Molecular dynamics investigations on a quantum system in a thermostat

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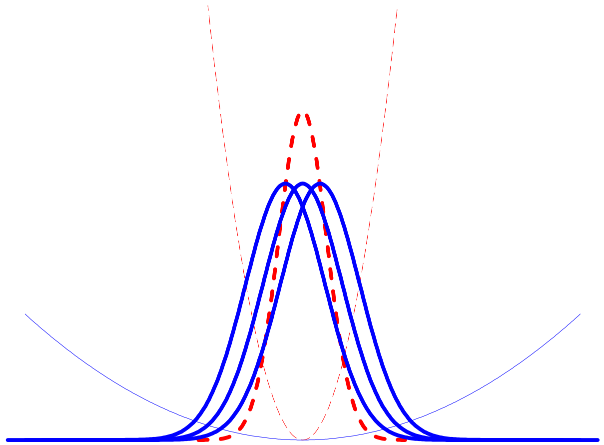

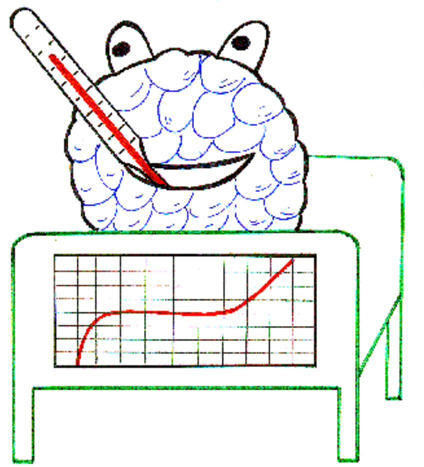

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Problem

Canonical ensemble

$$Z(T) = \mathrm{tr}\left(\exp\left\{-\frac{\underset{\sim}{H}}{k_B T}\right\}\right) \quad = \quad \int \mathrm{d}\mu(Q)\,\langle\, Q \,|\, \exp\left\{-\frac{\underset{\sim}{H}}{k_B T}\right\} |\, Q \,\rangle$$

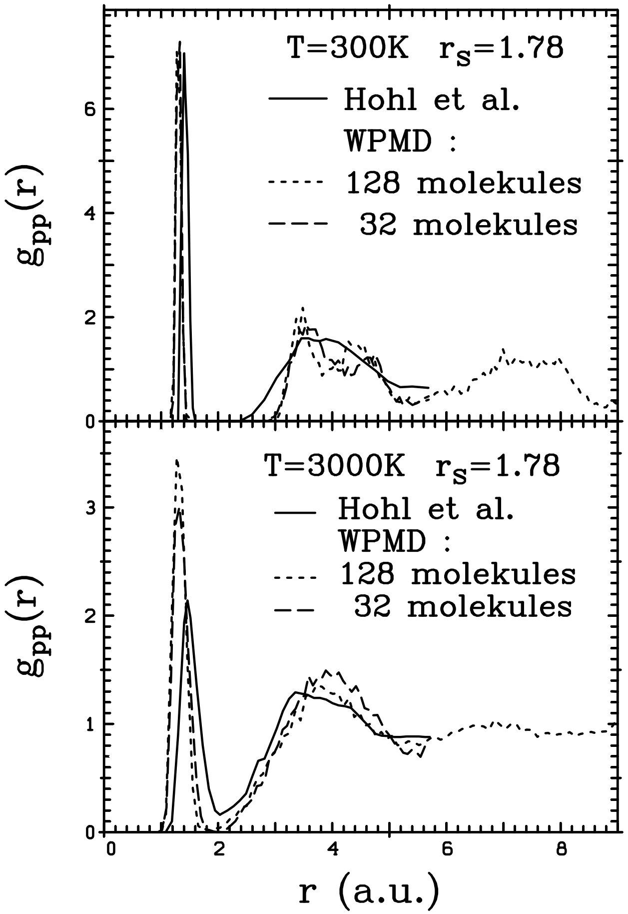
- calculation of $Z(T)$ impossible due to two-body interaction
- replace ensemble averages by time averages

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

- exact quantum dynamics also not known
- use approximate dynamics instead ⇒ Molecular Dynamics for Fermions

Example

Atomic physics – solid hydrogen[a]



- electrons described by wave packet molecular dynamics
- protons classical
- temperature via equipartition theorem for protons $\surd$

[a] D. Klakow, C. Toepffer, P.-G. Reinhard, Phys. Lett. **A192** (1994) 55

Classical Mechanics
Nosé–Hoover–Thermostat

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

$$\frac{d}{dt}\,\vec{r}_i = \frac{\vec{p}_i}{m_i}\;, \quad \frac{d}{dt}\,\vec{p}_i = -\frac{\partial V}{\partial \vec{r}_i} - \xi\,\vec{p}_i\;, \quad \frac{d}{dt}\,\xi = \frac{1}{M_s}\left(\sum_i \frac{\vec{p}_i^{\,2}}{2m_i} - \frac{3N}{2}k_B T\right)$$

- 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
- there is no equipartition theorem for quantum systems

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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

Time-Dependent Variational Principle

TDVP[a] with trial state $|\, Q(t)\,\rangle = |\, \{q_\mu(t)\}\,\rangle$:

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

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

Euler–Lagrange equations in their most general form:

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

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

- 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

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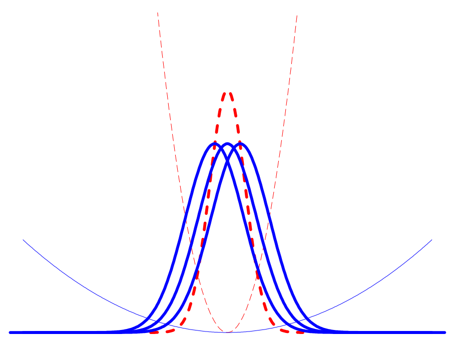
[a] P. Kramer, M. Saraceno, Lecture Notes in Physics **140**, Springer, Berlin (1981)

Coupling to a Thermometer



- **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
  $\underset{\sim}{H}_{\mathrm{Th}} = \underset{\sim}{T}_{\mathrm{Th}} + \underset{\sim}{V}_{\mathrm{Th}}$,

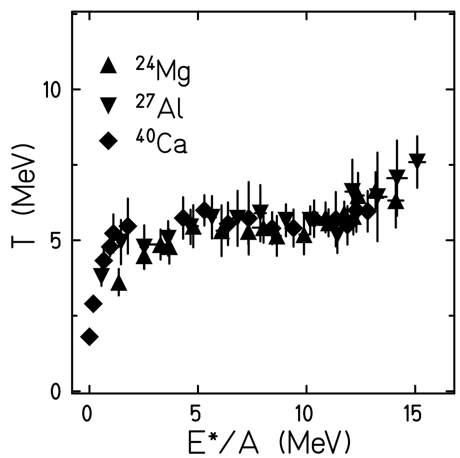
- **coupling** of all nucleons to the thermometer wave packet:
  $\underset{\sim}{V}_{\mathrm{N-Th}}, \quad \underset{\sim}{H} = \underset{\sim}{H}_{\mathrm{N}} + \underset{\sim}{H}_{\mathrm{Th}} + \underset{\sim}{V}_{\mathrm{N-Th}}\,, \quad |\,Q(t)\,\rangle = |\,\mathit{nucleus}\,\rangle \otimes |\,\mathit{thermometer}\,\rangle$,

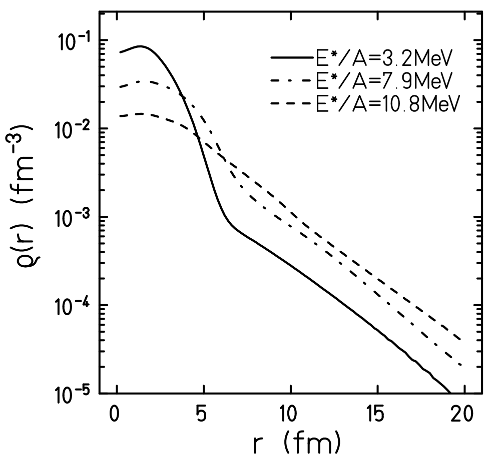
- **time-averaging:**
  $E_{\mathrm{Th}} = \overline{\langle\, \underset{\sim}{H}_{\mathrm{Th}}\,\rangle}\,, \quad E^{*} = \overline{\langle\, \underset{\sim}{H}_{\mathrm{N}} - E_0\,\rangle}\,,$

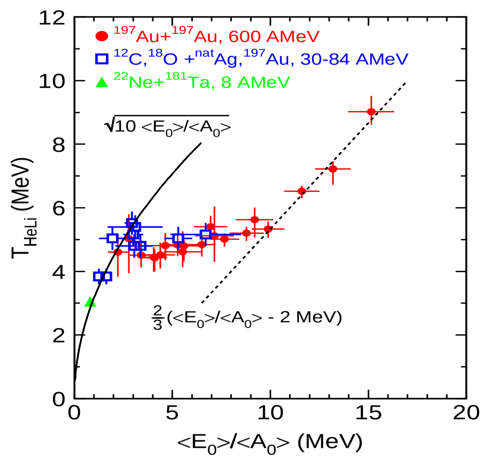
- **zeroth law:** both subsystems approach the same T

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

Nuclear liquid-gas phase transition







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

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

Thermostat I

Total system:

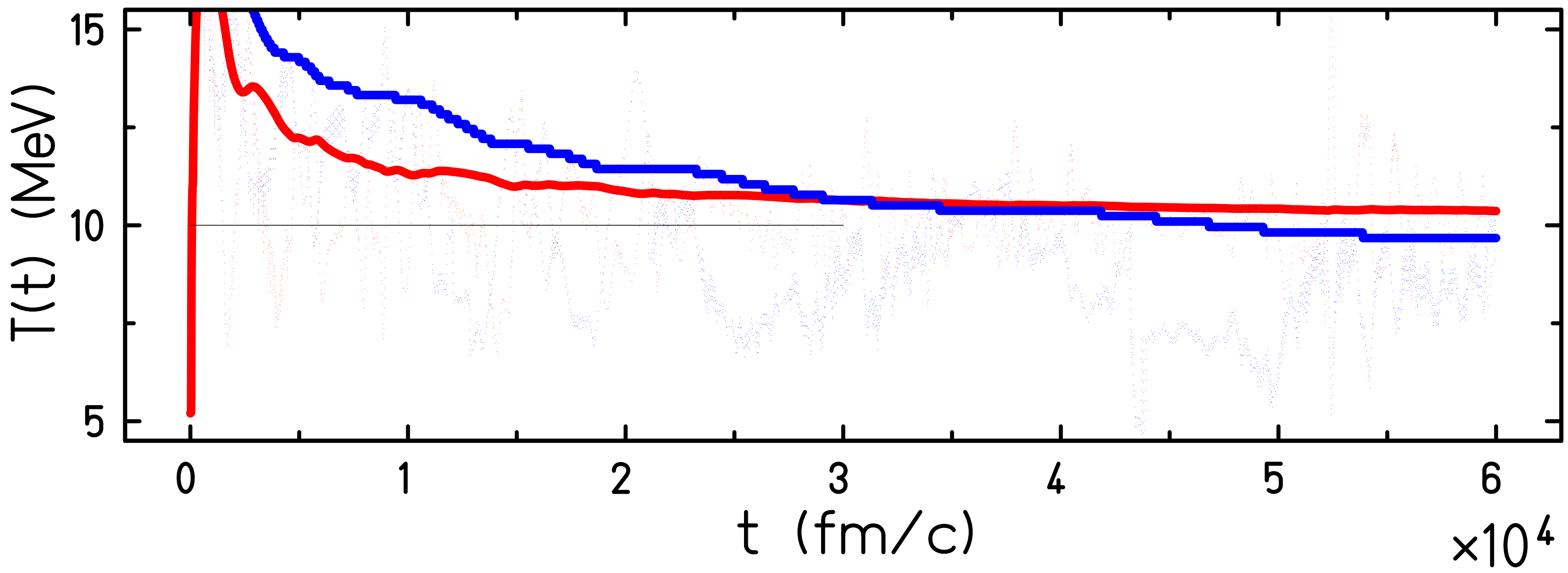
$$|\,Q(t)\,\rangle \quad = \quad |\,system(t)\,\rangle \otimes |\,thermometer(t)\,\rangle$$

Complex time steps:

$$d\tau = dt - i d\beta \ , \quad d\beta \propto (T_{th} - T)/T_{th} \ , \quad |\,Q(t)\,\rangle \to |\,Q(t + d\tau)\,\rangle$$

- T desired temperature
- T_{th} temperature measured by the thermometer
- $d\beta > 0 \ \Rightarrow$ cooling; $\quad d\beta < 0 \ \Rightarrow$ heating

Thermostat II



Fermions in a harmonic oscillator:

- actual temperatures – pointed lines
- time averaged temperatures – solid lines
- thermometer – red lines, fermions – blue lines

The End

Summary

- thermodynamic properties can be extracted from time evolution via coupling to a thermometer and time averaging
- a thermostat can be defined using a coupled thermometer and a feedback mechanism with complex time steps
- approximate time evolution with wave packet dynamics sufficient for gross properties

Literature

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2. H. Feldmeier, Nucl. Phys. A **515** (1990) 147
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5. H. Feldmeier, J. Schnack, Rev. Mod. Phys. (2000), to appear in July
6. J. Schnack, Physica A **259** (1998) 49
7. J. Schnack, Europhysics Letters **45** (1999) 647
8. http://obelix.physik.uni-osnabrueck.de/∼schnack/