Molecular Dynamics for Fermions

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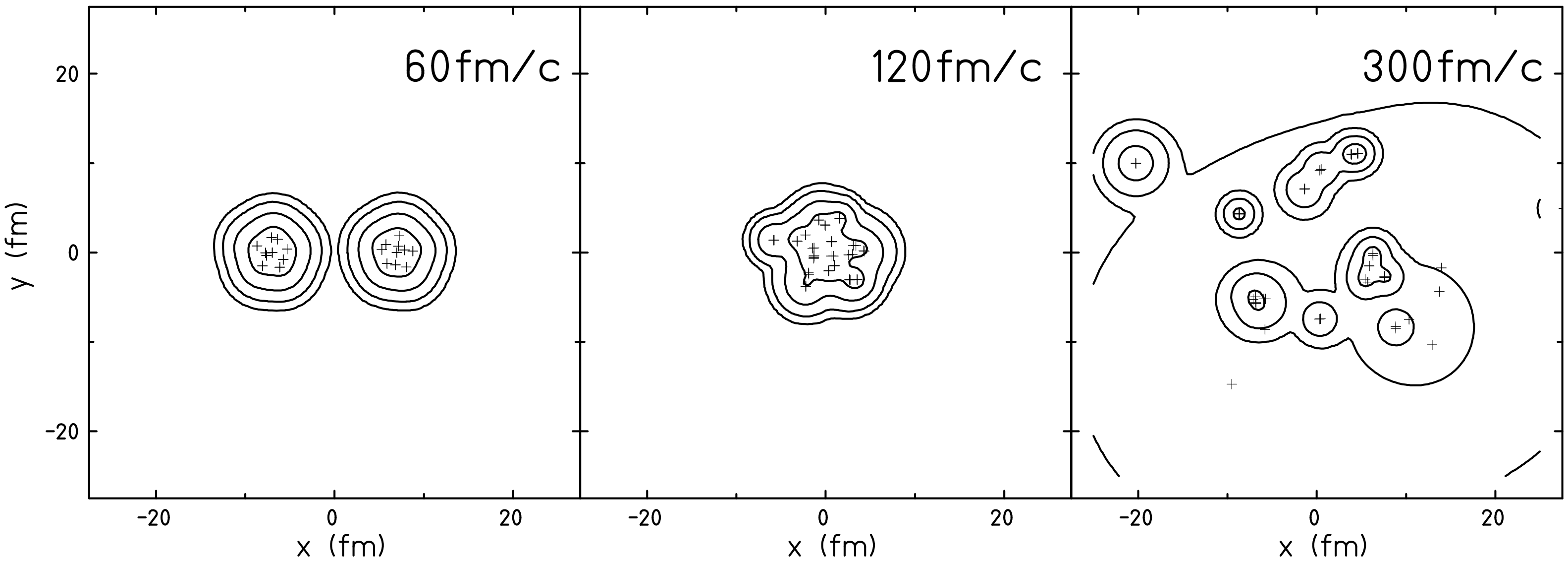
Aim

Description of many-fermion systems like atomic nuclei, plasmas or atomic gases in magnetic traps in terms of dynamics and thermodynamics.



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

Why molecular dynamics for fermions?

Multifragmentation reactions:

- large fluctuations in the final results;
- cannot be accounted for with TDHF, because nucleons are to fast ($\varepsilon > \varepsilon_F \approx 30\,\mathrm{MeV}$);
- no common mean field established;
- molecular dynamics better suited.

Molecular dynamics:

- molecular dynamics means: single-particle states always localized;
- “trajectory” calculations for fermions;
- quantum mechanically necessary ingredients: Heisenberg uncertainty principle, Pauli exclusion principle;
- dynamics will be non-linear through localization.

Systematic creation of a model

1. **Trial state:**
   - definition of a trial state which has the necessary degrees of freedom;
   - working with quantum states automatically guarantees the Heisenberg uncertainty principle;
   - using antisymmetrized states automatically guarantees the Pauli principle.
2. **Ground states:**
   - Ritz variational principle defines ground states;
   - aim: reasonable (nuclear) ground state properties like binding energy and rms radius;
   - usually phenomenological interaction suited for choice of trial states.
3. **Dynamics:**
   - time-dependent variational principle defines dynamics;
   - aim: dynamics should cover the phenomena of the desired energy range, i.e. fusion, deeply inelastic reactions, evaporation, fragmentation, vaporisation.
4. **Open problems:**
   - restricted dynamics causes barriers in Hilbert space;
   - due to localization no tunneling or branching.

Applications

Nuclear physics

- **Classical Molecular Dynamics (CMD):** Pauli and possibly Heisenberg potential to correct for missing quantum features; applied to collisions;
- **Quantum Molecular Dynamics (QMD):** product state of gaussian wave packets and Pauli potential to mock effects of antisymmetrization; wide spread in nuclear physics because simple; applied to collisions;
- **Antisymmetrized Molecular Dynamics (AMD):** Slater determinant of gaussian wave packets with fixed width (coherent states); applied to collisions;
- **Fermionic Molecular Dynamics (FMD):** Slater determinant of gaussian wave packets with time-dependent width; applied to collisions and thermodynamics;

Atomic physics

- **Classical Molecular Dynamics:** many groups worldwide; description of atomic clusters etc.;
- **Quantum Molecular Dynamics:** product state of gaussian wave packets and Pauli potential to mock effects of antisymmetrization; description of Hydrogen plasma.

Time-Dependent Variational Principle

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

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

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)

Conservation laws

1. Generalized Poisson Brackets

$\underset{\sim}{B}$ be a time-independent operator, $\mathcal{H} = \langle\, Q(t) \,|\, \underset{\sim}{H} \,|\, Q(t) \,\rangle$

$$\frac{d}{dt}\,\mathcal{B}(t) \quad = \quad \frac{d}{dt}\,\langle\, Q(t) \,|\, \underset{\sim}{B} \,|\, Q(t) \,\rangle = \sum_{\nu} \dot{q}_{\nu} \frac{\partial}{\partial q_{\nu}}\,\mathcal{B} = \sum_{\mu,\nu} \frac{\partial\,\mathcal{H}}{\partial q_{\mu}}\,\mathcal{A}^{-1}_{\mu\nu} \frac{\partial\,\mathcal{B}}{\partial q_{\nu}} \quad =: \{\mathcal{H}, \mathcal{B}\}$$

2. Conservation Laws

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

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

  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 $\underset{\sim}{H}$

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

  Relates the choice 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.

Example 1 – Schrödinger Equation

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

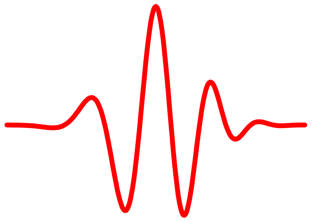
$$\begin{aligned} |\, Q \,\rangle &= |\, \rho_1, \rho_2, \cdots, \pi_1, \pi_2, \cdots \rangle = \sum_n c_n \,|\, n \,\rangle \equiv \sum_n \frac{1}{\sqrt{2}} (\rho_n + i\pi_n) \,|\, n \,\rangle \\ \mathcal{L} &= -\sum_n \rho_n \dot{\pi}_n - \mathcal{H}(\rho_1, \rho_2, \cdots, \pi_1, \pi_2, \cdots) + \text{ total time derivative} \end{aligned}$$

$$\frac{d}{dt} \, \pi_n = -\frac{\partial \, \mathcal{H}}{\partial \, \rho_n} \quad \text{and} \quad \frac{d}{dt} \, \rho_n = \frac{\partial \, \mathcal{H}}{\partial \, \pi_n}$$

These classical looking equations of motion are equivalent to the time-dependent Schrödinger equation and provide the full quantum solution (if $\{ \,|\, n \,\rangle\}$ is complete).

Example 2 – WPMD, QMD

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



$$\begin{aligned} |\, Q \,\rangle &= |\, \vec{r}_1,\vec{p}_1 \,\rangle \otimes |\, \vec{r}_2,\vec{p}_2 \,\rangle \otimes \cdots \otimes |\, \vec{r}_N,\vec{p}_N \,\rangle \\ \langle\, \vec{x} \,|\, \vec{r}_k\,,\vec{p}_k \,\rangle &= \left(\frac{1}{\pi a_0}\right)^{3/4} \exp\left\{ -\frac{(\vec{x} - \vec{r}_k)^2}{2\,a_0} + i\,\vec{p}_k \cdot \vec{x} \right\} \end{aligned}$$

$$\mathcal{L} = -\sum_{k=1}^{N} \vec{r}_k\,\dot{\vec{p}}_k - \mathcal{H}(\vec{r}_1,\vec{p}_1,\dots,\vec{r}_N,\vec{p}_N) \;\Rightarrow\; \frac{d}{dt}\,\vec{p}_k = -\frac{\partial\,\mathcal{H}}{\partial\,\vec{r}_k} \quad \text{and} \quad \frac{d}{dt}\,\vec{r}_k = \frac{\partial\,\mathcal{H}}{\partial\,\vec{p}_k}$$

- product state describes distinguishable particles; most classical MD;
- impact of Pauli principle on dynamics sometimes mocked by additional terms in $\mathcal{H}(\vec{r}_1,\vec{p}_1,\dots,\vec{r}_N,\vec{p}_N)$ – "Pauli potential";
- E.J. Heller, J. Chem. Phys. **62** (1975) 1544

Example 3 – EQMD

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

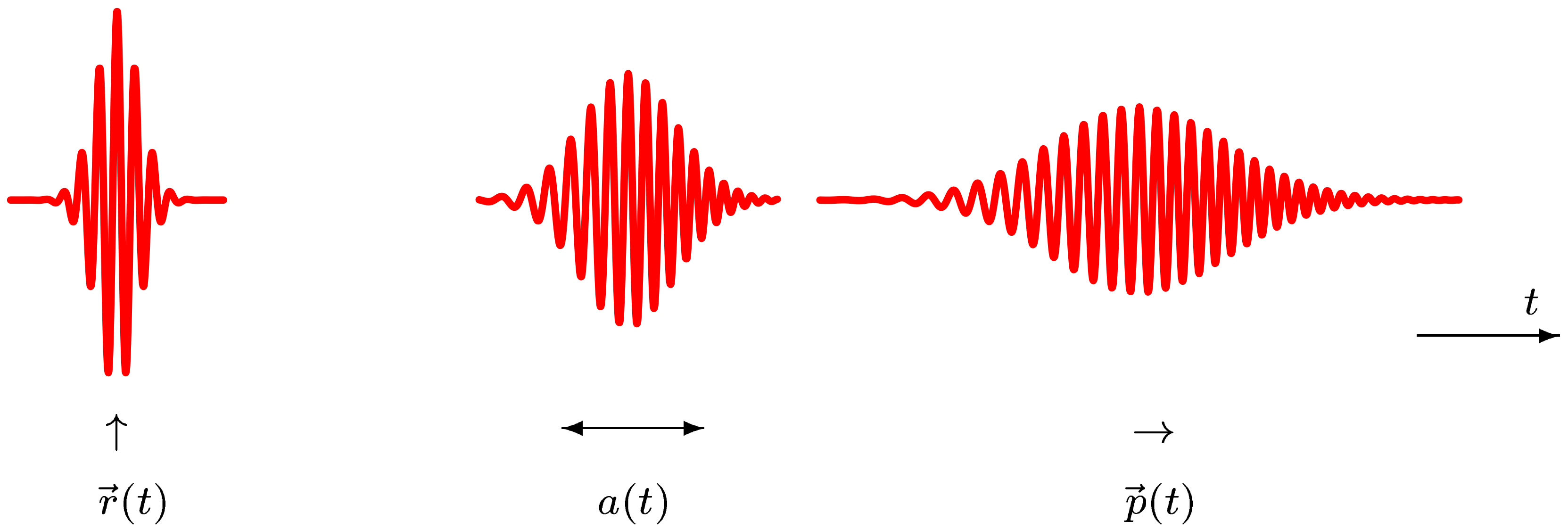
$$\begin{aligned} |\, Q \,\rangle &= |\, \vec{r}_1, \vec{p}_1, a_1 \,\rangle \otimes \cdots \otimes |\, \vec{r}_N, \vec{p}_N, a_N \,\rangle \\ \langle\, \vec{x} \,|\, \vec{r}_l, \vec{p}_l, a_l \,\rangle &= \left(2\pi \frac{a_l^* \, a_l}{a_l^* + a_l} \right)^{-3/4} \exp\left\{ - \frac{(\vec{x} - \vec{r}_l)^2}{2 \, a_l} + i \, \vec{p}_l \cdot \vec{x} \right\} \end{aligned}$$

The width parameter $a_l(t)$ is a first non-classical degree of freedom.

Example 3 – Free motion

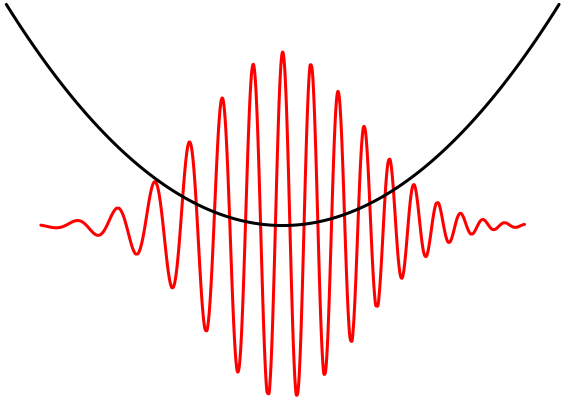
$$\langle \vec{x} \,|\, \vec{r}_l, \vec{p}_l, a_l \rangle = \left(2\pi \, \frac{a_l^* \, a_l}{a_l^* + a_l} \right)^{-3/4} \exp\left\{ - \frac{(\vec{x} - \vec{r}_l)^2}{2\, a_l} + i \, \vec{p}_l \cdot \vec{x} \right\}$$

$$\frac{d}{dt} \, \vec{r}_l = \frac{\vec{p}_l}{m_l} \, , \quad \frac{d}{dt} \, \vec{p}_l = 0 \, , \quad \frac{d}{dt} \, a_l = \frac{i}{m_l}$$



Example 3 – Non-interacting particles moving in a harmonic oscillator

$$\langle \vec{x} \,|\, \vec{r}_l, \vec{p}_l, a_l \,\rangle \quad = \quad \left(2\pi \, \frac{a_l^* \, a_l}{a_l^* + a_l} \right)^{-3/4} \exp\left\{ - \frac{(\vec{x} - \vec{r}_l)^2}{2\, a_l} + i\, \vec{p}_l \cdot \vec{x} \right\}$$



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

$$\frac{d}{dt}\, a_l = \frac{i}{m_l} - i m_l \, \omega^2 \, a_l^2$$

Oscillation of the wave-packet centres $(\vec{r}_l(t), \vec{p}_l(t))$ as well as of the widths $a_l(t)$.

Example 4 – FMD

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

Fermionic Molecular Dynamics (FMD)[a]**:**

$$\begin{aligned} |\, Q(t) \,\rangle \quad &\propto \quad \frac{1}{N!} \sum_{\pi} \mathrm{sgn}(\pi)\ \ |\, q_{\pi(1)}(t) \,\rangle \otimes \cdots \otimes |\, q_{\pi(N)}(t) \,\rangle \\ \langle\, \vec{x} \,|\, q_l(t) \,\rangle \quad &= \quad \langle\, \vec{x}\ |\, \vec{r}_l, \vec{p}_l, a_l, \chi_l, \phi_l \,\rangle = \exp\left\{ -\frac{(\vec{x}\ - \vec{r}_l)^2}{2\, a_l} + i\, \vec{p}_l \cdot \vec{x} \right\} \otimes |\, \chi_l(t), \phi_l(t) \,\rangle \otimes |\, m_t(l) \,\rangle \end{aligned}$$

- antisymmetrized many-body state: a priori Pauli principle
- exact for free motion and common harmonic oscillator

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[a] H. Feldmeier, Nucl. Phys. A **515** (1990) 147;
H. Feldmeier, J. Schnack, Rev. Mod. Phys. **72** (2000) 655

FMD – Expectation values

Inverse overlap matrix:

Wave packets $|\, q_k \,\rangle$ 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:

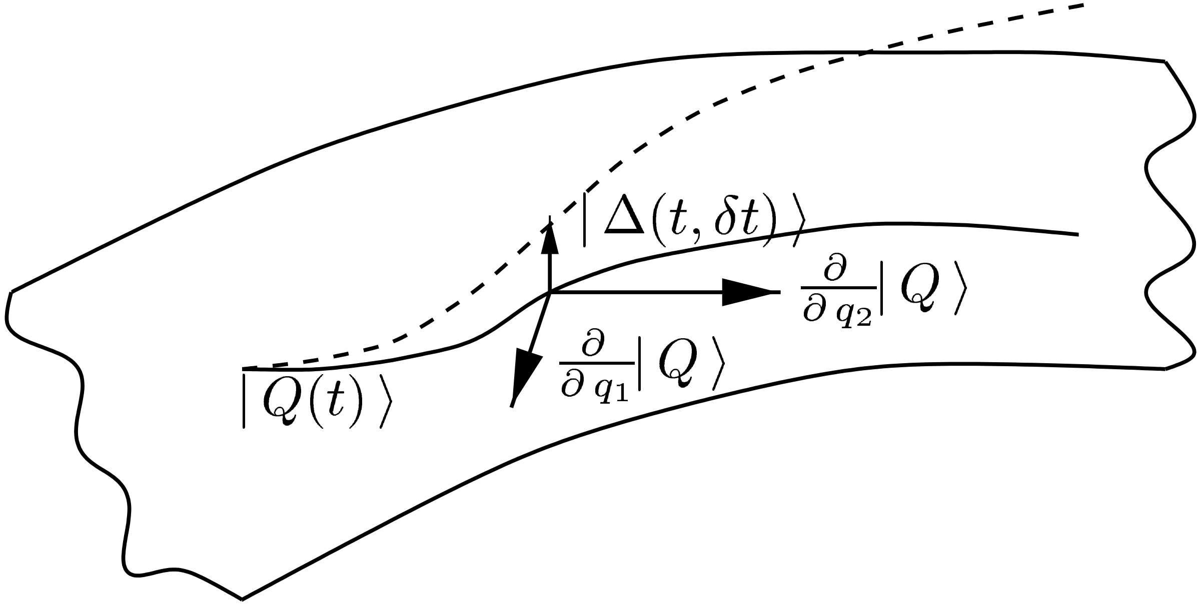
$$\langle\, Q \,|\, \underset{\sim}{T} \,|\, Q \,\rangle = \sum_{k,l}^{N} \langle\, q_k \,|\, \underset{\sim}{t} \,|\, q_l \,\rangle \; \mathcal{O}_{lk}$$

Two-body interaction:

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

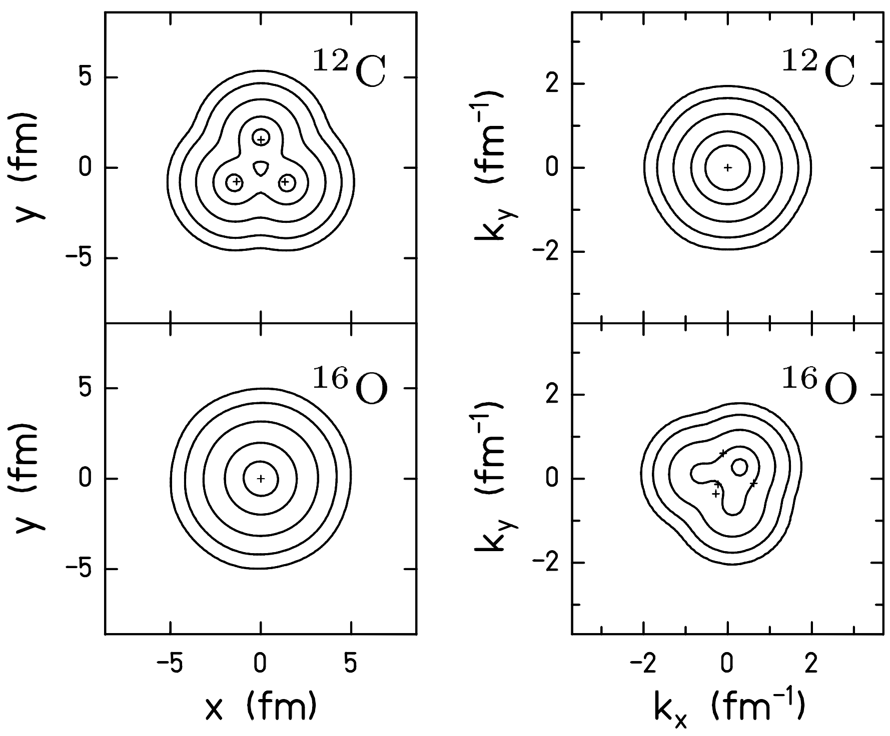
$\Longrightarrow$ Total effort scales with N^4,
in classical MD or for simple product states with N^2.

Error due to restriction of the wave function



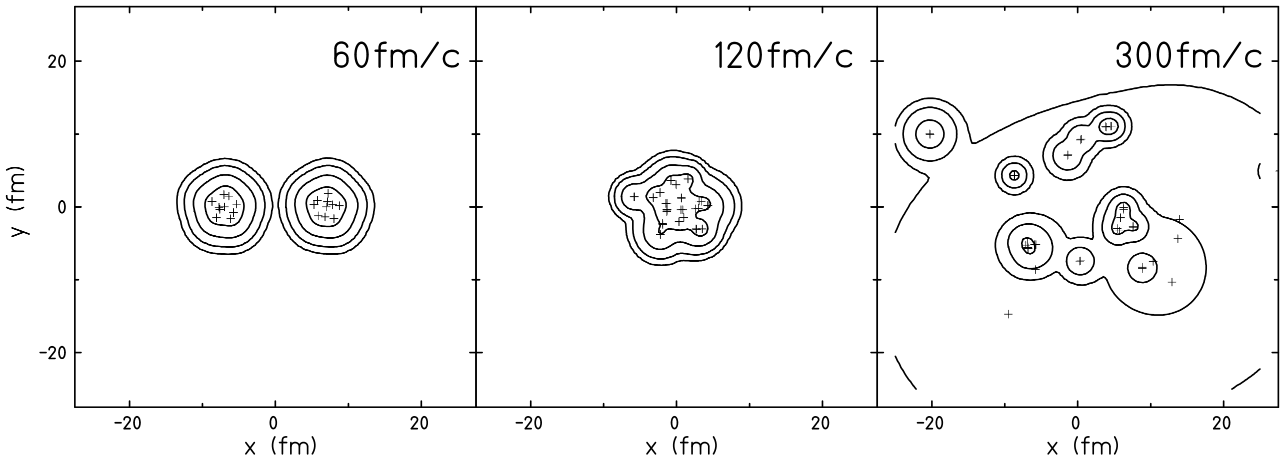
The error $|\,\Delta(t,\delta t)\,\rangle = \exp(-i\underset{\sim}{H}\delta t)\,|\,Q(t)\,\rangle - |\,Q(t+\delta t)\,\rangle$ is orthogonal to all tangent states $\frac{\partial}{\partial\, q_\nu}|\,Q\,\rangle$. Thus the TDVP-evolved state has the minimum distance $\langle\,\Delta(t,\delta t)\,|\,\Delta(t,\delta t)\,\rangle$ to the exact solution.

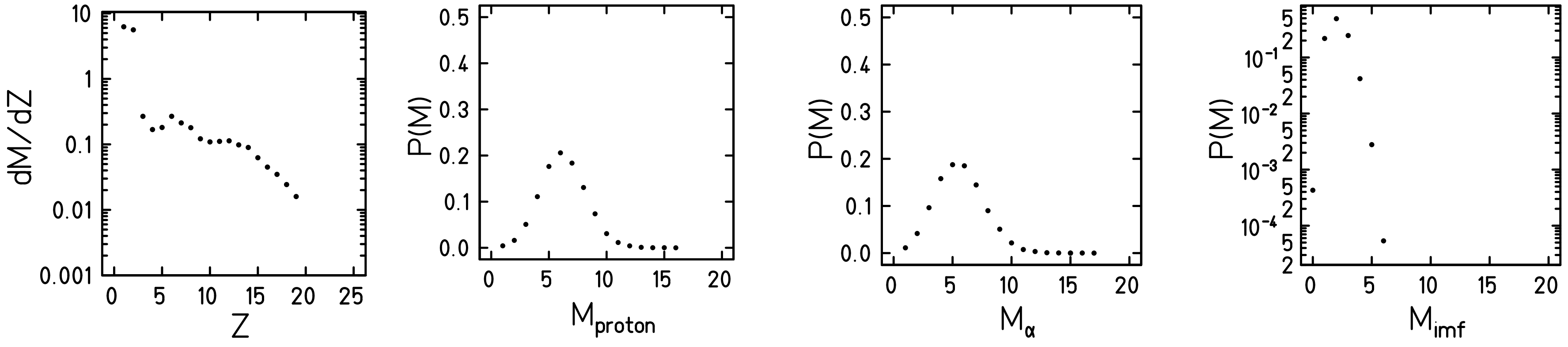
Ground States



- ground state $\mid Q\,\rangle$ lowest one in energy (Ritz variational principle)
- $\frac{\partial}{\partial q_\mu}\ \langle\, Q \mid \underset{\sim}{H} \mid Q\,\rangle = 0 \quad \forall q_\mu$
- $\Longrightarrow\ \dot{q}_\mu = 0 \quad \forall q_\mu$, stationary
- for experts: take care of centre of mass motion
- phenomenological interaction suited for choice of trial states; short range repulsion & long range attraction
- graphics shows single-particle density for selected nuclear ground states

Multifragmentation



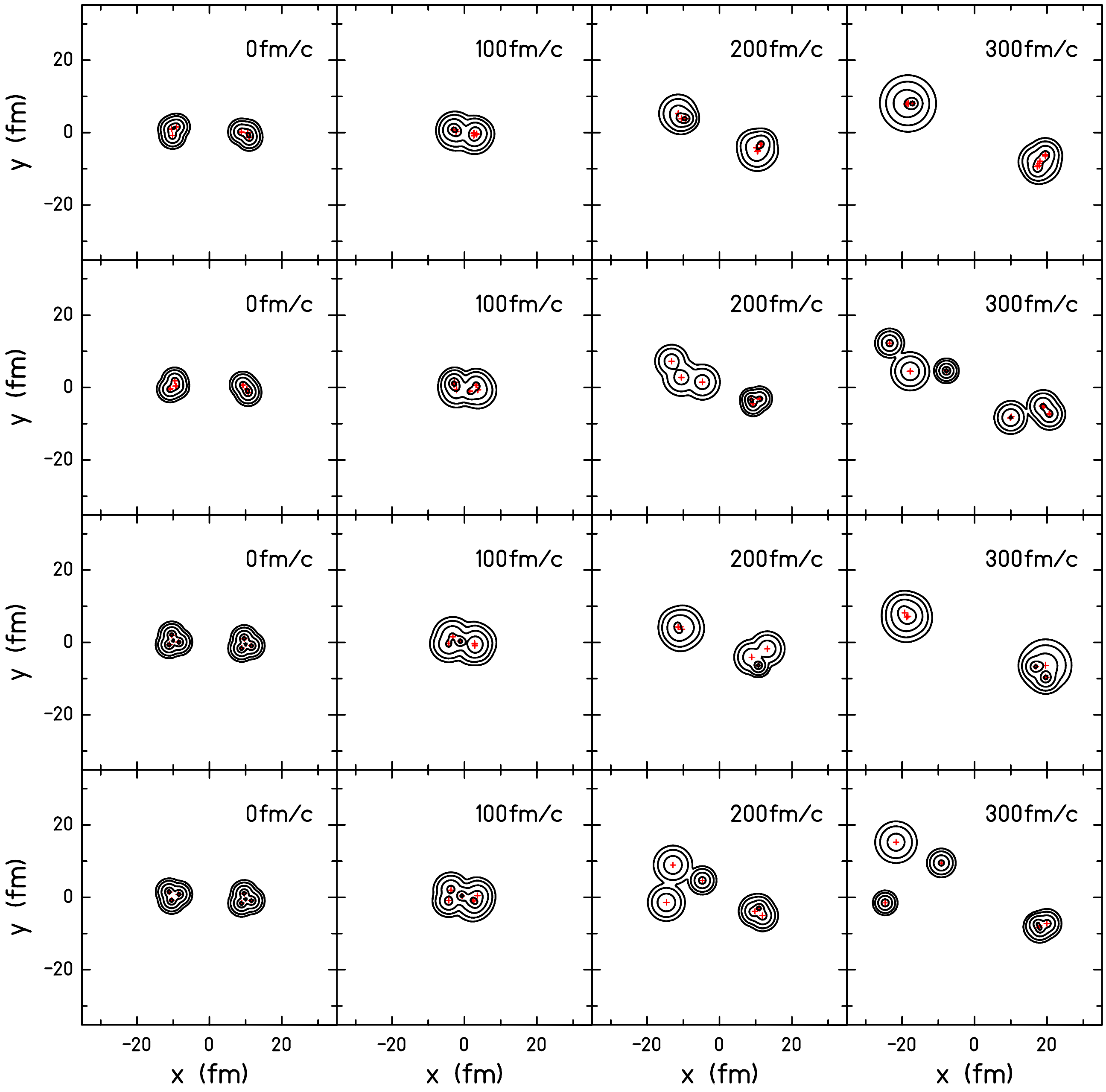


^{40}Ca-^{40}Ca at $E_{Lab} = 35A\,\mathrm{MeV}$

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

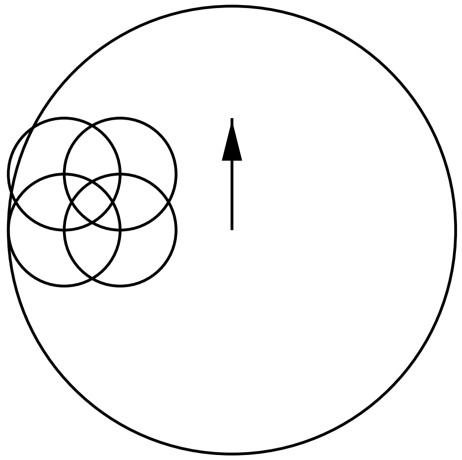
Event Ensemble

- 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: $|\,Q\,;\vec{\Omega}_1,\vec{\Omega}_2\,\rangle$.
  The same holds for the impact parameter.
- Within the ensemble large fluctuations arise.



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

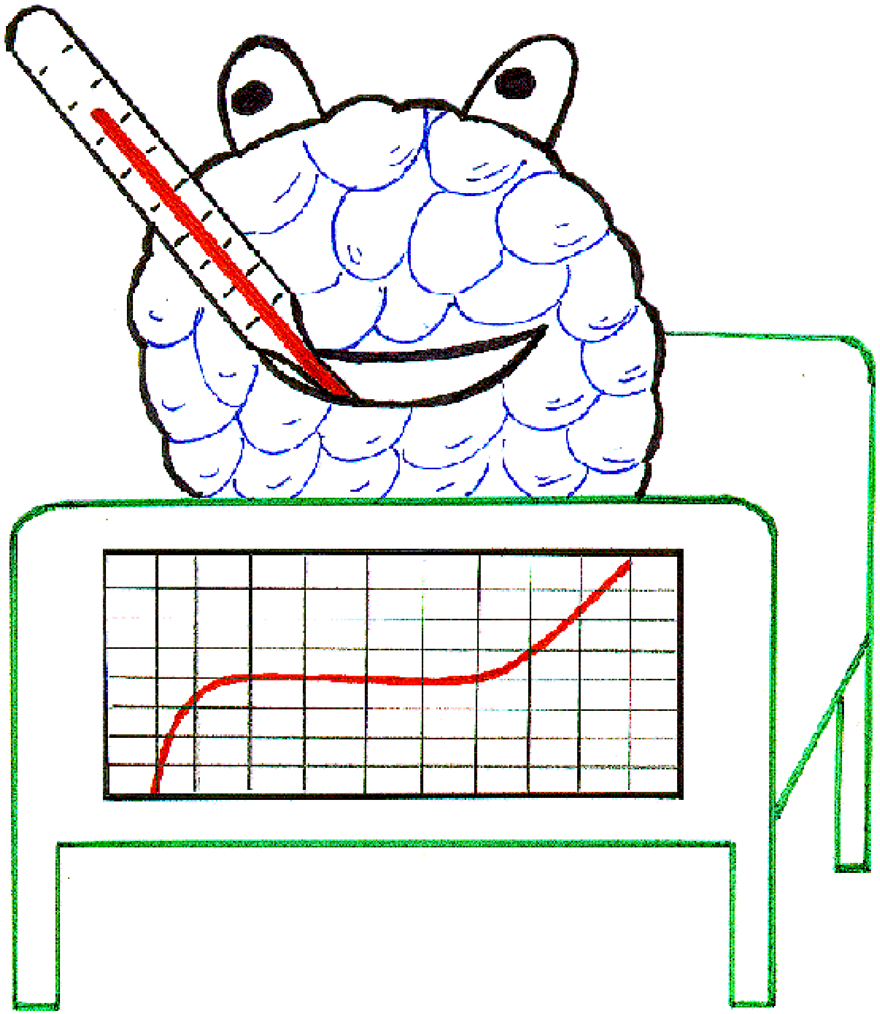
Open questions



Pictorial scetch of a four particle cluster and a passing wave packet.

- localization implies that a wave packet moves always as a whole and does not split;
- in quantum mechanics the wave packet may split with parts getting attached to the four particle cluster;
- localization also implies that the wave packet cannot tunnel;
- idea: quantum branching;
- jumps $\mid Q_i(t)\,\rangle \rightarrow \mid Q_j(t)\,\rangle$ with a probability amplitude related to the residual hamiltonian; not realized up to now, only reasonable probability distributions utilized;
- problems: conservation laws, small probabilities.

Thermodynamics



Thermostated molecular dynamics

Canonical ensemble

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

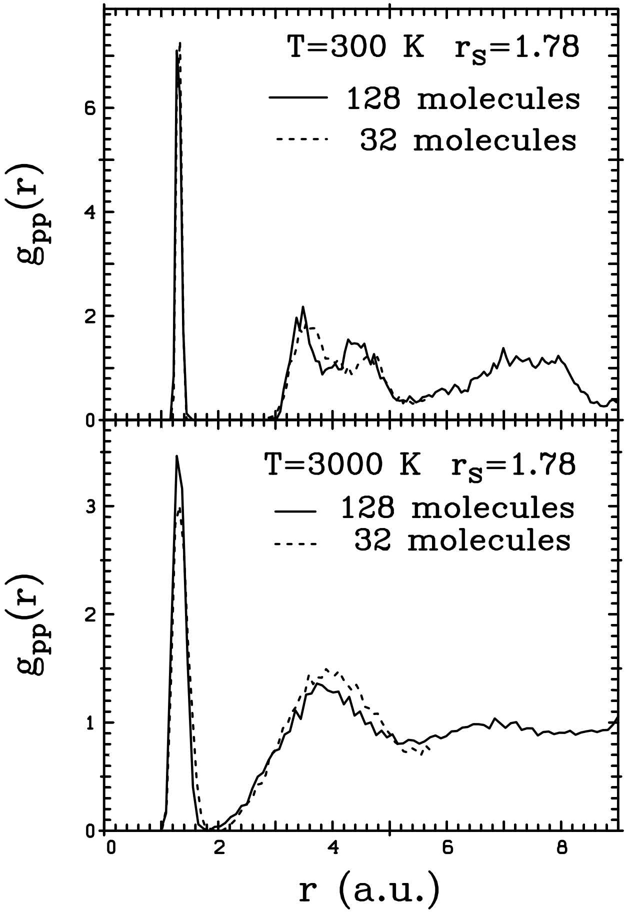
- calculation of $Z(T)$ impossible due to two-body interaction
- replace ensemble averages by time averages

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

- 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 $\surd$

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[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
- $\left(\sum_i \frac{\vec{p}_i^{\,2}}{2m_i} - \frac{3N}{2}k_B T\right) > 0 \quad \Rightarrow$ cooling
- $\left(\sum_i \frac{\vec{p}_i^{\,2}}{2m_i} - \frac{3N}{2}k_B T\right) < 0 \quad \Rightarrow$ heating
- there is no equipartition theorem for quantum systems

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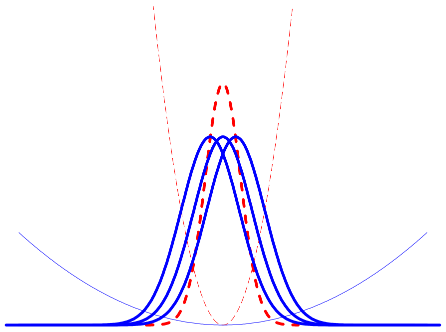
[a] W.G. Hoover, Phys. Rev. **A31** (1985) 1685

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

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

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

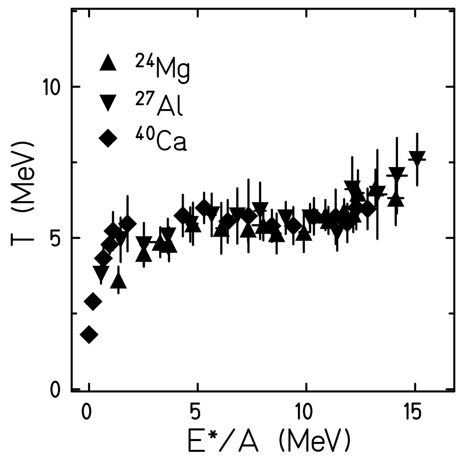
- **coupling** of all nucleons to the thermometer wave packet:
  $\underset{\sim}{V}_{\mathrm{N-Th}}, \quad \underset{\sim}{H} = \underset{\sim}{H}_{\mathrm{N}} + \underset{\sim}{H}_{\mathrm{Th}} + \underset{\sim}{V}_{\mathrm{N-Th}} \,, \quad |\, Q(t)\, \rangle = |\, nucleus\, \rangle \otimes |\, thermometer\,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

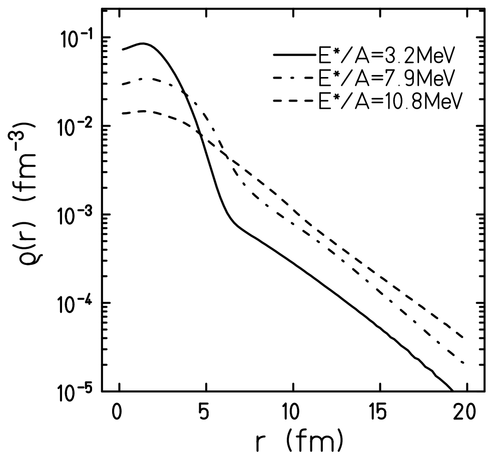
- **time-averaging:**
  $E_{\mathrm{Th}} = \overline{\langle\, \underset{\sim}{H}_{\mathrm{Th}}\, \rangle} \,, \quad E^* = \overline{\langle\, \underset{\sim}{H}_{\mathrm{N}} - E_0\, \rangle} \,,$

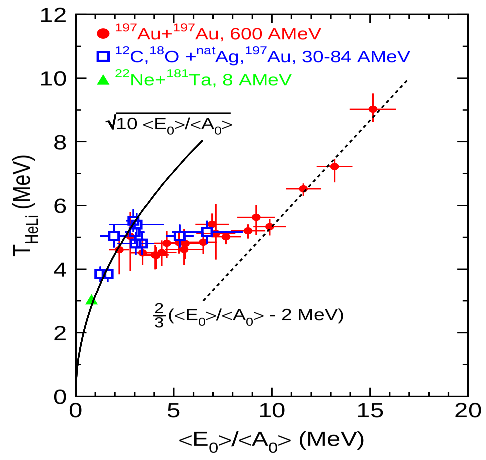
- **zeroth law:** both subsystems approach the same T

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

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

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

Thermostat I

Total system:

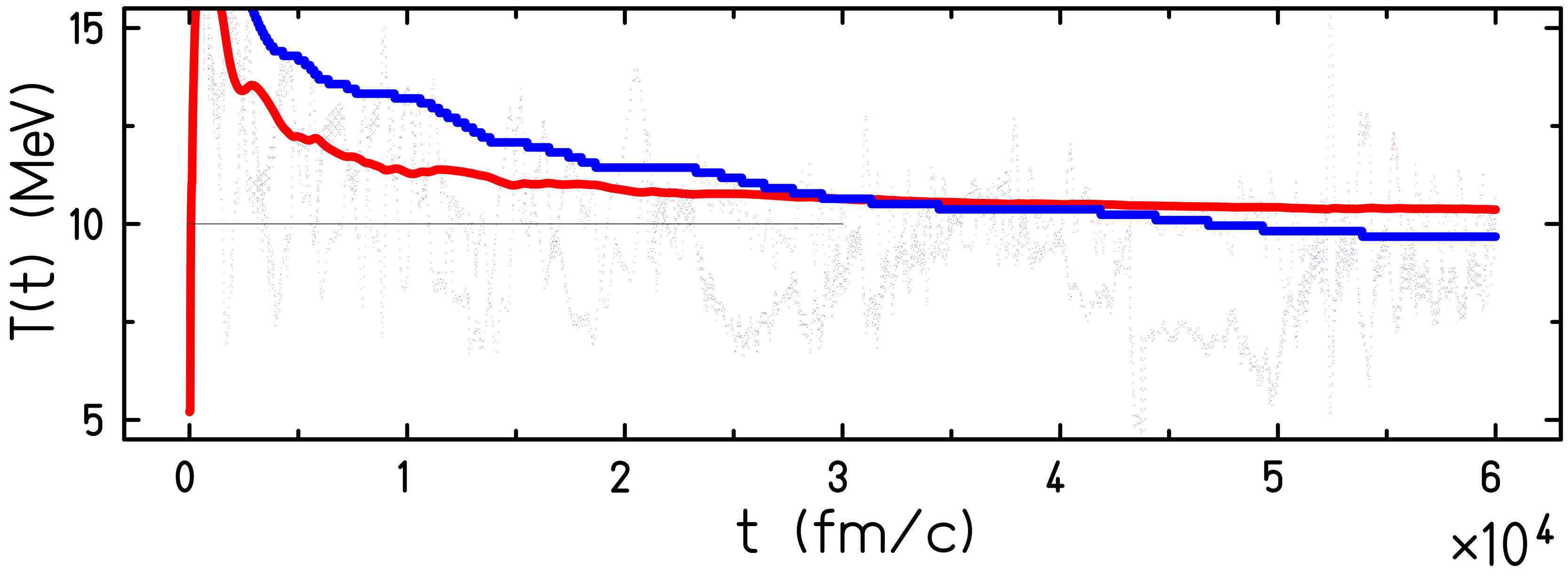
$$|\,Q(t)\,\rangle \quad = \quad |\,system(t)\,\rangle \otimes |\,thermometer(t)\,\rangle$$

Complex time steps:

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

- 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

Summary

Dynamics

- 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

Thermodynamics

- 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

Problems to solve

- tunneling, branching
- realistic interactions
- reliable thermostats

Literature

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5. H. Feldmeier, J. Schnack, Rev. Mod. Phys. **72** (2000) 655
6. J. Schnack, Physica A **259** (1998) 49
7. J. Schnack, Europhysics Letters **45** (1999) 647
8. H. Feldmeier, T. Neff, R. Roth, J. Schnack, Nucl. Phys. A **632** (1998) 61
9. http://obelix.physik.uni-osnabrueck.de/∼schnack/