Realistic Interactions and Configuration Mixing

in

FMD

H. Feldmeier, Thomas Neff, R. Roth, J. Schnack

Overview

FMD Model

- The FMD model
- Multifragmentation in FMD

Realistic Interactions

- Effective vs. Realistic interactions
- The Unitary Correlator Operator Method
- Groundstate results for the ATS3M Interaction

Configuration Mixing

- Multiconfiguration Calculations
- Quantum Branching

The FMD model

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

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

Dynamics

Variational Principle

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

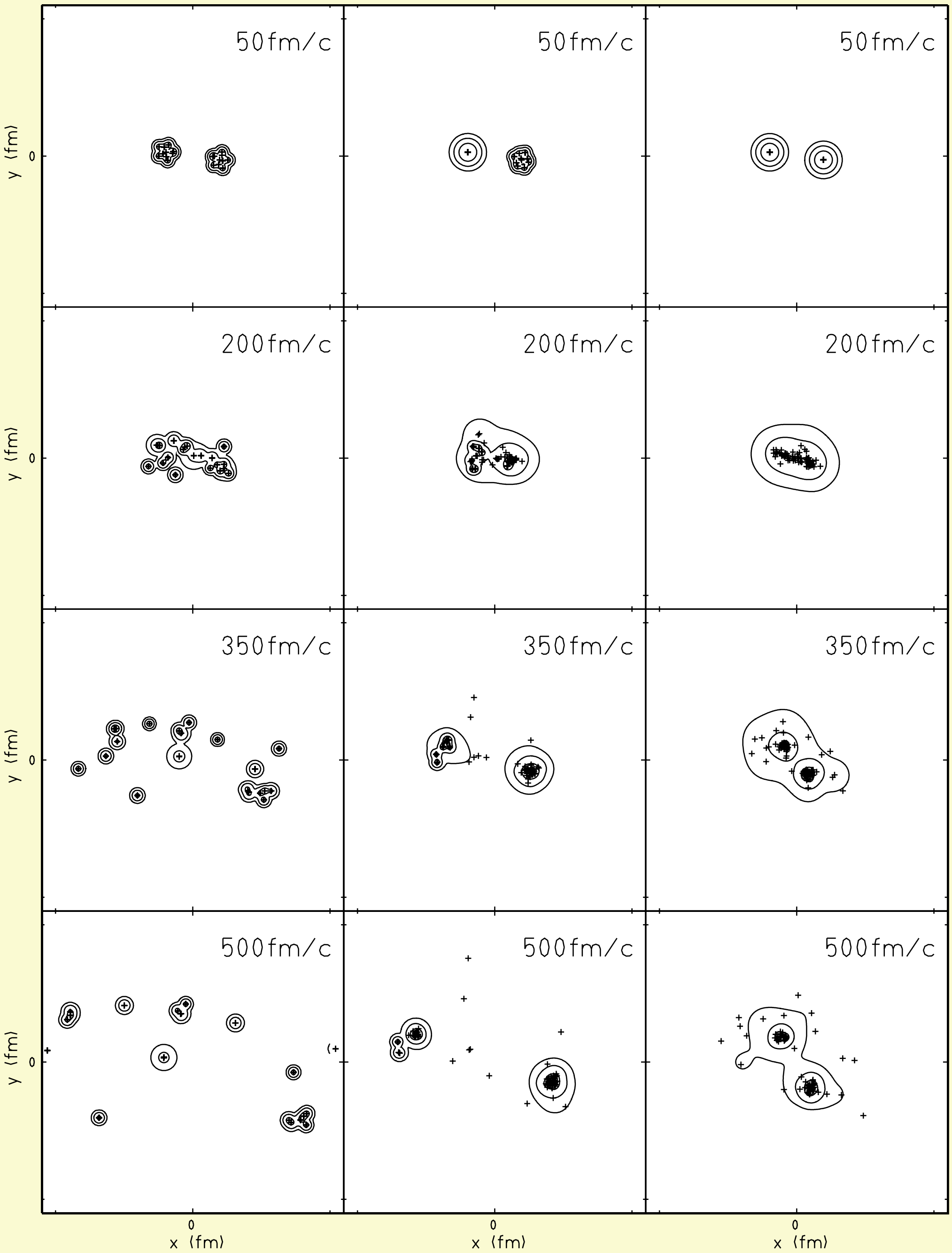
Equations of motion

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

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

Multifragmentation in FMD

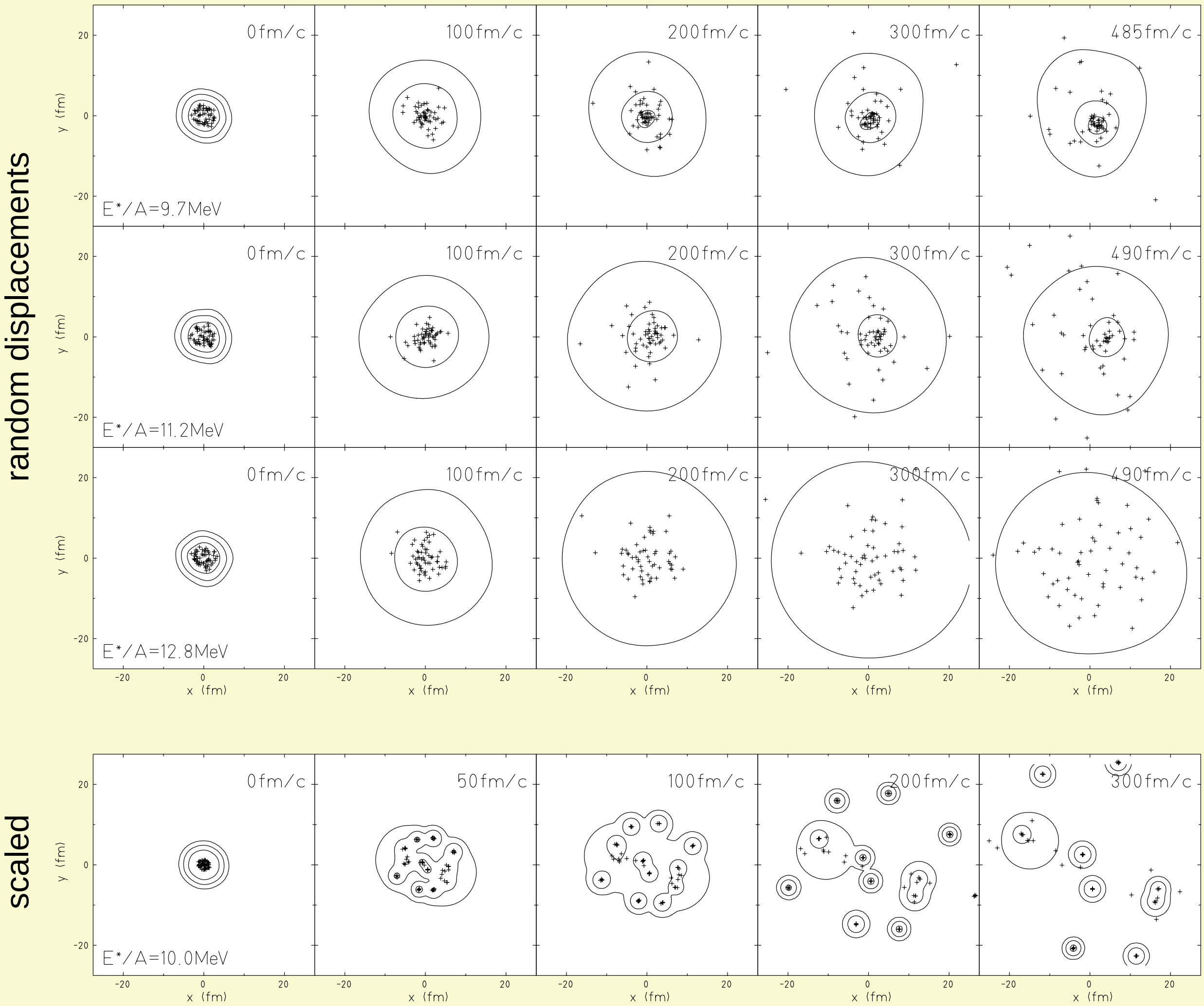
^{40}Ca on ^{40}Ca at $E_{lab} = 35\,A\,$MeV and $b = 2.75$ fm



- different configurations with very similar properties show strongly different behavior regarding multifragmentation
- in reaction dynamics initial correlations between nucleons play an important role and tend to survive during the collision process

Multifragmentation in FMD

Decay of excited Nuclei



- randomly excited states decay by evaporation of nucleons
- depending on the strength of the excitation a smaller or bigger residue remains
- excitations which do not completely destroy the spatial correlations between the nucleons lead to multifragmentation

Nuclear Interactions

Effective Interactions

Features

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

Problems

- don’t saturate for bigger nuclei
- ambiguities – 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 potentials with repulsive core and tensor parts

Unitary Correlator

How to address the core

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

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

Unitary Correlator

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

$$\left| \hat{Q} \right\rangle = \underset{\sim}{C} \left| Q \right\rangle, \qquad \hat{B} = \underset{\sim}{C}^\dagger \underset{\sim}{B} \underset{\sim}{C}$$

- correlated kinetic energy gives momentum-dependent and potential like two-body contributions

Correlation as a coordinate transformation

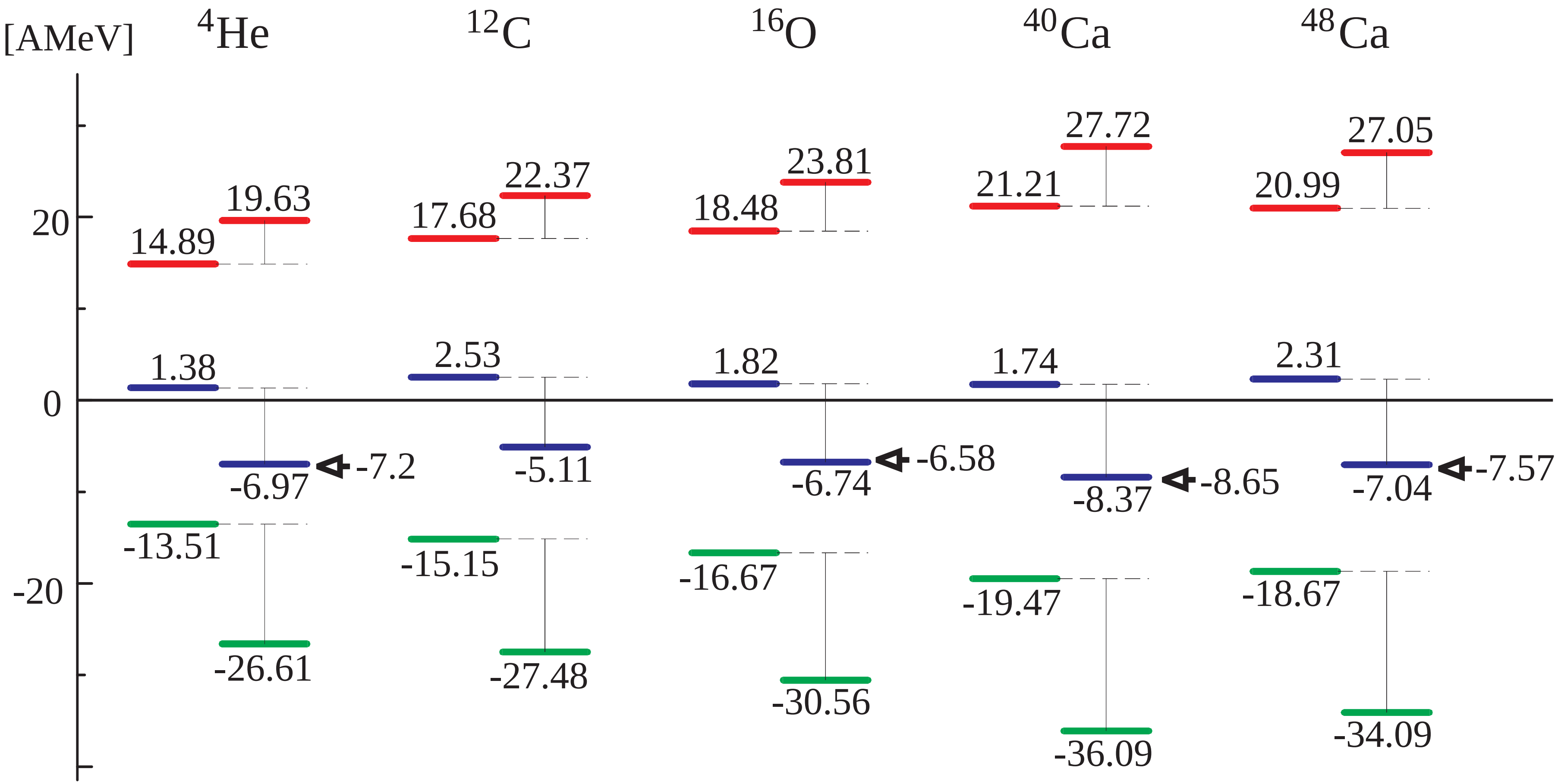
define correlation functions R_+ and R_-

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

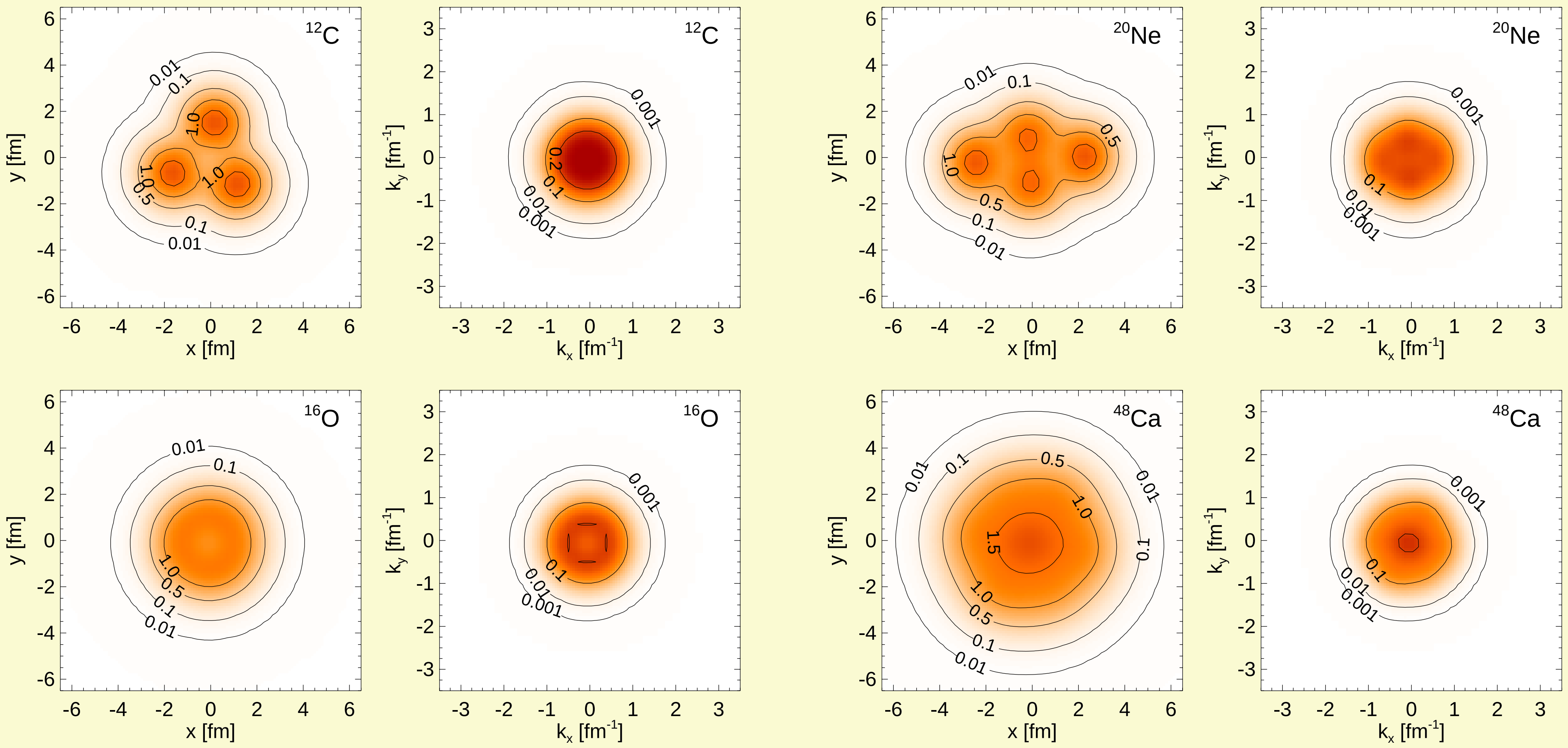
correlated wavefunction using coordinate transformation

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

Afnan-Tang S3M results



Afnan-Tang S3M results



Multiconfiguration Calculations

Improve FMD description

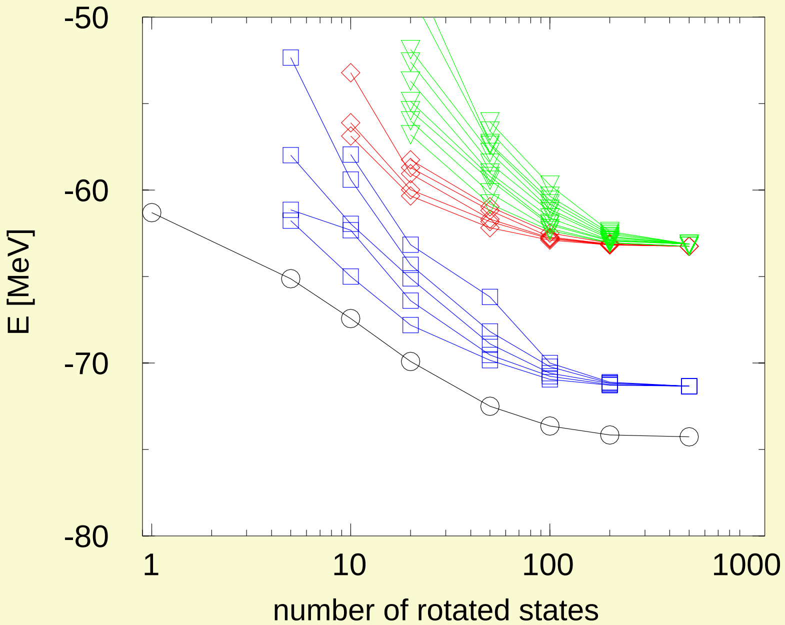
- address intrinsically deformed ground states
- describe long-range correlations beyond the mean-field

Multiconfiguration FMD

diagonalize Hamiltonian in a set $\{|\hat{Q}^i\rangle\}$ of (nonorthogonal) FMD states, leads to generalized eigenvalue problem

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

diagonalization in a set of randomly rotated ^{12}C FMD states



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

Ideas about Quantum Branching

- Multiconfigration calculations show that the exact state is a superposition of many FMD states
- Dynamical calculations (only central interactions up to now) with shell-model like groundstates which show no multifragmentation indicate that there is a necessity for quantum branching. A better description of the state should also have components with a clustered structure. These components can lead to multifragmentation.
- Therefore allow many configurations for the dynamical description

- Quantum Branching should be derived from the TDVP

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

- if $\big| \hat{Q}(t) \big\rangle$ is the exact solution no branching should happen
- the branching to another trajectory should be determined by the perturbation operator

$$i \sum_{\nu} \dot{q}_{\nu} \frac{\partial}{\partial q_{\nu}} - \underset{\sim}{H}$$

which describes the difference between the FMD and the exact time-evolution

Summary

Fermionic Molecular Dynamics

Pauli Principle, Gaussian Wave Packets, TDVP

Fragmentation in FMD

importance of initial many-body correlations,
dependence on interactions and structure of states

ambiguities in phenomenological interactions, therefore start from

Realistic Interactions in FMD

central correlators for short-range repulsion work well,
tensor correlator is under investigation

$$\underset{\sim}{C}_{Tensor} = \exp\left\{ -s(x) \left(3(\vec{\sigma}_1 \cdot \vec{x})(\vec{\sigma}_2 \cdot \frac{\partial}{\partial \vec{x}}) - (\vec{\sigma}_1 \cdot \vec{\sigma}_2)(\vec{x} \cdot \frac{\partial}{\partial \vec{x}}) \right) + 1 \leftrightarrow 2 \right\}$$

Multiconfiguration Calculations

better descpription of groundstate properties

Quantum Branching

branching between FMD trajectories should improve description of multifragmentation,
methods for treatment of quantum branching are being developed (conservation laws)