Nuclear Structure

in

FMD

Thomas Neff

FMD attributes

Fermionic

$$\left|\,\hat{Q}\,\right\rangle = \underset{\sim}{C}\,\underset{\sim}{\mathcal{A}}\left(\left|\,q_1\,\right\rangle \otimes \cdots \otimes \left|\,q_A\,\right\rangle\right)$$

- Unitary Correlator $\underset{\sim}{C}$
- antisymmetrized A-particle state

Molecular

$$\left\langle\,\vec{x}\,\middle|\,q\,\right\rangle = \left\langle\,\vec{x}\,\middle|\,a,\vec{b},\chi,\xi\,\right\rangle = \exp\{-\frac{(\vec{x}-\vec{b})^2}{2a}\}\left|\,\chi\,\right\rangle \otimes \left|\,\xi\,\right\rangle$$

Dynamics

Variational Principle

$$\delta \int dt \frac{\left\langle\,\hat{Q}\,\middle|\,i\frac{d}{dt} - \underset{\sim}{H}\,\middle|\,\hat{Q}\,\right\rangle}{\left\langle\,\hat{Q}\,\middle|\,\hat{Q}\,\right\rangle} = 0$$

Equations of motion

$$i\sum_{\nu} \mathscr{C}_{\mu\nu}\,\dot{q}_{\nu} = \frac{\partial \mathscr{H}}{\partial q_{\mu}^{\star}}$$

$$\mathscr{C}_{\mu\nu} = \frac{\partial}{\partial q_{\mu}^{\star}}\frac{\partial}{\partial q_{\nu}} \ln\left\langle\,\hat{Q}\,\middle|\,\hat{Q}\,\right\rangle \qquad \mathscr{H} = \frac{\left\langle\,\hat{Q}\,\middle|\,\underset{\sim}{H}\,\middle|\,\hat{Q}\,\right\rangle}{\left\langle\,\hat{Q}\,\middle|\,\hat{Q}\,\right\rangle}$$

Nuclear Interactions

Effective Interactions

Features

- ✔ describe groundstate properties of (light) nuclei
- ✔ can be used with Slater determinants

Problems

- ✘ don't saturate
- ✘ no momentum dependence, dynamical processes
- ✘ ambiquities – different interactions reproduce comparable groundstate properties

Realistic Interactions

Features

- ✔ reproduce N-N-phase-shifts and deuteron properties
- ✔ based on meson-exchange
- ✔ spin-orbit-, tensor- and momentum-dependent parts of interaction

Problems

- ✘ Slater determinants are not suited for hard-core potentials and tensor-interactions

Unitary Correlator

How to address the hard-core problem

- in the spirit of the Jastrow correlation functions suppress the relative wave-function of two nucleons at short distances

Unitary Correlator

- ✔ no normalization problems – can be used easily in dynamics
- ✔ allows construction of correlated operators

$$\left| \hat{Q} \right\rangle = \underset{\sim}{C} \left| Q \right\rangle$$

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

Correlated wave function

$$\left\langle \vec{X}, \vec{x} \middle| \underset{\sim}{C} \middle| \Phi \right\rangle = \left\langle \vec{X}, \vec{x} \middle| e^{-i\underset{\sim}{S}} \middle| \Phi \right\rangle = \exp\left\{ -\frac{1}{2} s'(x) - \frac{s(x)}{x} - s(x) \frac{\partial}{\partial x} \right\} \left\langle \vec{X}, \vec{x} \middle| \Phi \right\rangle$$

- ✔ correlator shifts the wave function in the relative coordinate out of the core region

Correlation as a coordinate transformation

define correlation functions R_+ and R_-

$$\int_x^{R_-(x)} \frac{dt}{s(t)} = -1 \,, \qquad \int_x^{R_+(x)} \frac{dt}{s(t)} = +1$$

correlated wavefunction using coordinate transformation

$$\left\langle \vec{X}, \vec{x} \middle| \underset{\sim}{C} \middle| \Phi \right\rangle = \frac{R_+(x) \sqrt{R_+{}'(x)}}{x} \left\langle \vec{X}, \frac{\vec{x}}{x} R_+(x) \middle| \Phi \right\rangle$$

Unitary Correlator

Particle Number Expansion

- correlated interaction has components of higher particle order
- in FMD only contributions up to second order are taken into account
- estimations of three-particle contributions by R. Roth

$$\hat{\underset{\sim}{B}} = \hat{\underset{\sim}{B}}^{[1]} + \hat{\underset{\sim}{B}}^{[2]} + \hat{\underset{\sim}{B}}^{[3]} + \dots$$

$$\hat{\underset{\sim}{B}}^{[1]} = \sum_{k,k'} \langle \, k \, | \, \underset{\sim}{C}^{\dagger} \underset{\sim}{B} \underset{\sim}{C} \, | \, k' \, \rangle \, \underset{\sim}{a}_{k}^{\dagger} \underset{\sim}{a}_{k'} = \sum_{k,k'} \langle \, k \, | \, \underset{\sim}{B} \, | \, k' \, \rangle \, \underset{\sim}{a}_{k}^{\dagger} \underset{\sim}{a}_{k'}$$

$$\hat{\underset{\sim}{B}}^{[2]} = \frac{1}{4} \sum_{\substack{k_1,k_2 \\ k_1',k_2'}} {}_a\langle \, k_1, k_2 \, | \, \underset{\sim}{C}^{\dagger} \underset{\sim}{B} \underset{\sim}{C} - \hat{\underset{\sim}{B}}^{[1]} \, | \, k_1', k_2' \, \rangle_a \, \underset{\sim}{a}_{k_1}^{\dagger} \underset{\sim}{a}_{k_2}^{\dagger} \underset{\sim}{a}_{k_2'} \underset{\sim}{a}_{k_1'}$$

Unitary Correlator

Correlated Potential

$$\hat{V}^{[2]}(x) = V(R_+(x))$$

Correlated Kinetic Energy

$$\hat{\underset{\sim}{T}}^{[1]} = \underset{\sim}{T} \qquad \hat{\underset{\sim}{T}}^{[2]} = \hat{\underset{\sim}{T}}_r^{[2]} + \hat{\underset{\sim}{T}}_{\vec{r}}^{[2]} + \hat{\underset{\sim}{T}}_{pot}^{[2]}$$

$$\left\langle \vec{X},\vec{x} \right| \hat{\underset{\sim}{T}}_r^{[2]} \left| \vec{X}',\vec{x}' \right\rangle = \frac{\overleftarrow{\partial}}{\partial x} \frac{\delta(\vec{X}-\vec{X}')\,\delta(\vec{x}-\vec{x}')}{2\mu_r^\star(x)} \frac{\overrightarrow{\partial}}{\partial x'}$$

$$\left\langle \vec{X},\vec{x} \right| \hat{\underset{\sim}{T}}_{\vec{r}}^{[2]} \left| \vec{X},\vec{x} \right\rangle = \frac{\overleftarrow{\partial}}{\partial \vec{x}} \frac{\delta(\vec{X}-\vec{X}')\,\delta(\vec{x}-\vec{x}')}{2\mu(x)} \frac{\overrightarrow{\partial}}{\partial \vec{x}'}$$

$$\frac{1}{2\mu_r^\star(x)} = \frac{1}{m}\left(\frac{1}{R_+'(x)^2} - \frac{x^2}{R_+(x)^2}\right), \qquad \frac{1}{2\mu(x)} = \frac{1}{m}\left(\frac{x^2}{R_+(x)^2} - 1\right)$$

$$\hat{\underset{\sim}{T}}_{pot}^{[2]} = \hat{U}^{[2]}(x) = \frac{1}{m}\frac{1}{R_+'(x)^2}\left(\frac{1}{2}\frac{R_+'''(x)}{R_+'(x)} - \frac{5}{4}\left(\frac{R_+''(x)}{R_+'(x)}\right)^2 + 2\frac{R_+''(x)}{xR_+'(x)}\right)$$

Evaluation of Matrix Elements

Gaussian Integrals

- Gaussian integrals can be evaluated analytically
- interactions are parametrized by Gaussians
- for analytical and numerical work it is important to find a compact form of the two-body Gaussian integral

$$G(|\vec{x}_1 - \vec{x}_2|) = \exp\left\{ -\frac{(\vec{x}_1 - \vec{x}_2)^2}{2\kappa} \right\}$$

$$\left\langle a_k \vec{b}_k, a_l \vec{b}_l \,\middle|\, \underset{\sim}{G} \,\middle|\, a_m \vec{b}_m, a_n \vec{b}_n \right\rangle = R_{km} R_{ln} \left(\frac{\kappa}{\alpha_{klmn} + \kappa} \right)^{3/2} \exp\left\{ -\frac{\vec{\rho}_{klmn}^{\,2}}{2(\alpha_{klmn} + \kappa)} \right\}$$

$$\alpha_{klmn} = \frac{a_k^\star a_m}{a_k^\star + a_m} + \frac{a_l^\star a_n}{a_l^\star + a_n}, \qquad \vec{\rho}_{klmn} = \frac{a_m \vec{b}_k^\star + a_k^\star \vec{b}_m}{a_k^\star + a_m} - \frac{a_n \vec{b}_l^\star + a_l^\star \vec{b}_n}{a_l^\star + a_n}$$

$$R_{km} = \left\langle a_k \vec{b}_k \,\middle|\, a_m \vec{b}_m \right\rangle, \qquad R_{ln} = \left\langle a_l \vec{b}_l \,\middle|\, a_n \vec{b}_n \right\rangle$$

- from this Gaussian integral, all matrix elements for two-body interactions are derived

Evaluation of Matrix Elements

Central Interaction

$$\left\langle \vec{X},\vec{x} \,\middle|\, \underset{\sim}{V} \,\middle|\, \vec{X},\vec{x} \right\rangle = V(x) = \sum_i \gamma_i G^i(x)$$

$$\left\langle a_k\vec{b}_k, a_l\vec{b}_l \,\middle|\, \underset{\sim}{V} \,\middle|\, a_m\vec{b}_m, a_n\vec{b}_n \right\rangle = \sum_i \gamma_i G^i_{klmn}$$

Tensor and Spin-Orbit Interaction

$$\underset{\sim}{V}_T = V_T(\underset{\sim}{x})\,\underset{\sim}{S}_{12} \qquad V_T(x) = \sum_i \gamma_i x^2 G^i(x) \qquad \underset{\sim}{V}_{LS} = V_{LS}(\underset{\sim}{x})\left(\underset{\sim}{\vec{x}} \times \frac{1}{i}\frac{\partial}{\partial \vec{x}}\right)\cdot \underset{\sim}{\vec{S}} \qquad V_{LS}(x) = \sum_i \gamma_i G^i(x)$$

$$\left\langle a_k\vec{b}_k\chi_k, a_l\vec{b}_l\chi_l \,\middle|\, \underset{\sim}{V}_T \,\middle|\, a_m\vec{b}_m\chi_m, a_n\vec{b}_n\chi_n \right\rangle = \left[3\left(\vec{\sigma}_{km}\cdot\vec{\rho}_{klmn}\right)\left(\vec{\sigma}_{ln}\cdot\vec{\rho}_{klmn}\right) - \left(\vec{\sigma}_{km}\cdot\vec{\sigma}_{ln}\right)\vec{\rho}^{\,2}_{klmn}\right]\sum_i \left(\frac{\kappa_i}{\alpha_{klmn}+\kappa_i}\right)^2 G^i_{klmn}$$

$$\left\langle a_k\vec{b}_k\chi_k, a_l\vec{b}_l\chi_l \,\middle|\, \underset{\sim}{V}_{LS} \,\middle|\, a_m\vec{b}_m\chi_m, a_n\vec{b}_n\chi_n \right\rangle = \left(\vec{\rho}_{klmn}\times\vec{\pi}_{klmn}\right)\cdot\vec{S}_{klmn}\sum_i \gamma_i \left(\frac{\kappa_i}{\alpha_{klmn}+\kappa_i}\right) G^i_{klmn}$$

Evaluation of Matrix Elements

Correlated Kinetic Energy

$$\frac{1}{2\mu(x)} \cong \sum_i \gamma_i\, G^i(x), \qquad \frac{1}{2\mu_r^\star(x)} \cong \sum_i \gamma_i\, x^2\, G^i(x)$$

$$\left\langle a_k \vec{b}_k, a_l \vec{b}_l \,\middle|\, \underset{\sim}{\hat{T}}{}_{\vec{r}}^{[2]} \,\middle|\, a_m \vec{b}_m, a_n \vec{b}_n \right\rangle \cong$$

$$\sum_i \gamma_i \left[\vec{\pi}_{klmn}^{\,2} - \frac{\theta_{klmn}}{2(\alpha_{klmn}+\kappa_i)} (\vec{\rho}_{klmn} \cdot \vec{\pi}_{klmn}) + \frac{\theta_{klmn}}{4(\alpha_{klmn}+\kappa_i)^2} \vec{\rho}_{klmn}^{\,2} + \frac{3}{4} \left(\lambda_{klmn} - \frac{\theta_{klmn}}{\alpha_{klmn}+\kappa_i} \right) \right] G^i_{klmn}$$

$$\left\langle a_k \vec{b}_k, a_l \vec{b}_l \,\middle|\, \underset{\sim}{\hat{T}}{}_{r}^{[2]} \,\middle|\, a_m \vec{b}_m, a_n \vec{b}_n \right\rangle \cong$$

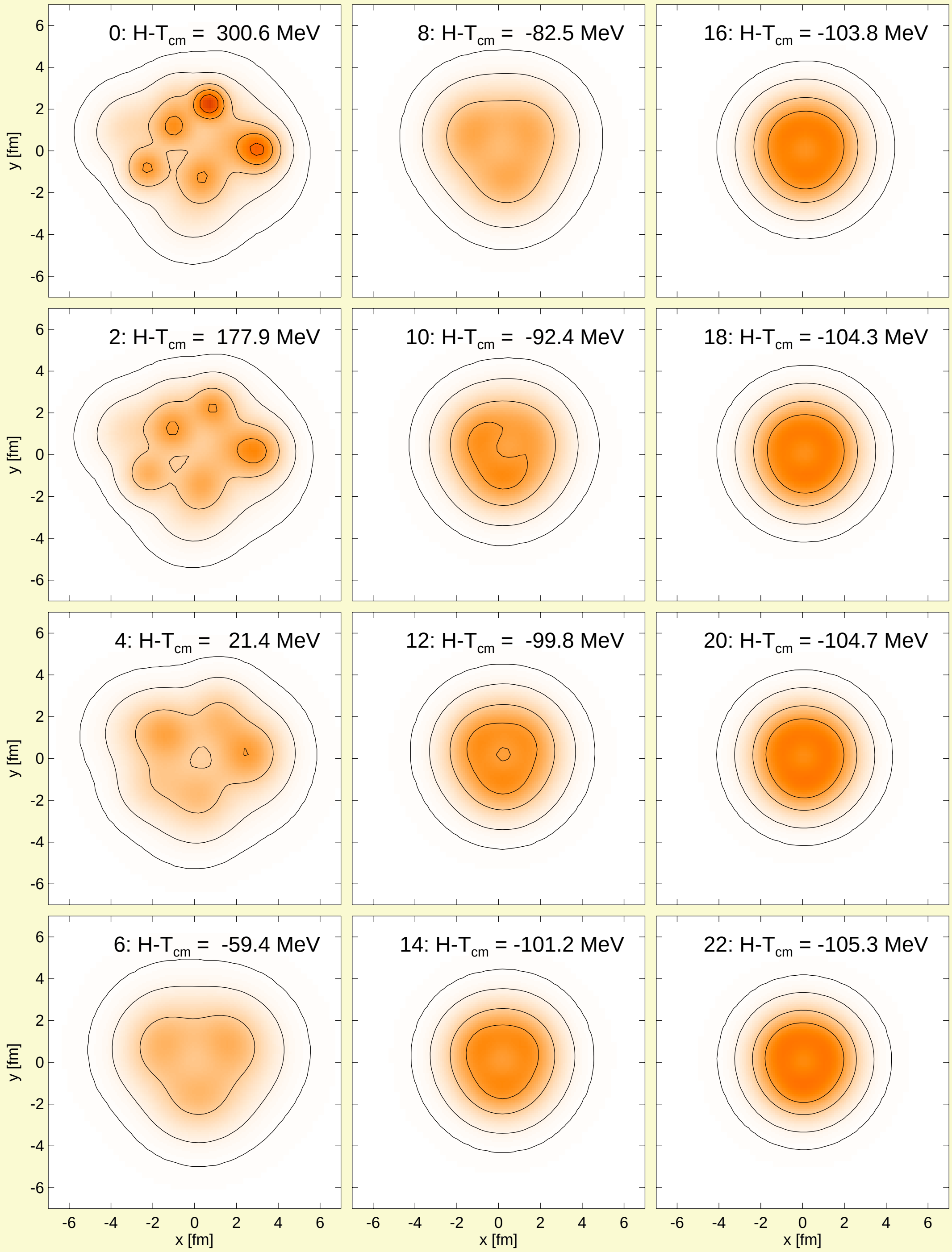
$$\sum_i \gamma_i \left[\left(\frac{\kappa_i}{\alpha_{klmn}+\kappa_i} \right)^2 \times \left((\vec{\rho}_{klmn} \cdot \vec{\pi}_{klmn})^2 - \frac{\beta_{klmn}}{2(\alpha_{klmn}+\kappa_i)} (\vec{\rho}_{klmn} \cdot \vec{\pi}_{klmn}) \vec{\rho}_{klmn}^{\,2} + \frac{\theta_{klmn}}{4(\alpha_{klmn}+\kappa_i)^2} \vec{\rho}_{klmn}^{\,4} \right) \right.$$

$$+ \frac{\alpha_{klmn}\kappa_i}{\alpha_{klmn}+\kappa_i} \left(\vec{\pi}_{klmn}^{\,2} - \frac{\beta_{klmn}}{2(\alpha_{klmn}+\kappa_i)} (\vec{\rho}_{klmn} \cdot \vec{\pi}_{klmn}) + \frac{\theta_{klmn}}{4(\alpha_{klmn}+\kappa_i)^2} \vec{\rho}_{klmn}^{\,2} \right)$$

$$- 2 \left(\frac{\kappa_i}{\alpha_{klmn}+\kappa_i} \right)^2 \left(\frac{\theta_{klmn}}{\alpha_{klmn}+\kappa_i} \vec{\rho}_{klmn}^{\,2} - \beta_{klmn} (\vec{\rho}_{klmn} \cdot \vec{\pi}_{klmn}) \right)$$

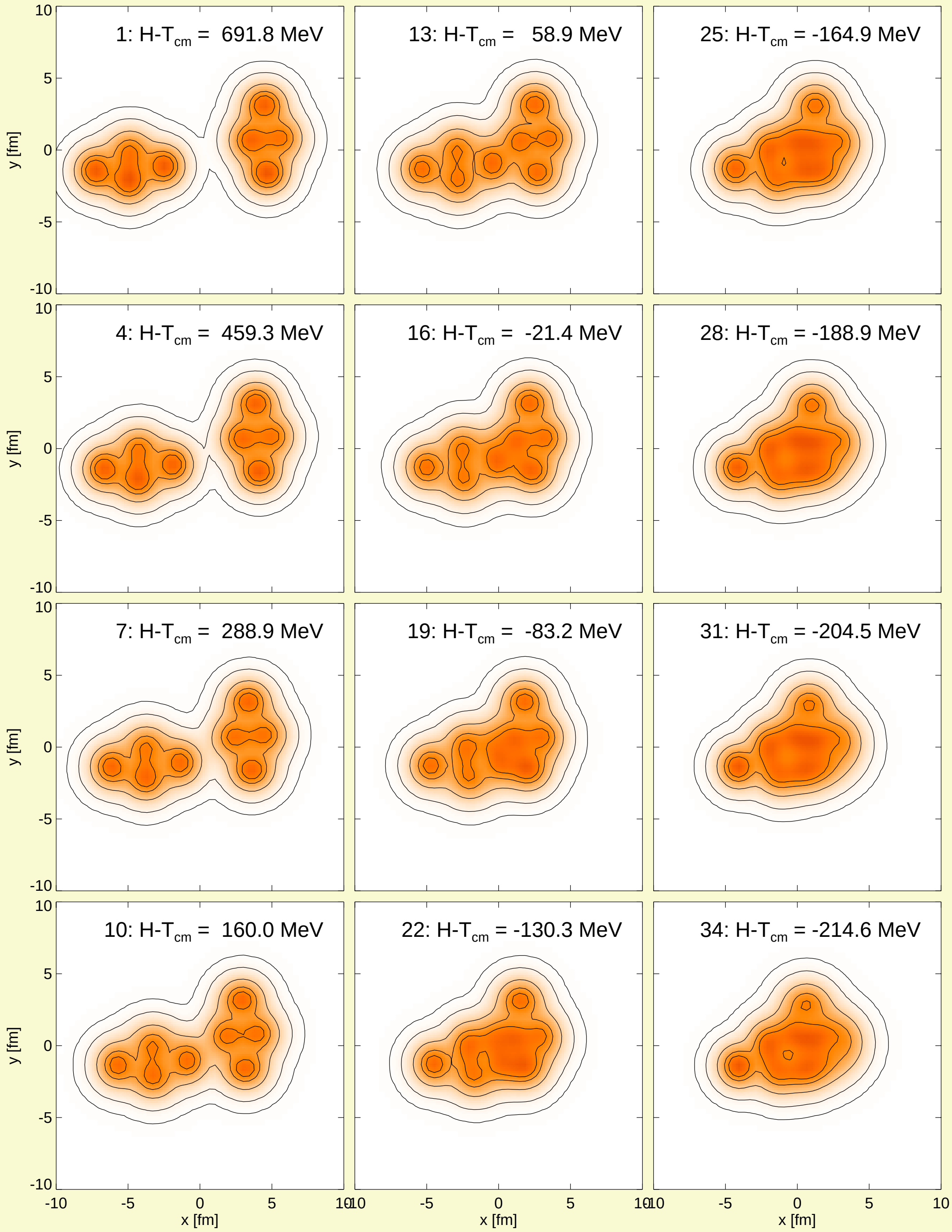
$$\left. + \frac{1}{4} \left(\lambda_{klmn} - \frac{\theta_{klmn}}{\alpha_{klmn}+\kappa_i} \right) \left(\left(\frac{\kappa_i}{\alpha_{klmn}+\kappa_i} \right)^2 \vec{\rho}_{klmn}^{\,2} + 3 \frac{\alpha_{klmn}\kappa_i}{\alpha_{klmn}+\kappa_i} \right) + 3\theta_{klmn} \left(\frac{\kappa_i}{\alpha_{klmn}+\kappa_i} \right)^2 \right] G^i_{klmn}$$

Searching the Ground State



- Minimization of ground state energy of ^{16}O with quasi-Newton-method

“frictional cooling”



- finding a starting point for ^{40}Ca groundstate by collision of two ^{20}Ne with frictional cooling

Probing the Unitary Correlator

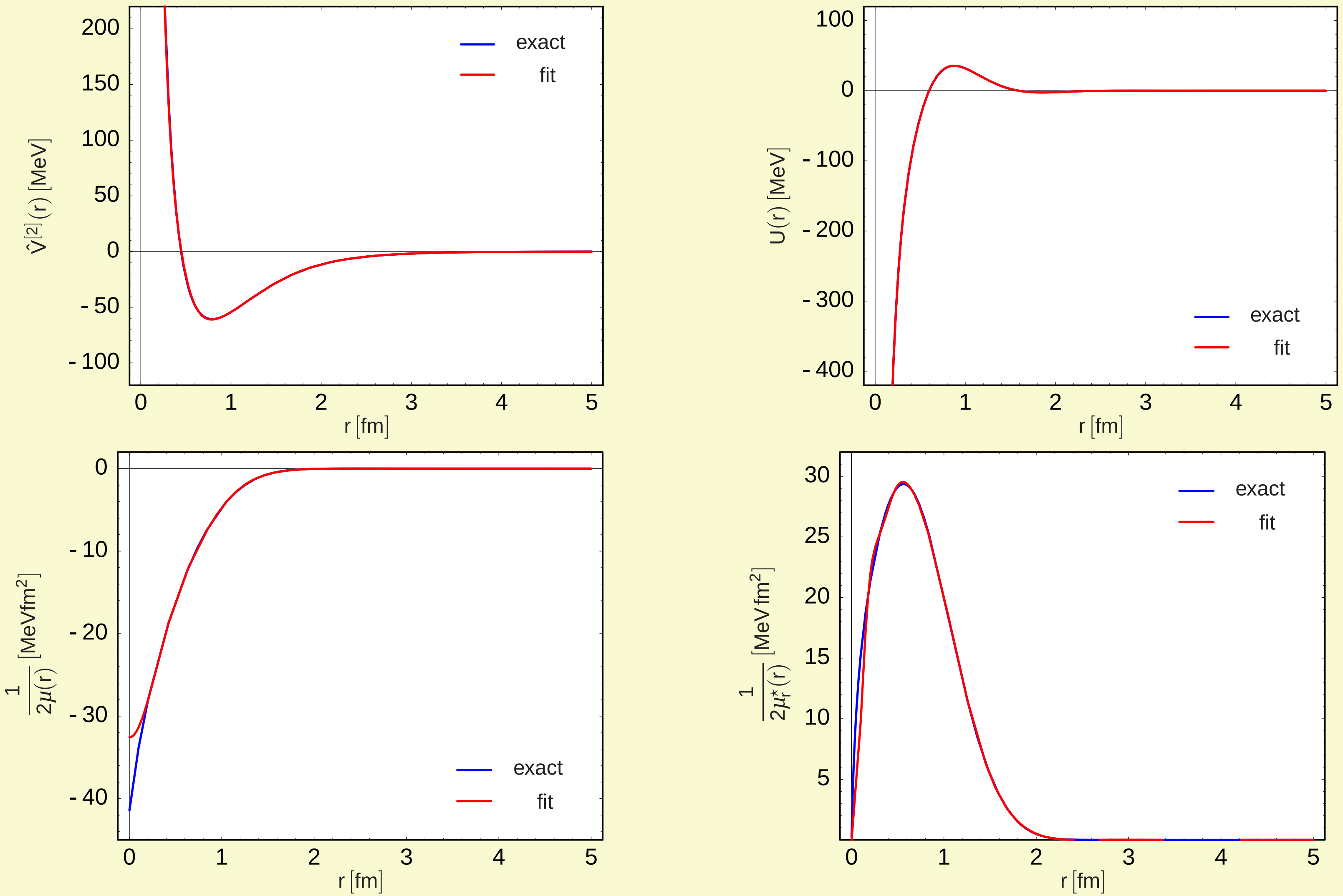
Malfiet V Interaction

- pure Wigner potential with a core
- used as a benchmark for many-body models
- overbinds strongly for heavy nuclei

Afnan-Tang S3M interaction

- central potential with spin- and isospin-dependence to reproduce deuteron and triton properties
- additional repulsive term added in odd channels, gives reasonable results for heavier nuclei

Malfliet V interaction

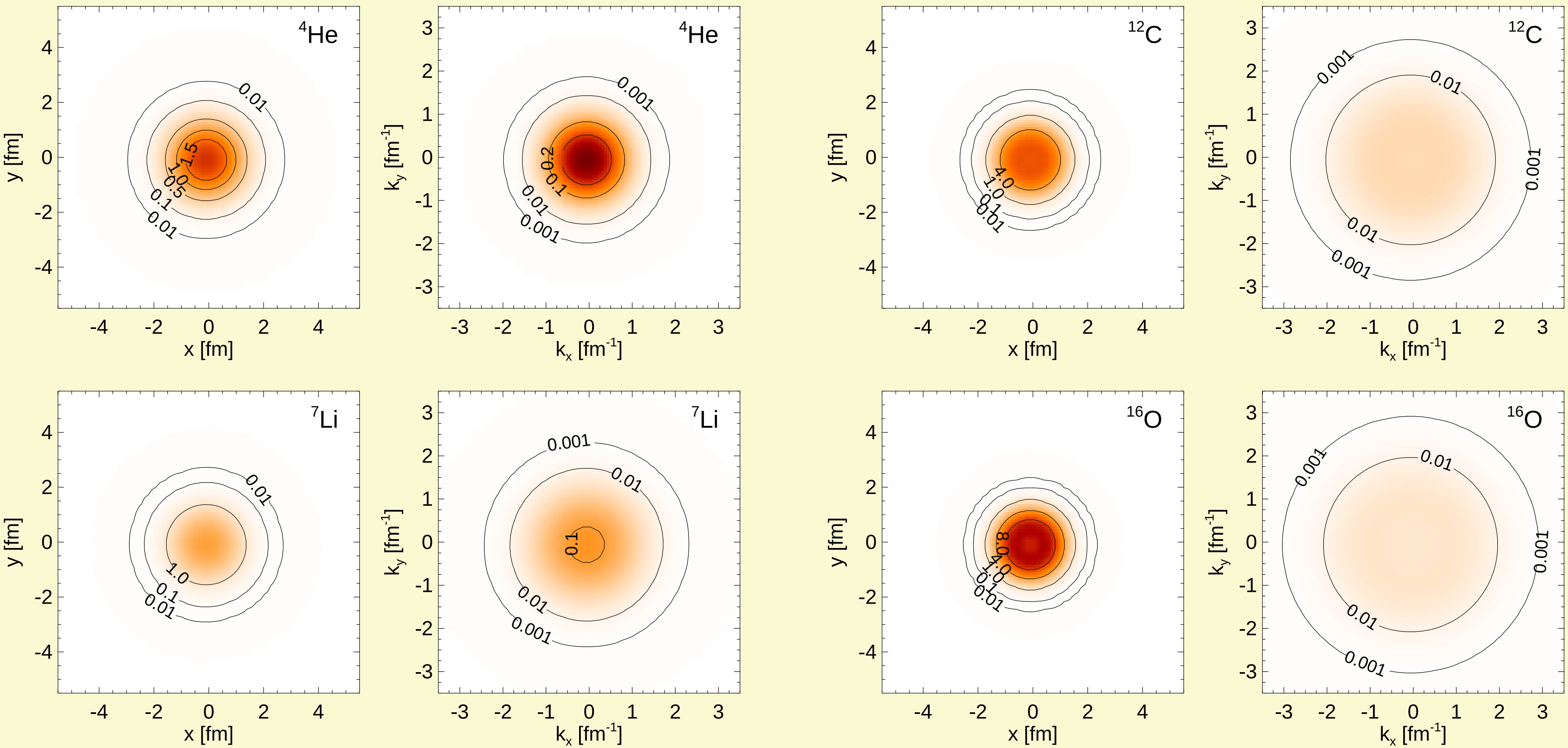


Malfliet V results

	FMD correlated			*FMD uncorrelated*			*SVM*	*VMC*
	$\langle \hat{\underset{\sim}{T}}^{[2]}_{int} \rangle$	$\langle \hat{\underset{\sim}{V}}^{[2]} \rangle$	E_B	$\langle \underset{\sim}{T}_{int} \rangle$	$\langle \underset{\sim}{V} \rangle$	E_B	E	E
^{3}H	35.13	-41.62	-6.49	30.04	-23.56	6.48	-8.25	-8.27
^{4}He	75.60	-106.09	-30.49	60.34	-50.34	10.00	-31.36	-31.3
^{5}He	127.62	-170.07	-42.45	103.95	-86.65	17.30	-43.48	-42.98
^{6}He	193.56	-259.55	-65.99	156.78	-132.36	24.42	-66.30	-66.34
^{6}Li	198.46	-264.52	-66.06	161.53	-137.76	23.76		
^{7}Li	290.96	-395.34	-104.38	235.04	-208.35	26.69	-83.40	
^{8}Be	392.63	-551.11	-158.48	312.26	-284.12	28.14		
^{12}C	942.50	-1500.01	-557.51	698.02	-688.12	9.90		
^{16}O	1673.30	-2952.07	-1278.77	1154.30	-1202.54	-48.24		-1194

- estimation of three-body contributions gives only small values, even for ^{16}O
- very significant increase in binding energy due to correlator
- good agreement with other calculations

Malfliet V results

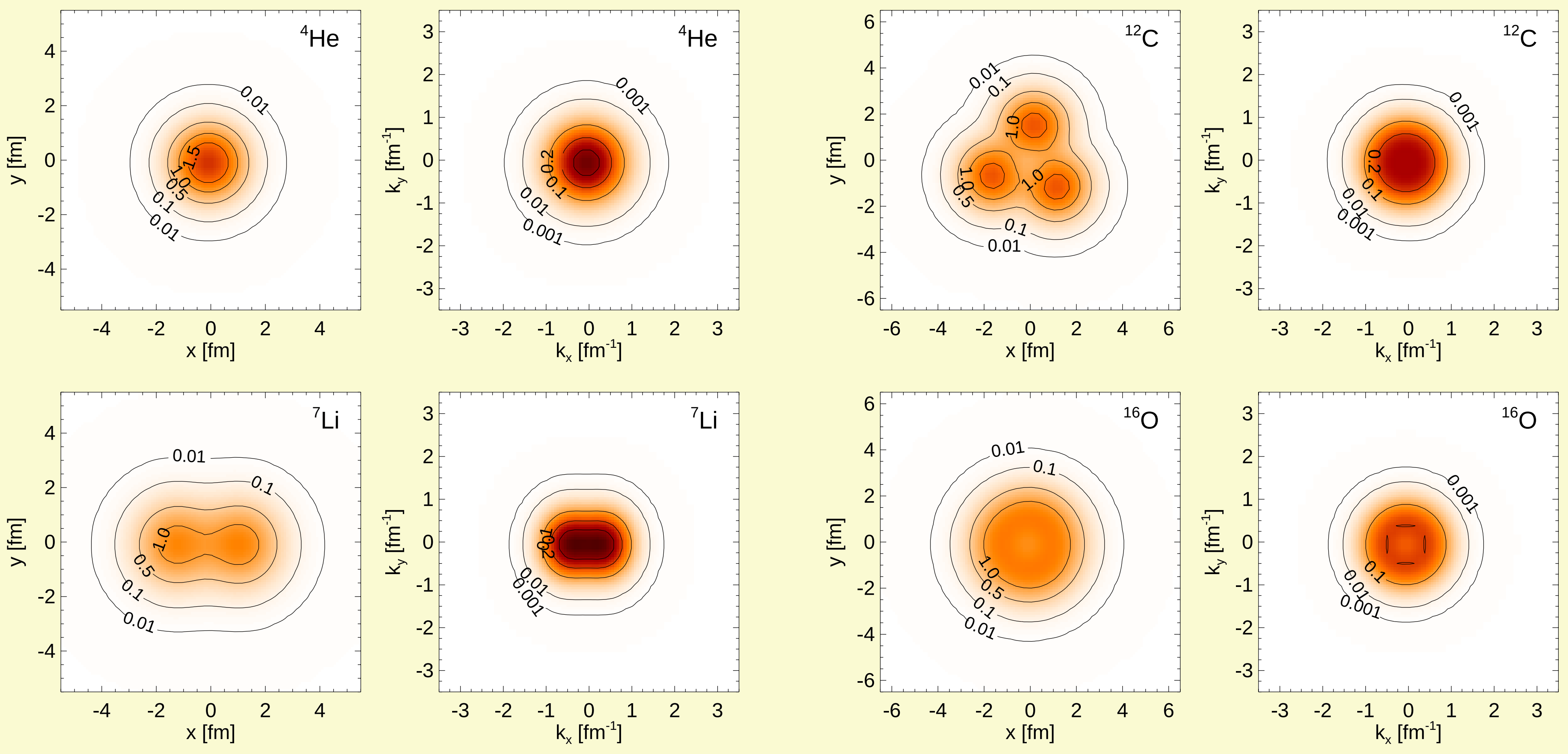


Afnan-Tang S3M results

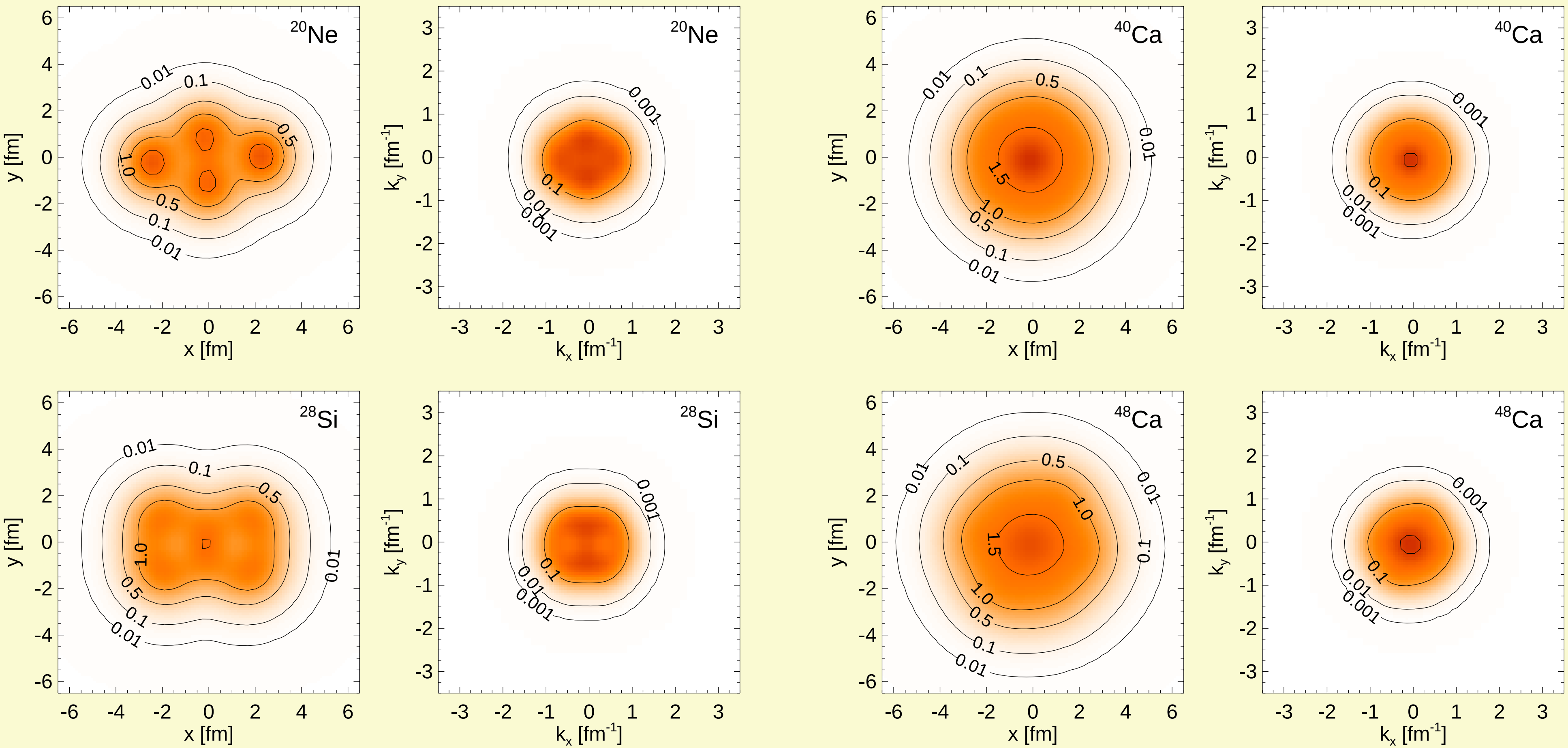
	FMD correlated			*FMD uncorrelated*			*VJ*	*FHNC*	*CBF*
	$\langle \underset{\sim}{\hat{T}}_{int}^{[2]} \rangle$	$\langle \underset{\sim}{\hat{V}}^{[2]} \rangle$	E_B	$\langle \underset{\sim}{T}_{int} \rangle$	$\langle \underset{\sim}{V} \rangle$	E_B	E_B	E_B	E_B
^{4}He	78.5	-106.4	-27.9	59.6	-54.1	5.5	-24.2		
^{6}He	88.9	-100.9	-12.0	73.0	-59.6	13.4			
^{7}Li	124.8	-145.9	-21.1	101.2	-85.3	17.0			
^{12}C	268.5	-329.8	-61.3	212.2	-181.9	30.3			-25.8
^{16}O	381.0	-488.9	-107.9	296.7	-266.7	29.1	-107.7	-105.3	-96.3
^{20}Ne	502.5	-630.0	-127.5	391.4	-341.6	49.8			
^{28}Si	705.4	-896.1	-190.7	549.3	-494.6	54.8			
^{40}Ca	1108.7	-1443.6	-334.9	848.5	-778.7	69.8	-335.6	-350.0	-346.0
^{48}Ca	1298.4	-1636.1	-337.7	1007.4	-896.4	111.0			-363.4

- correlator gives binding
- good agreement with other methods

Afnan-Tang S3M results



Afnan-Tang S3M results



Improvements for Nuclear Structure

one-particle state

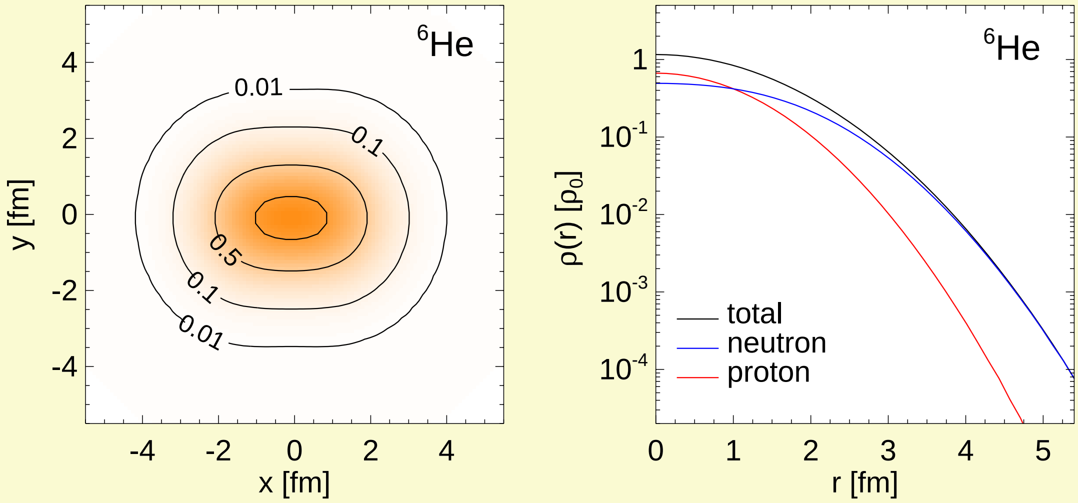
- superposition of two or three Gaussian wave packets per one-particle state
- should describe exponential tail of neutron density in halo nuclei
- tested with ATS3M He isotopes

many-particle state

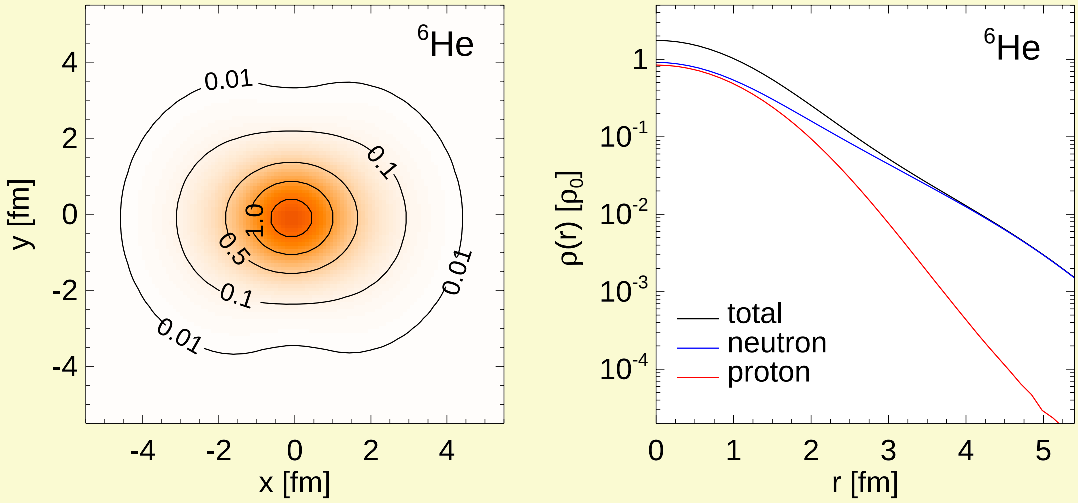
- multiconfiguration calculations with FMD
- address intrinsically deformed ground states
- describe long-range correlations beyond the mean-field
- tested with ATS3M ^{12}C

Halo Nuclei

One gaussian per one-particle state



Two gaussians per one-particle state



- ✔ exponential tail of neutron density in the surface
- ✔ α-core reappears
- ✔ gained 3.5 MeV in binding energy

Multiconfiguration FMD

diagonalize Hamiltonian in a set

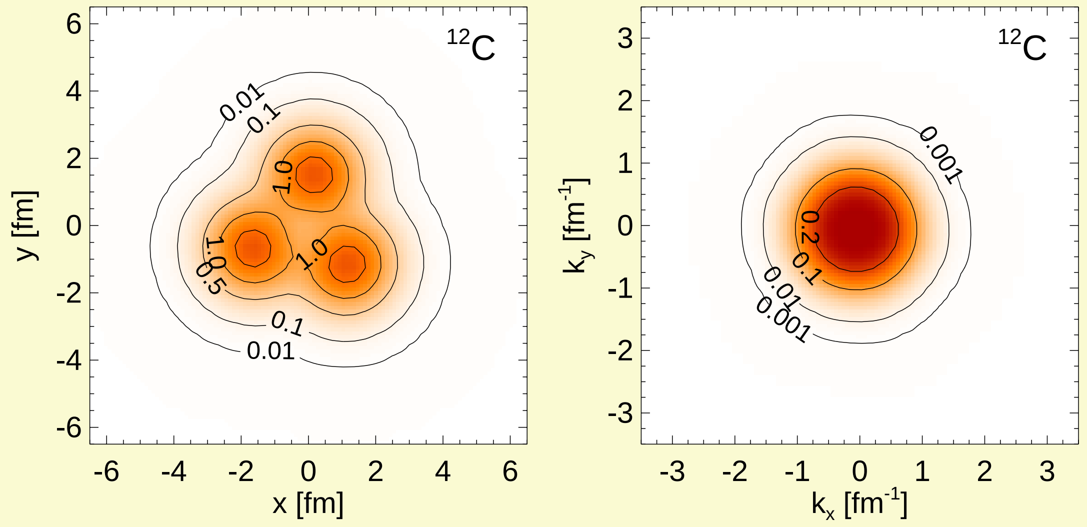
$$\left\{ \left| \hat{Q}^i \right\rangle \right\}$$

of (nonorthogonal) FMD states, leads to generalized eigenvalue problem

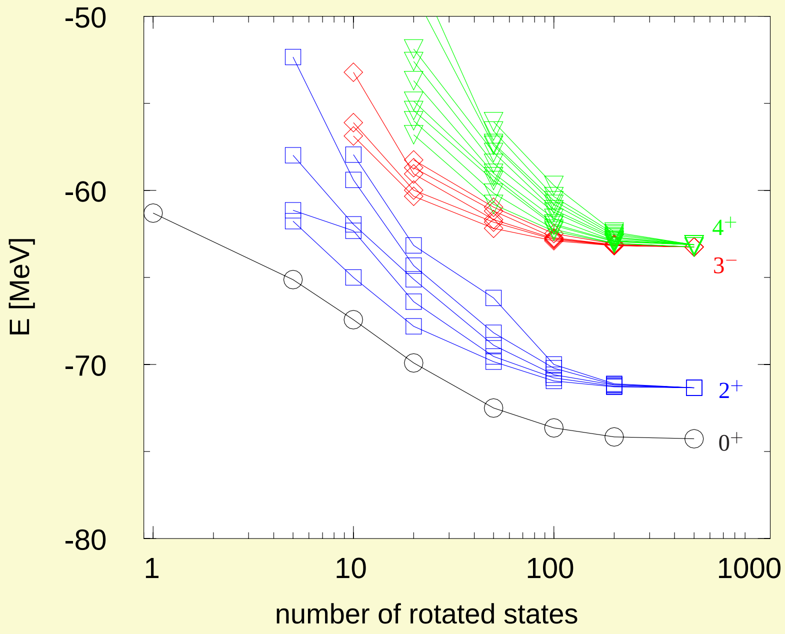
$$\sum_j \left\langle \hat{Q}^i \right| \underset{\sim}{H} \left| \hat{Q}^j \right\rangle c_j^\alpha = E^\alpha \sum_j \left\langle \hat{Q}^i \middle| \hat{Q}^j \right\rangle c_j^\alpha$$

Multiconfiguration FMD

FMD groundstate of ^{12}C is intrinsically deformed



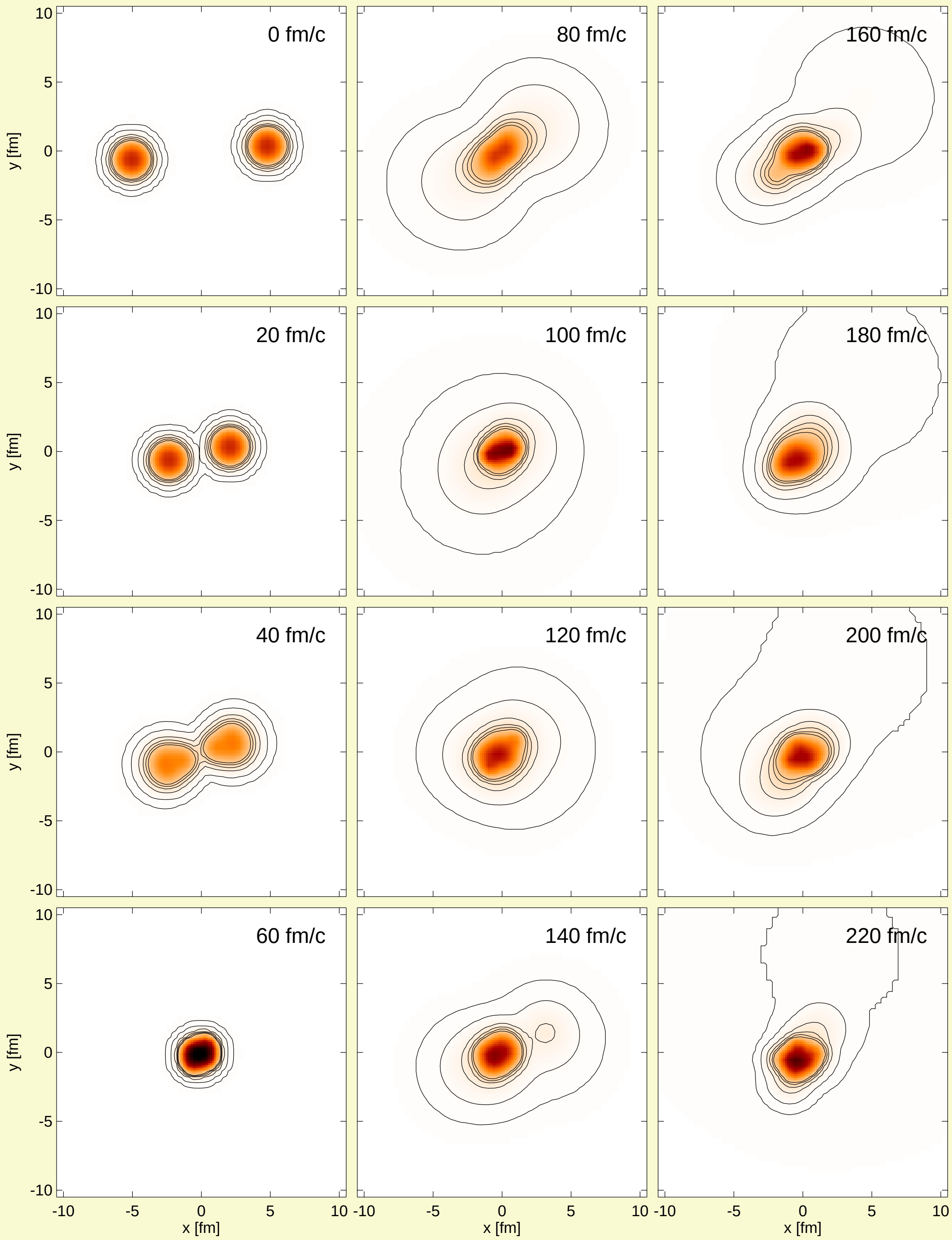
diagonalization in a set of randomly rotated states



- ✔ big increase in binding energy
- ✔ eigenstates of angular momentum and parity states
- ✔ spectrum of rotational excitations

MTV reactions

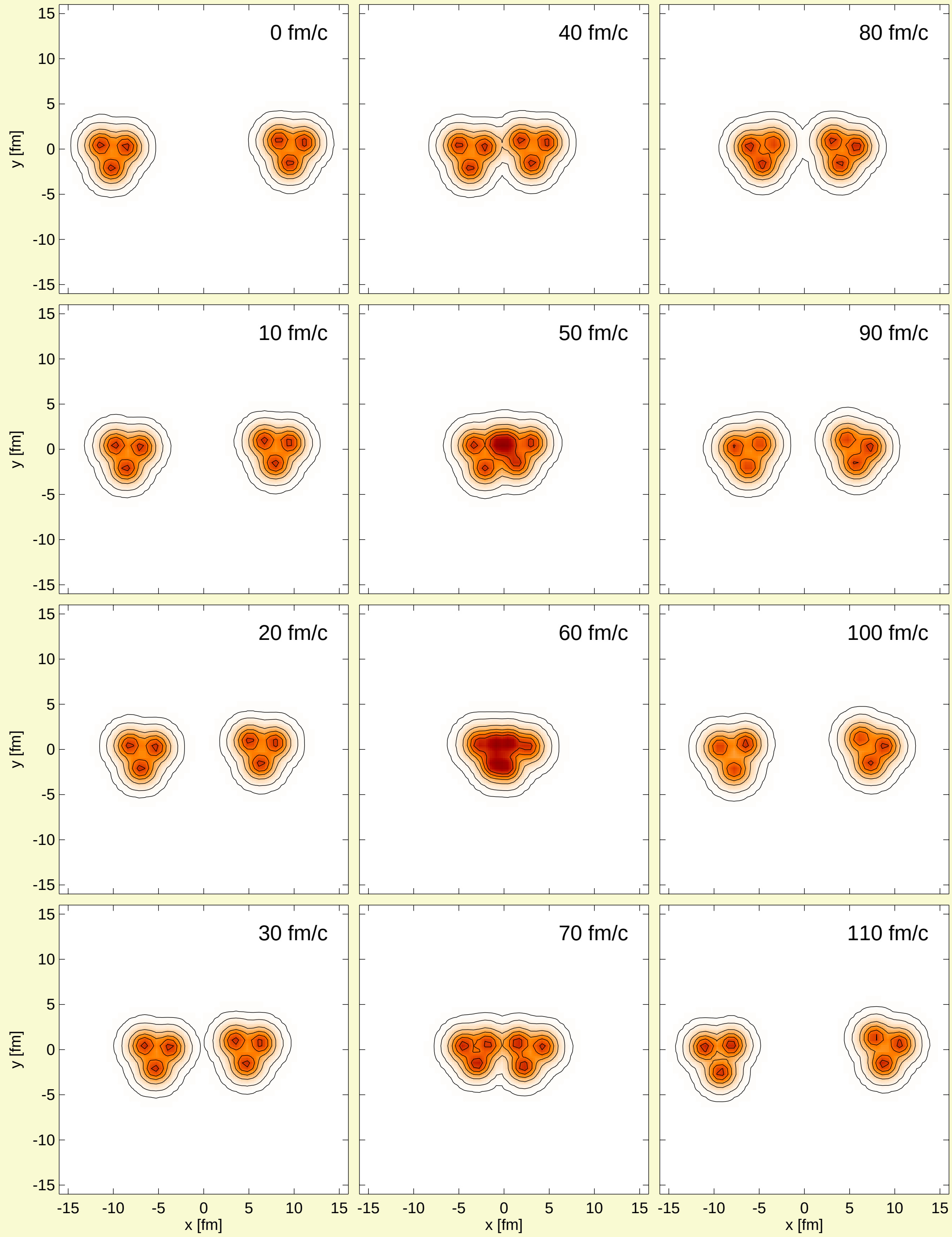
^{12}C on ^{12}C at $E_{lab} = 35\,A\,\mathrm{MeV}$ and $b = 1.0$ fm



▶ MTV-Potential leads to *fusion*

ATS3M reactions

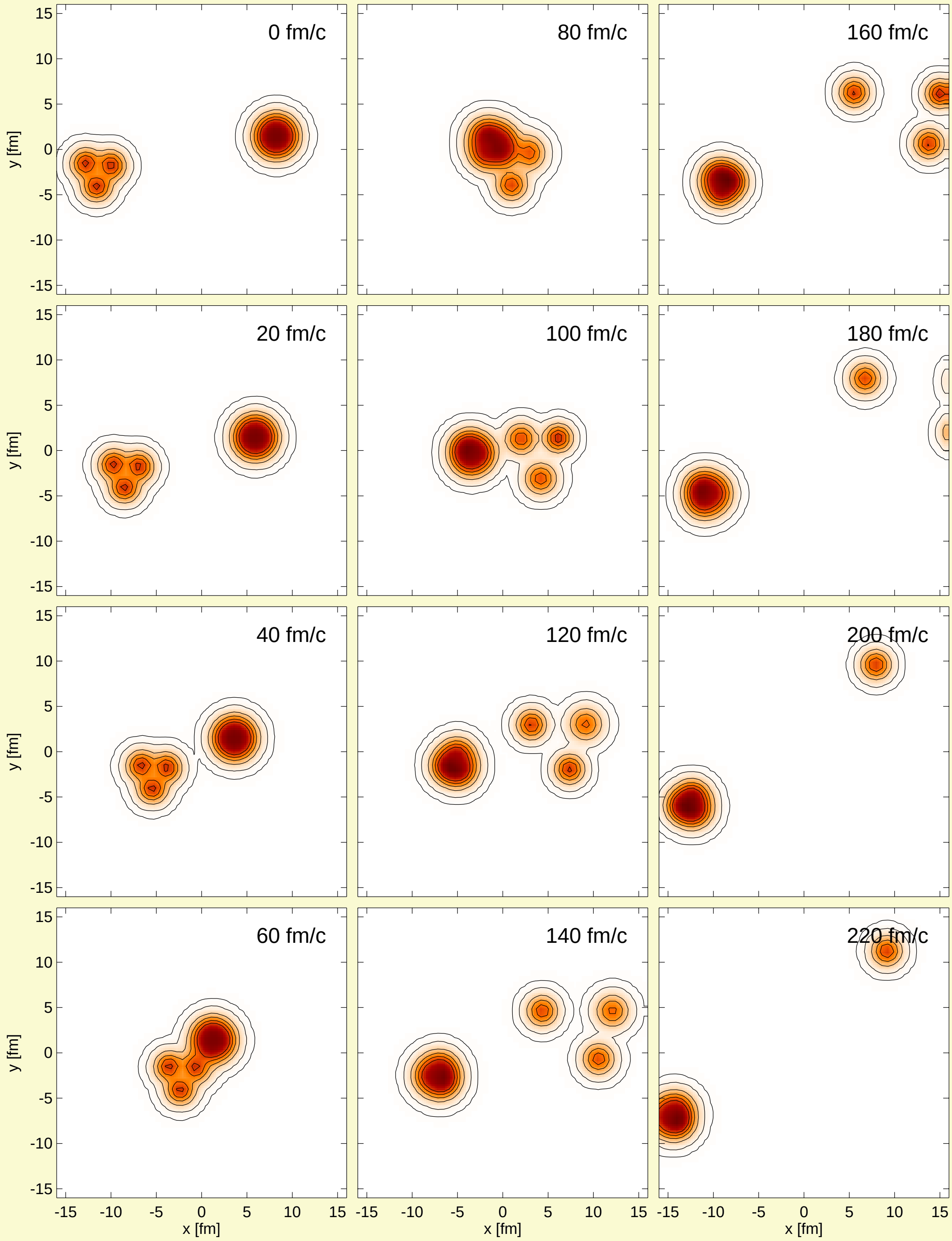
^{12}C on ^{12}C at $E_{lab} = 50\,A\,$MeV and $b = 0.5$ fm



- ATS3M-Potential is *transparent* in most cases

ATS3M reactions

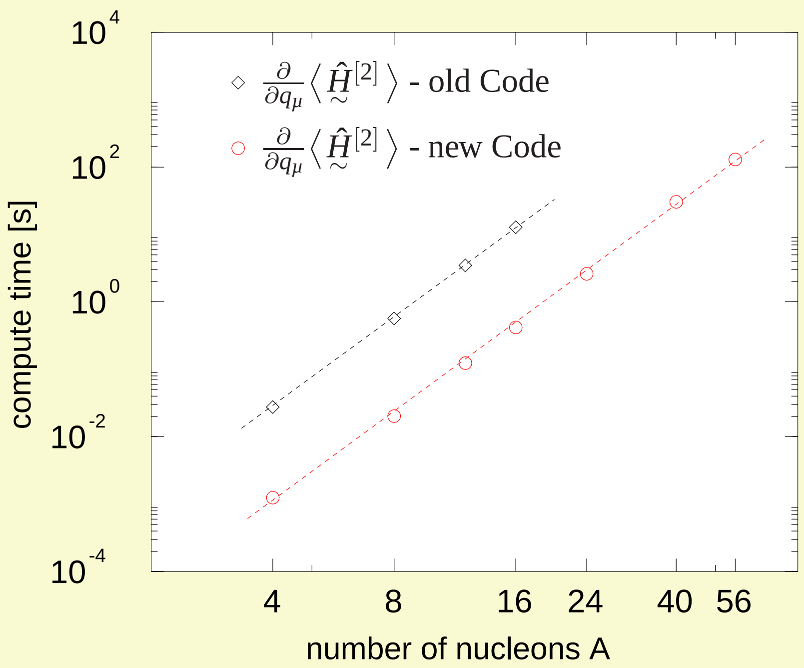
^{12}C on ^{16}C at $E_{lab} = 35\,A\,$MeV and $b = 4.0$ fm



- ATS3M-Potential allows *fragmentation* only in peripheral collisions and with preformed fragments

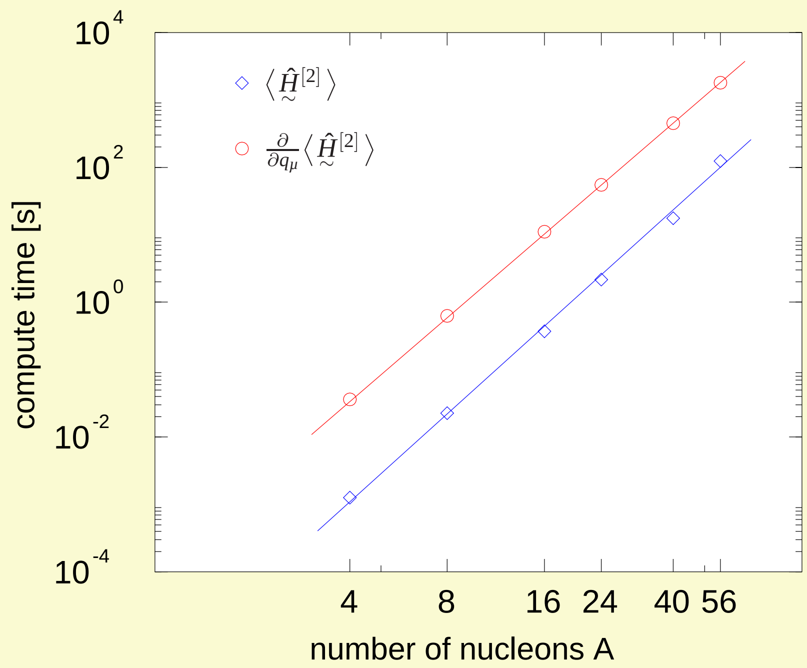
Benchmarks

old and *new* FMD code in comparision



- increase of performance for matrix elements by an order of magnitude
- memory consumption reduced by an order of magnitude

expectation values and *gradients*



- compute time increases with A^4
- gradients are much more expensive than expectation values

Summary and Outlook

New FMD code

- ✔ completely rewritten from scratch, platform independent, C and Fortran
- ✔ matrix elements for $\underset{\sim}{V}$, $\underset{\sim}{V}_T$, $\underset{\sim}{V}_{LS}$, $\underset{\sim}{V}_3$ and correlated kinetic energy $\underset{\sim}{\hat{T}}$
- ✔ allows superposition of Gaussians in the single-particle state
- ✔ allows multiconfiguration calculations
- ✔ speed and memory consumption improvements

Realistic Interactions

- ► hard-core central interactions can be treated with the Unitary Correlator
- ► Spin-Orbit- and Tensor-Interactions included in code
- ► adapted Spin-Orbit- and Tensor-Correlators are necessary

Improvements of the One-Particle States

- ► use of several Gaussians per one-particle state describe exponential tail of nuclear density – halo nuclei

Multiconfiguration Calculations

- ► projection on parity and angular momentum eigenstates is possible
- ► alternatively use multiconfiguration FMD to diagonalize Hamiltonian in basis of rotated and reflected FMD state
- ► multiconfiguration calculations with set of FMD states (nonorthogonal basis) can be used to improve FMD solutions
- ► a scheme for choosing the optimal basis states has to be developed

Summary and Outlook

Nuclear Structure

- realistic interactions induce short and long range correlations
  - mean-field – several Gaussians
  - short range – unitary correlator
  - long range – configuration mixing
- systematic study of nuclear structure including neutron-rich nuclei using the flexible nature of FMD states with compact core states, wide halo states, no model assumptions about core and halo, configuration mixing to include many-body correlations, pairing
- either effective interactions as used in other models or realistic interactions using unitary correlator
- tensor- and spin-orbit correlators are the topic of present investigations