Fermionic Molecular Dynamics for Nuclear Ground States, Dynamics and Thermodynamics

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Intention of FMD

Ground states:

- reasonable nuclear ground state properties like binding energy and rms radius
- phenomenological interaction
- antisymmetrization, shell effects

Dynamics:

- heavy ion collisions below particle production threshold
- fusion, deeply inelastic reactions, evaporation, fragmentation, vaporisation
- large fluctuations

Means:

- Slater determinant of Gaussian wave packets, one per nucleon, as trial state
- Ritz variational principle for ground states
- time-dependent variational principle for reactions
- "trajectory" calculations for fermions

Advancement of FMD

Short range correlations

- realistic nucleon-nucleon interaction, short range repulsion
- suppression of wave function at short relative distances
- high momentum components, hard scattering
- description by a unitary correlation operator

Long and medium range correlations

- improvement of the surface
- important for weakly bound systems, like halo nuclei
- superposition of single-particle wave packets or Slater determinants

Thermodynamics

- thermodynamic properties of small quantum systems
- nuclear liquid gas phase transition, caloric curve
- coupling of the system to a thermometer

Contents

Time-dependent variational principle

- equations of motion
- constants of motion
- good generators

Fermionic Molecular Dynamics

- trial state (Slater determinant)
- ground state (interactions, examples)
- dynamics (instructive examples, role of width, event ensemble, reactions)
- short range correlations
- thermodynamics (thermostatics, time averaging, caloric curve)

Time-Dependent Variational Principle

TDVP[a]**:**

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

A variation of $\langle \, Q(t) \, |$ in the complete Hilbert space yields the Schrödinger equation.

Euler–Lagrange equations in their most general form:

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

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

- trial state $| \, Q(t) \, \rangle = | \, \{ q_\mu(t) \} \, \rangle$
- variation in the set of Slater determinants leads to TDHF
- variation with localized single-particle states leads to various kinds of quantum molecular dynamics models

[a] P. Kramer, M. Saraceno, Lecture Notes in Physics **140**, Springer, Berlin (1981)

Conservation Laws

1. Generalized Poisson Brackets

$\underset{\sim}{B}$ be a time-independent operator.

$$\frac{d}{dt}\,\mathcal{B}(t) = \frac{d}{dt}\,\langle\, Q(t) \mid \underset{\sim}{B} \mid Q(t)\,\rangle = \sum_{\nu} \dot{q}_{\nu}\,\frac{\partial}{\partial q_{\nu}}\,\mathcal{B}$$

$$= \sum_{\mu,\nu} \frac{\partial\,\mathcal{H}}{\partial q_{\mu}}\,\mathcal{A}^{-1}_{\mu\nu}\,\frac{\partial\,\mathcal{B}}{\partial q_{\nu}} =: \{\mathcal{H},\mathcal{B}\}$$

2. Conservation Laws

- for time-independent operators $\underset{\sim}{B}$

  $$\frac{d}{dt}\,\mathcal{B}(t) = 0 \;\text{ if }\; \{\mathcal{H},\mathcal{B}\} = \sum_{\mu,\nu} \frac{\partial\,\mathcal{H}}{\partial q_{\mu}}\,\mathcal{A}^{-1}_{\mu\nu}\,\frac{\partial\,\mathcal{B}}{\partial q_{\nu}} = 0$$

  obviously for $\underset{\sim}{H}$ since $\mathcal{A}$ and $\mathcal{A}^{-1}$ skew symmetric

- for generators $\underset{\sim}{G}$ which do not map out of the set of trial states and commute with $\underset{\sim}{H}$

  $$\frac{d}{dt}\,\mathcal{G}(t) = \{\mathcal{H},\mathcal{G}\} = \langle\, Q(t) \mid i\,[\,\underset{\sim}{H},\underset{\sim}{G}\,]\;\mid Q(t)\,\rangle$$

  Relates the choise of the trial state to possible conservation laws, e.g. total momentum conservation is possible if a translated trial state is again a valid trial state.

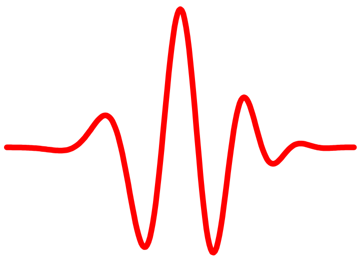
Fermionic Molecular Dynamics (FMD)

Many-body state (Slater determinant):

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

Single-particle state (Gaussian wave packet):

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



$\vec{b}(t) = \vec{r}(t) + i a(t) \vec{p}(t)$

$\vec{r}(t)$: mean position

$\vec{p}(t)$: mean momentum

$a(t)$: complex width, $a = a_R + i\, a_I$

$\chi(t), \phi(t)$: spin angles

m_t : Isospin–3–component

Special expectation values:

$$
\langle\, \underset{\sim}{\vec{x}}\,\rangle = \vec{r} \quad , \quad \langle\, \underset{\sim}{\vec{k}}\,\rangle = \vec{p}
$$

$$
(\Delta x)^2 = \frac{3}{2}\,\frac{a_R^2 + a_I^2}{a_R} \quad , \quad (\Delta k)^2 = \frac{3}{2}\,\frac{1}{a_R}
$$

Expectation values

Inverse overlap matrix

Wave packets $\mid q_k \rangle$ are not orthogonal, therefore expectation values involve an inverse overlap matrix $\mathcal{O}$.

$$\left(\mathcal{O}^{-1}\right)_{kl} := \langle\, q_k \,|\, q_l \,\rangle$$

Kinetic energy

$$\langle\, Q \,|\, \underset{\sim}{T} \,|\, Q \,\rangle = \sum_{k,l}^{A} \langle\, q_k \,|\, \underset{\sim}{t} \,|\, q_l \,\rangle\, \mathcal{O}_{lk}$$

Two-body interaction

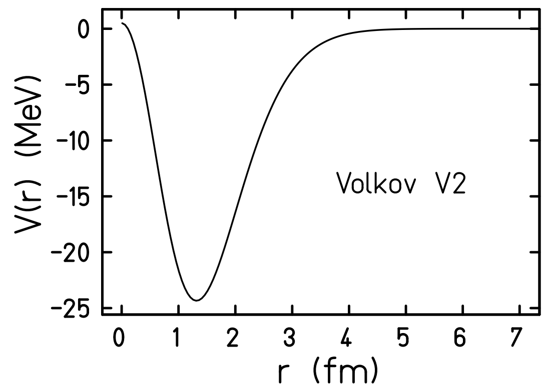
$$\langle\, Q \,|\, \underset{\sim}{V} \,|\, Q \,\rangle = \frac{1}{2} \sum_{k,l,m,n}^{A} \langle q_k q_l |\, \underset{\sim}{v} \,| q_m q_n \rangle \left(\mathcal{O}_{mk}\mathcal{O}_{nl} - \mathcal{O}_{ml}\mathcal{O}_{nk} \right)$$

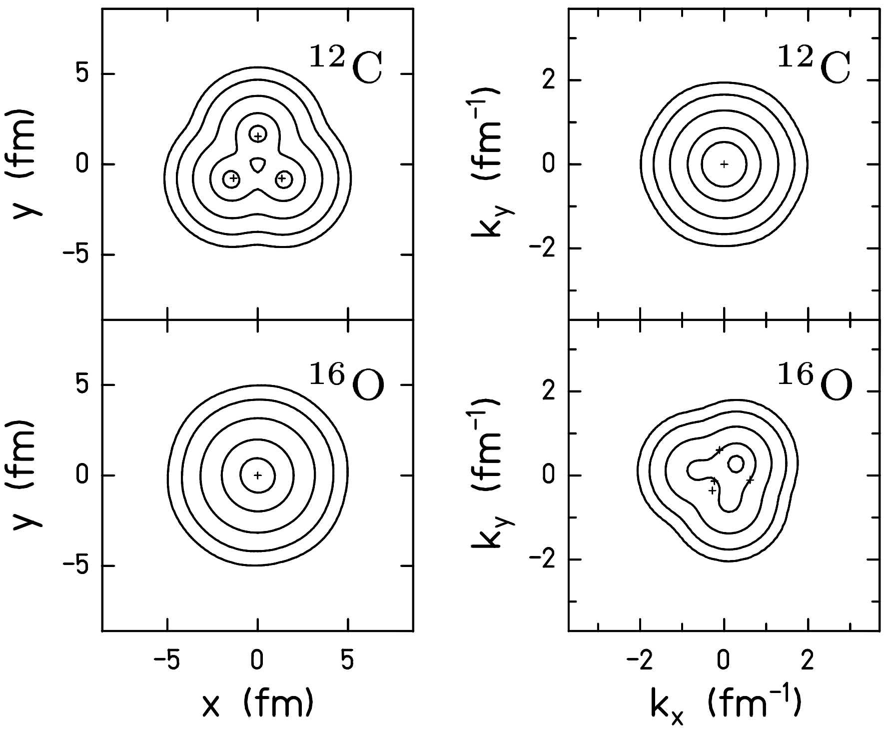
$\Longrightarrow$ Total effort scales with A^4.

Nuclear Ground States

- ground state $|\, Q\, \rangle$ lowest one in energy
- $\frac{\partial}{\partial q_\mu} \langle\, Q \,|\, \underset{\sim}{H} \,|\, Q\, \rangle = 0 \quad \forall q_\mu$
- $\Longrightarrow \dot{q}_\mu = 0 \quad \forall q_\mu$, stationary
- for experts: take care of centre of mass motion

Simple phenomenological potential





Dynamics

Equations of motion

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

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

Trial state

$$\begin{aligned}
|\, Q(t) \,\rangle &= \frac{1}{\langle\, \widehat{Q}(t) \,|\, \widehat{Q}(t) \,\rangle^{\frac{1}{2}}}\ |\, \widehat{Q}(t) \,\rangle \\
|\, \widehat{Q}(t) \,\rangle &= \frac{1}{A!} \sum_\pi \mathrm{sgn}(\pi)\ \ |\, q_{\pi(1)}(t) \,\rangle \otimes \cdots \otimes \ |\, q_{\pi(A)}(t) \,\rangle \\
\langle\, \vec{x} \,|\, q(t) \,\rangle &= \exp\left\{ -\frac{(\,\vec{x} - \vec{b}(t)\,)^2}{2\,a(t)} \right\} \otimes |\, \chi(t), \phi(t) \,\rangle \otimes |\, m_t \,\rangle
\end{aligned}$$

- $\mathcal{A}_{\mu\nu}$ skewsymmetric
- antisymmetrization affects dynamics via $\mathcal{A}_{\mu\nu}$ (metric) and $\langle\, Q(t) \,|\, \underset{\sim}{H} \,|\, Q(t) \,\rangle$ (exchange terms)

FMD: Special Solutions

Free motion:

$$\underset{\sim}{h}(l) = \frac{\underset{\sim}{\vec{k}}^2(l)}{2m} \quad \Rightarrow \quad \frac{d}{dt}\,\vec{b}_l = 0\ , \quad \frac{d}{dt}\,a_l = \frac{i}{m}$$

$$\frac{d}{dt}\,\vec{p}_l = 0 \quad , \quad \frac{d}{dt}\,\vec{r}_l = \frac{\vec{p}_l}{m}$$

Common harmonic oscillator potential:

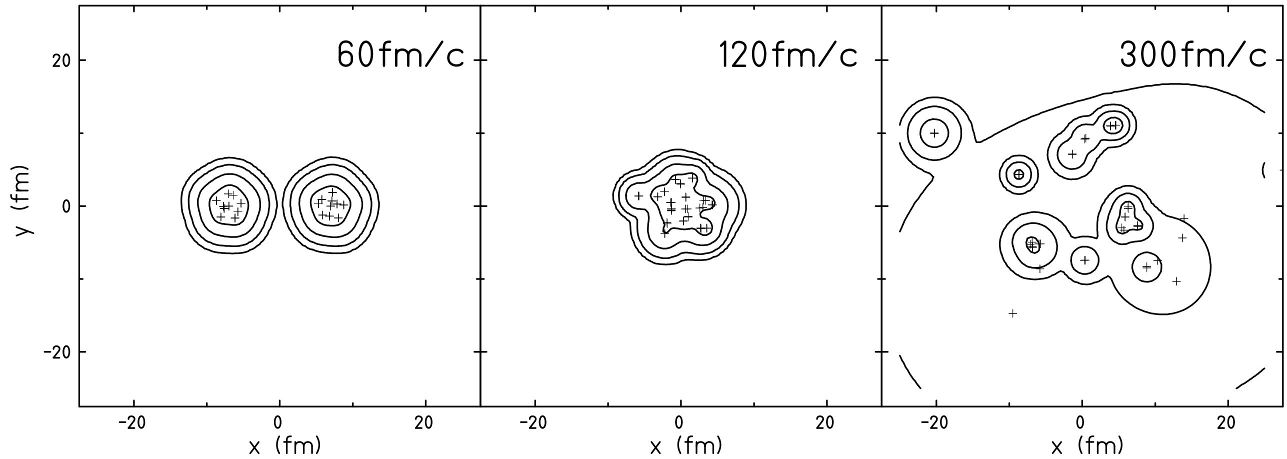
$$\underset{\sim}{h}(l) = \frac{\underset{\sim}{\vec{k}}^2(l)}{2m} + \frac{1}{2}\,m\omega^2\,\underset{\sim}{\vec{x}}^2(l) \quad \Rightarrow \quad \frac{d}{dt}\,\vec{b}_l = -im\omega^2 a_l \vec{b}_l$$

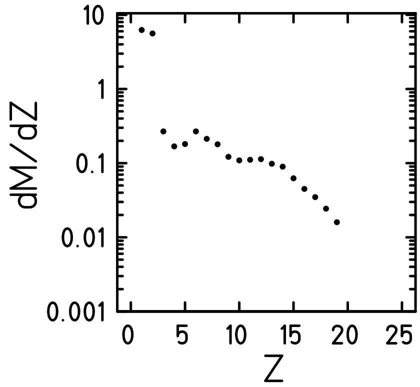
$$\frac{d}{dt}\,a_l = -im\omega^2 a_l^2 + \frac{i}{m}$$

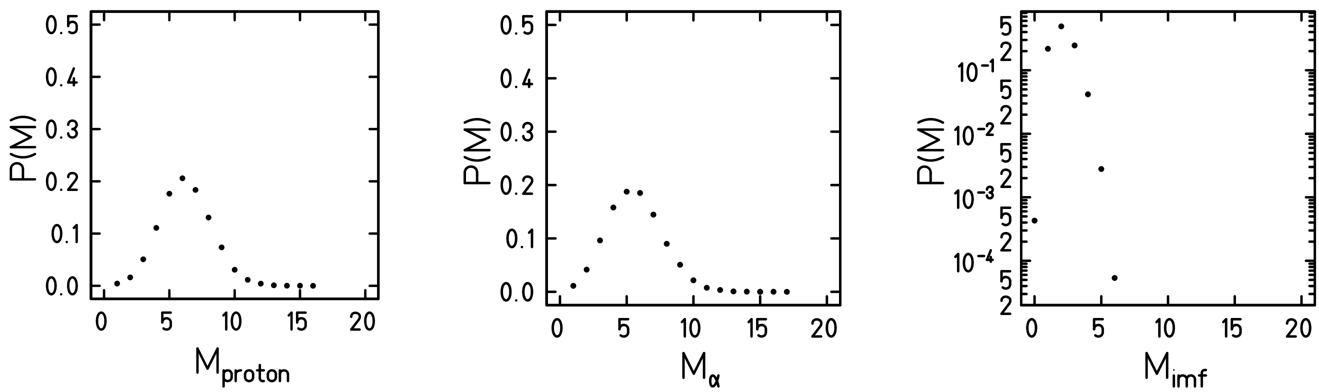
$$\frac{d}{dt}\,\vec{r}_l = \frac{\vec{p}_l}{m} \quad , \quad \frac{d}{dt}\,\vec{p}_l = -m\omega^2 \vec{r}_l$$

- both solutions coincide with the exact solution of the Schrödinger equation,
- both solutions remain the same irrespective of whether we describe bosons, fermions or distinguishable particles,
- without time-dependent complex width $a(t)$ spurious scattering occurs!

Multifragmentation - I





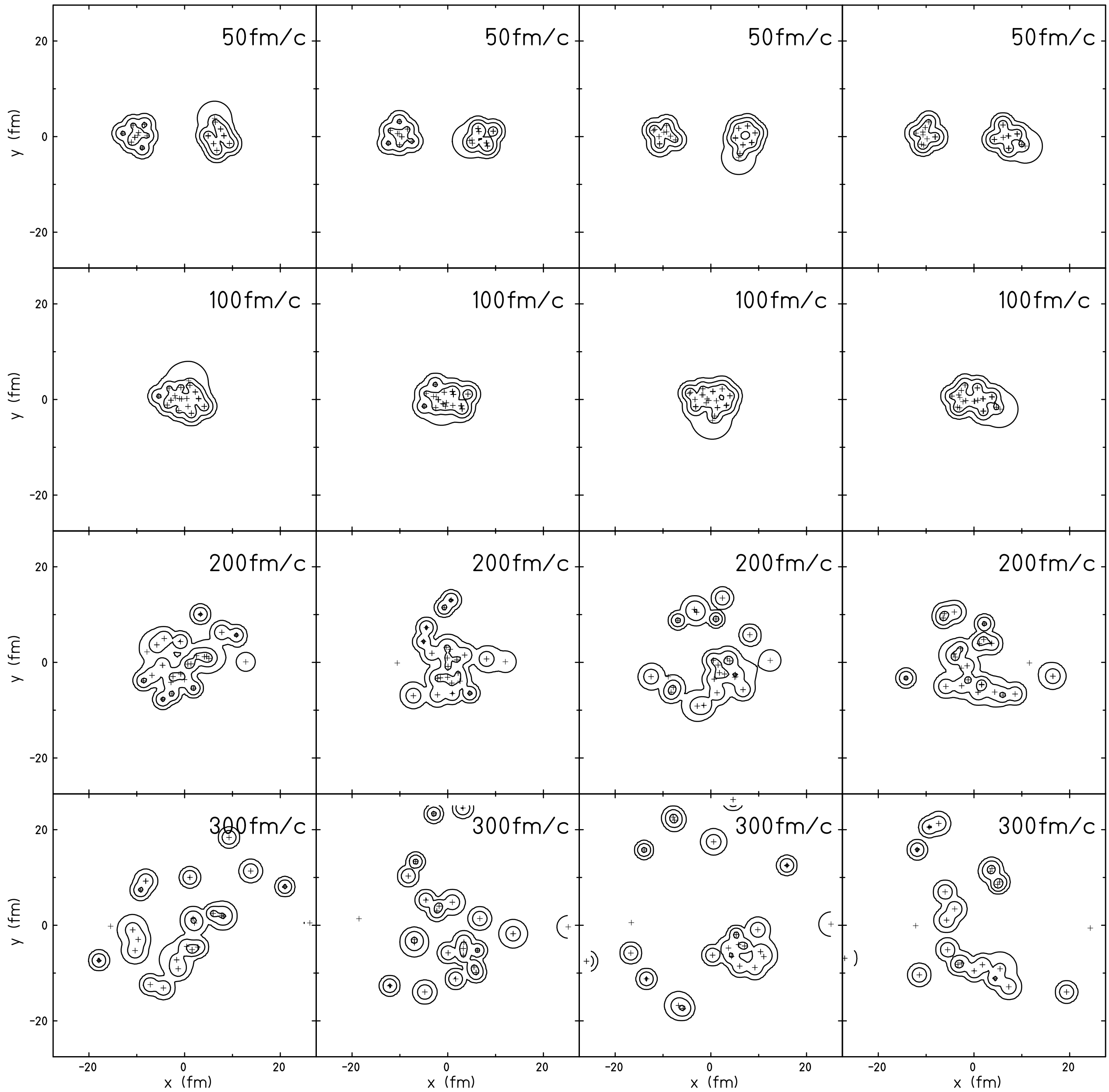


^{40}Ca-^{40}Ca at $E_{Lab} = 35A\,$MeV

K. Hagel et al., Phys. Rev. **C50** (1994) 2017

Multifragmentation - II

^{19}F–^{27}Al at $E_{Lab} = 32A$ MeV and $b = 0.5$ fm:



Role of Dynamical Width Parameter

Important Degree of Freedom for Evaporation and Fragmentation

- A packet with fixed width carries always ≈ 10 MeV zero–point energy.

- A packet with time–dependent width "pays binding with zero–point energy", i.e., it spreads in coordinate space (little overlap) and shrinks in momentum space (less zero–point energy).

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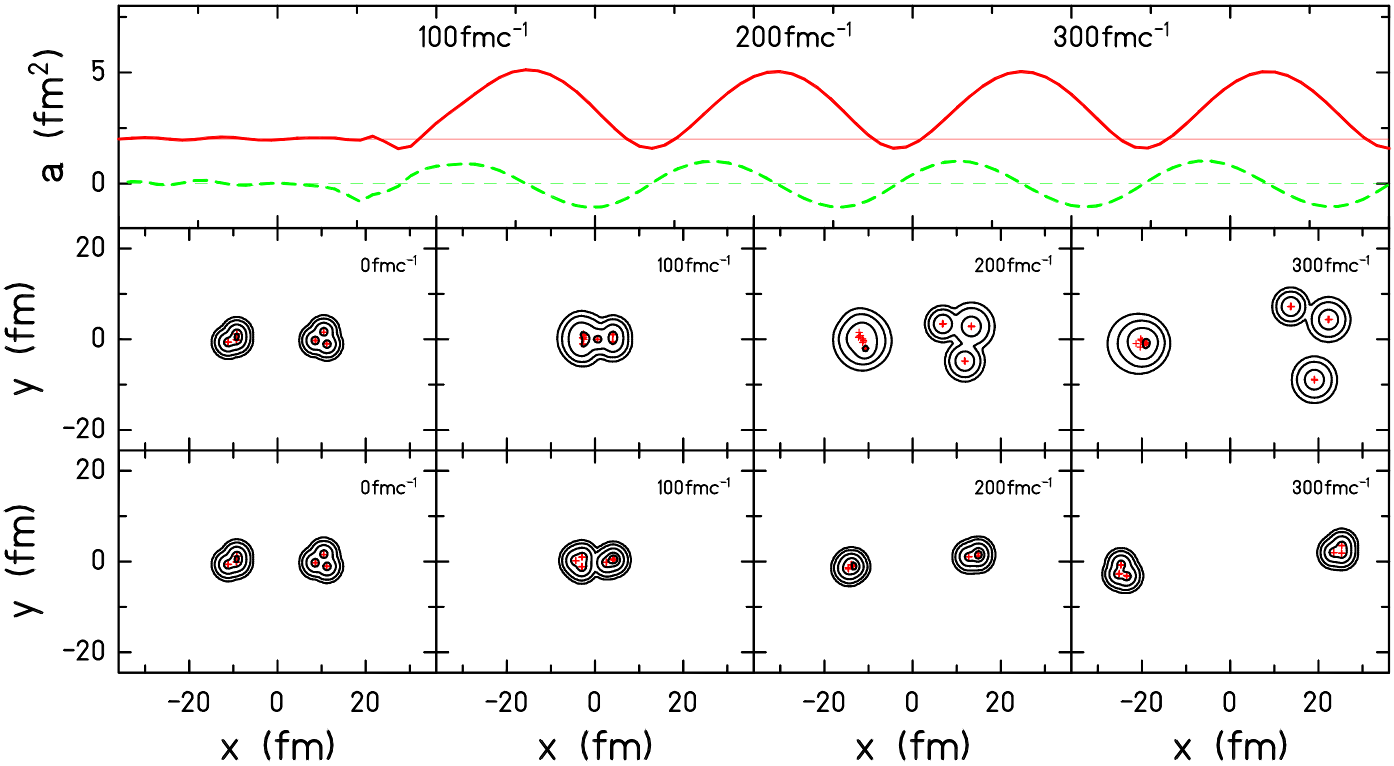
^{12}C–^{12}C (Dynamical & Fixed Width)

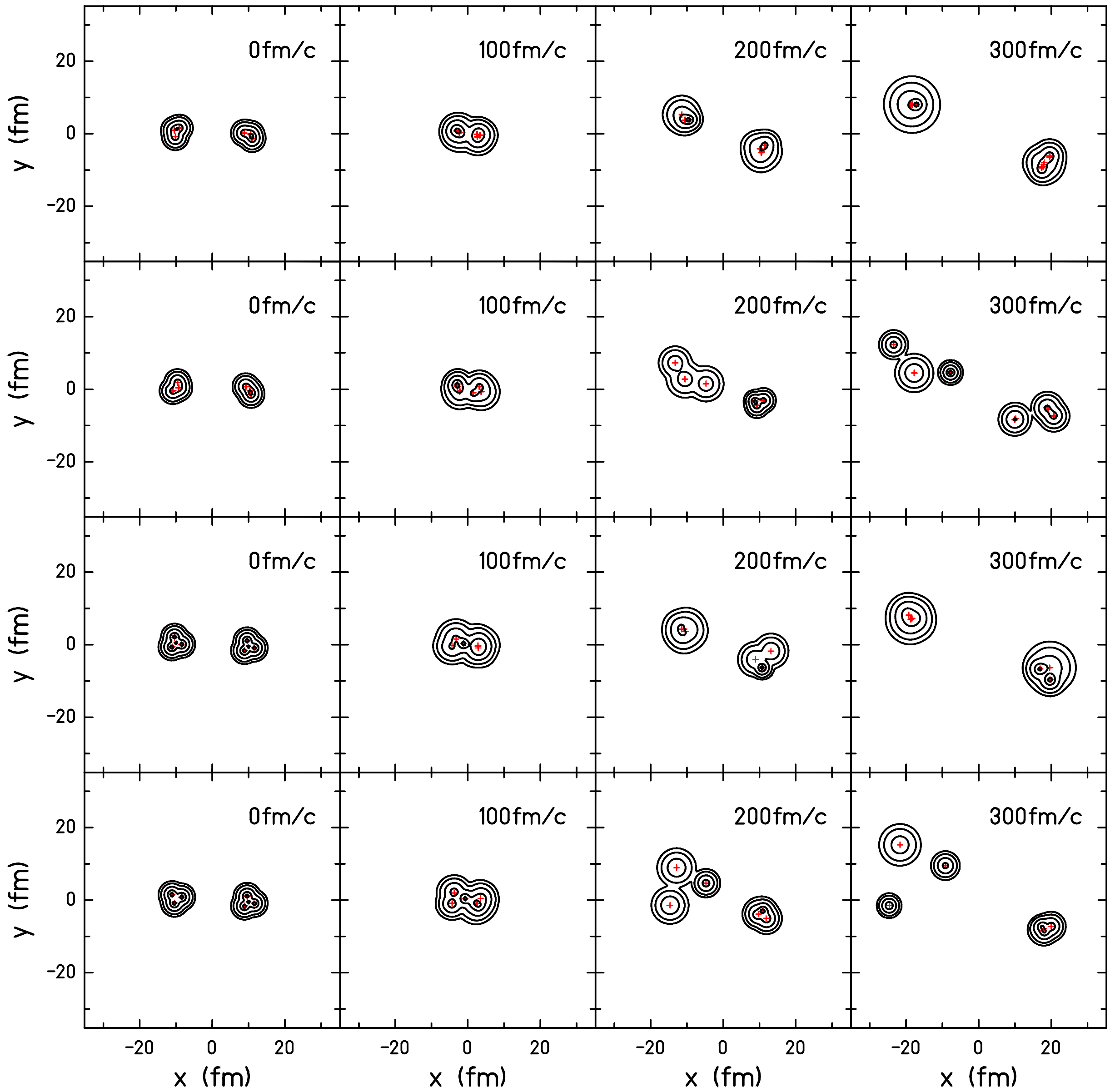


Event Ensemble

- FMD ground states have to be treated like intrinsically deformed Hartree–Fock states.

- The event ensemble consists of all orientations of the two initial ground states: $\mid Q\,; \vec{\Omega}_1, \vec{\Omega}_2\,\rangle$.
  The same holds for the impact parameter.

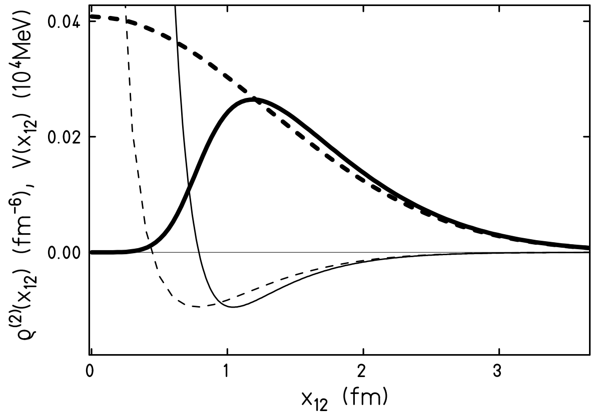
- Within the ensemble large fluctuations arise.

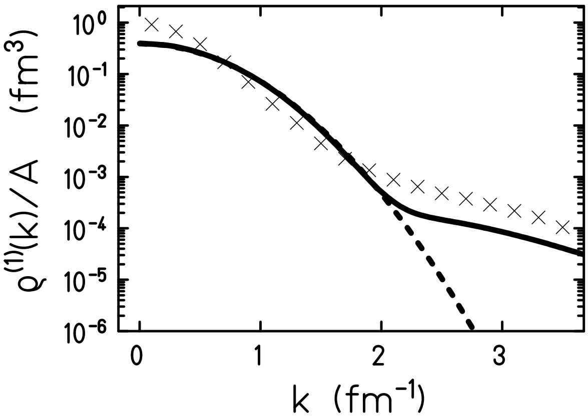


^{12}C-^{12}C at $E_{Lab} = 28.7A\,\mathrm{MeV}$

Unitary Correlation Operator Method

Problem: short range repulsion (e.g. ^{4}He)





Solution: UCOM

- general method to introduce correlations
- idea: suppression of wave function for small relative distances (like Jastrow), but
- unitary and state independent

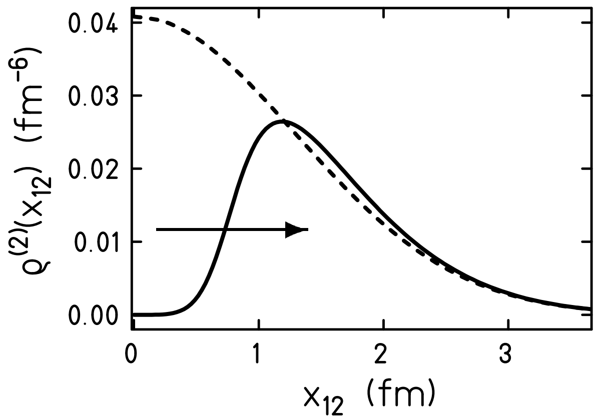
$$|\,\Psi\,\rangle = \underset{\sim}{C}\ |\,\Phi\,\rangle\ , \quad \underset{\sim}{C}^\dagger \underset{\sim}{C} = \underset{\sim}{\mathbb{1}}$$

$$\langle\,\Psi\,|\,\underset{\sim}{B}\,|\,\Psi\,\rangle = \langle\,\Phi\,|\,\underset{\sim}{C}^\dagger \underset{\sim}{B}\,\underset{\sim}{C}\,|\,\Phi\,\rangle = \langle\,\Phi\,|\,\underset{\sim}{B}_{\mathrm{cor}}\,|\,\Phi\,\rangle$$

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

UCOM

Mode of action



Distant-dependent radial shift

$$\langle\, \vec{x}_1\ \vec{x}_2 \,|\, \underset{\sim}{C} \,|\, \Phi \,\rangle$$

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

FMD + UCOM

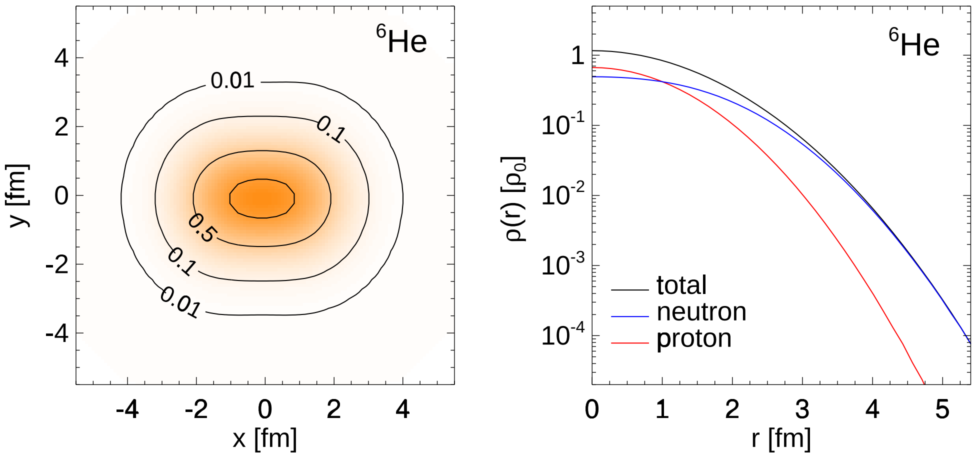
- $\underset{\sim}{C}\ \,|\, Q(t) \,\rangle$ as new trial state
- use of realistic potentials, like BONN, with strong short range repulsion and tensor contributions
  $V_T \propto \frac{3}{r^2}(\vec{\sigma}_1 \cdot \vec{r})(\vec{\sigma}_2 \cdot \vec{r}) - \vec{\sigma}_1 \cdot \vec{\sigma}_2$
- fix correlation operator e.g. at small systems
- cluster expansion for operators, two-body approximation; three-body terms small for nuclear systems, but not for atom-atom potentials[a]

[a] Robert Roth, Diplomarbeit, TU Darmstadt (1998)

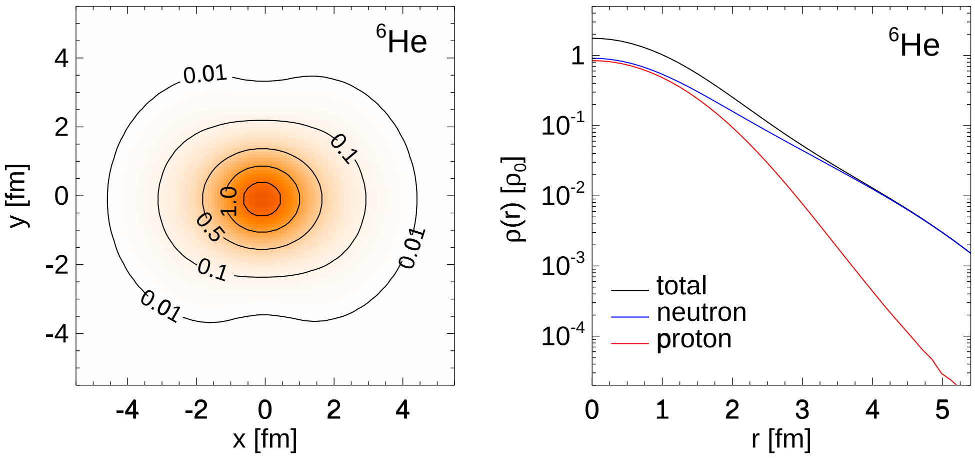
Short and Medium Range Correlations

Superposition of single-particle states or Slater determinants[a]

One gaussian per single-particle state



Two gaussians per single-particle state



- realistic density distribution and correlations, improvement of the surface, gain in binding energy
- with configuration mixing of many Slater determinants long range correlations

[a] Thomas Neff, Diplomarbeit, TU Darmstadt (1998)

Thermodynamics

Canonical ensemble

$$
\begin{aligned}
\underset{\sim}{R} &= \exp\left\{-\frac{1}{T}\underset{\sim}{H}\right\} \\
Z &= \mathrm{tr}\left(\exp\left\{-\frac{1}{T}\underset{\sim}{H}\right\}\right)
\end{aligned}
$$

- Z cannot be evaluated for realistic $\underset{\sim}{H}$
- Idea: replace ensemble average by time average
- Problem: allthough trial states span the Hilbert space, approximate dynamics needs not to be ergodic!

Time averaging of an operator $\underset{\sim}{B}$:

$$
\overline{\langle \underset{\sim}{B} \rangle} = \lim_{t_2\to\infty} \frac{1}{(t_2 - t_1)} \int_{t_1}^{t_2} \mathrm{d}t \, \langle\, Q(t) \,|\, \underset{\sim}{B} \,|\, Q(t) \,\rangle
$$

Classical Mechanics
Hoover–Nosé–Thermostat

Introduction[a b c] **of a pseudo friction coefficient ξ:**

$$
\begin{aligned}
\frac{d}{dt}\,\vec{r}_{\,i} &= \frac{\vec{p}_{\,i}}{m_i} \\
\frac{d}{dt}\,\vec{p}_{\,i} &= -\frac{\partial V}{\partial \vec{r}_{\,i}} - \xi\,\vec{p}_{\,i} \\
\frac{d}{dt}\,\xi &= \frac{1}{M_s}\left(\sum_i \frac{\vec{p}_{\,i}^{\,2}}{2m_i} - \frac{3N}{2}k_B T\right)
\end{aligned}
$$

- this special thermostat uses the equipartition theorem
- $\left(\sum_i \frac{\vec{p}_{\,i}^{\,2}}{2m_i} - \frac{3N}{2}k_B T\right) > 0 \quad \Rightarrow \quad$ cooling
- $\left(\sum_i \frac{\vec{p}_{\,i}^{\,2}}{2m_i} - \frac{3N}{2}k_B T\right) < 0 \quad \Rightarrow \quad$ heating
- does not work in quantum mechanics, equipartition theorem does not exist

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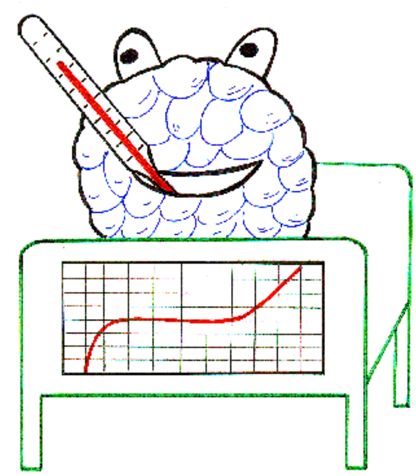
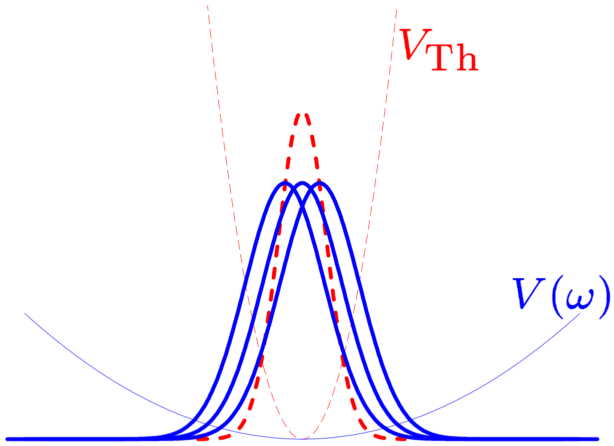
[a] W.G. Hoover, Phys. Rev. **A31** (1985) 1685

[b] S. Nosé, Prog. of Theor. Phys. Suppl. **103**(1991) 1

[c] D. Kusnezov, A. Bulgac, W. Bauer, Ann. of Phys. **204** (1990) 155

Coupling to a Thermometer





Procedure:

- **excited nucleus:** self-bound liquid drop in a large container (harmonic oscillator)
  $\underset{\sim}{H}_{\mathrm{N}} = \underset{\sim}{T}_{\mathrm{N}} + \underset{\sim}{V}_{\mathrm{NN}} + \underset{\sim}{V}(\omega)$,

- **thermometer:** single wave packet in a second oscillator with ω_{Th}, ideal gas thermometer
  $\underset{\sim}{H}_{\mathrm{Th}} = \underset{\sim}{T}_{\mathrm{Th}} + \underset{\sim}{V}_{\mathrm{Th}}$,

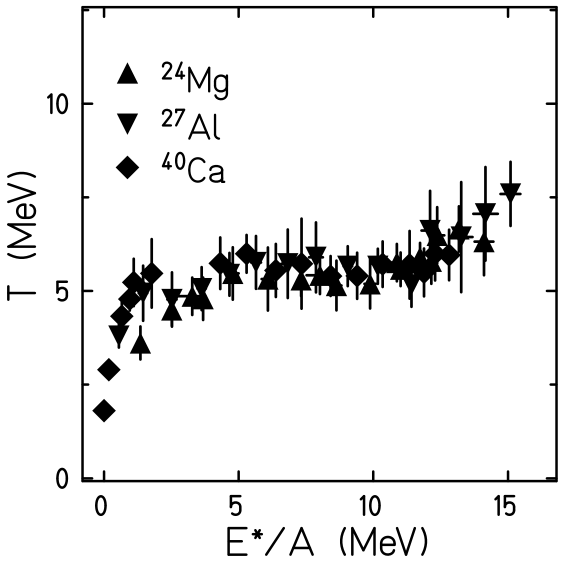
- **coupling** of all nucleons to the thermometer wave packet:
  $\underset{\sim}{V}_{\mathrm{N-Th}}$, $\quad \underset{\sim}{H} = \underset{\sim}{H}_{\mathrm{N}} + \underset{\sim}{H}_{\mathrm{Th}} + \underset{\sim}{V}_{\mathrm{N-Th}}$,

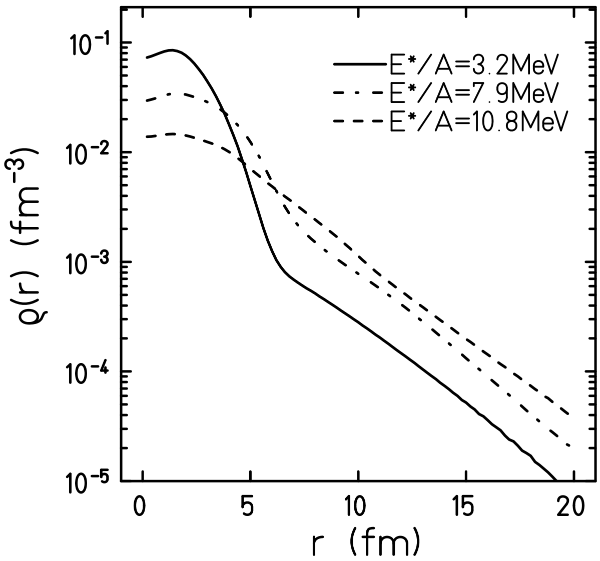
  $\mid Q(t) \,\rangle = \;\mid \textit{nucleus} \,\rangle \otimes \;\mid \textit{thermometer} \,\rangle$,

- **time-averaging:**
  $$E_{\mathrm{Th}} = \overline{\langle\, \underset{\sim}{H}_{\mathrm{Th}} \,\rangle}\Big|_{\langle \underset{\sim}{H} \rangle} \;, \qquad E^* = \overline{\langle\, \underset{\sim}{H}_{\mathrm{N}} - E_0 \,\rangle}\Big|_{\langle \underset{\sim}{H} \rangle} \;,$$

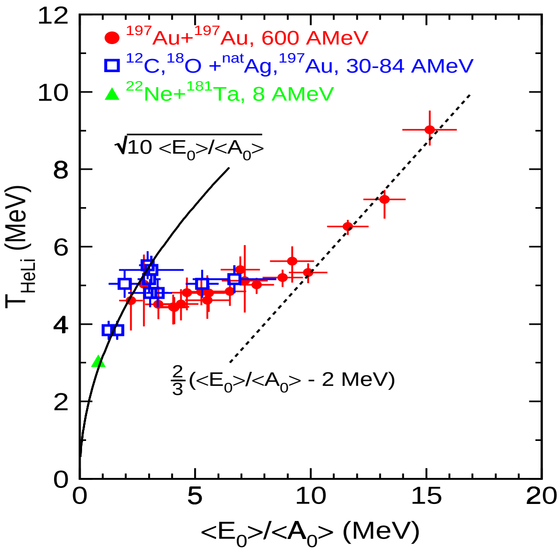
- **zeroth law:** both subsystems approach the same T
  $$T = \omega_{Th} \left[\ln \left(\frac{E_{\mathrm{Th}} + \frac{3}{2}\omega_{Th}}{E_{\mathrm{Th}} - \frac{3}{2}\omega_{Th}} \right) \right]^{-1}$$

Caloric Curve





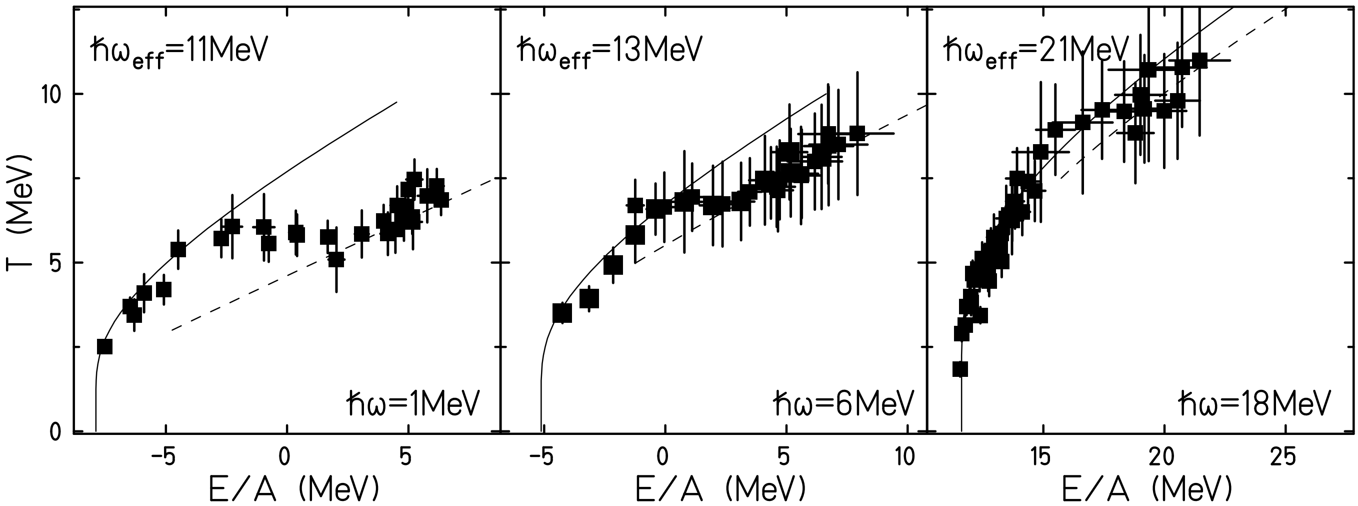
J. Pochodzalla et al., Phys. Rev. Lett. 75 (1995) 1040:



- simulation: equilibrium due to evolution in container over long time, ideal gas thermometer
- experiment: event–ensemble shows equilibrium properties, chemical thermometer

Caloric Curve
Critical Temperature

Critical temperature of ^{16}O:



- ω serves as external parameter like volume or pressure
- critical point: latent heat vanishes
- system finite and charged: $T_c = T_c(N, Z)$

Summary

- TDVP allows approximate quantum time evolution
- system ($\underset{\sim}{H}$) and observables of interest determine how sophisticated trial state $|\, Q(t)\, \rangle$ must be
- FMD: $|\, Q(t)\, \rangle$ is Slater determinant of Gaussian wave packets; trial state may be improved with UCOM and configuration mixing
- FMD describes nuclear ground states and dynamics, e.g. fusion, evaporation, deeply inelastic reactions, fragmentation
- thermodynamic properties can be extracted from time evolution via thermometer and time averaging
- FMD describes an equilibrium caloric curve of finite nuclear systems and a nuclear liquid gas phase transition

Problems to solve

- tunneling, branching
- tensor correlations

FMD Literature

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   Contents: Statistical Properties of Fermionic Molecular Dynamics

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   Contents: The nuclear liquid-gas phase transition within Fermionic Molecular Dynamics

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   Contents: Unitary Correlation Operator Method