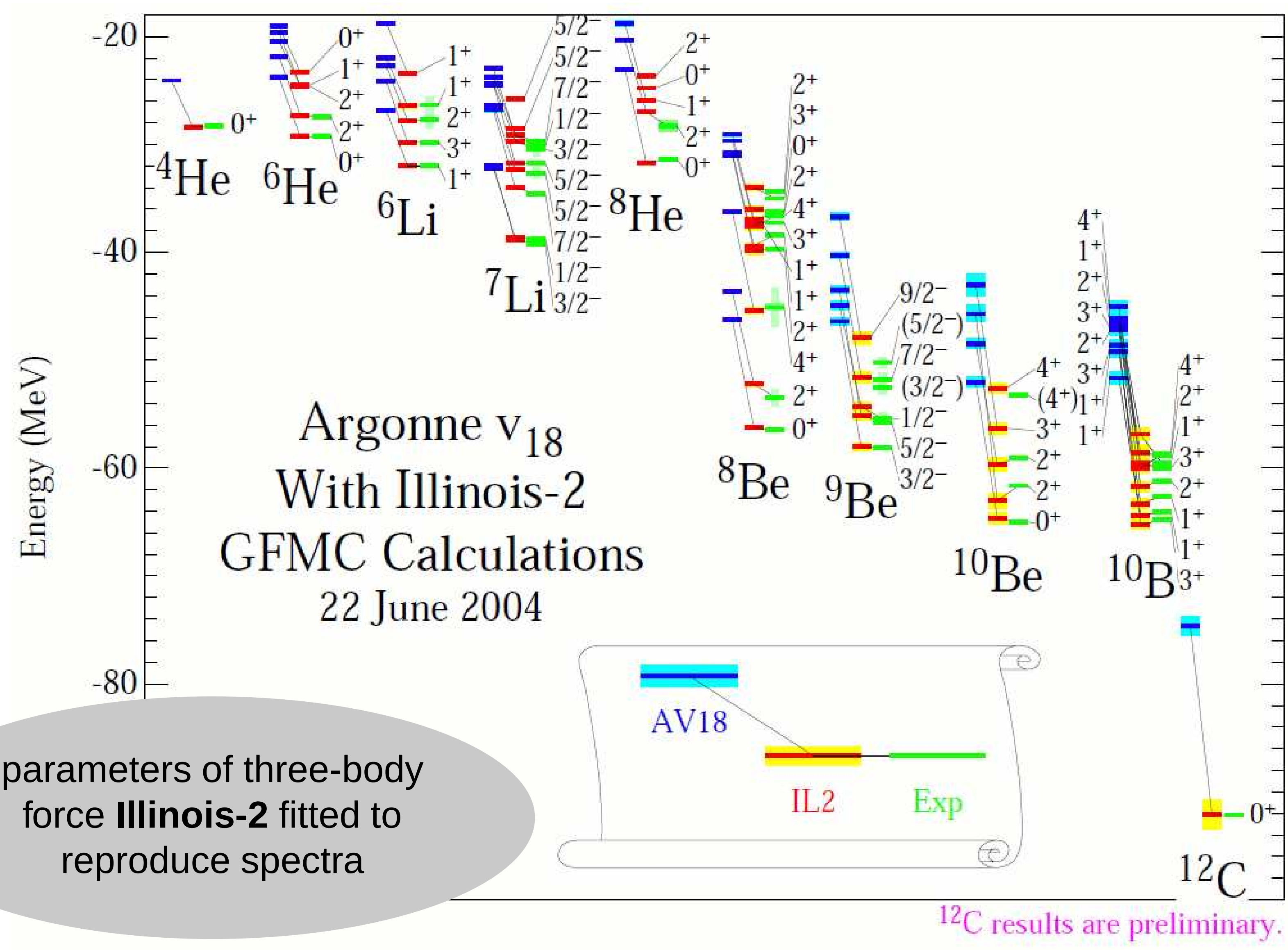
four charge dependent and charge asymmetric terms

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2, \qquad \mathbf{p} = \tfrac{1}{2}(\mathbf{p}_1 - \mathbf{p}_2)$$

$$\mathbf{L} = \mathbf{r}\times\mathbf{p}, \qquad \mathbf{S} = \tfrac{1}{2}(\boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2)$$

$$S_{12} = 3(\boldsymbol{\sigma}_1\cdot\hat{\mathbf{r}})(\boldsymbol{\sigma}_2\cdot\hat{\mathbf{r}}) - \boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2$$

Green's Function Monte Carlo



parameters of three-body force **Illinois-2** fitted to reproduce spectra

Wiringa, Pieper, PRL **89** (2002) 182501

Unitary Correlation Operator Method

Central and Tensor Correlations

Unitary Correlation Operator

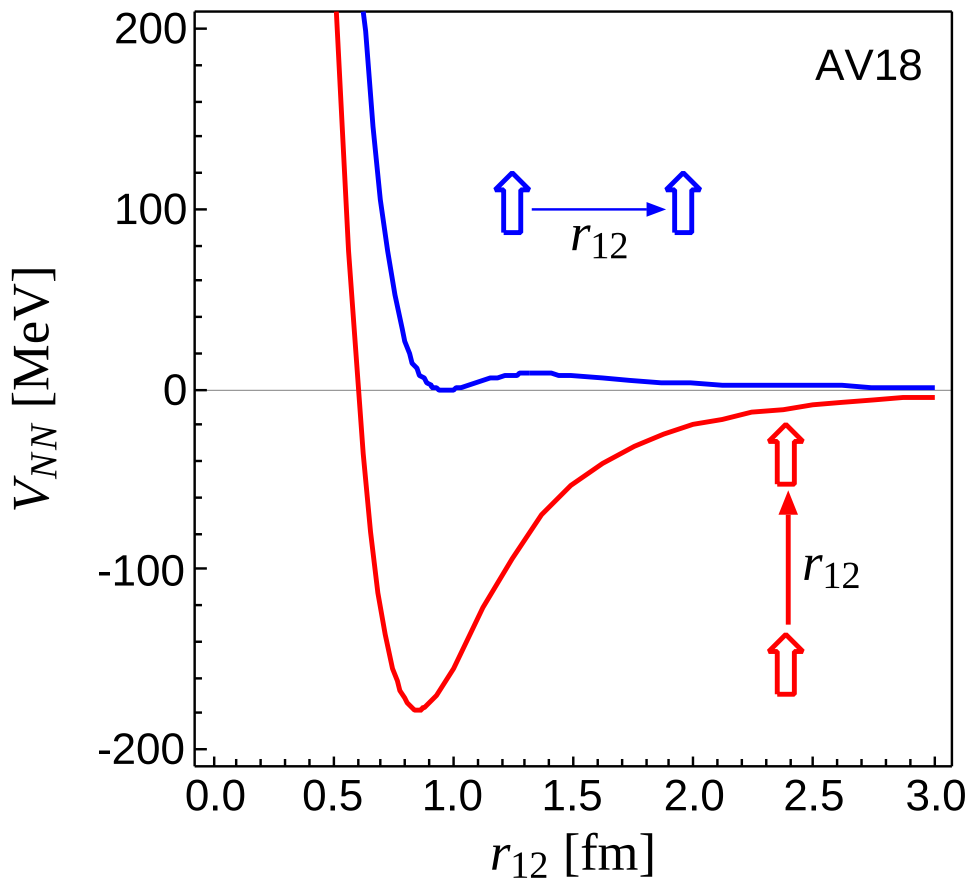
Interaction in Momentum Space

***ab initio* Calculations**

Nuclear Force

Argonne V18 (T=0)

spins aligned parallel or perpendicular to the relative distance vector



- strong repulsive core: nucleons can not get closer than ≈ 0.5 fm

➨ **central correlations**

- strong dependence on the orientation of the spins due to the tensor force

➨ **tensor correlations**

the nuclear force will induce
strong short-range correlations
in the nuclear wave function

One- and Two-Body Densities

(Diagonal) One-body density

$$\rho^{(1)}(\mathbf{r}) = \sum_{m_t,m_s} \left\langle \Psi \middle| \underset{\sim}{a}^{\dagger}_{m_s,m_t}(\mathbf{r})\, \underset{\sim}{a}_{m_s,m_t}(\mathbf{r}) \middle| \Psi \right\rangle$$

Probability to find a nucleon at position $\mathbf{r}$

(Diagonal) Two-body density

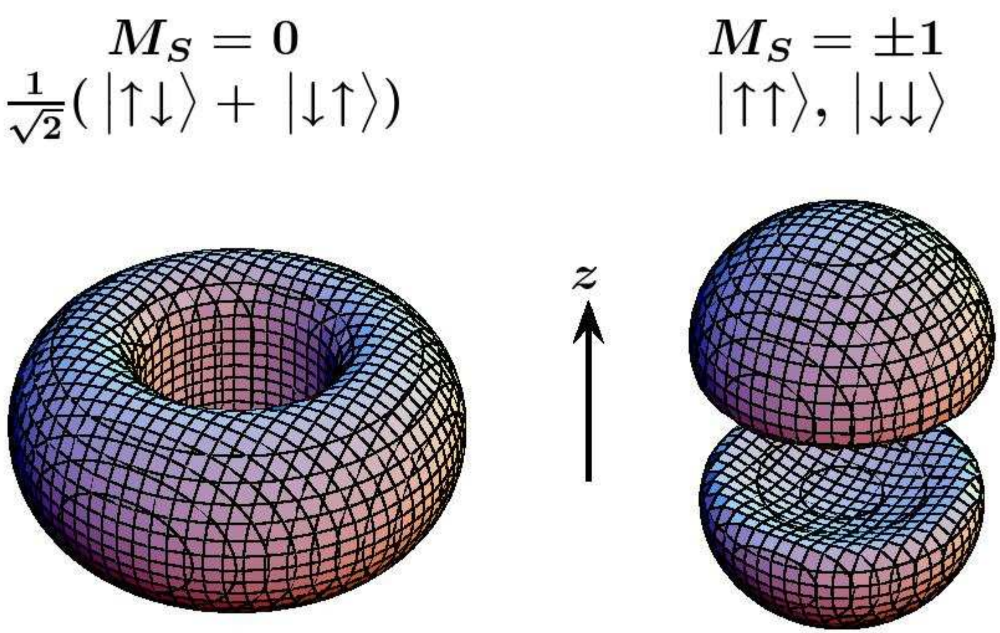
$$\rho^{(2)}_{S,M_S;T,M_T}(\mathbf{r},\mathbf{r}') = \sum_{m_s,m_s'} C\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & S \\ m_s & m_s' & M_S \end{pmatrix} \sum_{m_t,m_t'} C\begin{pmatrix} \frac{1}{2} & \frac{1}{2} & T \\ m_t & m_t' & M_T \end{pmatrix} \left\langle \Psi \middle| \underset{\sim}{a}^{\dagger}_{m_s,m_t}(\mathbf{r})\, \underset{\sim}{a}^{\dagger}_{m_s',m_t'}(\mathbf{r}')\, \underset{\sim}{a}_{m_s',m_t'}(\mathbf{r}')\, \underset{\sim}{a}_{m_s,m_t}(\mathbf{r}) \middle| \Psi \right\rangle$$

$$\rho^{(2)}_{S,M_S;T,M_T}(\mathbf{r}) = \int d^3R\, \rho^{(2)}_{S,M_S;T,M_T}(\tfrac{1}{2}\mathbf{R}+\mathbf{r}, \tfrac{1}{2}\mathbf{R}-\mathbf{r})$$

Probability to find **two nucleons** at a relative distance $\mathbf{r}$

Deuteron

Spin-projected two-body density $\rho^{(2)}_{S=1,M_S,T=0}(\mathbf{r})$ (isodensity plot)



"Donut" "Dumbbell"

density at small distances suppressed

➨ **central correlations**

density depends strongly on spin orientation

➨ **tensor correlations**

these **short-range Correlations** can not be described with product states (Slater determinants)

Realistic and Effective Nucleon-Nucleon Interactions

Realistic Interactions

- reproduce scattering data and deuteron properties
- meson-exchange (Bonn), phenomenological (AV18), χ-PT (Idaho)
- **repulsive core** and **tensor force** induce **strong short-range correlations**

Effective Interactions

- phenomenological effective interactions describe many properties of nuclear systems like energies, radii, spectra successfully using simple many-body wave functions (HF, shell model, microscopic cluster models)
- No-Core Shell Model uses Lee-Suzuki transformation in oscillator basis
- G-matrix and V_{lowk} derive effective interaction in momentum space

Our approach

- derive **effective interaction** from **realistic interaction** by explicitly including correlations with **unitary correlation operator** $\underset{\sim}{C} = \underset{\sim}{C}_{\Omega}\underset{\sim}{C}_{r}$ formulated in **coordinate space**

➨ correlated (effective) interaction

$$\hat{\underset{\sim}{H}} = \underset{\sim}{C}^{\dagger}\underset{\sim}{H}\underset{\sim}{C}$$

Unitary Transformation

transform eigenvalue problem

$$\underset{\sim}{H} \left| \hat{\Psi}_n \right\rangle = E_n \left| \hat{\Psi}_n \right\rangle$$

with the unitary operator $\underset{\sim}{C}$

$$\left| \hat{\Psi}_n \right\rangle = \underset{\sim}{C} \left| \Psi_n \right\rangle, \quad \underset{\sim}{C}^{-1} = \underset{\sim}{C}^{\dagger}$$

into the equivalent eigenvalue problem

$$\underset{\sim}{\hat{H}} \left| \Psi_n \right\rangle = (\underset{\sim}{C}^{\dagger} \underset{\sim}{H} \underset{\sim}{C}) \left| \Psi_n \right\rangle = E_n \left| \Psi_n \right\rangle$$

finally solve eigenvalue problem in a (small) model space $\left\{ \left| \Psi_n \right\rangle, n = 1, \ldots, N \right\}$

“pre-diagonalization”

correlator $\underset{\sim}{C}$ describes short-range correlations that are very similar (for the states in the model space)

correlator $\underset{\sim}{C}$ admixes component
from outside the model space

it does not project on the model space

The Unitary Correlation Operator

Two-Body Correlations

- two-body generator

$$\underset{\sim}{C} = e^{-i\underset{\sim}{G}}, \qquad \underset{\sim}{G} = \sum_{i<j} \underset{\sim}{g}_{ij}$$

Correlator $\underset{\sim}{C}$

should conserve translational, rotational and Galilei invariance

cluster decomposition principle should be fulfilled

Cluster Expansion

correlated operators $\hat{\underset{\sim}{A}} = \underset{\sim}{C}^\dagger \underset{\sim}{A} \underset{\sim}{C}$ are no longer operators with definite particle number

- decompose correlated operator into irreducible k-body operators

$$\hat{\underset{\sim}{A}} = \hat{\underset{\sim}{A}}^{[1]} + \hat{\underset{\sim}{A}}^{[2]} + \cdots$$

Two-Body Approximation

$$\hat{\underset{\sim}{T}}^{C2} = \hat{\underset{\sim}{T}}^{[1]} + \hat{\underset{\sim}{T}}^{[2]}, \qquad \hat{\underset{\sim}{V}}^{C2} = \hat{\underset{\sim}{V}}^{[2]}$$

✘ correlation range should be smaller than mean distance of nucleons

Spin-Isospin Dependence

nuclear interaction strongly depends on spin and isospin

$$\underset{\sim}{v} = \sum_{S,T} \underset{\sim}{v}_{ST} \underset{\sim}{\Pi}_{ST}$$

- different correlations in the respective channels

$$\underset{\sim}{g} = \sum_{S,T} \underset{\sim}{g}_{ST} \underset{\sim}{\Pi}_{ST}$$

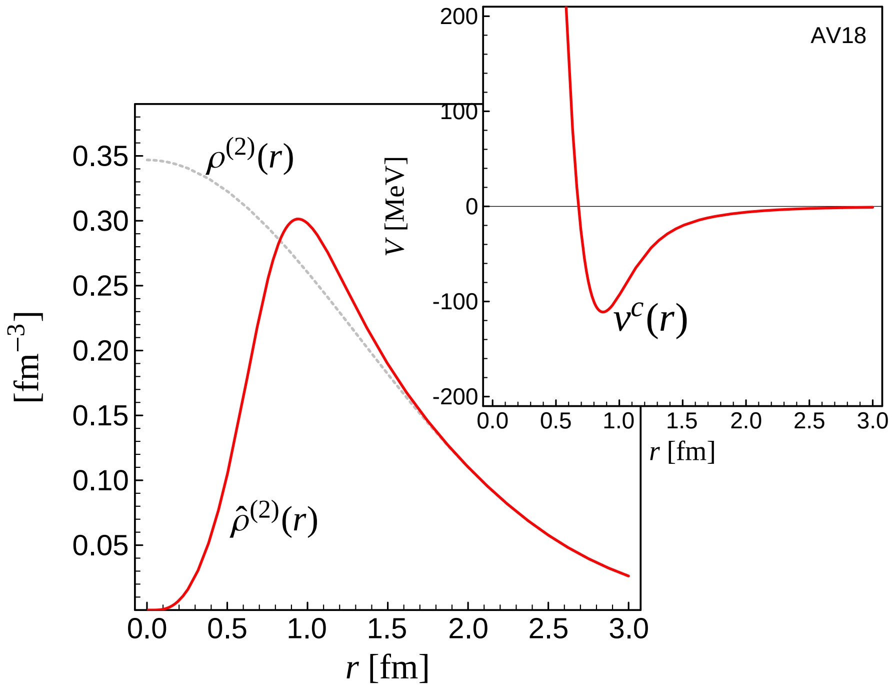
- correlated interaction in two-body space

$$\hat{\underset{\sim}{v}} = \sum_{S,T} \left(e^{i\underset{\sim}{g}_{ST}} \underset{\sim}{v}_{ST} e^{-i\underset{\sim}{g}_{ST}} \right) \underset{\sim}{\Pi}_{ST}$$

Central Correlations

repulsion at short distances

➨ probability density of nucleons in the repulsive core strongly suppressed



Radial Shift

➨ correlator shifts nucleons out of core

radial shift generated by radial momentum p_r

$$\underset{\sim}{g}_r \overset{\mathbf{r}}{\Rightarrow} \frac{1}{2}\{p_r s(r) + s(r) p_r\}, \quad p_r = \frac{1}{i}\left(\frac{1}{r} + \frac{\partial}{\partial r}\right)$$

Correlation Function

use correlation function $R_\pm(r)$ instead of shift function $s(r)$

$$\pm 1 = \int_r^{R_\pm(r)} \frac{d\xi}{s(\xi)}, \quad R_\pm(r) \approx r \pm s(r)$$

Correlated Wave function

$$\left\langle \mathbf{X}, \mathbf{r} \middle| \underset{\sim}{c}_r \middle| \Phi \right\rangle = \frac{R_-(r)}{r} \sqrt{R'_-(r)} \left\langle \mathbf{X}, R_-(r)\hat{\mathbf{r}} \middle| \Phi \right\rangle$$

Tensor Operators

$$S_{12}(\mathbf{a},\mathbf{b}) = 3(\boldsymbol{\sigma}_1\cdot\mathbf{a})(\boldsymbol{\sigma}_2\cdot\mathbf{b}) - (\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)(\mathbf{a}\cdot\mathbf{b})$$
$$= 3\left\{a^{(1)}\,b^{(1)}\right\}^{(2)}\cdot S^{(2)}$$
$$= 3\sqrt{5}\left\{(ab)^{(2)}\otimes S^{(2)}\right\}^{(0)}$$

$$S_{12}(\hat{\mathbf{r}},\hat{\mathbf{r}}) = 3\,Y^{(2)}\cdot S^{(2)}$$

couple two operators

$$\left\{A^{(j_1)}\,B^{(j_2)}\right\}^{(j)}_q \equiv \sum_{m_1,m_2} \mathrm{C}\left(\begin{array}{cc|c} j_1 & j_2 & j \\ m_1 & m_2 & q \end{array}\right) A^{(j_1)}_{m_1}\,B^{(j_2)}_{m_2}$$

couple spins to a tensor of rank 1

$$S^{(1)} = \frac{1}{2}\left(\sigma^{(1)}\otimes 1 + 1\otimes\sigma^{(1)}\right)$$

or to a tensor of rank 2

$$S^{(2)} = \left\{S^{(1)}\,S^{(1)}\right\}^{(2)}$$

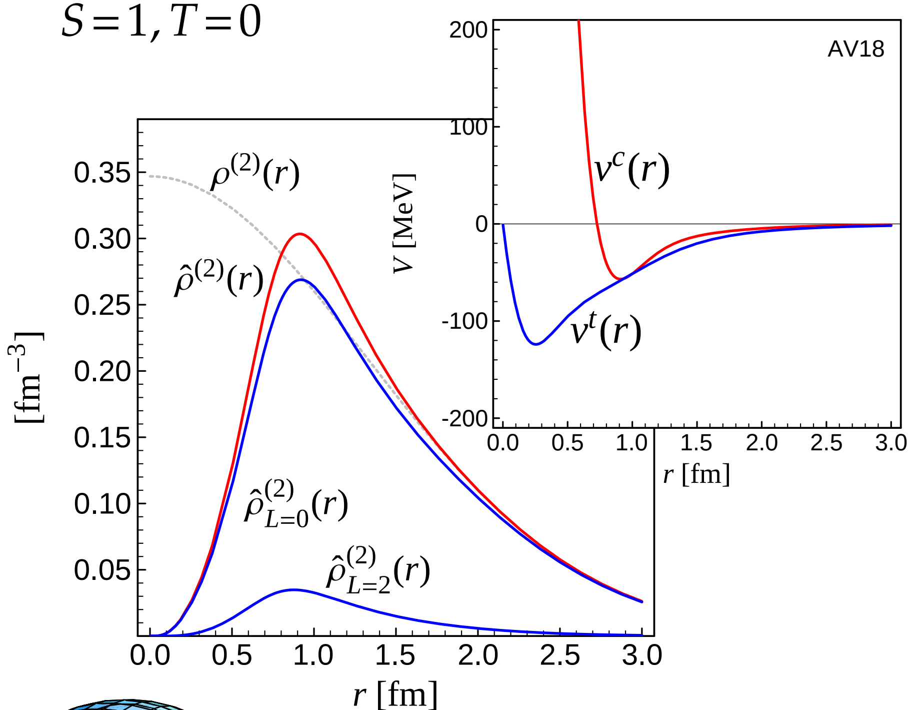
tensor operators are scalar operators
$\left\langle JM \middle| S_{12}(\mathbf{a},\mathbf{b}) \middle| J'M' \right\rangle \propto \delta_{J,J'}\delta_{M,M'}$

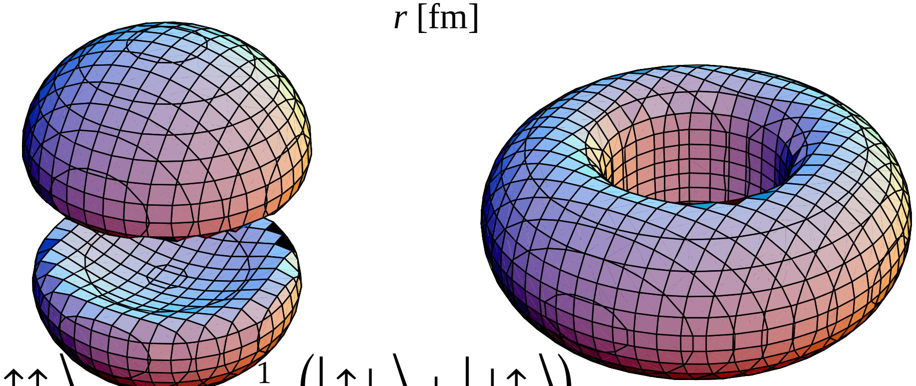
but they couple different orbital angular momenta
$\left\langle (L1)JM \middle| S_{12}(\mathbf{a},\mathbf{b}) \middle| (L'1)JM \right\rangle \neq 0$ for $|L-L'| = 0, 2$

Tensor Correlations

➨ tensor force admixes higher angular momenta

$S=1, T=0$





$\left|\uparrow\uparrow\right\rangle$ $\quad \frac{1}{\sqrt{2}}\left(\left|\uparrow\downarrow\right\rangle + \left|\downarrow\uparrow\right\rangle\right)$

Perpendicular Shift

➨ correlator aligns density with spin

perpendicular shift generated by $s_{12}(\mathbf{r}, \mathbf{p}_\Omega)$

$$\underset{\sim}{g}_\Omega \overset{\mathbf{r}}{\Rightarrow} \vartheta(r) s_{12}(\mathbf{r}, \mathbf{p}_\Omega), \qquad \mathbf{p} = \mathbf{p}_r + \mathbf{p}_\Omega$$

$$s_{12}(\mathbf{r}, \mathbf{p}_\Omega) = \frac{3}{2}(\boldsymbol{\sigma}_1 \cdot \mathbf{p}_\Omega)(\boldsymbol{\sigma}_2 \cdot \mathbf{r}) + \frac{3}{2}(\boldsymbol{\sigma}_1 \cdot \mathbf{r})(\boldsymbol{\sigma}_2 \cdot \mathbf{p}_\Omega)$$

$s_{12}(\mathbf{r}, \mathbf{p}_\Omega)$	$\left\|(J-1,1)J\right\rangle$	$\left\|(J1)J\right\rangle$	$\left\|(J+1,1)J\right\rangle$
$\left\langle (J-1,1)J\right\|$	0	0	$-3i\sqrt{J(J+1)}$
$\left\langle (J,1)J\right\|$	0	0	0
$\left\langle (J+1,1)J\right\|$	$3i\sqrt{J(J+1)}$	0	0

Correlated Wave function

$$\left\langle r \middle| \underset{\sim}{c}_\Omega \middle| \varphi; (J,1)J \right\rangle = \varphi(r) \left| (J,1)J \right\rangle$$

$$\left\langle r \middle| \underset{\sim}{c}_\Omega \middle| \varphi; (J\mp1,1)J \right\rangle = \cos\left(\theta^{(J)}(r)\right) \varphi(r) \left| (J\mp1,1)J \right\rangle$$
$$\pm \sin\left(\theta^{(J)}(r)\right) \varphi(r) \left| (J\pm1,1)J \right\rangle$$

$$\theta^{(J)}(r) = 3\sqrt{J(J+1)}\,\vartheta(r)$$

Tensor Correlated Interaction

Tensor Correlated Operators

- Baker-Campbell-Hausdorff

$$\tilde{c}_{\Omega}^{\dagger}\tilde{a}\tilde{c}_{\Omega} = e^{i\tilde{g}_{\Omega}}\tilde{a}e^{-i\tilde{g}_{\Omega}} = e^{\mathsf{L}_{\Omega}}\tilde{a}, \quad \mathsf{L}_{\Omega} = \left[\tilde{g}_{\Omega}, \circ\right]_{-}$$

$$s_{12}(\mathbf{l},\mathbf{l}) = 3(\boldsymbol{\sigma}_1\cdot\mathbf{l})(\boldsymbol{\sigma}_2\cdot\mathbf{l}) - (\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2)\mathbf{l}^2 \, .$$

$$\bar{s}_{12}(\mathbf{p}_{\Omega},\mathbf{p}_{\Omega}) = 2r^2 s_{12}(\mathbf{p}_{\Omega},\mathbf{p}_{\Omega}) + s_{12}(\mathbf{l},\mathbf{l}) - \frac{1}{2}s_{12}(\hat{\mathbf{r}},\hat{\mathbf{r}})$$

$$\left[g_{\Omega}, p_r^2\right]_{-} = i\left(p_r\vartheta'(r) + \vartheta'(r)p_r\right)s_{12}(\mathbf{r},\mathbf{p}_{\Omega})$$

$$\left[g_{\Omega},\left[g_{\Omega}, p_r^2\right]_{-}\right]_{-} = -2\vartheta'(r)^2\left[(18 + 6\,\mathbf{l}^2)\Pi_1 + \frac{45}{2}\mathbf{l}\cdot\mathbf{s} + \frac{3}{2}s_{12}(\mathbf{l},\mathbf{l})\right]$$

$$\left[g_{\Omega},\left[g_{\Omega},\left[g_{\Omega}, p_r^2\right]_{-}\right]_{-}\right]_{-} = 0$$

$$\left[g_{\Omega},\Pi_1\right]_{-} = 0$$

$$\left[g_{\Omega}, s_{12}(\hat{\mathbf{r}},\hat{\mathbf{r}})\right]_{-} = i\vartheta(r)\left[-24\,\Pi_1 - 18\,\mathbf{l}\cdot\mathbf{s} + 3\,s_{12}(\hat{\mathbf{r}},\hat{\mathbf{r}})\right]$$

$$\left[g_{\Omega}, \mathbf{l}\cdot\mathbf{s}\right]_{-} = i\vartheta(r)\left[-\bar{s}_{12}(\mathbf{p}_{\Omega},\mathbf{p}_{\Omega})\right]$$

$$\left[g_{\Omega}, \mathbf{l}^2\right]_{-} = i\vartheta(r)\left[2\,\bar{s}_{12}(\mathbf{p}_{\Omega},\mathbf{p}_{\Omega})\right]$$

$$\left[g_{\Omega}, s_{12}(\mathbf{l},\mathbf{l})\right]_{-} = i\vartheta(r)\left[7\,\bar{s}_{12}(\mathbf{p}_{\Omega},\mathbf{p}_{\Omega})\right]$$

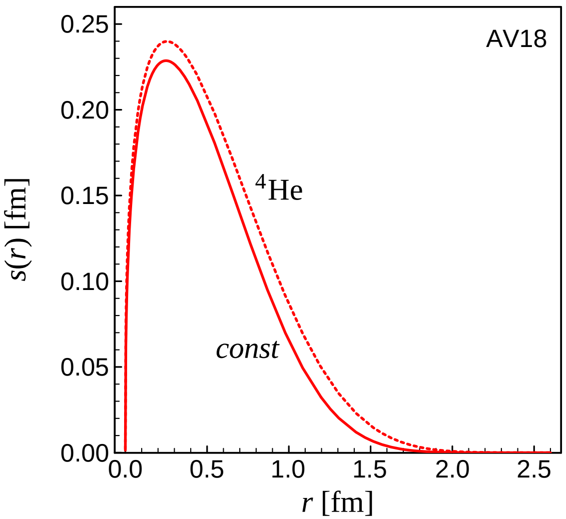
$$\left[g_{\Omega}, \bar{s}_{12}(\mathbf{p}_{\Omega},\mathbf{p}_{\Omega})\right]_{-} = i\vartheta(r)\left[(96\,\mathbf{l}^2 + 108)\Pi_1 + (36\,\mathbf{l}^2 + 153)\,\mathbf{l}\cdot\mathbf{s} + 15\,s_{12}(\mathbf{l},\mathbf{l})\right]$$

- evaluate $e^{\mathsf{L}_{\Omega}}$ in truncated operator space

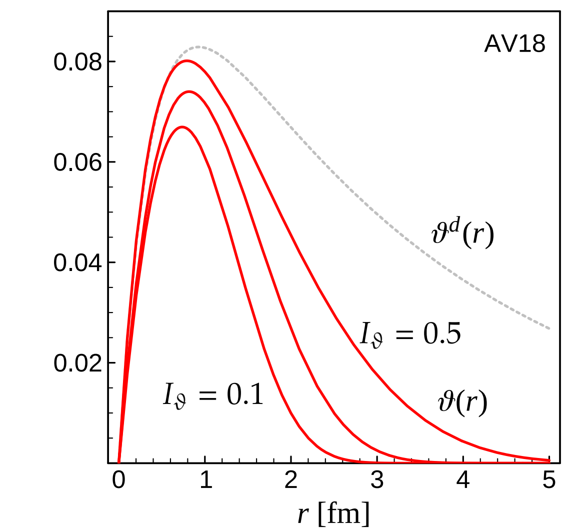
- use in HF or FMD calculations

Determine Correlation Functions

Central Correlations



Tensor Correlations



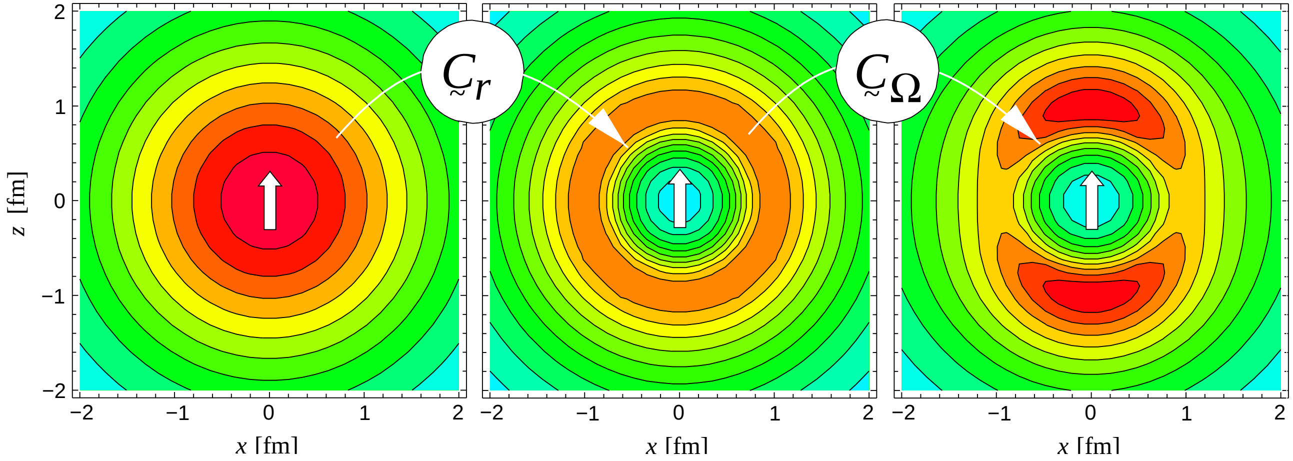
- determine $s(r)$ und $\vartheta(r)$ in each spin-isospin channel by minimizing the energy in the two-body system

$$\min_{s(r),\vartheta(r)} \left\langle \phi^{ST}_{trial} \middle| \underset{\sim}{C}_r^\dagger \underset{\sim}{C}_\Omega^\dagger \underset{\sim}{H} \underset{\sim}{C}_\Omega \underset{\sim}{C}_r \middle| \phi^{ST}_{trial} \right\rangle$$

- correlation functions depend only weakly on the trial wave function
- restrict the range of the tensor correlations in the $S=1, T=0$ channel (parameter I_ϑ)

Correlated Two-Body Densities and Energies

two-body densities



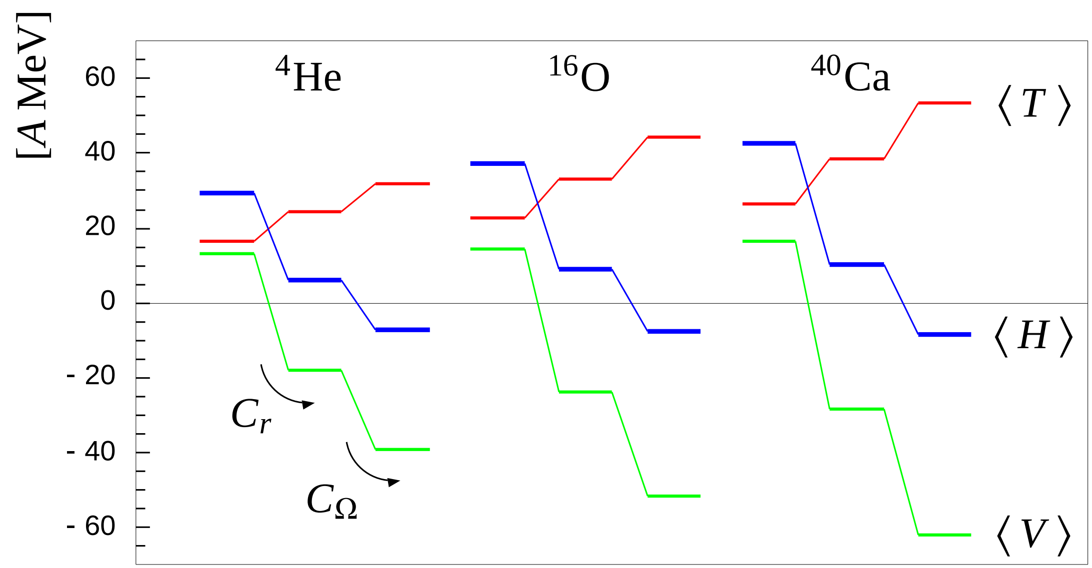
$\rho^{(2)}_{S,T}(\mathbf{r}_1 - \mathbf{r}_2) \quad S = 1, M_S = 1, T = 0$

central correlator $\underset{\sim}{C}_r$ shifts density out of the repulsive core

tensor correlator $\underset{\sim}{C}_\Omega$ aligns density with spin orientation

energies

$0\hbar\omega$ Harmonic Oscillator

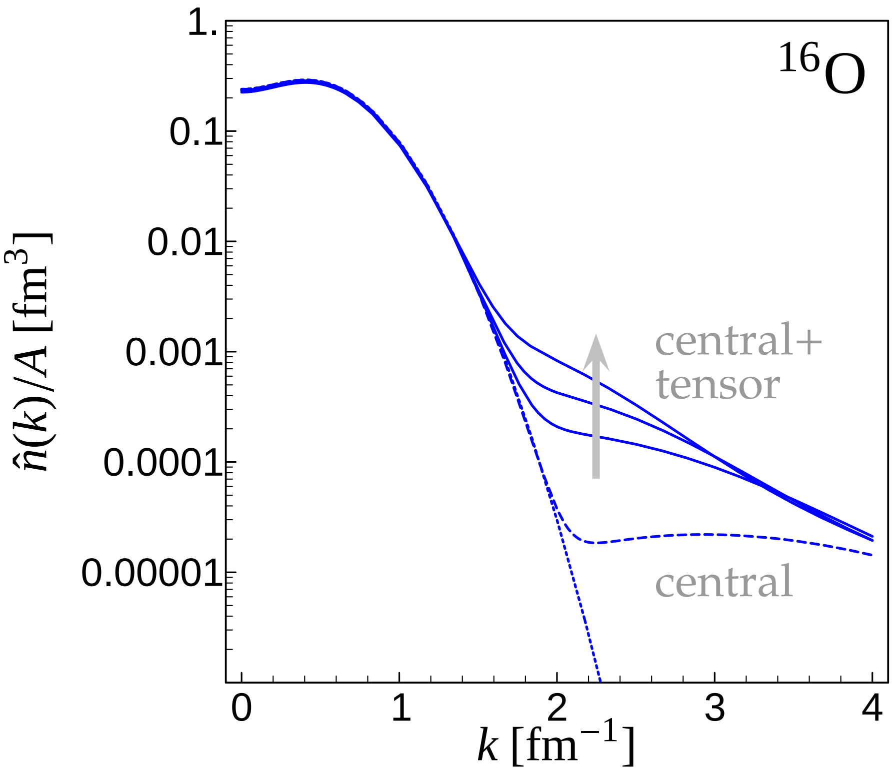


both central and tensor correlations are essential for binding

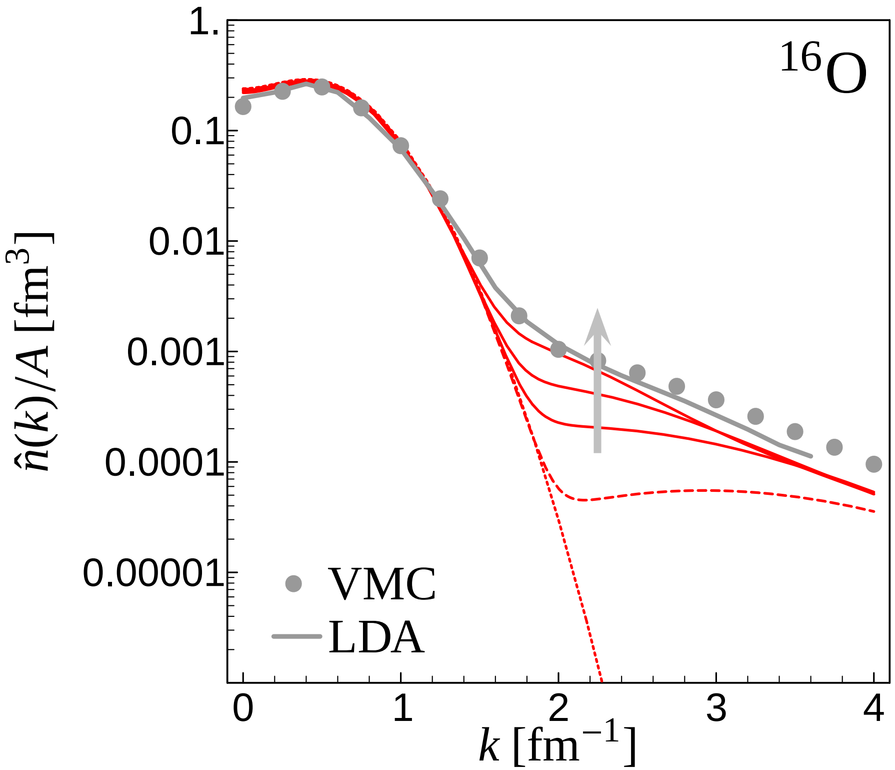
Nucl. Phys. **A713** (2003) 311

Nucleon Momentum Distributions

Bonn-A



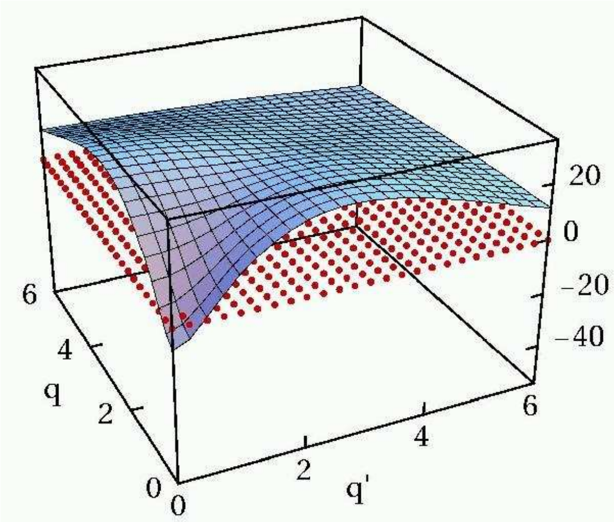
Argonne V18



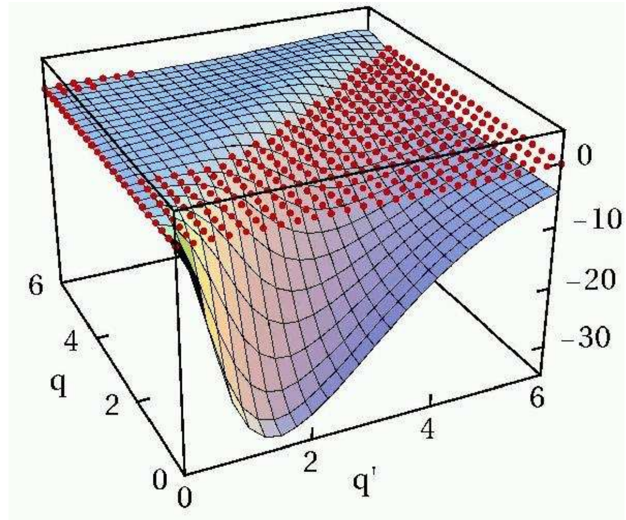
- correlations induce high-momentum components
- large contributions by tensor correlations
- dependence on the correlation range at the Fermi surface

Correlated Interaction in Momentum Space

$^3S_1$ bare

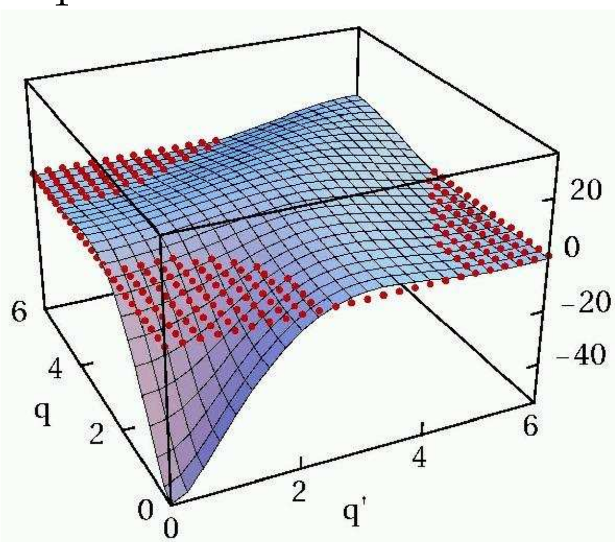


$^3S_1$ - $^3D_1$ bare

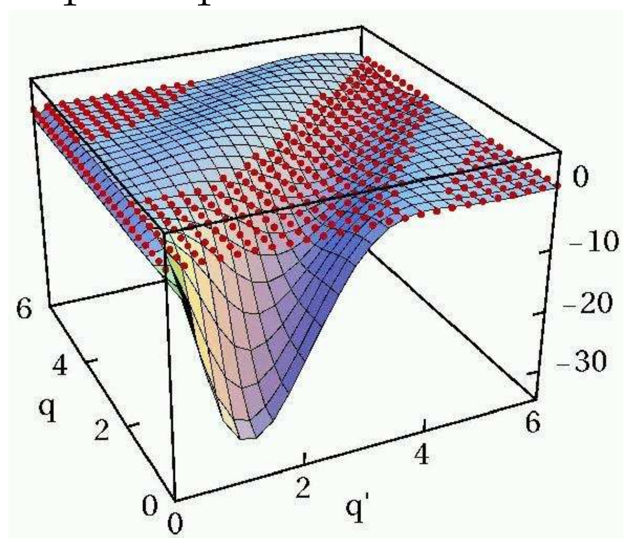


correlated interaction is **more attractive** at low momenta

$^3S_1$ correlated



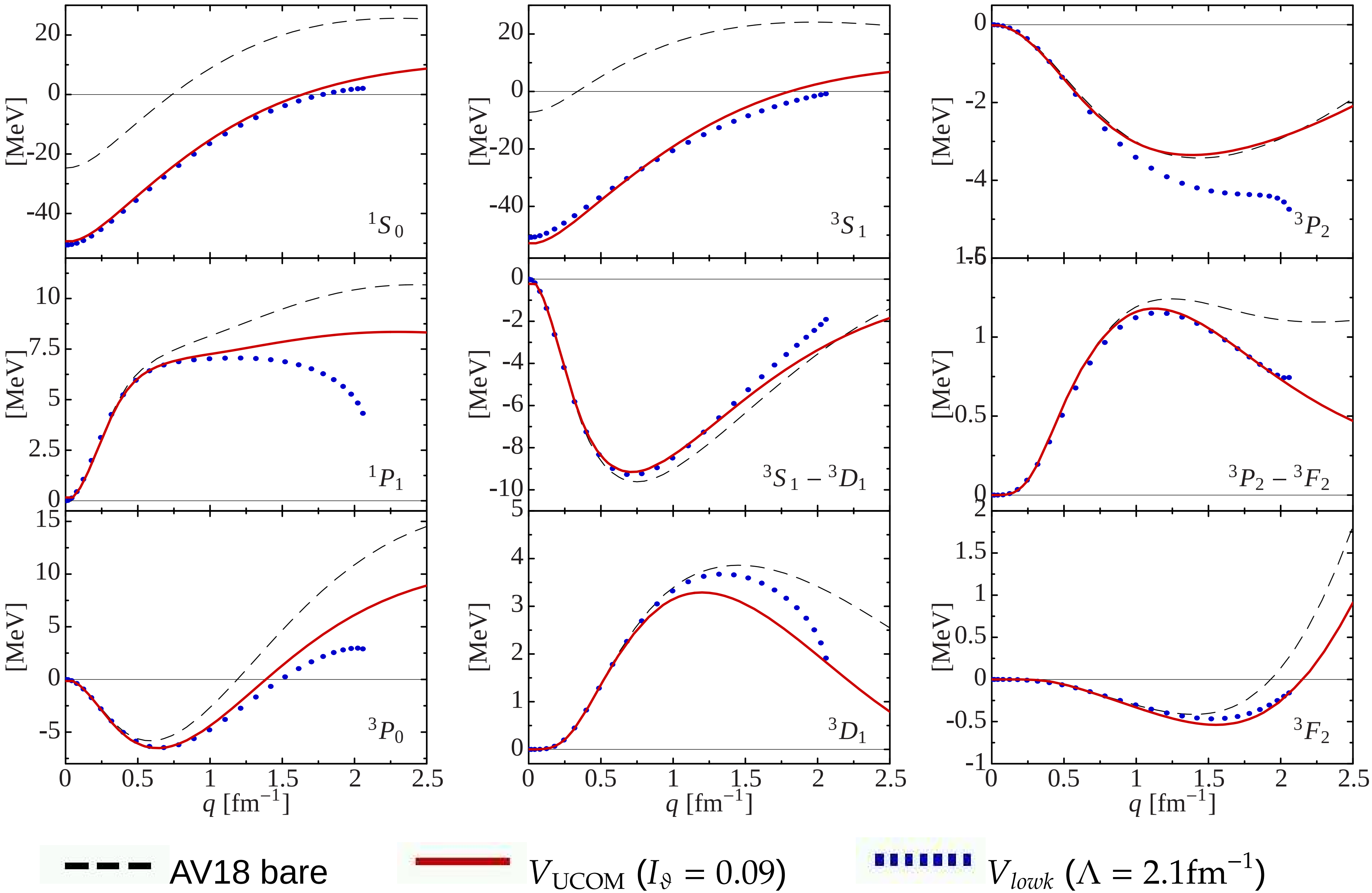
$^3S_1$ - $^3D_1$ correlated



off-diagonal matrix elements connecting low- and high-momentum states are **strongly reduced**

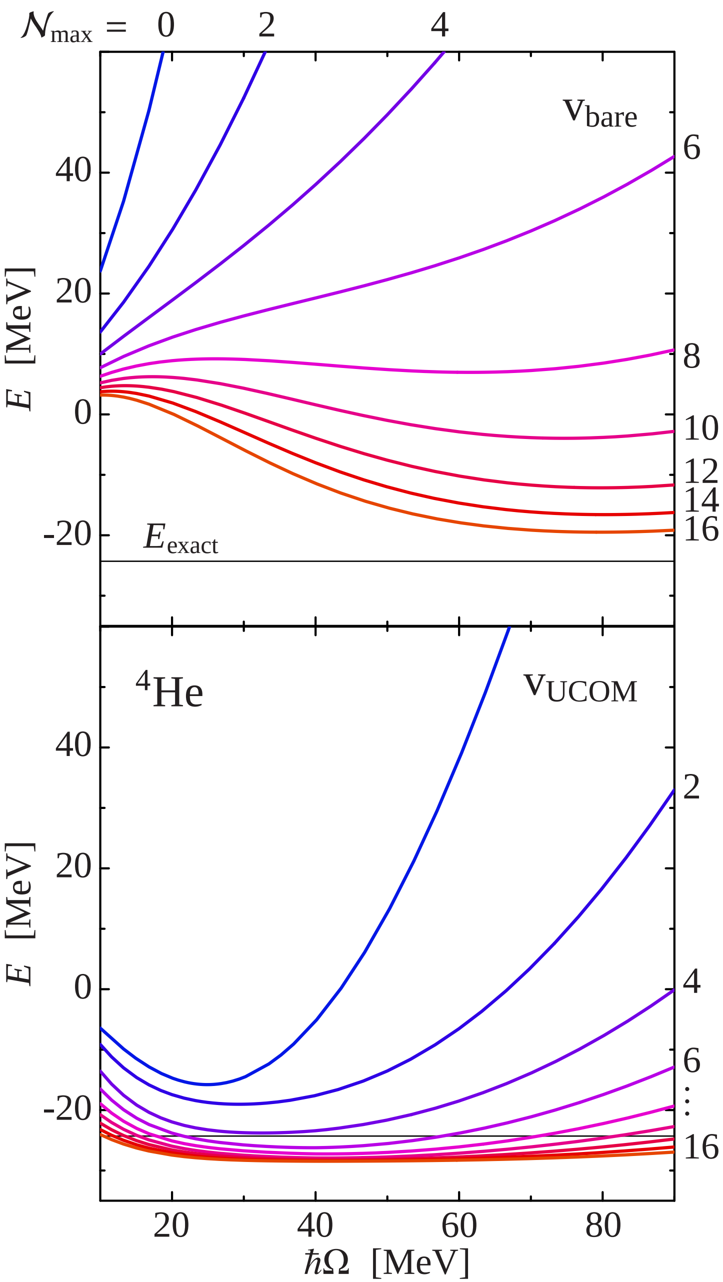
Phys. Rev. **C72** (2005) 034002

Correlated Interaction in Momentum Space



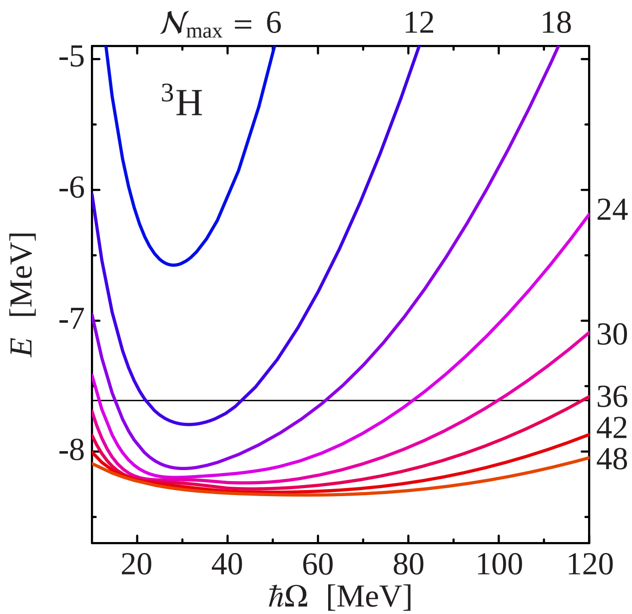
Bogner, Kuo, Schwenk, Phys. Rept. **386** (2003) 1

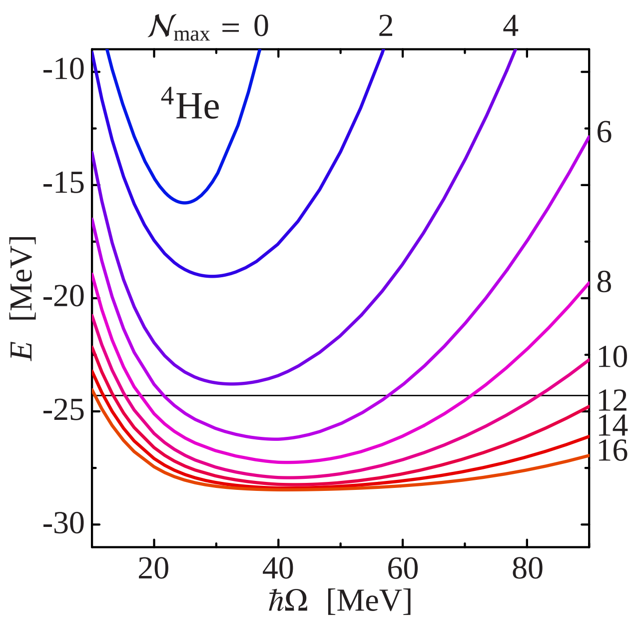
No-Core Shell Model Calculations

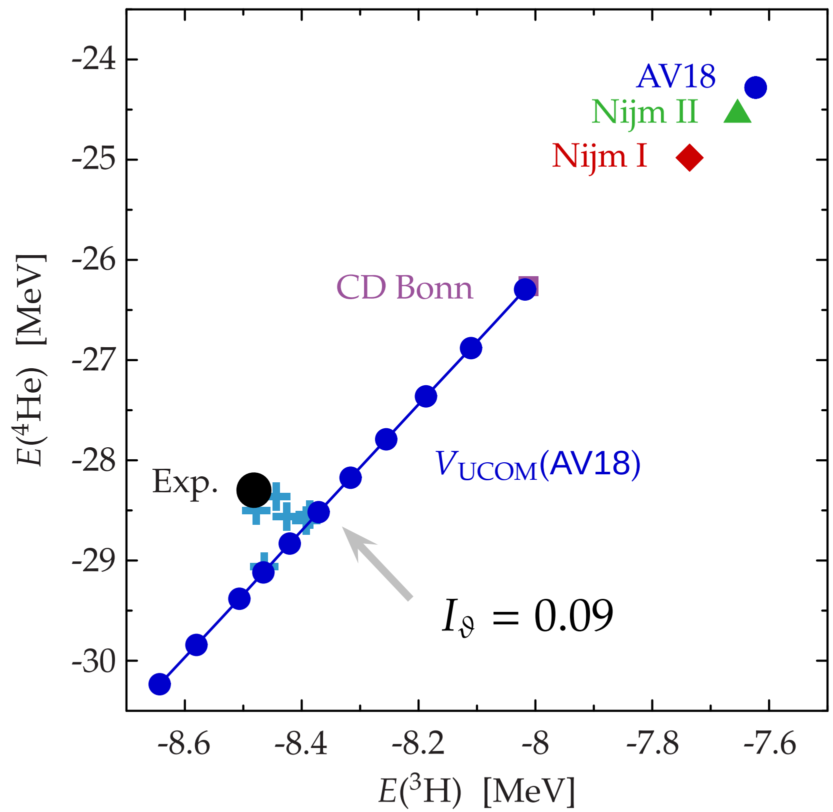


- use Jacobi-coordinate NCSM code by Petr Navrátil, LLNL for ^{3}He and ^{4}He (don't use Lee-Suzuki transformation)
- dramatically **improved convergence** compared to bare interaction
- **does not converge to exact result for bare interaction** due to omitted higher order terms $V^{[3]}_{UCOM}, \ldots$
- study the effect of higher order contributions as a function of tensor correlation range I_ϑ.

Tjon Line with NCSM



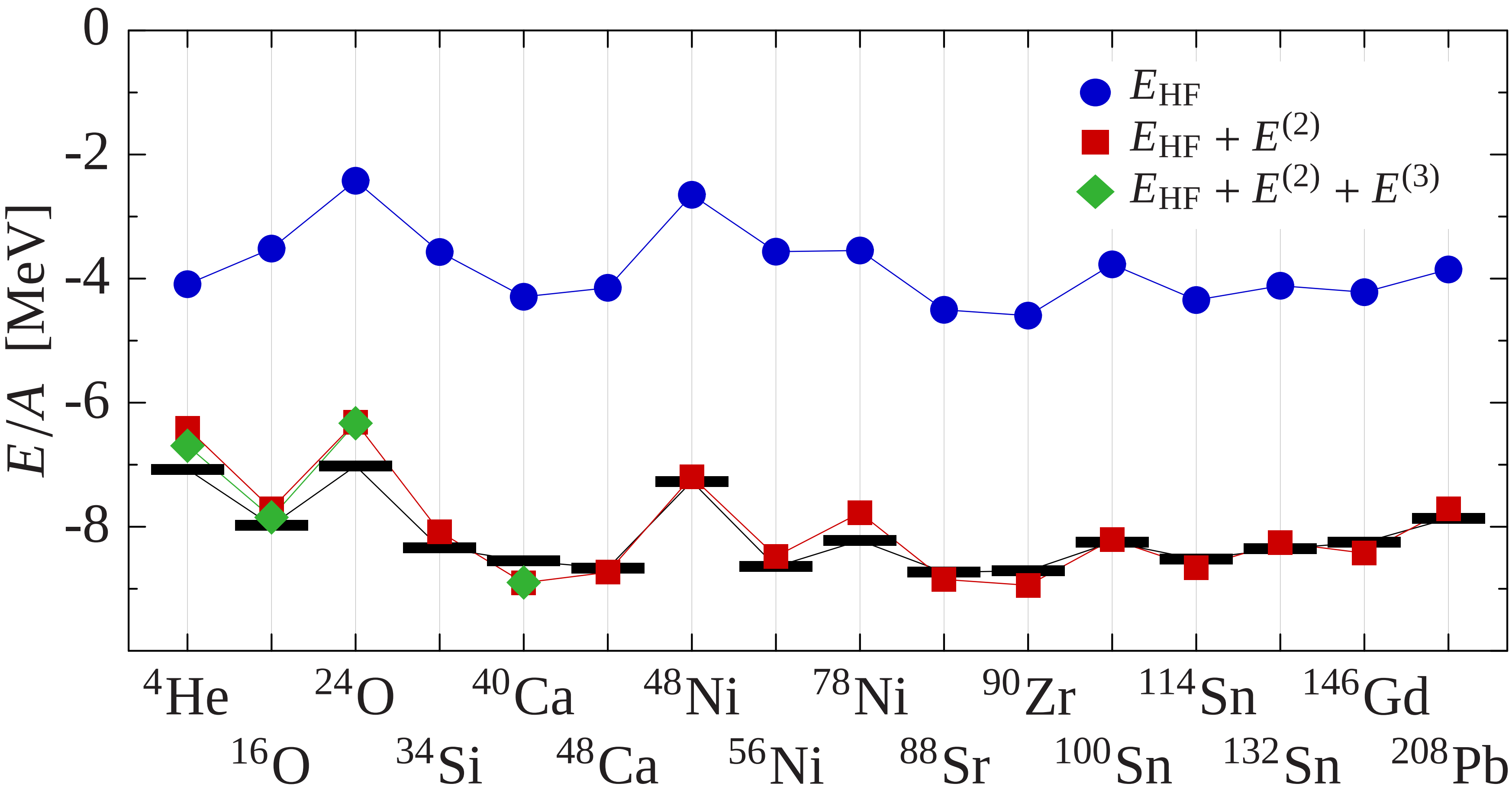




- choose tensor correlation range $I_\vartheta = 0.09$ such that **need for three-body forces is minimized**

➨ **different perspective**: don't try to reproduce the results with the bare interaction but consider **V_{UCOM} as a realistic potential** to describe experiment

HF and MBPT calculations

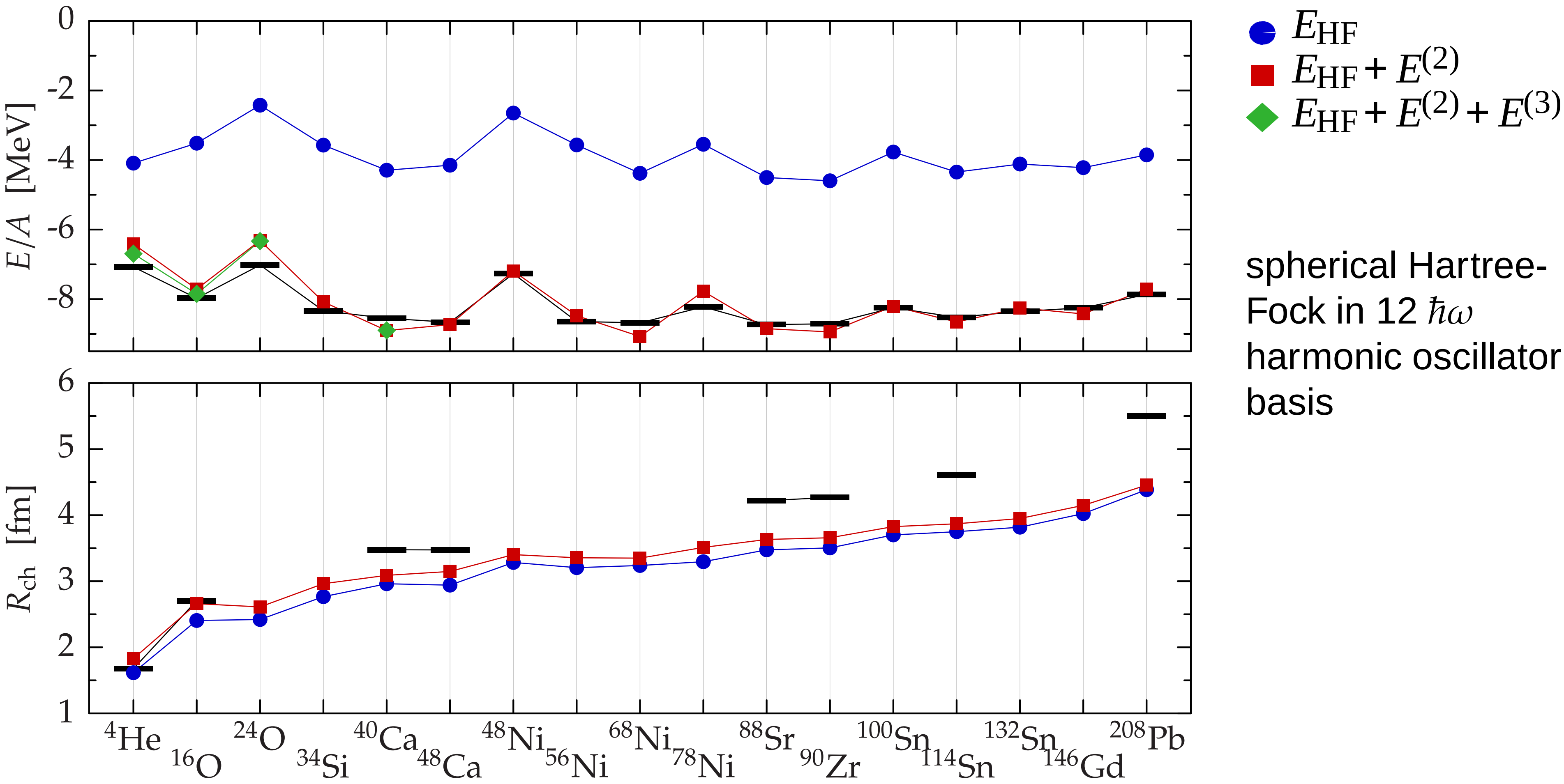


spherical Hartree-Fock in 12 $\hbar\omega$ harmonic oscillator basis

additional attraction mainly by **medium to long range tensor forces**

long-range correlations appear to be perturbative

Hartree-Fock and Many-Body Perturbation Theory



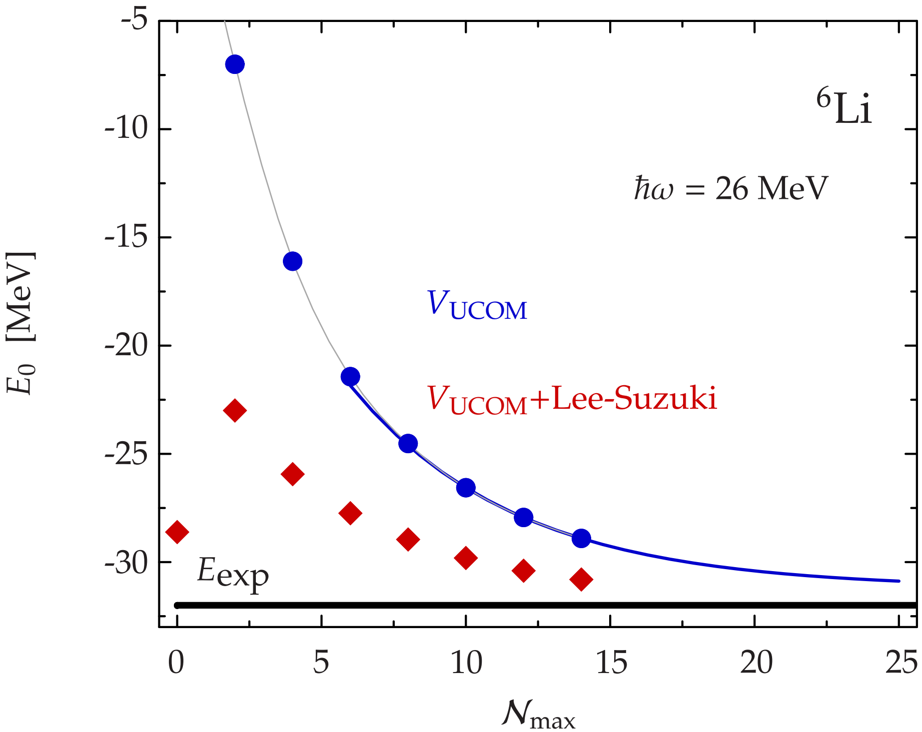
spherical Hartree-Fock in 12 $\hbar\omega$ harmonic oscillator basis

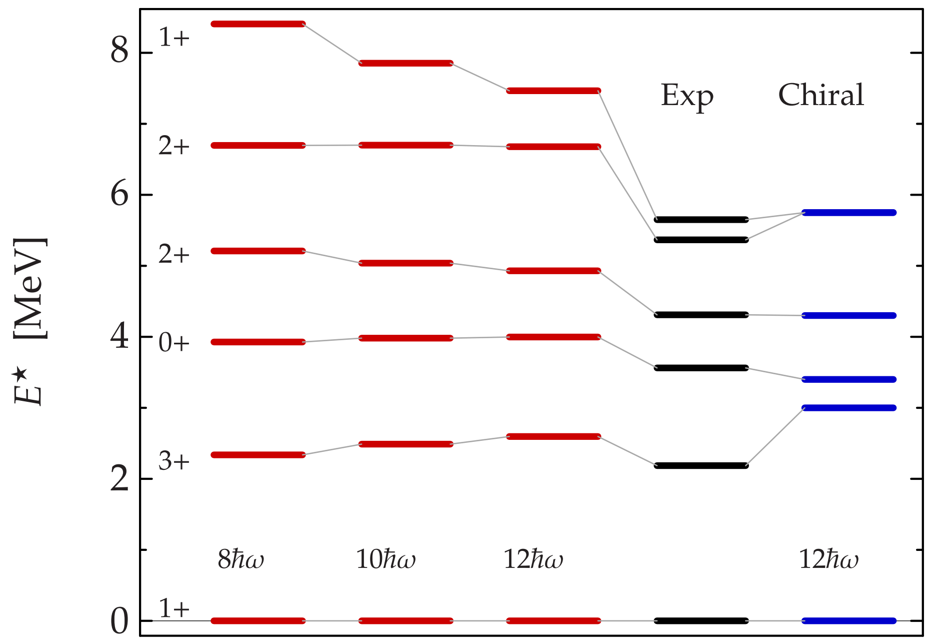
additional binding mainly due to **medium to long range tensor forces**

long-range correlations appear to be perturbative

problems with saturation indicate need for **three-body forces**

^{6}Li

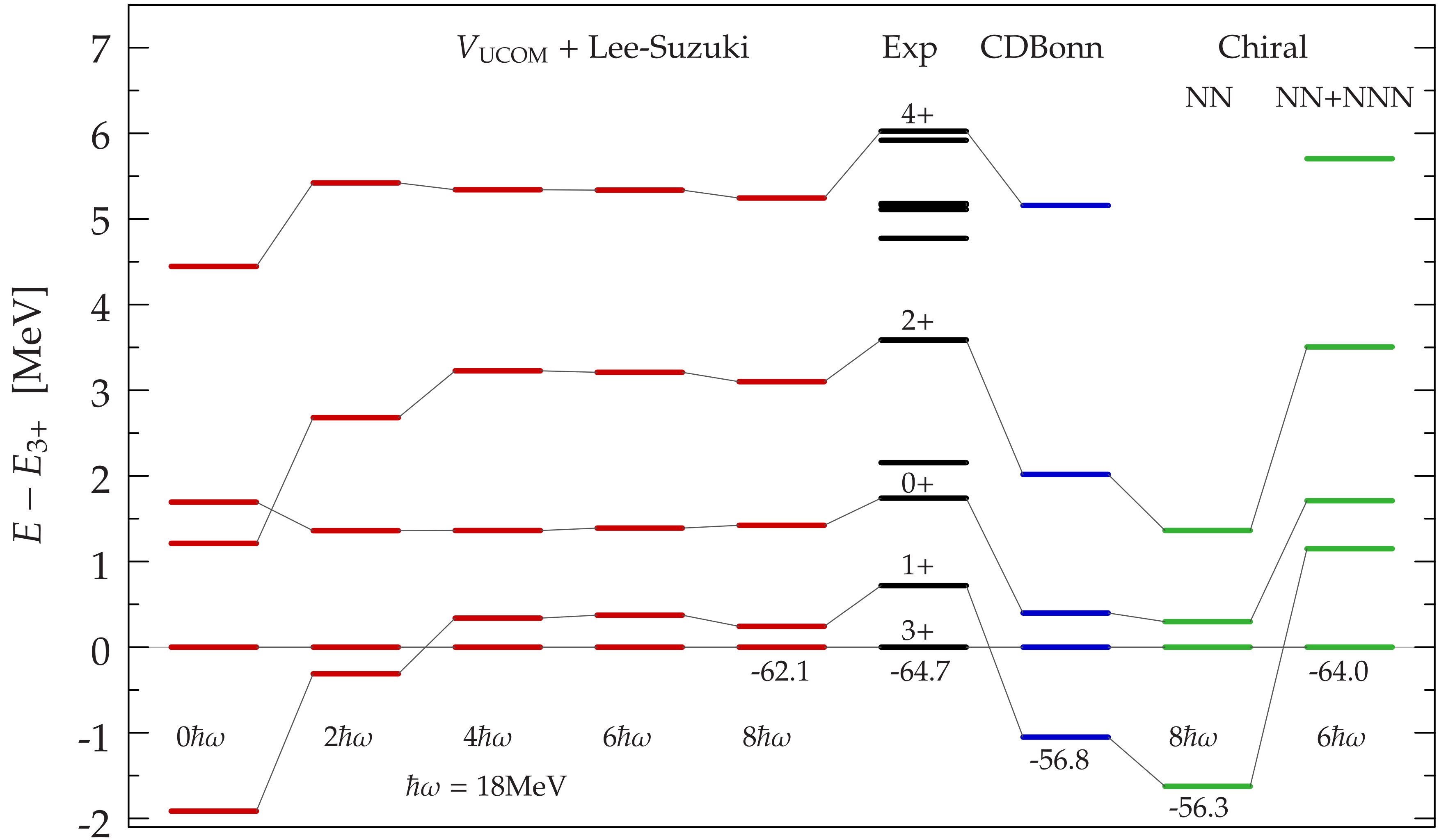




calculations by Petr Navrátil, LLNL

- NCSM calculations with “bare” V_{UCOM} and Lee-Suzuki effective interaction derived from V_{UCOM} show consistent convergence pattern
- Binding energy close to experiment
- Spectra with V_{UCOM} are of similar quality than with other modern NN forces

NCSM ^{10}B



calculations by Petr Navrátil, LLNL

- correct level ordering without three-body forces
- binding energy not too far from experiment