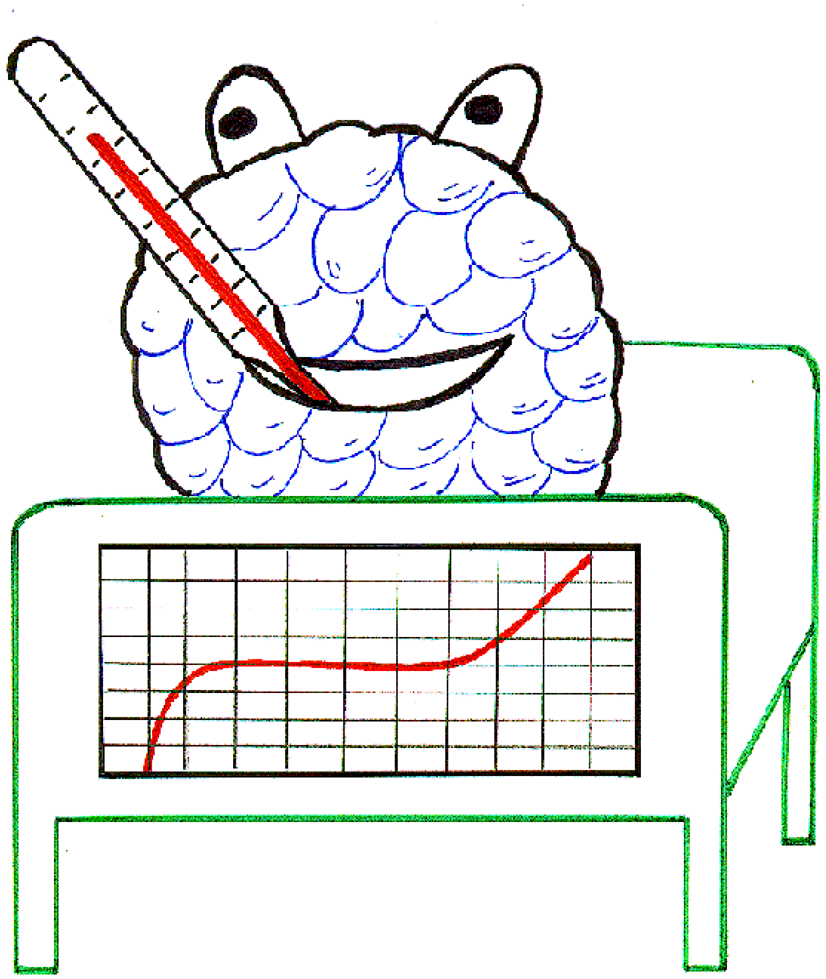
Statistical Properties of FMD and the Nuclear Liquid-Gas Phase Transition

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:** $0 \le \ E/A \ \le 100$MeV, fusion, incomplete fusion, dissipative reactions, fragmentation, sequential decay, evaporation

- **nuclear ground-state properties:** energies and radii, densities, short range correlations

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

---

Problems and Ansatz:

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

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

- dense system $\Leftrightarrow$ large overlap of wave packets
  $\Rightarrow$ no density-expansion possible

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

Contents

The Model:

- many-body state
- single-particle wave packet
- correlation operator
- equations of motion

Thermo*dynamic* **properties of the model:**

- ergodic ensemble: time-averaging
- example system: fermions in a harmonic oscillator
- identification of the temperature
- comparison: Fermi-Dirac versus Maxwell-Boltzmann

The nuclear liquid-gas phase transition in FMD:

- definition of a thermometer
- excited nucleus in a container potential

Model States

Uncorrelated many-body state (Slater determinant):

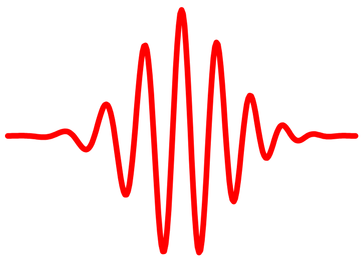
$$
\begin{aligned}
|\, Q(t)\,\rangle &= \frac{1}{\langle\, \widehat{Q}(t)\,|\,\widehat{Q}(t)\,\rangle^{\frac{1}{2}}}\ |\,\widehat{Q}(t)\,\rangle \\
|\,\widehat{Q}(t)\,\rangle &= \frac{1}{A!}\sum_{\pi} \mathrm{sgn}(\pi)\ |\, q_{\pi(1)}(t)\,\rangle \otimes \cdots \otimes |\, q_{\pi(A)}(t)\,\rangle
\end{aligned}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

Correlated many-body state:

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

Single-particle state (gaussian wave packet):

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



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

$\vec{r}(t)$: 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.

The Correlated Trial State

The unitary correlation operator $\underset{\sim}{C}$:

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

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:

$$\underset{\sim}{S} = \frac{1}{(2\pi)^6} \int \mathrm{d}^3x_1\ \mathrm{d}^3x_2\ \mathrm{d}^3k_1\ \mathrm{d}^3k_2 \int \mathrm{d}^3u_1\ \mathrm{d}^3u_2\ \mathrm{e}^{i\vec{k}_1\cdot\vec{u}_1}\mathrm{e}^{i\vec{k}_2\cdot\vec{u}_2}$$

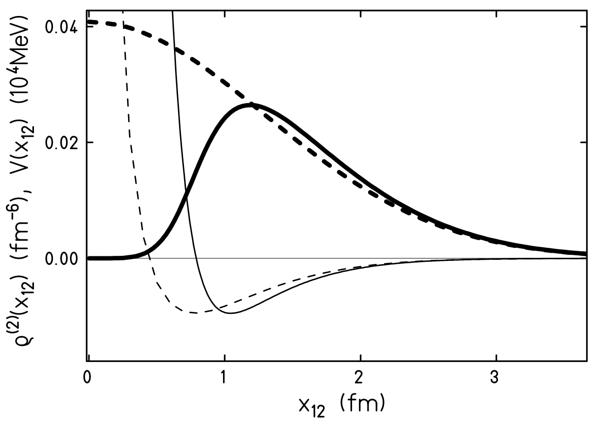
$$\times O(\vec{x}_1,\vec{x}_2;\vec{k}_1,\vec{k}_2)\ \underset{\sim}{\Psi}^\dagger(\vec{x}_1+\frac{\vec{u}_1}{2})\underset{\sim}{\Psi}^\dagger(\vec{x}_2+\frac{\vec{u}_2}{2})\underset{\sim}{\Psi}(\vec{x}_2-\frac{\vec{u}_2}{2})\underset{\sim}{\Psi}(\vec{x}_1-\frac{\vec{u}_1}{2})$$

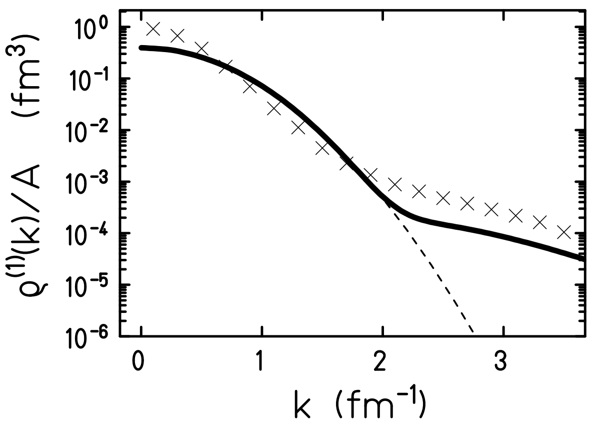
Translational, rotational and Galilei invariance:

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

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

Densities of ^{4}He:





Expectation Values

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

$$\langle \underset{\sim}{Q} \rangle = \langle Q \,|\, \underset{\sim}{C}^\dagger \underset{\sim}{Q}\, \underset{\sim}{C} \,|\, Q \rangle$$

- $\underset{\sim}{C}$ contains operators to all particle numbers
- $\underset{\sim}{C}^\dagger \underset{\sim}{Q}\, \underset{\sim}{C}$ ordered with respect to n-particle operators

$$\underset{\sim}{Q}_{\text{eff}} := \underset{\sim}{C}^\dagger \underset{\sim}{Q}\, \underset{\sim}{C} = \sum_{n=0}^{\infty} \underset{\sim}{Q}_{\text{eff}}^{(n)}$$

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

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

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

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

Equations of Motion

The time-dependent variational principle:

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

Euler–Lagrange equations in their most general form:

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

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

- purely geometrical object
- not depending on the Hamilton operator $\underset{\sim}{H}$
- not depending on the correlation operator $\underset{\sim}{C}$
- Pauli principle

Generalized Poisson brackets:

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

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

Thermodynamic Properties
Idea: Time-Averaging

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

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

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

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

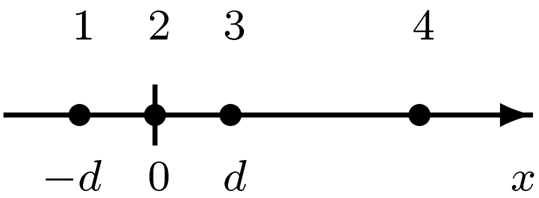
$$= \quad \lim_{t_2 \to \infty} \frac{1}{(t_2 - t_1)} \int_{t_1}^{t_2} \mathrm{d}t \; \langle\, Q(t) \,|\, \underset{\sim}{B} \,|\, Q(t) \,\rangle$$

- $|\, Q(t) \,\rangle$ trial state of the model,
- time–averaging instead of ensemble–averaging,
- ergodic assumption: $\underset{\sim}{R}_{\text{erg}}$ depends only on $\langle\, \underset{\sim}{H} \,\rangle$, but not on $|\, Q(t_1) \,\rangle$, $\underset{\sim}{H}$ or the equations of motion,
- $\langle\, \underset{\sim}{H} \,\rangle$ is a constant of motion,

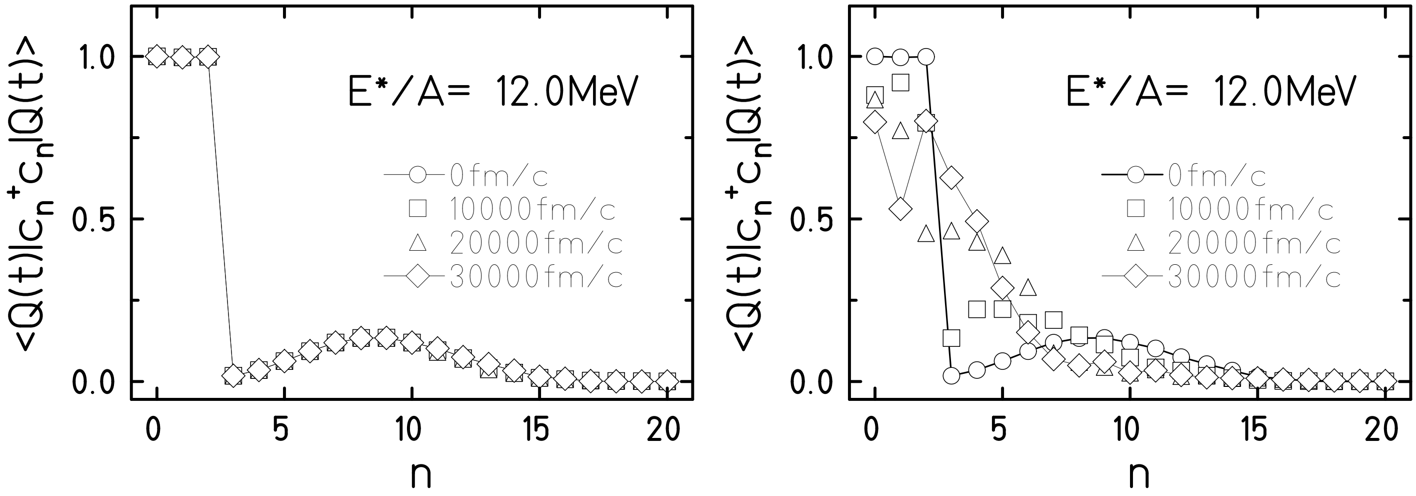
Example
1-dimensional Harmonic Oscillator

Initialization:

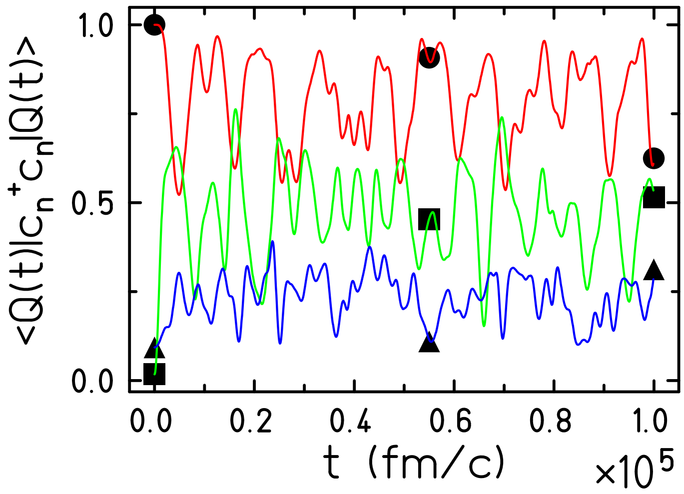
T (MeV)	E^*/A (MeV)
5	0.75
10	3.63
20	12.02
30	21.41



Time evolution without and with small interaction:

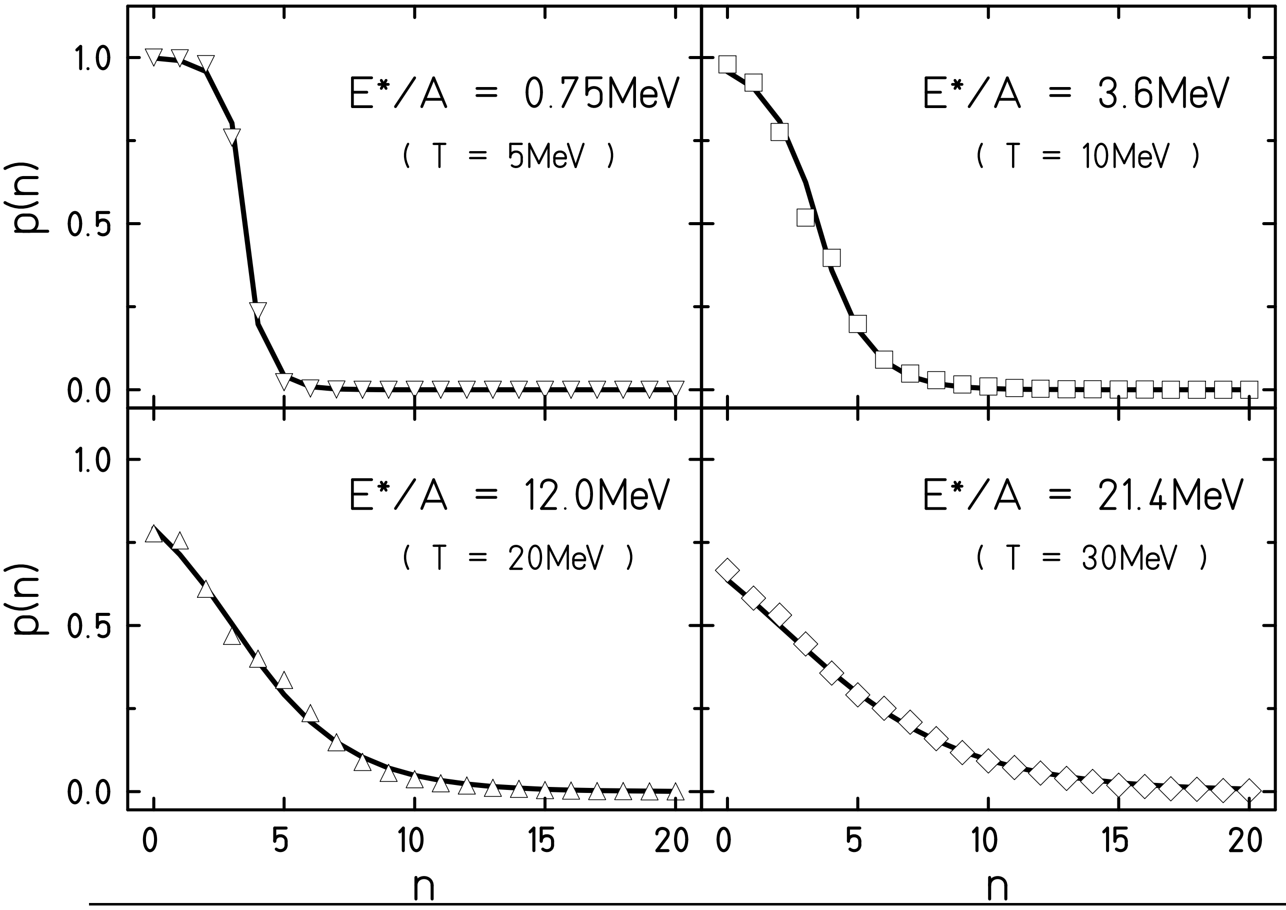


Time evolution of the occupation numbers:



Example
1-dimensional Harmonic Oscillator

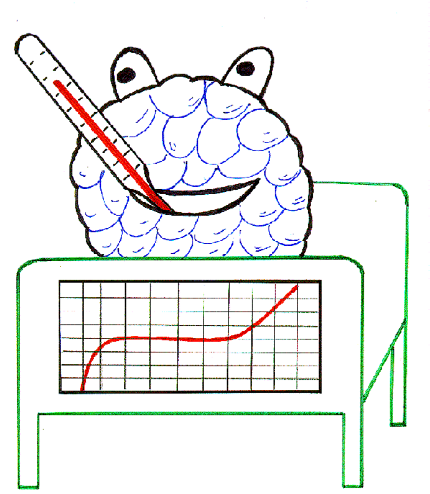
Occupation numbers in the ergodic ensemble:

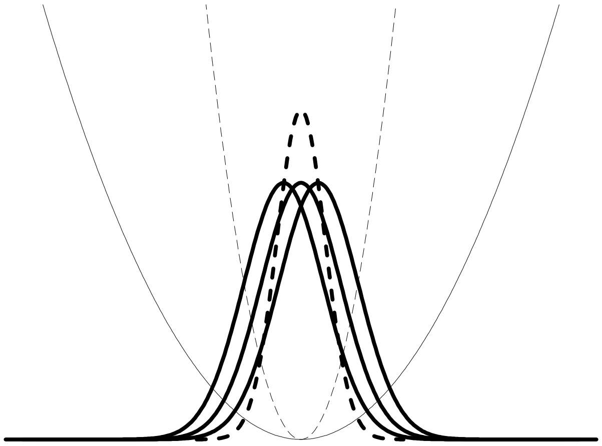


- time–averaging over about 2000 periods,
- ergodic and canonical ensemble give the same occupation numbers at the same excitation energy,
  $\Rightarrow$ correct relation between E and T
- FMD many–body trajectory covers the phase space according to Fermi–Dirac statistics.

Phase Transition – 1
Idea

Arrangement:





Procedure:

- time evolution of an excited nucleus in a container potential of a harmonic oscillator with small ω_C:
  $\underset{\sim}{H}_{\mathrm{N}} = \underset{\sim}{T}_{\mathrm{N}} + \underset{\sim}{V}_{\mathrm{NN}} + \underset{\sim}{V}_{\mathrm{C}}$,

- coupling of all nucleons to a single wave-packet in a second oscillator with ω_{Th}, this is the thermometer:
  $\underset{\sim}{H}_{\mathrm{Th}} = \underset{\sim}{T}_{\mathrm{Th}} + \underset{\sim}{V}_{\mathrm{Th}} + \underset{\sim}{V}_{\mathrm{N-Th}}$,

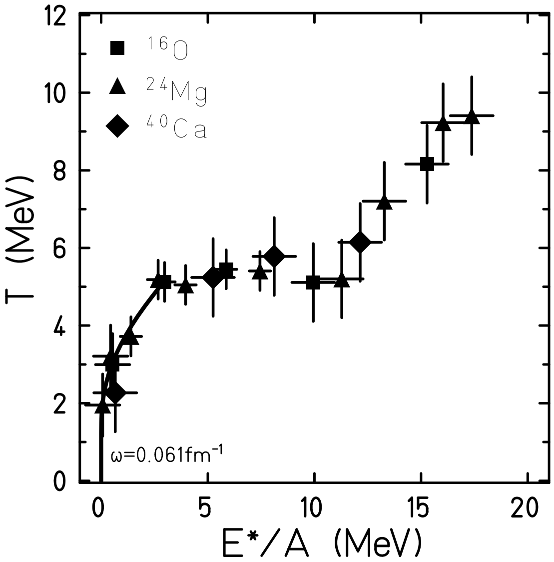
- time-averaging of the excitation energy of the thermometer wave-packet in its oscillator:
  $E_{\mathrm{Th}} = \overline{\langle \, \underset{\sim}{T}_{\mathrm{Th}} + \underset{\sim}{V}_{\mathrm{Th}} \, \rangle}\Big|_{\langle \, \underset{\sim}{H} \, \rangle}$,

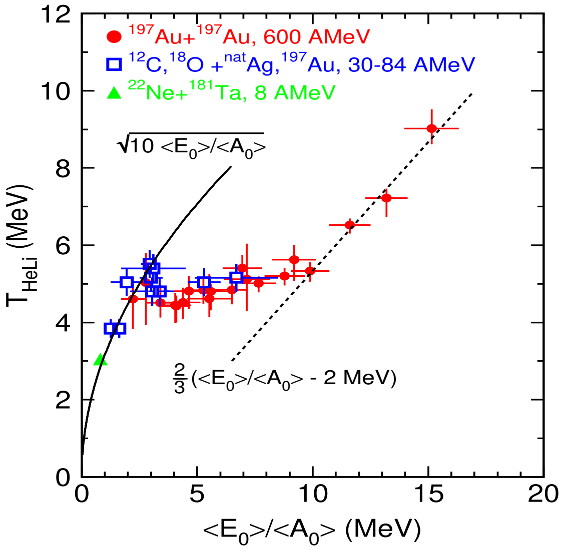
- ergodic assumption: both systems approach the same temperature

$$T = \omega \left[\ln \left(\frac{E_{\mathrm{Th}} + \frac{3}{2}\omega}{E_{\mathrm{Th}} - \frac{3}{2}\omega} \right) \right]^{-1}$$

Phase Transition – 2
Caloric Curve

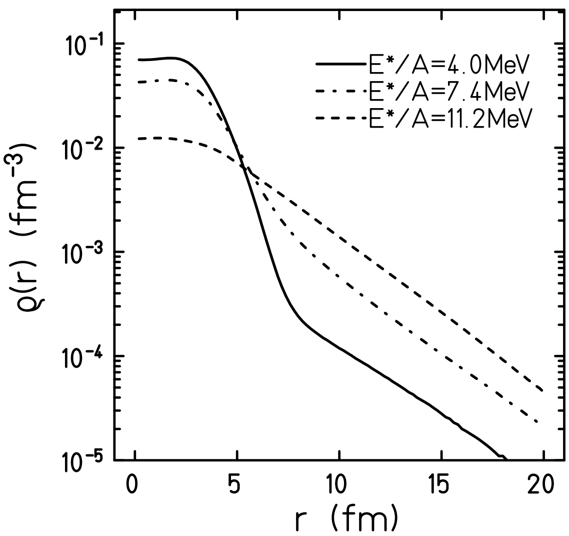
Caloric Curve for excited ^{16}O, ^{24}Mg and ^{40}Ca:





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

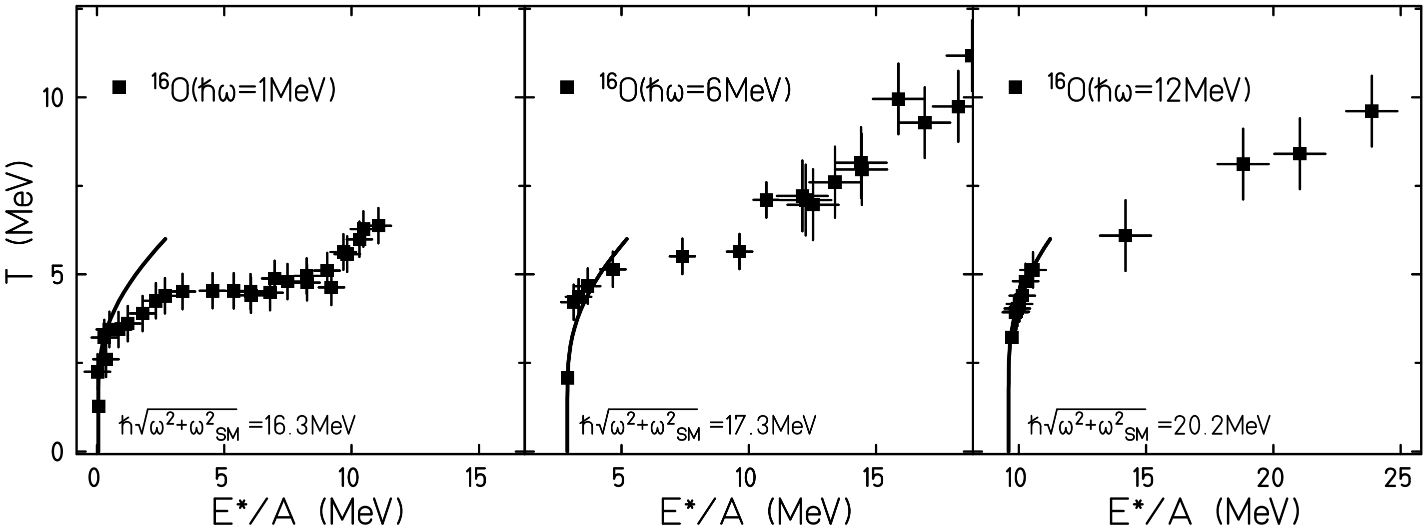
Radial distribution of the density (^{24}Mg):



- simulation: contained, thermodynamic equilibrium, slow
- experiment: in vacuum, nonequilibrium, fast

Phase Transition – 3
Critical Temperature

Critical temperature of ^{16}O:



Summary:

- FMD describes finite charged fermi systems
- Ansatz: correlated Slater determinant of single–particle Gaussian wave packets
- equations of motion and ground states follow from variational principles