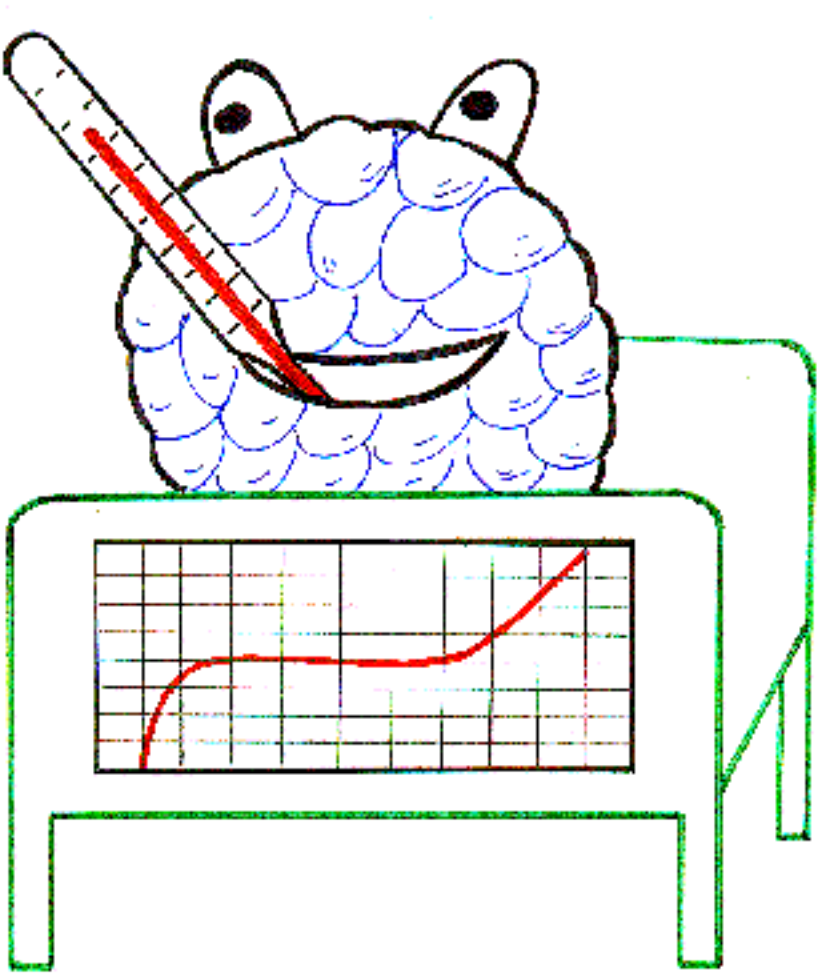
Fermionic Molecular Dynamics and the Nuclear Liquid-Gas Phase Transition

H. Feldmeier, T. Neff, R. Roth, J. Schnack;
GSI Darmstadt



H. Feldmeier, K. Bieler, J. Schnack, Nucl. Phys. **A586** (1995) 403

J. Schnack, H. Feldmeier, Nucl. Phys. **A601** (1996) 181

J. Schnack, PhD thesis, TH Darmstadt (1996)

Aim and Problems

Aim:

- **heavy-ion collisions:** $0 \leq \ E/A \ \leq 200$MeV, fusion, incomplete fusion, dissipative reactions, fragmentation, sequential decay, evaporation

- **nuclear ground-state properties:** energies and radii, densities, short range correlations;
  $\Rightarrow$ absolutely necessary condition

- **statistical properties of finite fermi systems:** definition of temperature for strongly interacting systems, phase transitions

---

Problems $\Rightarrow$ Ansatz:

- quantum objects $\Leftrightarrow$ Heisenberg uncertainty principle
  $\Rightarrow$ single-particle wave-packets

- fermions $\Leftrightarrow$ Pauli principle
  $\Rightarrow$ antisymmetrized many-body state

- hard core of NN-interaction $\Leftrightarrow$ short range correlations
  $\Rightarrow$ correlated trial state

Model States

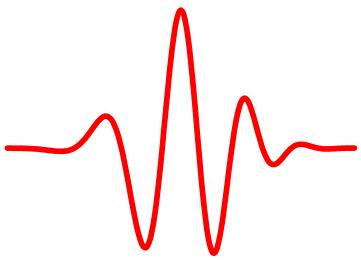
Uncorrelated many-body state (Slater determinant):

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

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

Single-particle states (gaussian wave packets):

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



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

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

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

$a(t)$: complex width

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

ξ : isospin 3-component

Gaussian wave packets are not orthogonal.

Equations of Motion

The time-dependent variational principle:

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

Euler–Lagrange equations in their most general form:

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

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

- purely geometrical object
- not depending on the Hamilton operator $\underset{\sim}{H}$
- Pauli principle in $\mathcal{A}_{\mu\nu}(Q(t))$ and exchange terms of $\langle \, Q(t) \, | \, \underset{\sim}{H} \, | \, Q(t) \, \rangle$

Thermodynamic Properties
Idea: Time-Averaging

Ergodic ensemble and statistical operator $\underset{\sim}{R}_{\rm erg}$:

$$\underset{\sim}{R}_{\rm erg} \quad := \quad \lim_{t_2 \to \infty} \frac{1}{(t_2 - t_1)} \int_{t_1}^{t_2} {\rm d}t \; |\, Q(t) \,\rangle\langle\, Q(t) \,|$$

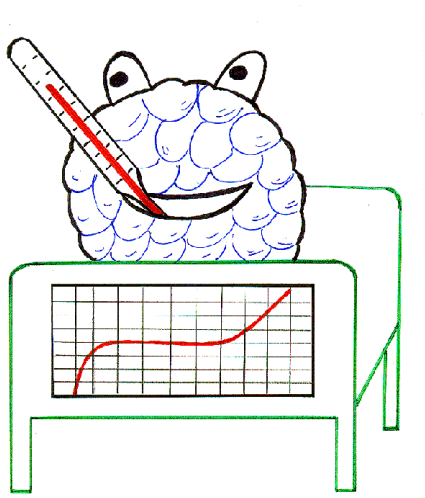
The ergodic mean of an operator $\underset{\sim}{B}$:

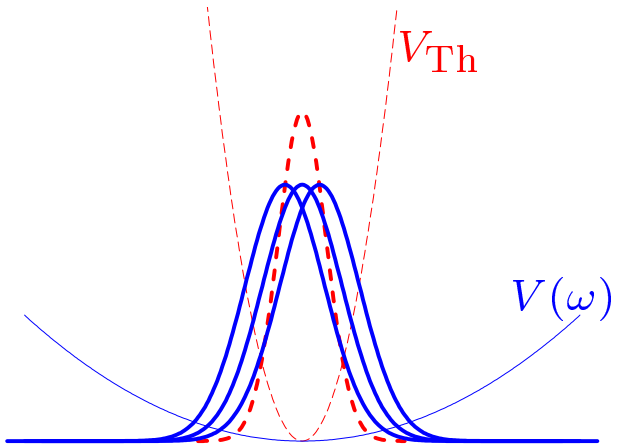
$$\overline{\langle\, \underset{\sim}{B} \,\rangle}\Big|_{\langle\, \underset{\sim}{H} \,\rangle} \quad := \quad {\rm Tr}\,(\underset{\sim}{R}_{\rm erg}\; \underset{\sim}{B})$$

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

- time–averaging instead of ensemble–averaging,
- ergodic assumption: $\underset{\sim}{R}_{\rm erg}$ depends only on $\langle\, \underset{\sim}{H} \,\rangle$ and $|\, Q(t) \,\rangle$ covers the available phase space,
- $\langle\, \underset{\sim}{H} \,\rangle$ is a constant of motion.

Phase Transition – 1
Idea





Procedure:

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

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

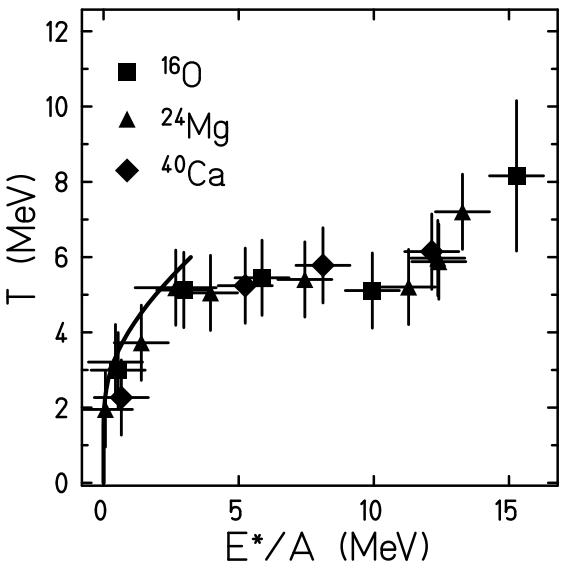
- **coupling** of all nucleons to the thermometer wave-packet:
  $\underset{\sim}{V}_{\rm N-Th}$, $\underset{\sim}{H} = \underset{\sim}{H}_{\rm N} + \underset{\sim}{H}_{\rm Th} + \underset{\sim}{V}_{\rm N-Th}$,
  $|\, Q(t) \,\rangle = |\, nucleus \,\rangle \otimes |\, thermometer \,\rangle$,

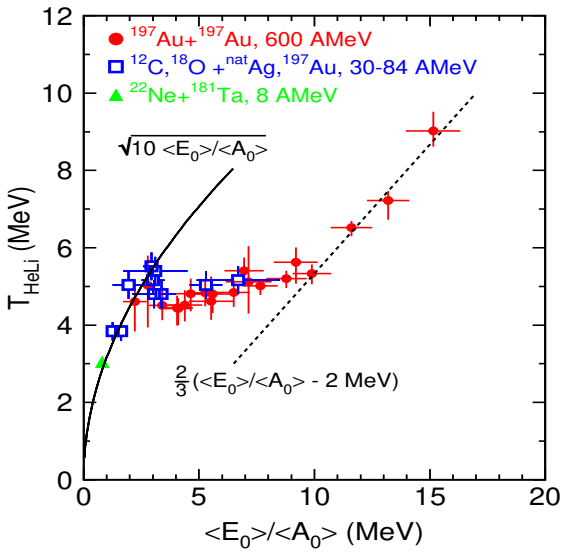
- **time-averaging:**
  $$E_{\rm Th} = \overline{\langle\, \underset{\sim}{H}_{\rm Th} \,\rangle}\Big|_{\langle\, \underset{\sim}{H} \,\rangle}, \qquad E^* = \overline{\langle\, \underset{\sim}{H}_{\rm N} - E_0 \,\rangle}\Big|_{\langle\, \underset{\sim}{H} \,\rangle},$$

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

Phase Transition – 2
Caloric Curve

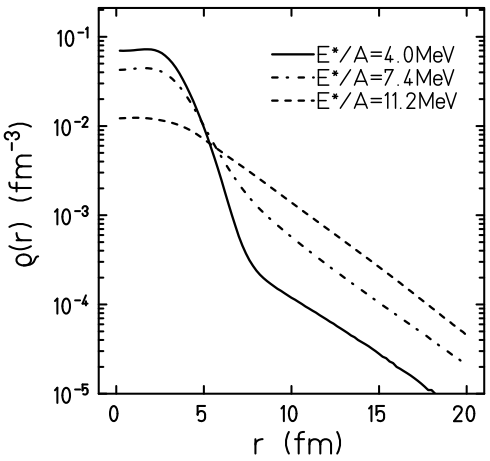
Caloric Curve for excited ^{16}O, ^{24}Mg and ^{40}Ca:





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

Radial distribution of the density (^{24}Mg):

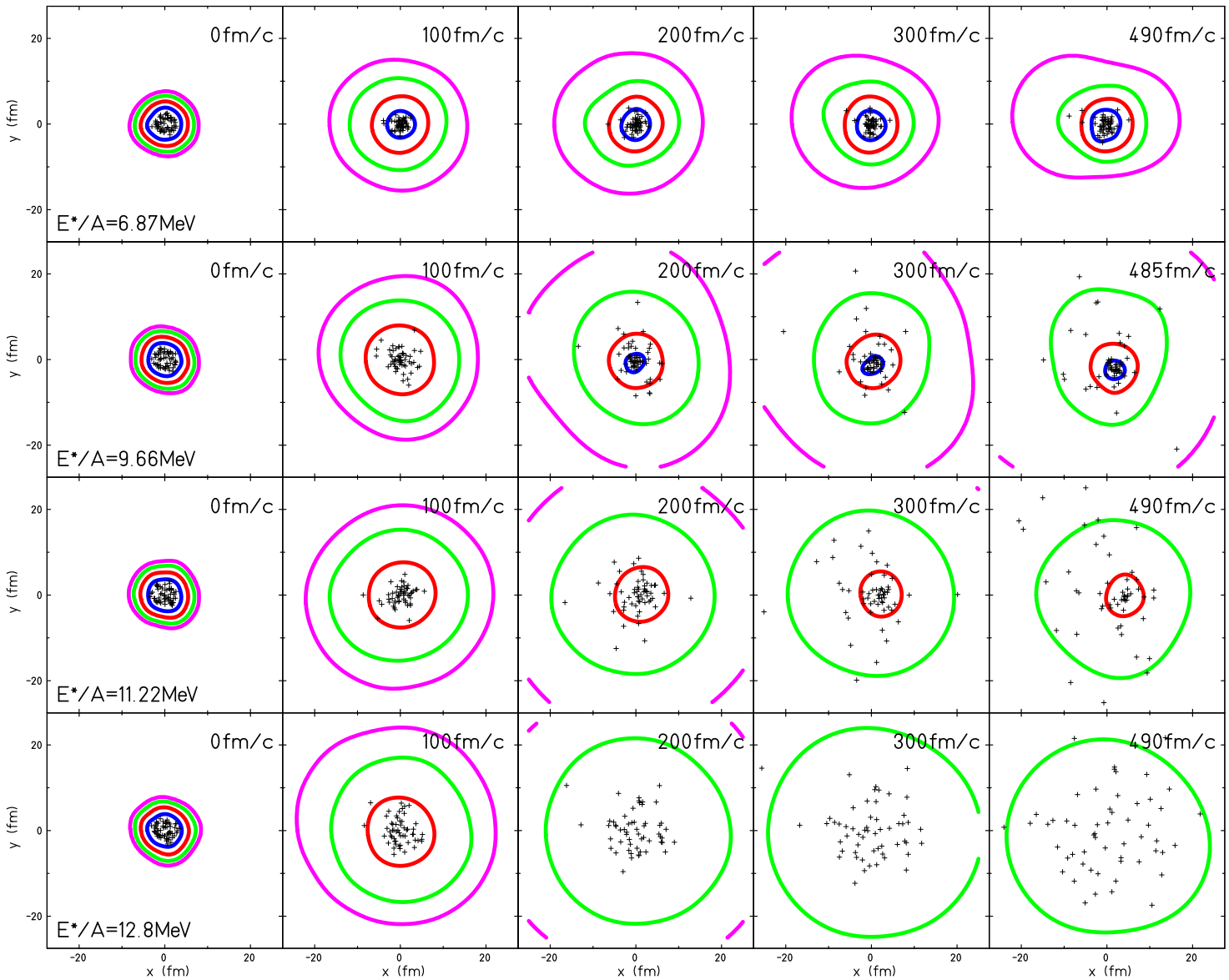


liquid drop

and vapour around

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

Randomly Excited ^{56}Fe



scale: 0.5, 0.1, 0.01, 0.001 (fm^{-2} ($\rho(\vec{x})$ integrated over z

- evolution without container,
- E^* ↑: evaporation $\longrightarrow$ blast,
- thermal expansion, small E^* contraction & residue, residue vanishes at $E^*/A \approx 11$MeV,
- no condensation in low density areas (real?)

Summary

- FMD describes finite charged fermi systems,
- ansatz: antisymmetrized many–body state of single–particle Gaussian wave packets,
- equations of motion and ground states follow from variational principles,
- liquid–gas phase transition of finite charged nuclei: first order, phase separation,
- randomly excited system: blast, no condensation in expanding low density, time too short to rebuild correlations,
- scaled system: low density, contraction, expansion, fragmentation; correlations survived partially,
  more randomness $\Rightarrow$ less multifragmentation,
- random $\neq$ thermal: coexistence region consists of droplets and vapour (not uniform)