Short Range Correlations in Fermionic Molecular Dynamics

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The fermionic molecular dynamics model is based on variational principles.

Ground states (Ritz variational principle):

$$0 = \frac{\partial}{\partial q_\mu} \langle Q | \underset{\sim}{H} | Q \rangle , \quad \forall q_\mu$$

Dynamics (time-dependent variational principle):

$$0 = \delta \int_{t_1}^{t_2} \mathrm{d}t \, \langle Q(t) | \left(i \frac{d}{dt} - \underset{\sim}{H} \right) | Q(t) \rangle$$

The physical system and the phenomena which shall be addressed determine the choice of the Hamilton operator $\underset{\sim}{H}$ and the trial state $| Q(t) \rangle$.

The uncorrelated FMD Trial State

Single nucleons are described by single-particle states which are gaussian wave packets localized in phase space (Heisenberg uncertainty principle):

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

$$\vec{b} = \vec{r} + ia\vec{p}$$

$\vec{r}$: mean position

$\vec{p}$: mean momentum

a : complex width

χ, ϕ : spin angles

ξ : isospin 3-component

A fermion system, e.g. a nucleus, is described by an antisymmetric many-body state (Pauli principle). In the most simple case this is a Slaterdeterminant:

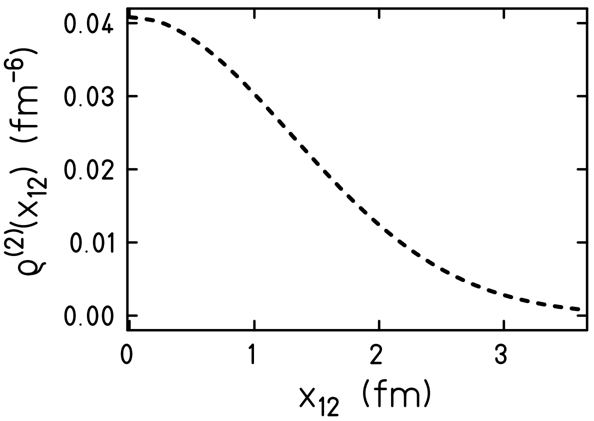
$$|\, Q \,\rangle = \frac{1}{\langle\, \widehat{Q} \,|\, \widehat{Q} \,\rangle^{\frac{1}{2}}} \; |\, \widehat{Q} \,\rangle$$

$$|\, \widehat{Q} \,\rangle = \frac{1}{A!} \sum_{\pi} \mathrm{sgn}(\pi) \; |\, q_{\pi(1)} \,\rangle \otimes \cdots \otimes \; |\, q_{\pi(A)} \,\rangle$$

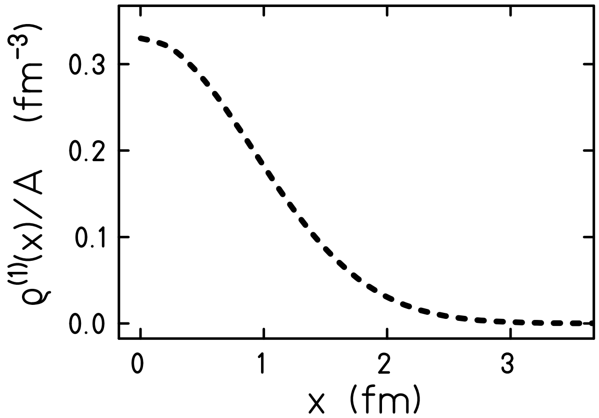
The Uncorrelated FMD Trial State ^{4}He

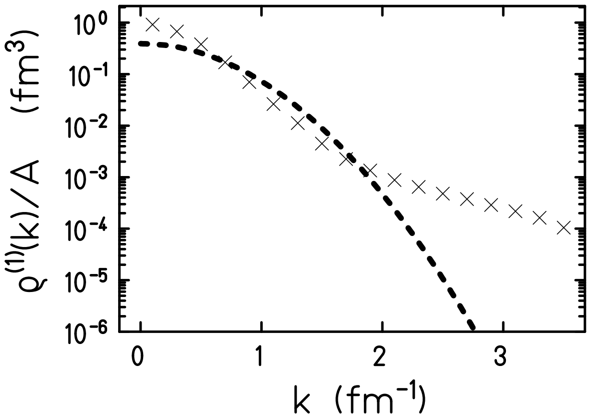
The uncorrelated trial state for the alpha particle is given by the product of 4 identical gaussians.

Two-body density as a function of the relative distance with the centre of mass kept fixed at zero:



One-body density in coordinate space (left) and in momentum space (right):





The experimental data points (right) show the occupation of higher momenta. This is a signature of short-range correlations induced by the strong repulsive core of the nucleon-nucleon interaction.

The Correlated FMD Trial State
^{4}He

Short-range correlations induced by the hard repulsion of the nucleon-nucleon interaction show up in various phenomena:

- ground states: saturation of the binding energy and of the one-body density in coordinate space, high momentum components in momentum space,
- heavy ion reactions: hard scattering of nucleons at short distances with large momentum transfer, stopping, thermalization

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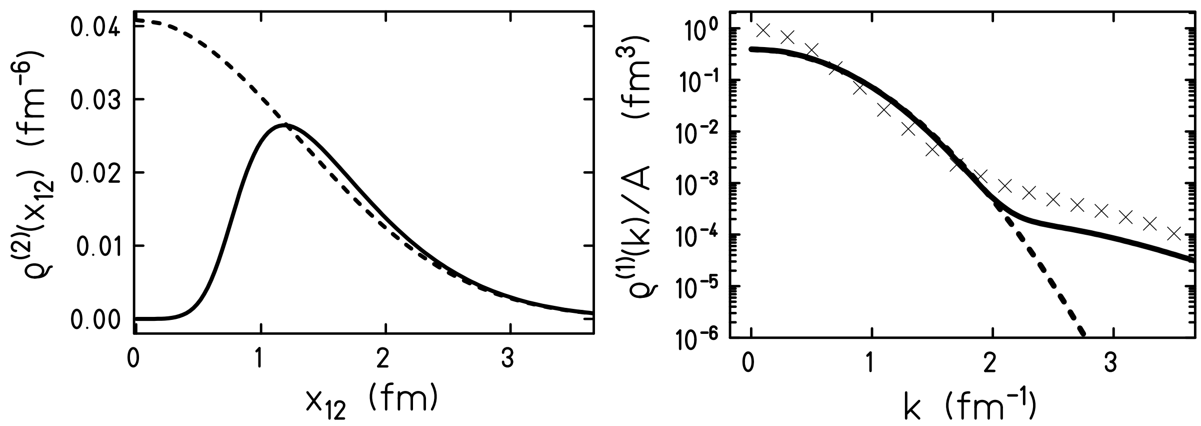
Correlated two-body density in coordinate space (left) and correlated one-body density in momentum space (right):



Contents

1. Ansatz of the correlated trial state:

- introduction of a unitary correlation operator,
- mode of action and examples,
- definition of a cluster expansion and the two-body approximation,
- expectation values of one- and two-body operators,
- relation between the correlator and the nucleon-nucleon interaction.

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2. Ground-state properties of nuclei:

- binding energies and charge radii of various isotopes.

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3. Dynamics:

- dissipative reaction of ^{19}F and ^{27}Al at $E_{\mathrm{Lab}} = 5.9\ A$ MeV,
- fragmentation reaction of ^{40}Ca and ^{40}Ca at $E_{\mathrm{Lab}} = 35\ A$ MeV.

The Correlated FMD Trial State Ansatz

The correlated FMD trial state is given by the action of a unitary, state-independent correlation operator on the uncorrelated trial state:

$$|\, Q(t)\, \rangle \Rightarrow \underset{\sim}{C}\, |\, Q(t)\, \rangle \;, \quad \underset{\sim}{C}^\dagger \underset{\sim}{C} = \underset{\sim}{1}$$

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unitary correlation $|\, \Psi(t)\, \rangle = \underset{\sim}{C}\, |\, \Phi(t)\, \rangle$**:**

$$\langle\, \Psi(t)\, |\, \underset{\sim}{B}\, |\, \Psi(t)\, \rangle = \langle\, \Phi(t)\, |\, \underset{\sim}{C}^\dagger \underset{\sim}{B}\, \underset{\sim}{C}\, |\, \Phi(t)\, \rangle = \langle\, \Phi(t)\, |\, \underset{\sim}{B}_{\mathrm{eff}}\, |\, \Phi(t)\, \rangle$$

Note: A correlation with Jastrow correlation functions is not unitary.

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state-independent correlation:

$$\begin{aligned} i\, \frac{d}{dt}\, |\, \Psi(t)\, \rangle &= \underset{\sim}{H}\, |\, \Psi(t)\, \rangle \\ i\, \frac{d}{dt}\, \underset{\sim}{C}\, |\, \Phi(t)\, \rangle &= \underset{\sim}{H}\underset{\sim}{C}\, |\, \Phi(t)\, \rangle \\ i\, \frac{d}{dt}\, |\, \Phi(t)\, \rangle &= \underset{\sim}{C}^\dagger \underset{\sim}{H}\underset{\sim}{C}\, |\, \Phi(t)\, \rangle = \underset{\sim}{H}_{\mathrm{eff}}\, |\, \Phi(t)\, \rangle \end{aligned}$$

The assumption that $\underset{\sim}{C}$ is state-independent is justified because the repulsive core suppresses the wave function for small relative distances like a boundary condition. In addition the action of $\underset{\sim}{C}$ is limited to short range and the density for which the model is designed is less than $2\rho_0$.

The Correlation Operator Mode of Action – 1

The unitary correlation operator is written using a hermitian generator:

$$\underset{\sim}{C} = \exp\{-i\underset{\sim}{S}\} \ , \quad \underset{\sim}{S}^\dagger = \underset{\sim}{S}$$

Since the correlations are of short range and the density is not too high, $\underset{\sim}{S}$ is a two-body operator and can be given in the Weyl-representation as:

$$\underset{\sim}{S} = \frac{1}{(2\pi)^6} \int \mathrm{d}^3x_1\ \mathrm{d}^3x_2\ \mathrm{d}^3k_1\ \mathrm{d}^3k_2 \int \mathrm{d}^3u_1\ \mathrm{d}^3u_2\ \mathrm{e}^{i\vec{k}_1\cdot\vec{u}_1}\mathrm{e}^{i\vec{k}_2\cdot\vec{u}_2}$$
$$\times O(\vec{x}_1,\vec{x}_2;\vec{k}_1,\vec{k}_2)\ \underset{\sim}{\Psi}^\dagger(\vec{x}_1+\frac{\vec{u}_1}{2})\underset{\sim}{\Psi}^\dagger(\vec{x}_2+\frac{\vec{u}_2}{2})\underset{\sim}{\Psi}(\vec{x}_2-\frac{\vec{u}_2}{2})\underset{\sim}{\Psi}(\vec{x}_1-\frac{\vec{u}_1}{2})$$

Translational, rotational and Galilei invariance:

$$O(\vec{x}_1,\vec{x}_2;\vec{k}_1,\vec{k}_2) = O(\vec{x}_{12};\vec{k}_{12}) = s(x_{12})\ \frac{\vec{x}_{12}}{x_{12}}\cdot\vec{k}_{12}$$

Coordinate representation:

$$\langle\, \vec{x}_1\ \vec{x}_2 \,|\, \underset{\sim}{C} \,|\, \Phi \,\rangle$$
$$= \exp\left\{ -\frac{1}{2}\ \frac{\partial\, s(x_{12})}{\partial\, x_{12}} - \frac{s(x_{12})}{x_{12}} - s(x_{12})\ \frac{\partial}{\partial\, x_{12}} \right\}\langle\, \vec{x}_1\ \vec{x}_2 \,|\, \Phi \,\rangle$$

$\underset{\sim}{C}$ performs a radial translation in the relative coordinate $\vec{x}_{12} = \vec{x}_1 - \vec{x}_2$ depending on the shift function $s(x_{12})$.

The Schematic Correlation Operator

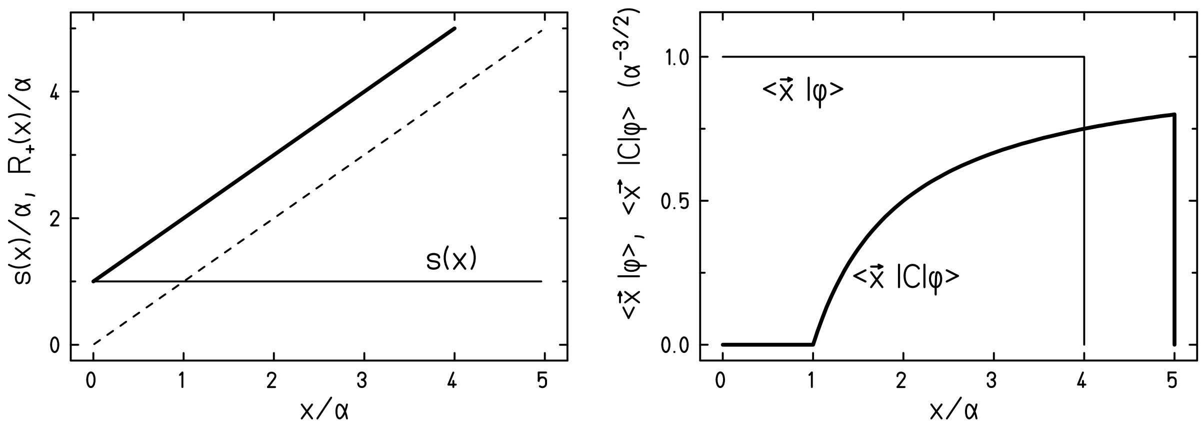
For the schematic correlation operator the function $s(x)$ is constant, i.e. the correlator has an infinite healing distance.

$$s(x) = \alpha$$

Correlated radial-symmetric two-body wave function $\langle\, \vec{x}\,|\,\phi\,\rangle = \phi(x)$:

$$\begin{aligned}
\langle\, \vec{x}\,|\,\underset{\sim}{C}\,|\,\phi\,\rangle &= e^{\left(-\frac{1}{2}\,\frac{\partial\, s(x)}{\partial\, x}\; - \frac{s(x)}{x} - s(x)\,\frac{\partial}{\partial\, x}\right)}\,\phi(x)\\
&= \exp\left\{-\frac{\alpha}{x} - \alpha\,\frac{\partial}{\partial\, x}\right\}\phi(x)\\
&= \Theta(x-\alpha)\,\frac{x-\alpha}{x}\;\phi(x-\alpha)
\end{aligned}$$

The correlation operator acts like a coordinate transformation: $x \mapsto R_-(x) = x - \alpha\ ;\ \ R_+(x) = (R_-)^{-1}(x)$.



The Correlation Operator Mode of Action – 2

Correlated relative wave function:

$$\langle\, \vec{x} \,|\, \underset{\sim}{C} \,|\, \phi \,\rangle = \frac{1}{\sqrt{x^2\; s(x)}}\; \exp\left\{ -s(x) \frac{\partial}{\partial\, x} \right\}\; \sqrt{x^2\; s(x)}\; \langle\, \vec{x} \,|\, \phi \,\rangle$$

$s(x)\frac{\partial}{\partial\, x} = \frac{\partial}{\partial\, y}$ — instead of $s(x)$-dependent translation perform a constant translation in a new coordinate $y = Y(x)$:

$$Y(x) = \int^{x} \frac{\mathrm{d}t}{s(t)} \quad , \quad y = \int^{R(y)} \frac{\mathrm{d}t}{s(t)}$$

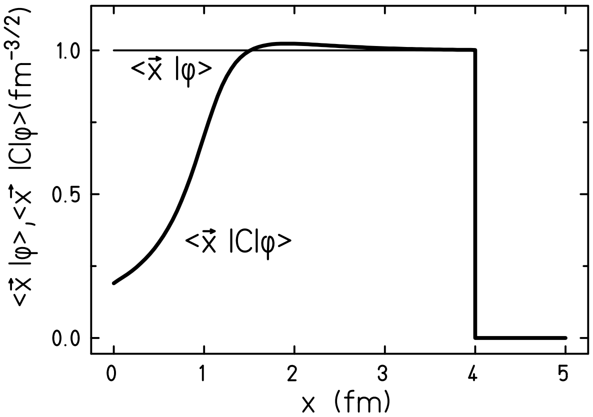
Correlated wave functions and expectation values can be expressed with the transformations $R_\pm$:

$$R_\pm = R(Y(x) \pm 1) \quad : \quad \int_{x}^{R_\pm(x)} \frac{\mathrm{d}t}{s(t)} = \pm 1$$

$$\begin{aligned}
\langle\, \vec{x} \,|\, \underset{\sim}{C} \,|\, \phi \,\rangle &= \Theta\big(R_-(x)\big)\; \frac{R_-(x)\sqrt{R_-'(x)}}{x}\; \langle\, R_-(x)\frac{\vec{x}}{x} \,|\, \phi \,\rangle \\
&= \Theta(r)\; \frac{r}{R_+(r)\sqrt{R_+'(r)}}\; \phi\,(\vec{r}) \;\;,\;\; r = R_-(x)
\end{aligned}$$

$$R_+(r) = r + \alpha \left(\tfrac{r}{\beta}\right) \mathrm{e}^{-\left(\frac{r}{\beta}\right)},$$

$$\alpha = 1.0\mathrm{fm}, \beta = 0.5\mathrm{fm}$$



The Correlation Operator Expectation Values

Expectation value of a local two-body interaction with respect to a relative wave function:

$$\langle\, \phi \,|\, \underset{\sim}{C}^{\dagger}\, \underset{\sim}{V}\, \underset{\sim}{C} \,|\, \phi \,\rangle = \int \mathrm{d}^3 x \,\langle\, \phi \,|\, \vec{x} \,\rangle\, V(R_+(x))\, \langle\, \vec{x} \,|\, \phi \,\rangle$$

The expectation value of the local two-body interaction with respect to the correlated state is equal to the expectation value of the transformed potential with respect to the uncorrelated state.

Expectation value of the kinetic energy with respect to a relativ wave function:

$$\langle\, \phi \,|\, \underset{\sim}{C}^{\dagger}\, \underset{\sim}{T}\, \underset{\sim}{C} \,|\, \phi \,\rangle = \frac{1}{2\mu} \int \mathrm{d}^3 r \, \left| \left(\frac{\partial}{\partial\, \vec{x}} \otimes \vec{r} \right) \cdot \frac{\partial}{\partial\, \vec{r}}\, \phi(\vec{r}) \right|^2$$

$$+ \frac{1}{2\mu} \int \mathrm{d}^3 r \;\, |\phi(\vec{r})|^2 \, \frac{1}{(R'_+(r))^2} \left[\frac{1}{2}\, \frac{R'''_+(r)}{R'_+(r)} - \frac{5}{4} \left(\frac{R''_+(r)}{R'_+(r)} \right)^2 + 2\, \frac{R''_+(r)}{r\, R'_+(r)} \right]$$

$$\vec{r} = R_-(x) \frac{\vec{x}}{x}$$

The expectation value of the kinetic energy of the relative motion includes two terms. The first one is a kinetic energy with an effective mass tensor, the second one the expectation value of a local potential.

The Cluster Expansion

Expectation value of an arbitrary operator $\underset{\sim}{O}$:

$$\langle \Psi | \underset{\sim}{O} | \Psi \rangle = \langle \Phi | \underset{\sim}{C}^\dagger \underset{\sim}{O} \underset{\sim}{C} | \Phi \rangle$$

Since $\underset{\sim}{C}$ contains operators to all particle numbers, $\underset{\sim}{C}^\dagger \underset{\sim}{O} \underset{\sim}{C}$ can be ordered with respect to n-particle operators.

Cluster expansion of $\underset{\sim}{O}_{\text{eff}} = \underset{\sim}{C}^\dagger \underset{\sim}{O} \underset{\sim}{C}$:

$$\underset{\sim}{O}_{\text{eff}} = \sum_{n=0}^{\infty} \underset{\sim}{O}_{\text{eff}}^{(n)}$$

$$\underset{\sim}{O}_{\text{eff}}^{(n)} = \frac{1}{n!} \sum_{k_1,\dots,k_n} \sum_{l_1,\dots,l_n} \langle k_1 \cdots k_n | \underset{\sim}{O}_{\text{eff}} - \sum_{m=0}^{n-1} \underset{\sim}{O}_{\text{eff}}^{(m)} | l_1 \cdots l_n \rangle \times \underset{\sim}{a}_{k_1}^\dagger \cdots \underset{\sim}{a}_{k_n}^\dagger \underset{\sim}{a}_{l_n} \cdots \underset{\sim}{a}_{l_1}$$

$$\Rightarrow \quad \langle \Psi | \underset{\sim}{O} | \Psi \rangle = \sum_{n=0}^{A} \mathrm{Tr}\left(\underset{\sim}{O}_{\text{eff}}^{(n)} \underset{\sim}{\rho}_0^{(n)} \right)$$

Two-body approximation ($n = 0, 1, 2$):

$$\langle \underset{\sim}{T} \rangle = \sum_{n=0}^{2} \mathrm{Tr}\left(\underset{\sim}{T}_{\text{eff}}^{(n)} \underset{\sim}{\rho}_0^{(n)} \right) = \mathrm{Tr}\left(\underset{\sim}{T} \underset{\sim}{\rho}_0^{(1)} \right) + \mathrm{Tr}\left(\left\{ \underset{\sim}{C}^\dagger \underset{\sim}{T} \underset{\sim}{C} - \underset{\sim}{T} \right\} \underset{\sim}{\rho}_0^{(2)} \right)$$

$$\langle \underset{\sim}{V} \rangle = \sum_{n=0}^{2} \mathrm{Tr}\left(\underset{\sim}{V}_{\text{eff}}^{(n)} \underset{\sim}{\rho}_0^{(n)} \right) = \mathrm{Tr}\left(\underset{\sim}{C}^\dagger \underset{\sim}{V} \underset{\sim}{C} \underset{\sim}{\rho}_0^{(2)} \right) = \mathrm{Tr}\left(\underset{\sim}{V} \underset{\sim}{C} \underset{\sim}{\rho}_0^{(2)} \underset{\sim}{C}^\dagger \right)$$

Two-Body Approximation
Densities

Uncorrelated trial state and densities:

$$|\,Q\,\rangle = \frac{1}{\langle\,\widehat{Q}\,|\,\widehat{Q}\,\rangle^{\frac{1}{2}}}\;|\,\widehat{Q}\,\rangle\;,\quad |\,\widehat{Q}\,\rangle = \frac{1}{A!}\sum_{\pi}\mathrm{sgn}(\pi)\;|\,q_{\pi(1)}\,\rangle\otimes\cdots\otimes\;|\,q_{\pi(A)}\,\rangle$$

$$\underset{\sim}{\rho}{}_0^{(2)} \;=\; \frac{1}{2}\sum_{k,l,m,n}^{A}\;|q_m q_n\rangle\Big(\mathcal{O}_{mk}\mathcal{O}_{nl}-\mathcal{O}_{ml}\mathcal{O}_{nk}\Big)\langle q_k q_l|$$

$$\underset{\sim}{\rho}{}_0^{(1)} \;=\; \sum_{k,l}^{A}\;|q_l\rangle\mathcal{O}_{lk}\langle q_k|\;\;,\qquad \left(\mathcal{O}^{-1}\right)_{kl} = \langle q_k|q_l\rangle$$

For single Slater determinant the uncorrelated two-body density can be expressed as the antisymmetric product of the one-body density. In this sense the system contains only correlations which are already in the one-body density.

Correlated trial state and densities:

$$|\,Q(t)\,\rangle \Rightarrow \underset{\sim}{C}\;|\,Q(t)\,\rangle$$

$$\underset{\sim}{\rho}{}^{(2)} = \underset{\sim}{C}\;\underset{\sim}{\rho}{}_0^{(2)}\underset{\sim}{C}^{\dagger} = \frac{1}{2}\sum_{k,l,m,n}^{A}\;\underset{\sim}{C}\;|q_m q_n\rangle\Big(\mathcal{O}_{mk}\mathcal{O}_{nl}-\mathcal{O}_{ml}\mathcal{O}_{nk}\Big)\langle q_k q_l|\;\underset{\sim}{C}^{\dagger}$$

$$\langle\,\vec{x}\,m_s\,m_t\,|\;\underset{\sim}{\rho}{}^{(1)}\;|\,\vec{x}'\;m_s'\;m_t'\,\rangle = \frac{2}{(A-1)}\int d^3x_2\sum_{m_{s2},m_{t2}}$$

$$\times\langle\,\vec{x}\,m_s\,m_t;\vec{x}_2\,m_{s2}\,m_{t2}\,|\;\underset{\sim}{\rho}{}^{(2)}\;|\,\vec{x}'\;m_s'\;m_t';\vec{x}_2\,m_{s2}\,m_{t2}\,\rangle$$

The correlated one-body density is no projection opeartor any longer, it contains fractional occupation numbers:
$(\underset{\sim}{\rho}{}^{(1)})^2 \neq \underset{\sim}{\rho}{}^{(1)}$, but $(\underset{\sim}{\rho}{}_0^{(1)})^2 = \underset{\sim}{\rho}{}_0^{(1)}$.

The Relation of Correlator and Potential

Local two-body interaction:

$$\frac{V(x)}{\mathrm{MeV}} = -10.5\frac{e^{-\mu x}}{\mu x} + 105.5\frac{e^{-2\mu x}}{\mu x} - 3187.8\frac{e^{-4\mu x}}{\mu x} + 9924.3\frac{e^{-6\mu x}}{\mu x}$$

$$-98.0\exp\left\{-\frac{x^2}{(1.4\mathrm{fm})^2}\right\}\ , \quad \text{with} \quad \mu = 0.7\mathrm{fm}^{-1}$$

Ansatz for the transformation:

$$R_+(r) = r + \alpha\left(\frac{r}{\beta}\right)^{\frac{1}{3}}\exp\left\{-\frac{r}{\beta}\right\}$$

Variation of the energy for ^{4}He:

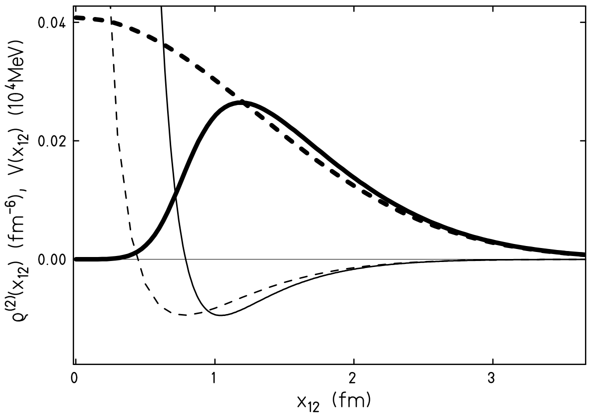
$$\mathcal{H}(\alpha,\beta,a) = \langle\, Q\,|\, \underset{\sim}{C}^\dagger(\alpha,\beta)\, \underset{\sim}{H}\, \underset{\sim}{C}(\alpha,\beta)\,|\, Q\,\rangle$$

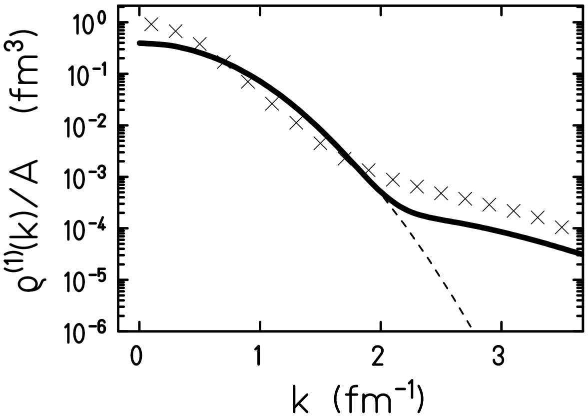
$$= \sum_k^A \langle q_k|\ \underset{\sim}{T}\ |q_k\rangle \mathcal{O}_{kk} + \frac{1}{2}\sum_{k\neq l}\langle q_k\, q_l|\ \left(\underset{\sim}{C}^\dagger \underset{\sim}{T}\ \underset{\sim}{C} - \underset{\sim}{T}\right)\ |q_k\, q_l\rangle \mathcal{O}_{kk}\mathcal{O}_{ll}$$

$$+\frac{1}{2}\sum_{k\neq l}\langle q_k\, q_l|\ \underset{\sim}{C}^\dagger \underset{\sim}{V}\ \underset{\sim}{C}\ |q_k\, q_l\rangle \mathcal{O}_{kk}\mathcal{O}_{ll}$$

$$\mathcal{H}(\alpha = 0.76\mathrm{fm}, \beta = 0.73\mathrm{fm}, a = 1.69\mathrm{fm}^2) = -28.5\ \mathrm{MeV}$$

Densities:





At This Point

- ansatz of a correlated antisymmetrized many-body trial state $\underset{\sim}{C} \,|\, Q(t) \,\rangle$,
- introduction of a unitary correlation operator $\underset{\sim}{C}$, which suppresses the many-body wave function for small relative distances of the nucleons,
- the unitary correlator performs a radial translation in the relative coordinate, which can be expressed in terms of a (non-linear) coordinate transformation,
- expectation values can be evaluated in a cluster expansion which is truncated after the two-body term,
- expectation value of the Hamilton operator: effective kinetic energy contains a two-body term, local two-body interaction is transformed; (technical approximation to get expressions in closed form and to speed up the computer simulation),
- with the variation of the energy for the ^{4}He the relation between the correlator and the nucleon-nucleon interaction is established and the correlator fixed,
- ground states,
- dynamics.

Ground States in Fermionic Molecular Dynamics

$$\mathcal{H}(Q) = \langle\, Q \,|\, \underset{\sim}{C}^\dagger \underset{\sim}{H}\, \underset{\sim}{C} \,|\, Q \,\rangle = \mathcal{T}(Q) + \mathcal{T}_{\mathrm{HC}}(Q) + \mathcal{V}(Q) + \mathcal{V}_{\mathrm{Coul}}(Q)$$

According to the Ritz variational principle the ground state of a nucleus is the state which is the lowest one in energy.

$$0 = \frac{\partial}{\partial q_\mu}\, \mathcal{H}(Q) \;, \quad \forall q_\mu$$

- since all generalized forces vanish the ground states are stationary,

$$\frac{d}{dt}\, q_\mu = 0 \;, \quad \forall q_\mu$$

- Fermi motion is reflected by $\rho^{(1)}(\vec{k})$; high momentum components,
- saturation of binding energies and density in coordinate space

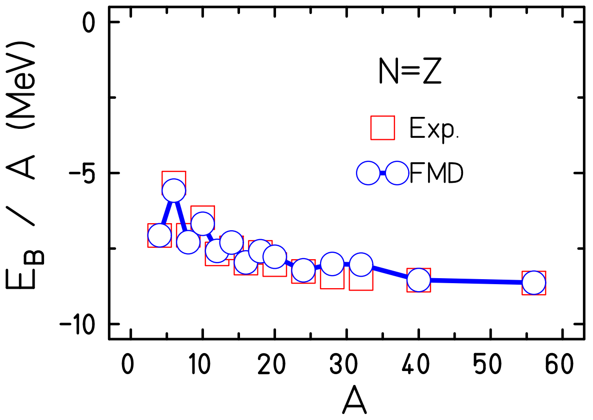
$$\mathcal{T}_{\mathrm{HC}}(Q) \propto k_F^2 A^2$$

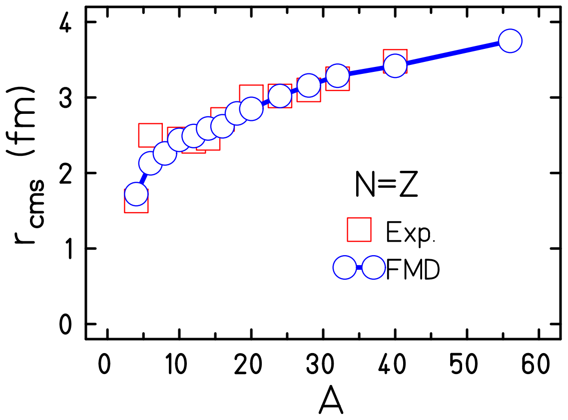
  nuclear matter: $\mathcal{T}(Q)/A \propto k_F^2$ repulsive, $\mathcal{V}(Q)/A \propto k_F^3$ attractive, $\mathcal{T}_{\mathrm{HC}}(Q)/A \propto k_F^5$ repulsive,

- intrinsically deformed ground states

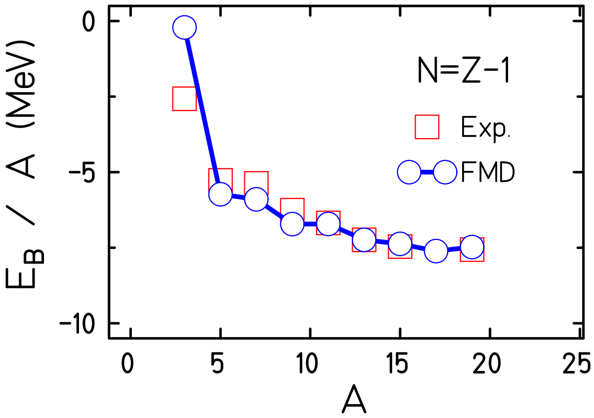
Ground States – 1

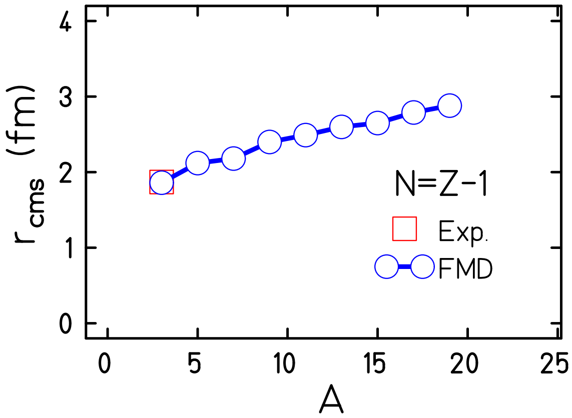
$N = Z$:



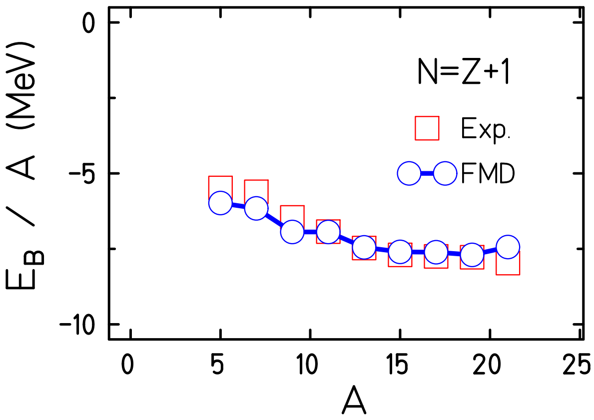


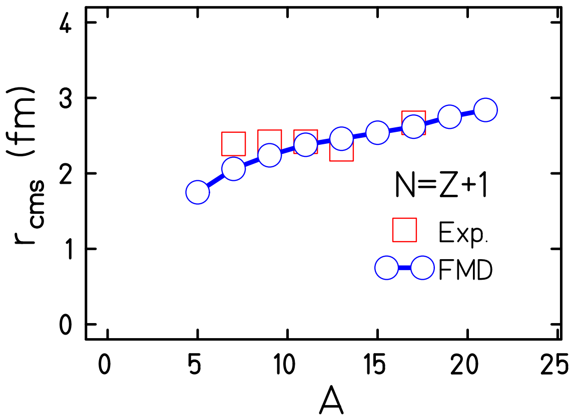
$N = Z - 1$:





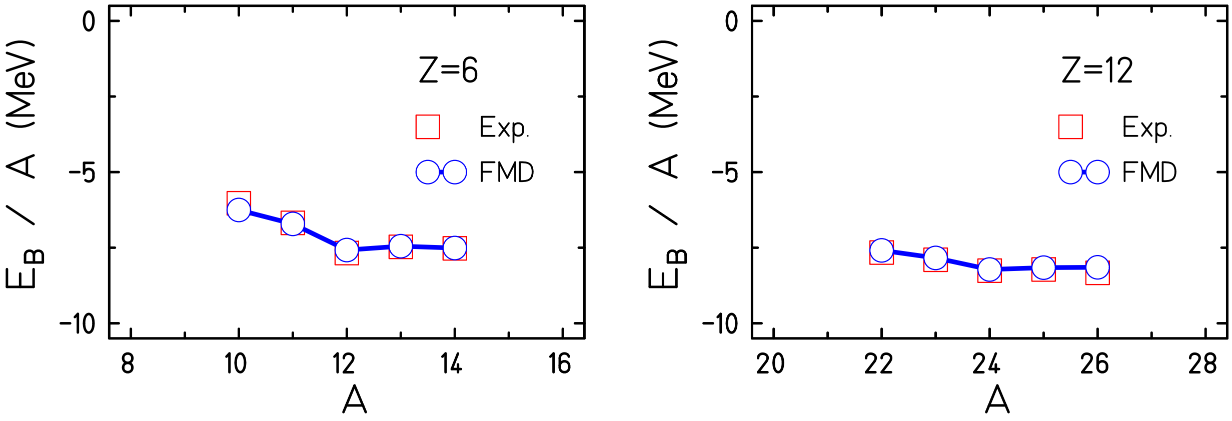
$N = Z + 1$:



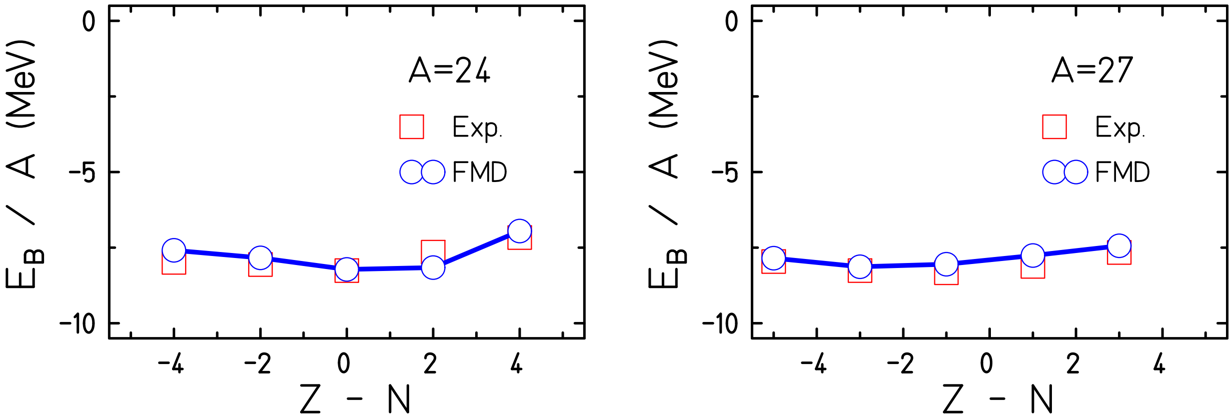


Ground States – 2

$Z = 6$**- and** $Z = 12$**-isotopes:**



$A = 24$**- and** $A = 27$**-isobares:**



Dynamics

$$\begin{aligned} 0 &= \delta \int_{t_1}^{t_2} \mathrm{d}t \, \langle\, Q(t) \,|\; \underset{\sim}{C}^{\dagger} \left(i\frac{d}{dt} - \underset{\sim}{H} \right) \underset{\sim}{C} \;|\, Q(t) \,\rangle \\ &= \delta \int_{t_1}^{t_2} \mathrm{d}t \left(\langle\, Q(t) \,|\, i\frac{d}{dt} \,|\, Q(t) \,\rangle - \langle\, Q(t) \,|\, \underset{\sim}{H}_{\mathrm{eff}} \,|\, Q(t) \,\rangle \right) \end{aligned}$$

Euler–Lagrange equations in their most general form:

$$\sum_{\nu} \mathcal{A}_{\mu\nu}(Q(t)) \; \dot{q}_{\nu} = -\frac{\partial}{\partial q_{\mu}} \; \langle\, Q(t) \,|\, \underset{\sim}{H}_{\mathrm{eff}} \,|\, Q(t) \,\rangle$$

$$\mathcal{A}_{\mu\nu}(Q(t)) = \frac{\partial^2 \langle\, Q(t) \,|\, i\frac{d}{dt} \;\; |\, Q(t) \,\rangle}{\partial \dot{q}_{\mu} \partial q_{\nu}} - \frac{\partial^2 \langle\, Q(t) \,|\, i\frac{d}{dt} \;\; |\, Q(t) \,\rangle}{\partial \dot{q}_{\nu} \partial q_{\mu}}$$

$\mathcal{A}_{\mu\nu}(Q(t))$ is a purely geometrical object depending only on the uncorrelated trial state $|\, Q(t) \,\rangle$, but not on $\underset{\sim}{H}$ or $\underset{\sim}{C}$!
The Pauli principle enters the equations of motion at the exchange terms of the energy and at the matrix $\mathcal{A}_{\mu\nu}(Q(t))$.

Generalized Poisson brackets:

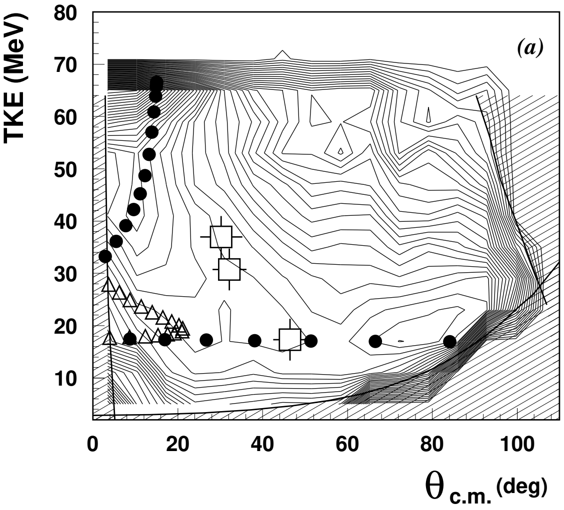
$$\mathcal{B}(t) = \langle\, Q(t) \,|\; \underset{\sim}{C}^{\dagger} \underset{\sim}{B} \, \underset{\sim}{C} \;|\, Q(t) \,\rangle$$

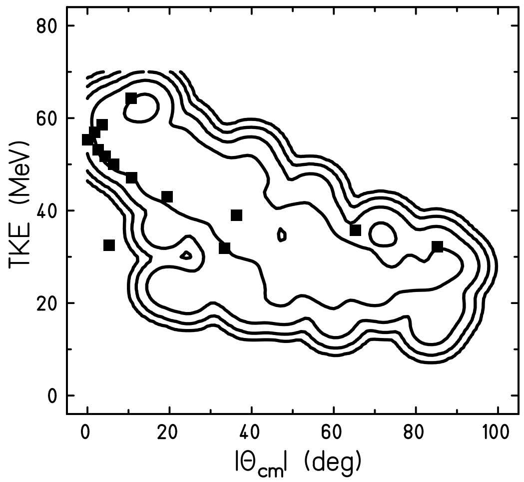
$$\frac{d}{dt}\, \mathcal{B}(t) = \sum_{\nu} \dot{q}_{\nu} \, \frac{\partial\, \mathcal{B}}{\partial q_{\nu}} \; = \sum_{\mu,\nu} \frac{\partial \mathcal{H}}{\partial q_{\mu}} \, \mathcal{A}^{-1}_{\mu\nu} \, \frac{\partial \mathcal{B}}{\partial q_{\nu}} = \{\mathcal{H}, \mathcal{B}\}$$

An expectation value $\mathcal{B}(t)$ is conserved if it commutes with $\mathcal{H}$, i.e. $\{\mathcal{H}, \mathcal{B}\} = 0$.

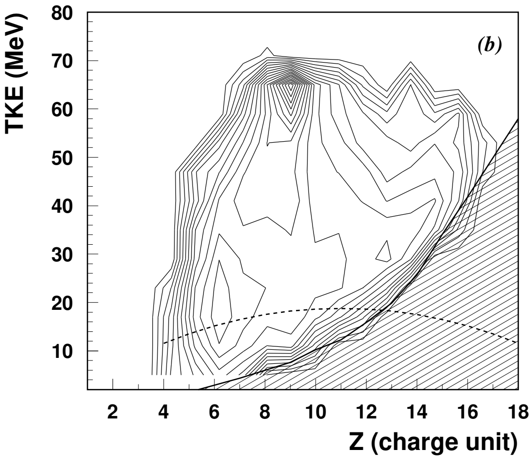
Dissipative Reaction

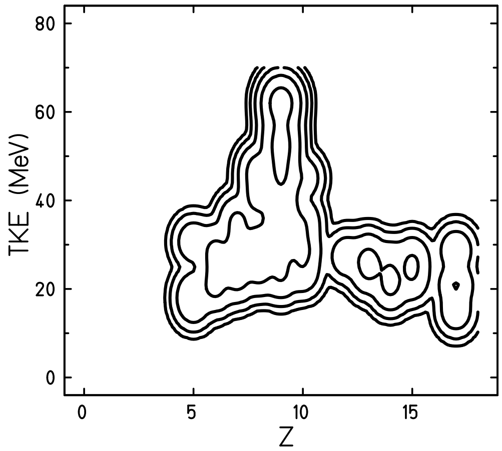
^{19}**F**–^{27}**Al**, $E = 5.9\ A$ **MeV:**





$$3^0 \leq \theta_{Lab} \leq 54^0$$





M. Petrovici et al.,

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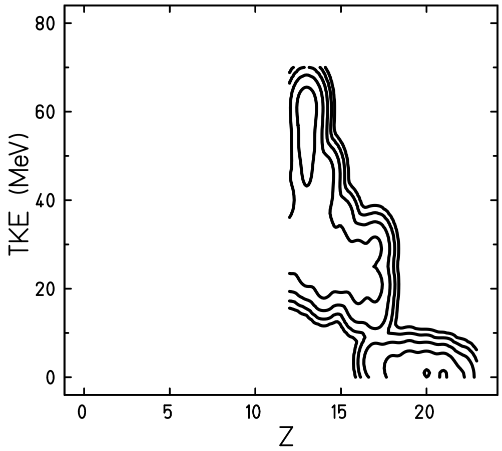
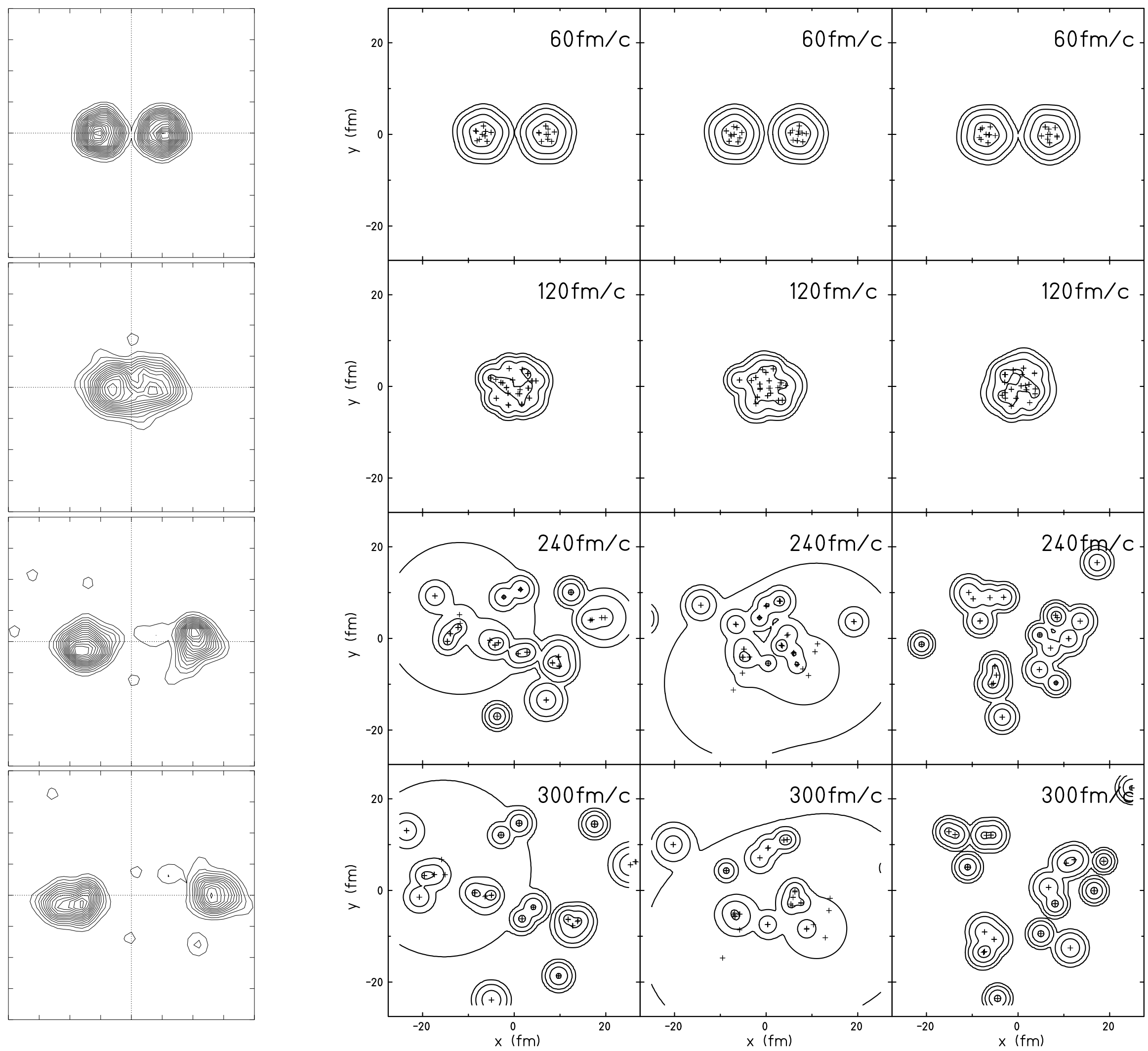


$$Z \geq 12$$

Fragmentation Reaction

^{40}**Ca**–^{40}**Ca,** $E = 35\ A$ **MeV:**



$b = 0$ fm, left: AMD with $t = 0, 60, 180, 240$fm$/c$, right: FMD

Summary and Outlook

Summary:

- introduction of a correlated trial state which is suppressed at short relative distances; the correlated trial is not a pure Slater determinant any longer; the one-body density is not a projection operator,
- unitary correlation operator; use of effective operators together with the uncorrelated trial state,
- cluster expansion; two-body approximation; Hamilton function for a simplified nucleon-nucleon interaction,
- ground states: correct binding energies and charge radii; saturation; high momentum tails,
- dynamics: fusion, dissipative reactions, fragmentation, evaporation; large fluctuations; hard collisions between nucleons,
- shortcomings of the simple potential: overemphasized alpha structure, maybe too repulsive.

Outlook:

- improvement of the used potential by taking a realistic nucleon-nucleon interaction (Bonn potential),
- evaluation of the ^{40}Ca–^{40}Ca fragmentation reaction and comparison with other models.