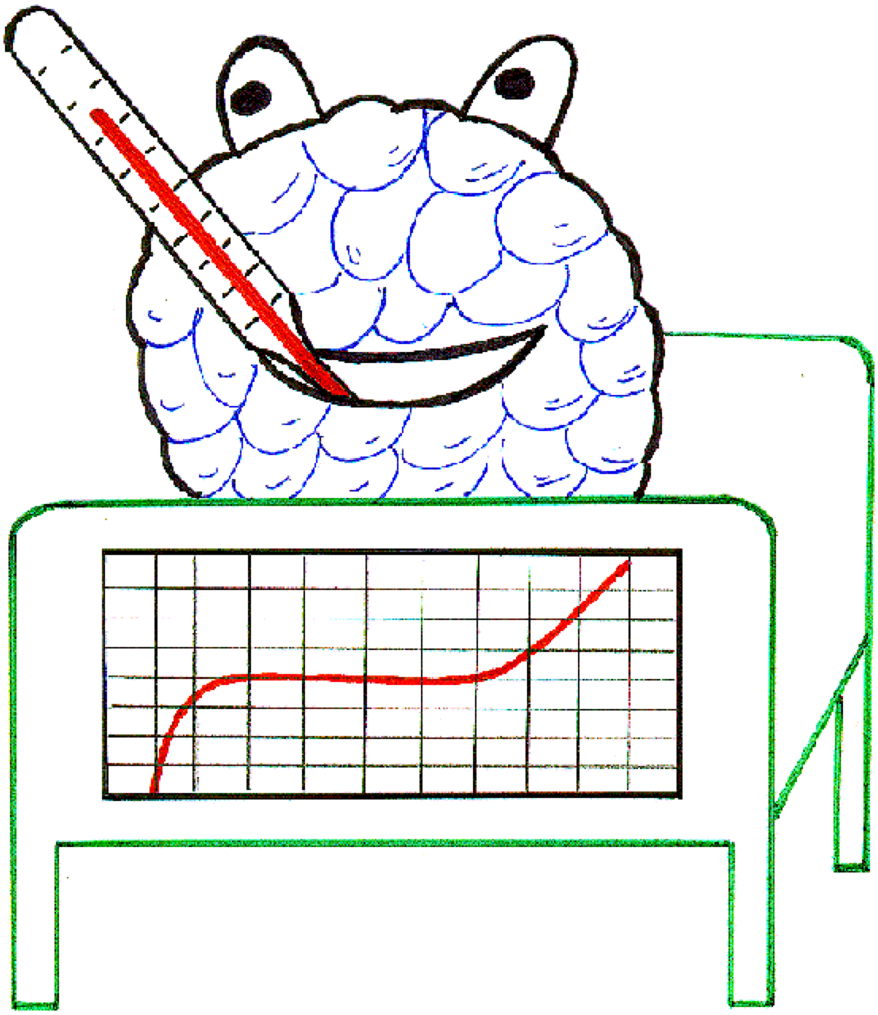
Statistical Properties of Fermionic Molecular Dynamics

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



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

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

Why ?

Why are statistical properties of a dynamical model important?

Dynamical microscopic models like FMD are designed to describe fragmentation reactions and especially the observed isotope multiplicities which to a large extend are governed by:

- the correct ground state properties (binding energies, shell effects),
- population of the Hilbert space with the correct weight of Fermi-Dirac statistics,
- thermalization properties induced by the nucleon-nucleon interaction.

Questions

What are the thermo*static* properties of the model?

- model states
- resolution of unity
- partition function

What are the 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

How can one investigate the caloric curve in FMD?

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

Thermostatic Properties – 1
Model States

Many-body state:

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

Single-particle state (gaussian wave packet):

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

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

$\vec{r}$: mean position

$\vec{p}$: mean momentum

a : complex width

χ, ϕ : spin angles

ξ : isospin 3-component

Gaussian wave packets are not orthogonal.

Thermostatic Properties – 2
Resolution of Unity

One-body space – coherent states (overcomplete):

$$\underset{\sim}{\vec{a}}\ |\,\vec{z}\,\rangle = \vec{z}\ |\,\vec{z}\,\rangle$$

$$\begin{aligned}
\underset{\sim}{\mathbb{1}}^{(1)} &= \int \frac{\mathrm{d}^3\mathrm{Re}\,(z)\ \mathrm{d}^3\mathrm{Im}\,(z)}{\pi^3}\ \frac{|\,\vec{z}\,\rangle\langle\,\vec{z}\,|}{\langle\,\vec{z}\,|\,\vec{z}\,\rangle} \\
&= \int \frac{\mathrm{d}^3 r\ \mathrm{d}^3 p}{(2\pi)^3}\ \frac{|\,q\,\rangle\langle\,q\,|}{\langle\,q\,|\,q\,\rangle}
\end{aligned}$$

Many-body space – resolution of unity:

$$\underset{\sim}{\mathbb{1}}^{(A)} = \int \mathrm{d}\mu(Q)\ |\,Q\,\rangle\langle\,Q\,|$$

$$\mathrm{d}\mu(Q) = \langle\,\hat{Q}\,|\,\hat{Q}\,\rangle \prod_{k=1}^{A} \frac{1}{\langle\,q_k\,|\,q_k\,\rangle}\,\frac{\mathrm{d}^3 r_k\ \mathrm{d}^3 p_k}{(2\pi)^3}$$

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

Inclusion of the width degree of freedom and spin and isospin is straightforward.

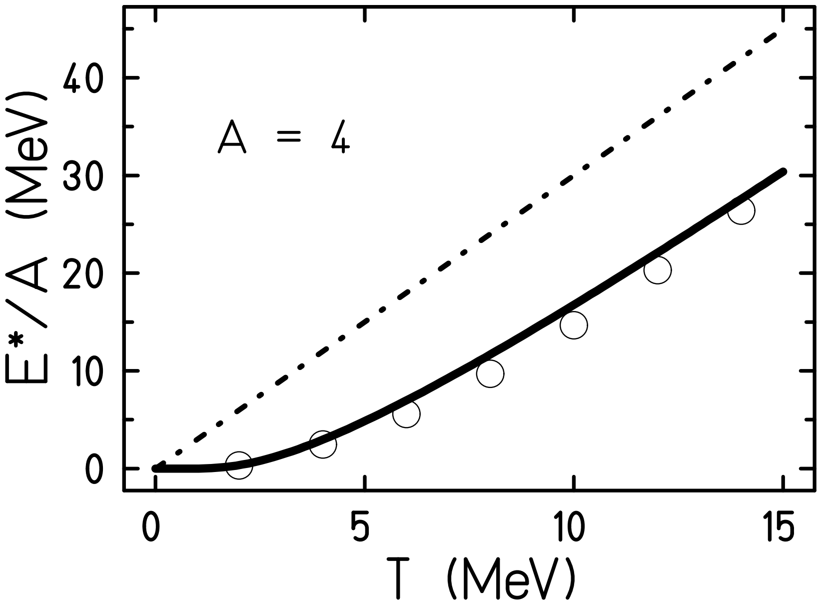
Thermostatic Properties – 3
Example: Canonical Ensemble

Identical fermions in a harmonic oscillator:

$$
\begin{aligned}
Z(\beta) &= \mathrm{Tr}\left(\mathrm{e}^{-\beta \underset{\sim}{H}}\right) = \int \mathrm{d}\mu(Q)\, \langle\, Q \,|\, \mathrm{e}^{-\beta \underset{\sim}{H}}\, |\, Q\,\rangle \\
&= \int \mathrm{d}\mu(Q)\, \frac{\det\left(\langle q_k|\ \exp\{-\beta\, \underset{\sim}{h}_{\mathrm{HO}}\}\, |q_l\rangle\right)}{\det\left(\langle q_k|q_l\rangle\right)}
\end{aligned}
$$

$$
\langle\langle\, \underset{\sim}{H}\, \rangle\rangle\Big|_{T} = -\frac{\partial}{\partial\beta}\ln(Z(\beta))
$$

Evaluation by Monte–Carlo:



Thermodynamic Properties – 1 The Problem

Equations of motion:

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

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

Example for a harmonic oscillator potential:

$$\underset{\sim}{h}(l) = \frac{\underset{\sim}{\vec{k}}^{\,2}(l)}{2m} + \frac{1}{2} \, m\omega^2 \, \underset{\sim}{\vec{x}}^{\,2}(l) \quad \Rightarrow \quad \begin{aligned} \frac{d}{dt} \, \vec{r}_l &= \frac{\vec{p}_l}{m} \\ \frac{d}{dt} \, \vec{p}_l &= -m\omega^2 \vec{r}_l \\ \frac{d}{dt} \, a_l &= -im\omega^2 a_l^2 + \frac{i}{m} \end{aligned}$$

Can one deduce the statistical properties from the equations of motion?

No!

E.g., in the example of the harmonic oscillator the equations of motion are the same for fermions, bosons and distinguishable particles.

Thermodynamic Properties – 2
Idea: Time-Averaging

The ergodic ensemble:

The statistical operator $\underset{\sim}{R}_{\text{erg}}$:

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

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

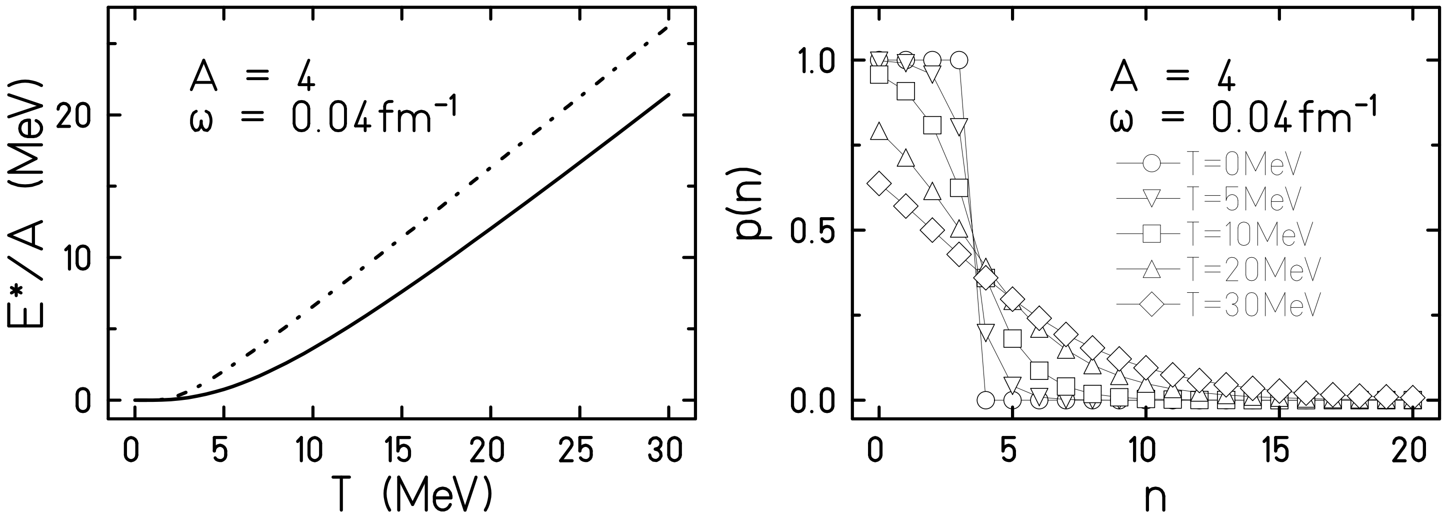
$$\overline{\langle\, \underset{\sim}{B}\,\rangle}\Big|_{\langle\, \underset{\sim}{H}\,\rangle} := \mathrm{Tr}\,(\underset{\sim}{R}_{\text{erg}}\; \underset{\sim}{B})$$

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

- Time–averaging instead of ensemble–averaging.
- If the ergodic assumption is fulfilled, the statistical operator should only depend on $\langle\, \underset{\sim}{H}\,\rangle$, but not on $|\, Q(t_1)\,\rangle$, $\underset{\sim}{H}$ or the equations of motion.
- Since $\langle\, \underset{\sim}{H}\,\rangle$ is a constant of motion, the average in the ergodic ensemble is always performed at the same expectation value of the Hamilton operator.

Thermodynamic Properties – 3
Canonical Ensemble

Excitation energy and occupation probabilities of 4 identical fermions in a harmonic oscillator:



$$E^* = \langle\langle \underset{\sim}{H} - E_0 \rangle\rangle\Big|_T = \sum_{k=1}^{A=4} \frac{\omega\, k}{2}\left[\coth\left(\frac{\omega\, k}{2\,T}\right) - 1\right] \;, \quad E_0 = 8\,\omega$$

$$p(n) = \langle\langle \underset{\sim}{c}_n^+ \underset{\sim}{c}_n \rangle\rangle\Big|_T \;, \quad \underset{\sim}{c}_n^+ \,|\,0\,\rangle = |\,n\,\rangle$$

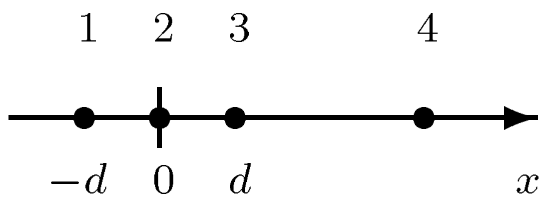
Now, compare the occupation numbers given by the canonical ensemble with those given by the ergodic ensemble at one excitation energy E^*, which is related to a temperature in the canonical ensemble.

$$\langle\langle \underset{\sim}{H} - E_0 \rangle\rangle\Big|_T = \overline{\langle \underset{\sim}{H} - E_0 \rangle}\Big|_{\langle \underset{\sim}{H} \rangle}$$

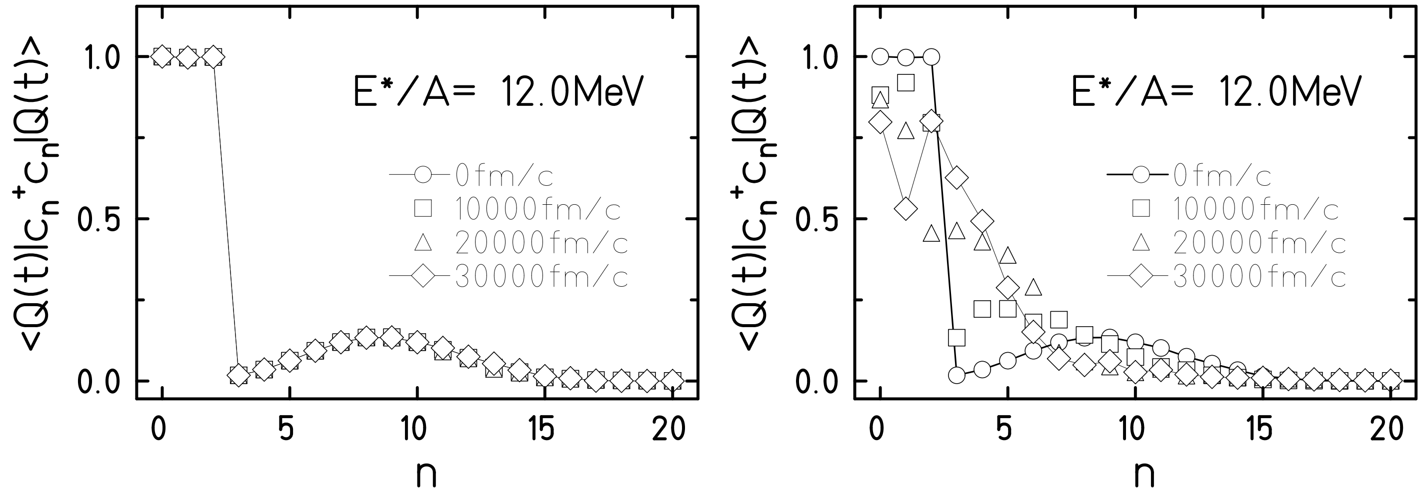
Thermodynamic Properties – 4
Time-Averaging

Initialization:

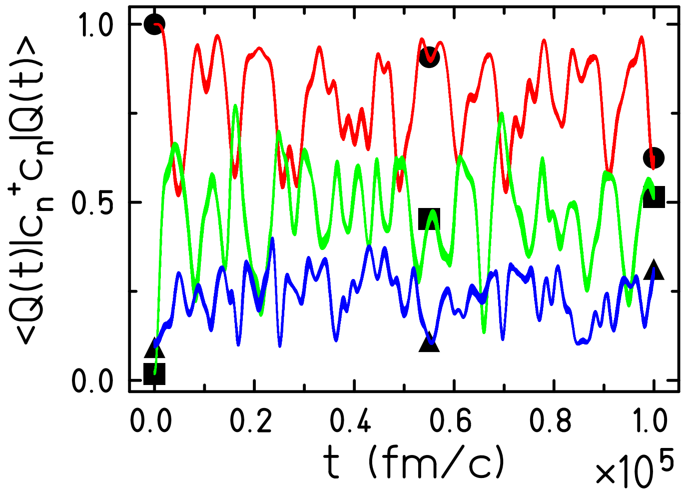
T (MeV)	E^*/A (MeV)
5	0.75
10	3.63
20	12.02
30	21.41



Time evolution without and with small interaction:

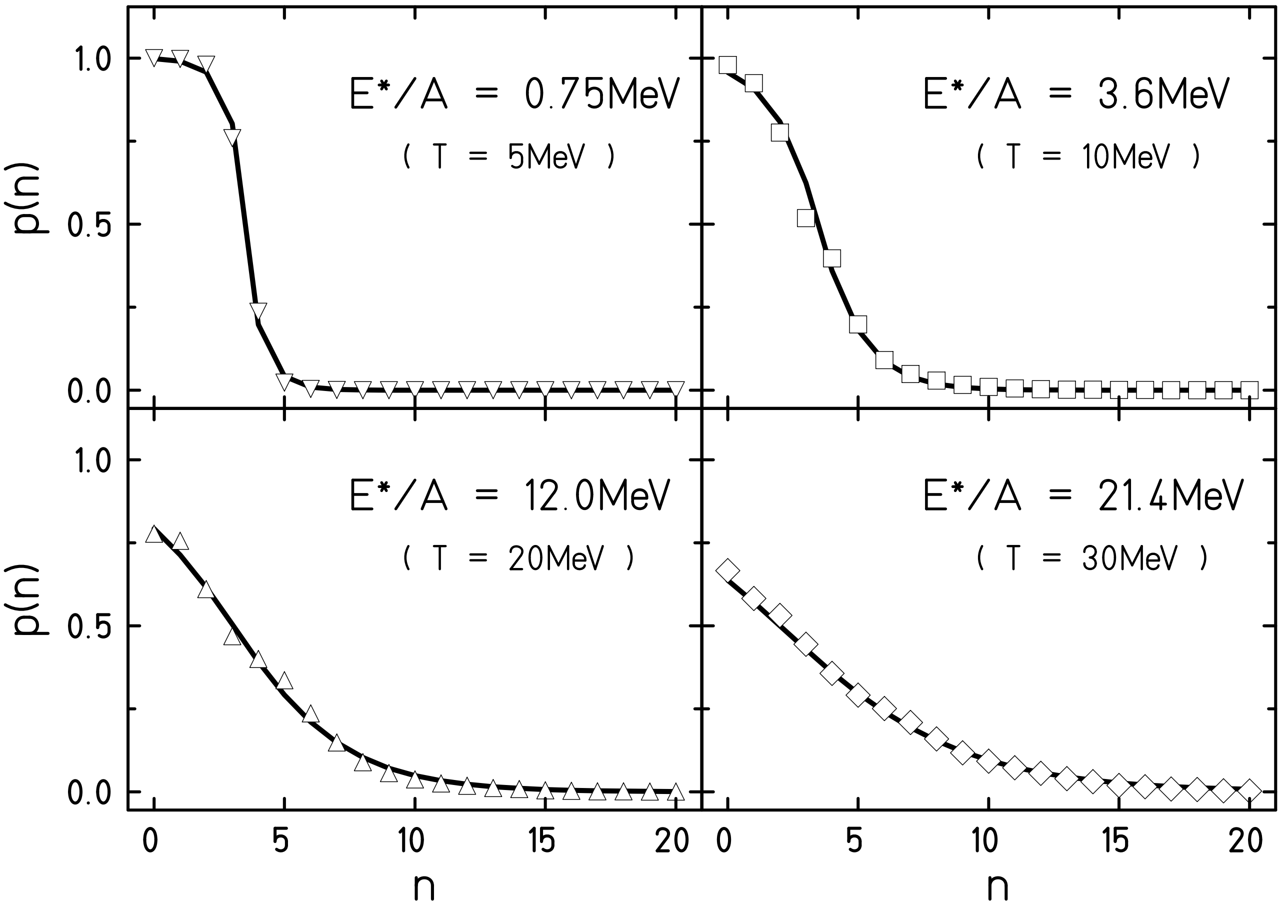


Time evolution of the occupation numbers:



Thermodynamic Properties – 5
Time-Averaged Occupation Numbers

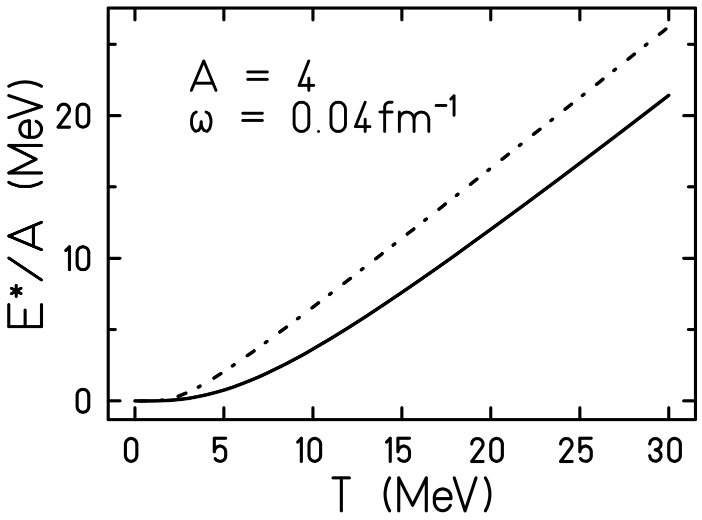
Occupation numbers in the ergodic ensemble:

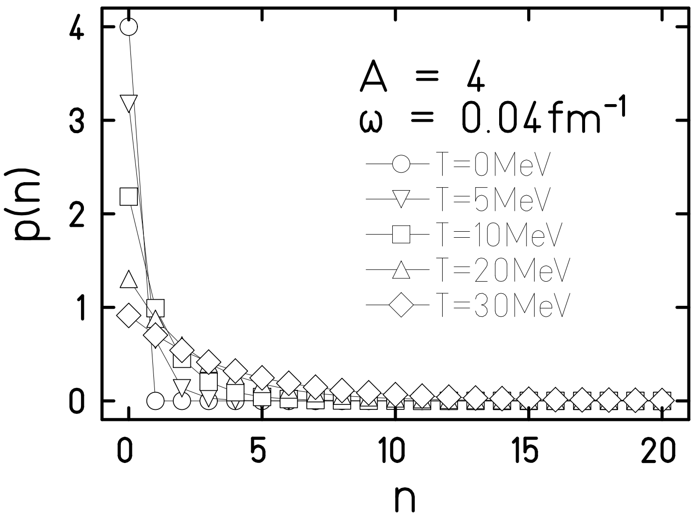


- Time–averaging is done over about 2000 periods.
- Numerically there is no difference between the occupation numbers in the ergodic and the canonical ensemble both taken at the same excitation energy. This equivalence attributes a temperature to the pure many–body state $\mid Q(t)\,\rangle$.
- The FMD many–body trajectory covers the phase space according to Fermi–Dirac statistics.

Thermodynamic Properties – 6
Product State

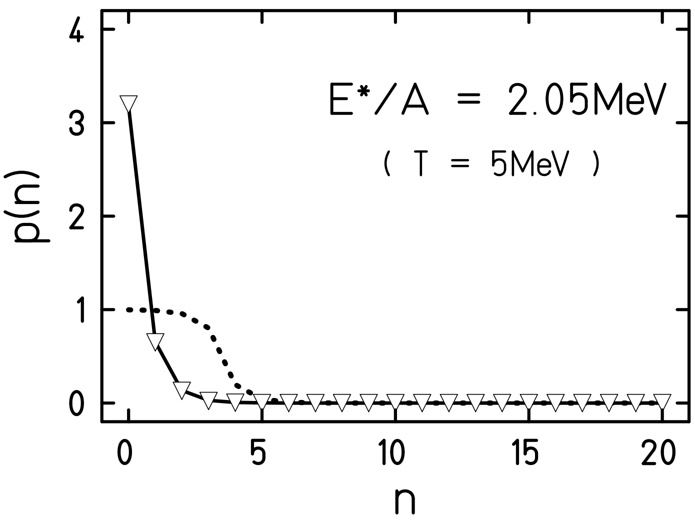
Excitation energy and occupation probabilities of 4 distinguishable particles in a harmonic oscillator:





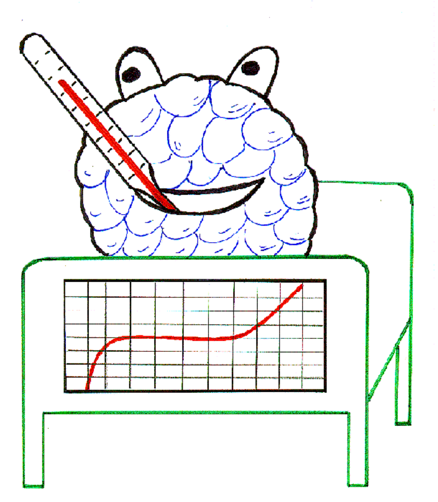
$$E^* = \langle\langle \underset{\sim}{H} - E_0 \rangle\rangle\Big|_T = 4\,\frac{\omega}{2}\left[\coth\left(\frac{\beta\,\omega}{2}\right) - 1\right] , \quad E_0 = 2\,\omega$$

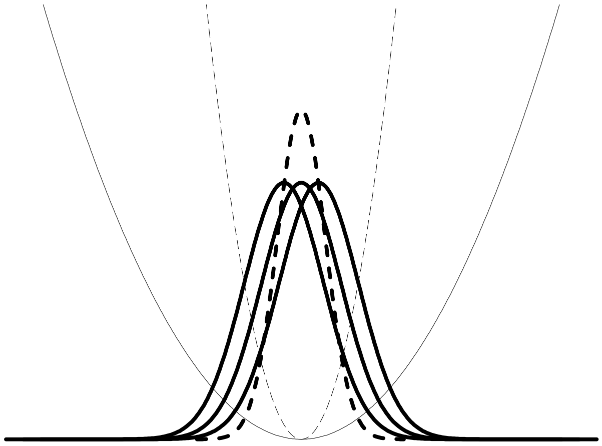
Time-averaged occupation numbers:



Phase Transition – 1
Idea

Arrangement:





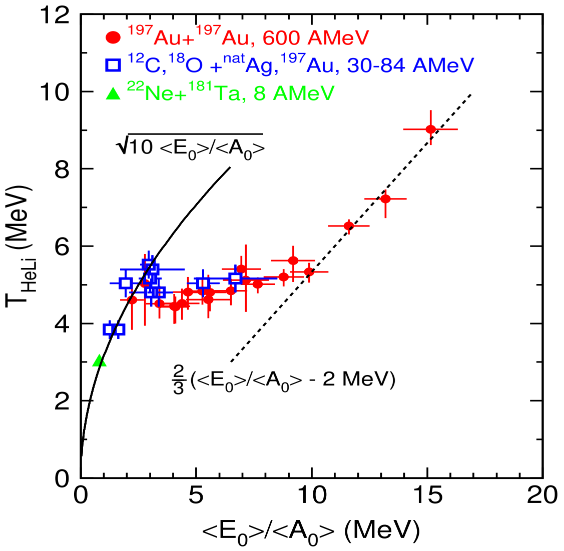
Procedure:

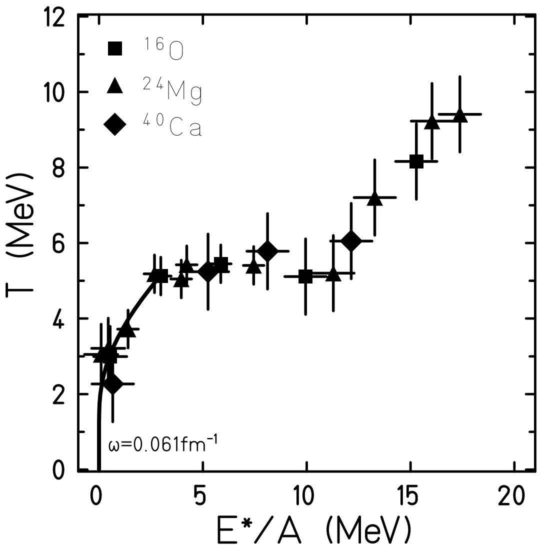
- time evolution of an excited nucleus in a container potential of a harmonic oscillator with small ω_C:
  $\underset{\sim}{H}_{\rm N} = \underset{\sim}{T}_{\rm N} + \underset{\sim}{V}_{\rm NN} + \underset{\sim}{V}_{\rm C}$,
- coupling of all nucleons to a single wave-packet in a second oscillator with ω_{Th}, this is the thermometer:
  $\underset{\sim}{H}_{\rm Th} = \underset{\sim}{T}_{\rm Th} + \underset{\sim}{V}_{\rm Th} + \underset{\sim}{V}_{\rm N-Th}$,
- time-averaging of the excitation energy of the thermometer wave-packet in its oscillator:
  $$E_{\rm Th} = \overline{\langle\, \underset{\sim}{T}_{\rm Th} + \underset{\sim}{V}_{\rm Th} \,\rangle}\Big|_{\langle \underset{\sim}{H} \rangle} \quad ,$$
- ergodic assumption: both systems approach the same temperature

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

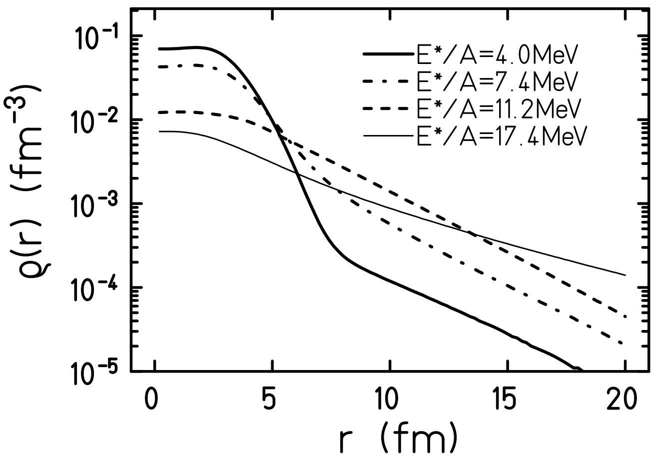
Phase Transition – 2
Caloric Curve

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





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



Open questions:

- detailed investigation on thermometer properties,
- A-dependence, $\underset{\sim}{V}_{\mathrm{NN}}$-dependence,
- relation of T and $T_{\mathrm{He,Li}}$,
- deexcitation in vacuum (non equilibrium process)

Statistical Properties of FMD
Summary

- FMD provides a complete set of model states which span the antisymmetric part of the Hilbert space, therefore thermo*static* properties can be expressed using FMD model states.

- FMD describes the thermo*dynamic* properties of interacting fermion systems which can be deduced by time-averaging in the ergodic ensemble. The many-body trajectory covers the Hilbert space according to Fermi–Dirac statistics.

- The identification of time-averaged mean values with ensemble means given by the canonical ensemble allows to attribute a temperature to the many-body system described by one time-dependent state.

- FMD provides a method to investigate the nuclear liquid-gas phase transition in a dynamical way.