Molecular Dynamics for Fermions

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Why molecular dynamics for fermions?
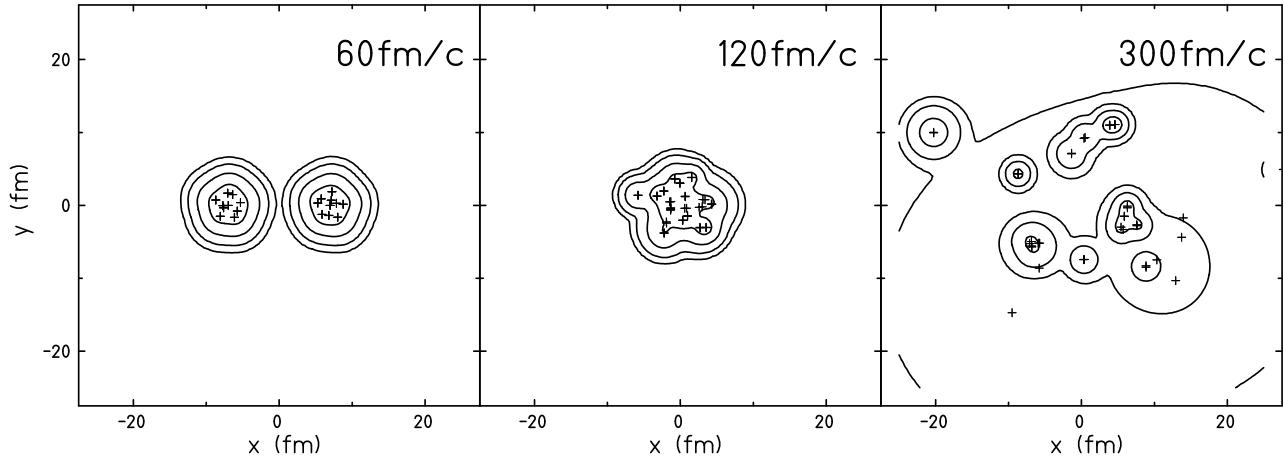
^{40}Ca-^{40}Ca-reaction at $E_{Lab} = 35 A$ MeV

Multifragmentation reactions:

- large fluctuations in the final results

- cannot be accounted for with TDHF, because nucleons are to fast ($\varepsilon > \varepsilon_F \approx 30$ MeV)

- no common mean field established

- molecular dynamics better suited

Means:

- "trajectory" calculations for fermions, non-linear dynamics through localization

- quantum mechanically necessary: Heisenberg uncertainty principle, Pauli exclusion principle

Creation of a model

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

Ground states:

- Ritz variational principle defines ground states

- aim: reasonable (nuclear) ground state properties like binding energy and rms radius

- usually phenomenological interaction

Dynamics:

- time-dependent variational principle defines dynamics

- aim: dynamics should cover fusion, deeply inelastic reactions, evaporation, fragmentation, vaporisation

- equations of motion non-linear, large fluctuations

Open problems:

- restricted dynamics causes barriers in Hilbert space

- due to localization no tunneling or branching

- thermodynamics ?

Applications

Nuclear physics

- Classical Molecular Dynamics (CMD)
  - e.g. Bondorf, Halbert (NBI); Wilets (Seattle), Randrup (Berkeley)
  - Pauli and possibly Heisenberg potential
- Quantum Molecular Dynamics (QMD)
  - Aichelin (Nantes); Stöcker (Frankfurt am Main); Maruyama (Japan)
  - product state of gaussian wave packets and Pauli potential
- Antisymmetrized Molecular Dynamics (AMD)
  - Horiuchi, Ono, Ohnishi (Japan)
  - Slater determinant of gaussian wave packets
- Fermionic Molecular Dynamics (FMD)
  - Feldmeier, Neff, Roth (GSI), Schnack (Osnabrück)
  - Slater determinant of gaussian wave packets, time-dependent width

Atomic physics

- Classical Molecular Dynamics
  - many groups worldwide
- Quantum Molecular Dynamics
  - Ebeling (Berlin); Klakow, Reinhard, Toepffer (Erlangen)

TDVP[a]:

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

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

Euler–Lagrange equations in their most general form:

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

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

- trial state $| \, Q(t) \, \rangle = | \, \{q_\mu(t)\} \, \rangle$
- 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, $\mathcal{H} = \langle\, Q(t)\,|\, \underset{\sim}{H}\, |\, Q(t)\,\rangle$

$$\frac{d}{dt}\, \mathcal{B}(t) \;\; = \;\; \frac{d}{dt}\, \langle\, Q(t)\,|\, \underset{\sim}{B}\, |\, Q(t)\,\rangle = \sum_{\nu} \dot{q}_{\nu} \frac{\partial}{\partial q_{\nu}}\, \mathcal{B}$$

$$= \;\; \sum_{\mu,\nu} \frac{\partial\, \mathcal{H}}{\partial q_{\mu}}\, \mathcal{A}_{\mu\nu}^{-1} \frac{\partial\, \mathcal{B}}{\partial q_{\nu}} \;\; =: \{\mathcal{H}, \mathcal{B}\}$$

2. Conservation Laws

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

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

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

TDVP:

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

Schrödinger equation:

$$
\begin{aligned}
|\, Q \,\rangle &= |\, \rho_1, \rho_2, \cdots, \pi_1, \pi_2, \cdots \,\rangle \\[2mm]
&= \sum_n c_n \,|\, n \,\rangle \equiv \sum_n \frac{1}{\sqrt{2}}(\rho_n + i\pi_n)\,|\, n \,\rangle \\[4mm]
\mathcal{L} &= -\sum_n \rho_n \dot{\pi}_n - \mathcal{H}(\rho_1, \rho_2, \cdots, \pi_1, \pi_2, \cdots) \\
&\quad + \text{total time derivative}
\end{aligned}
$$

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

Example 2 — QMD

TDVP:

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

Most classical quantum molecular dynamics[a]:

$$|Q\rangle = |\vec{r}_1, \vec{p}_1\rangle \otimes |\vec{r}_2, \vec{p}_2\rangle \otimes \cdots \otimes |\vec{r}_N, \vec{p}_N\rangle$$

$$\langle \vec{x} \,|\, \vec{r}_k, \vec{p}_k \rangle = \left(\frac{1}{\pi a_0}\right)^{3/4} \exp\left\{ -\frac{(\vec{x} - \vec{r}_k)^2}{2\,a_0} + i\,\vec{p}_k \cdot \vec{x} \right\}$$

$$\mathcal{L} = -\sum_{k=1}^{N} \vec{r}_k\, \dot{\vec{p}}_k - \mathcal{H}(\vec{r}_1, \vec{p}_1, \ldots, \vec{r}_N, \vec{p}_N)$$

$$\frac{d}{dt}\,\vec{p}_k = -\frac{\partial \mathcal{H}}{\partial \vec{r}_k} \quad \text{and} \quad \frac{d}{dt}\,\vec{r}_k = \frac{\partial \mathcal{H}}{\partial \vec{p}_k}$$

- product state describes distinguishable particles
- impact of Pauli principle on dynamics sometimes mocked by additional terms in $\mathcal{H}(\vec{r}_1, \vec{p}_1, \ldots, \vec{r}_N, \vec{p}_N)$ – Pauli potential
- statistics remains that of distinguishable particles

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[a]E.J. Heller, J. Chem. Phys. **62** (1975) 1544

Example 3 — LQMD

TDVP:

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

Molecular dynamics with more quantum effect:

$$|\, Q \,\rangle \quad = \quad |\, \vec{r}_1, \vec{p}_1, a_1 \,\rangle \otimes \cdots \otimes |\, \vec{r}_N, \vec{p}_N, a_N \,\rangle$$

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

Freely moving particles:

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

$$\frac{d}{dt}\, a_l \quad = \quad \frac{i}{m_l}$$

Particles moving in a harmonic oscillator:

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

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

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

Example 4 – FMD

TDVP:

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

Fermionic Molecular Dynamics (FMD)[a]:

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

$$\langle \, \vec{x} \, | \, q_l(t) \, \rangle \quad = \quad \langle \, \vec{x} \, | \, \vec{r}_l, \vec{p}_l, a_l, \chi_l, \phi_l \, \rangle$$

$$= \quad \exp\left\{ -\frac{(\vec{x} - \vec{r}_l)^2}{2\,a_l} + i\,\vec{p}_l \cdot \vec{x} \right\} \otimes | \, \chi_l(t), \phi_l(t) \, \rangle \otimes | \, m_t(l) \, \rangle$$

- a priori Heisenberg and Pauli principle
- coincides with solution of the Schrödinger equation for free motion and harmonic oscillator

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[a]H. Feldmeier, Nucl. Phys. **A515** (1990) 147

Results – Multifragmentation

^{19}F–^{27}Al at $E_{Lab} = 32A$ MeV and $b = 0.5$ fm:
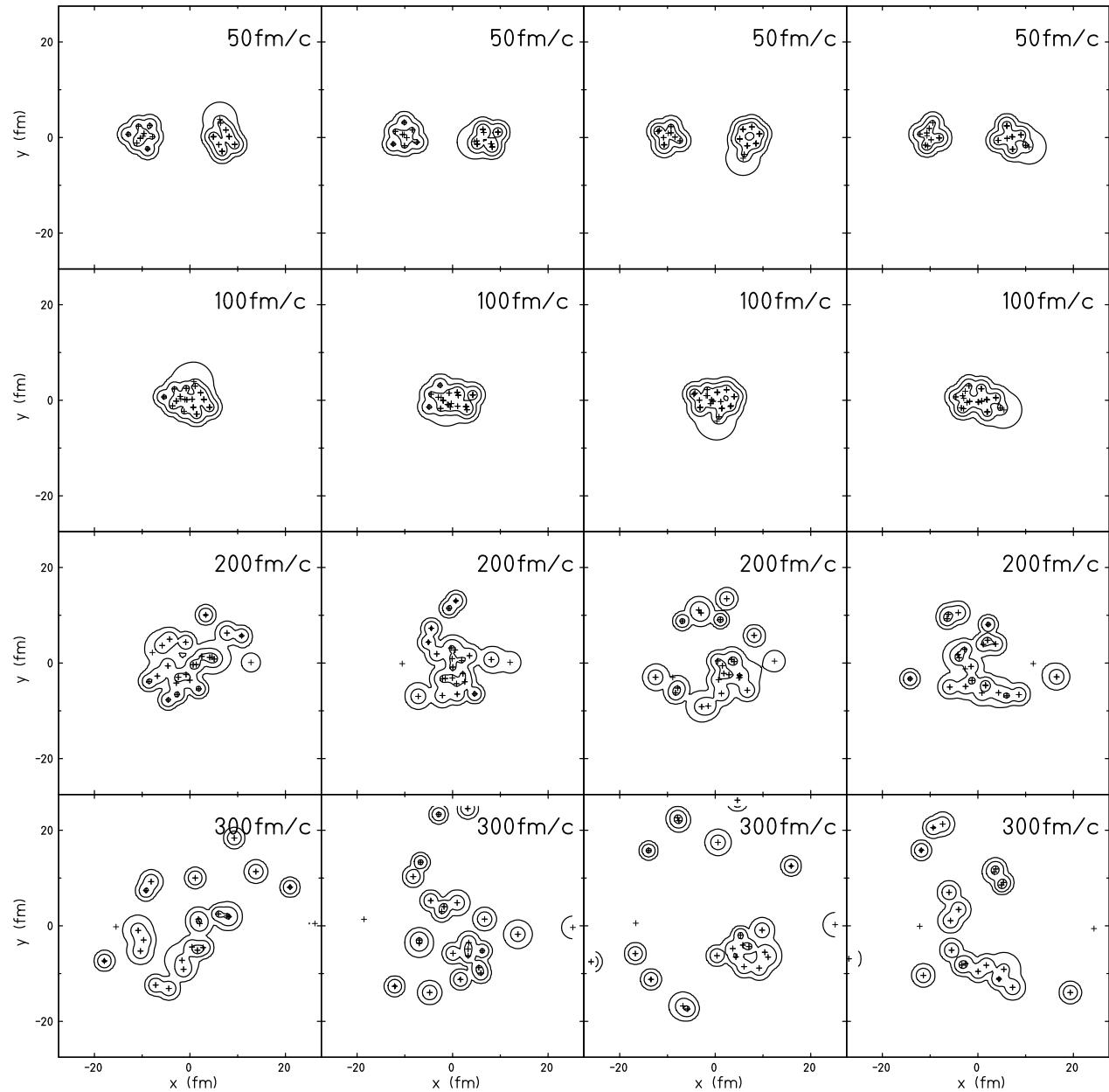
Error due to restriction of the wave function:
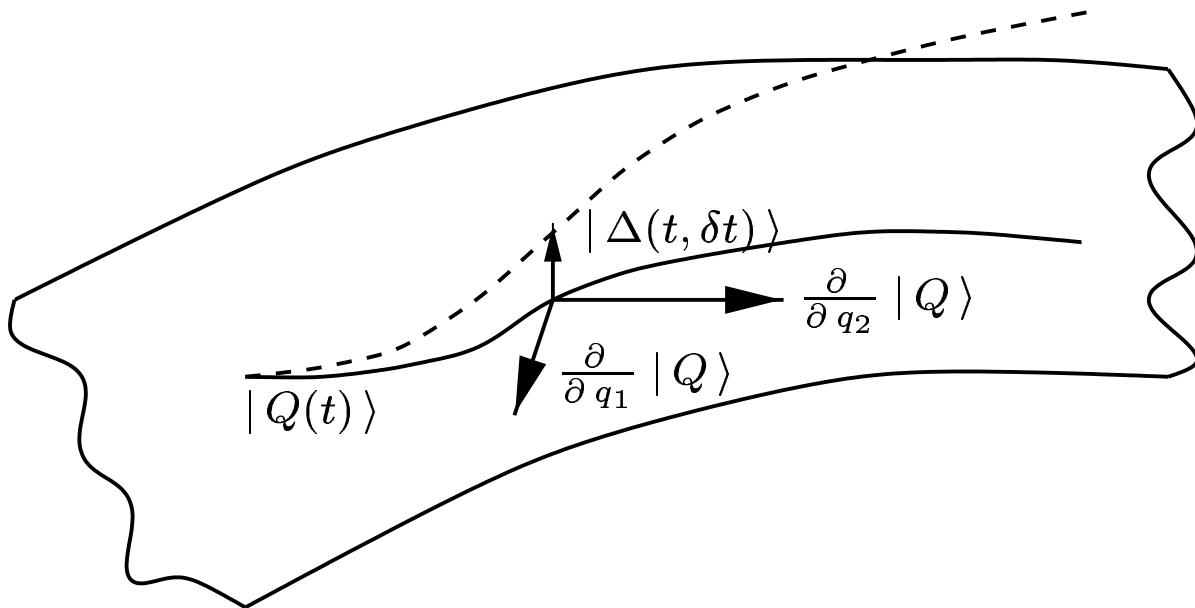
The error $|\Delta(t, \delta t)\rangle = \exp(-i\underset{\sim}{H}\delta t)\,|Q(t)\rangle - |Q(t+\delta t)\rangle$ is orthogonal to all tangent states $\frac{\partial}{\partial q_\nu}\,|Q\rangle$. Thus the TDVP-evolved state has the minimum distance $\langle\Delta(t, \delta t)\,|\,\Delta(t, \delta t)\rangle$ to the exact solution.

Open questions

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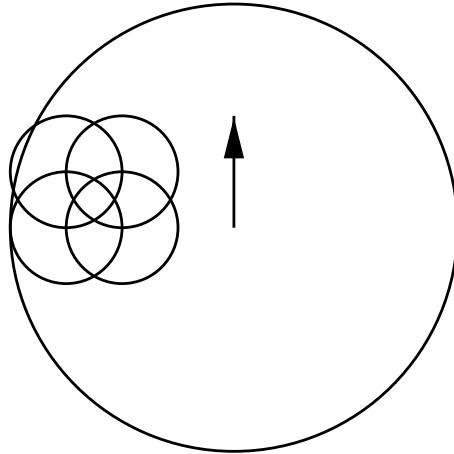
Pictorial scetch of a four particle cluster and a passing wave packet.

- 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

- idea: quantum branching

- jumps $|Q_i(t)\rangle \to |Q_j(t)\rangle$ 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 using restricted wave functions

Canonical ensemble

$$\underset{\sim}{R} \;\; = \;\; \frac{1}{Z} \exp\left\{ -\frac{\underset{\sim}{H}}{T} \right\}$$

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

- thermostatics: calculation of $Z(T)$

- if model states $|\,Q\,\rangle$ complete, $Z(T)$ correct, e.g. for gaussian wave packets

- Z cannot be evaluated for realistic $\underset{\sim}{H}$, one would like to replace ensemble averages by time averages

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

- Problem: allthough trial states span the Hilbert space, approximate dynamics needs not to be ergodic!
  And if limit exists, is it the right one?

Example

Atomic physics – solid hydrogen[a]

Plot showing $g_{pp}(r)$ versus r (a.u.). Top panel: T=300K, r_S=1.78; bottom panel: T=3000K, r_S=1.78. Legends: Hohl et al., WPMD: 128 molekules, 32 molekules.
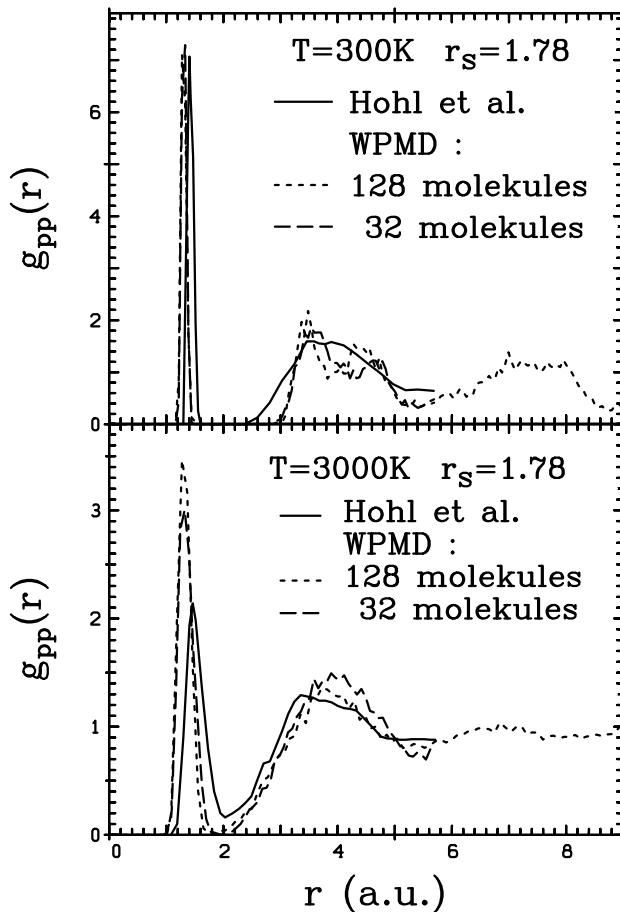
Proton pair distribution function $g(r)$

- electrons described by EQMD with Pauli potential

- protons classical

- temperature via equipartition theorem for protons $\sqrt{}$

- but in quantum mechanics equipartition theorem does not hold

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

Coupling to a Thermometer
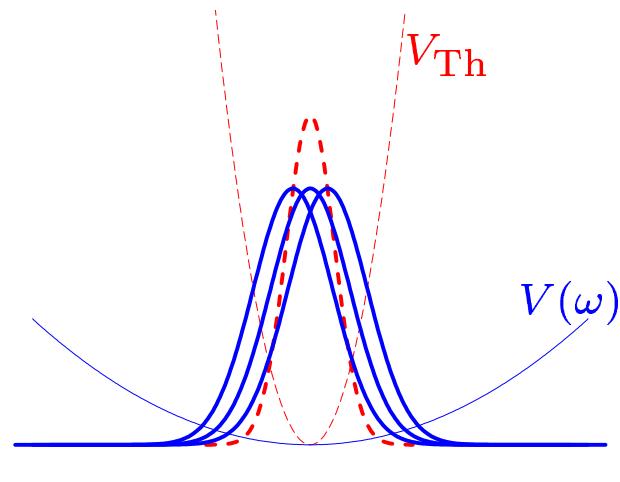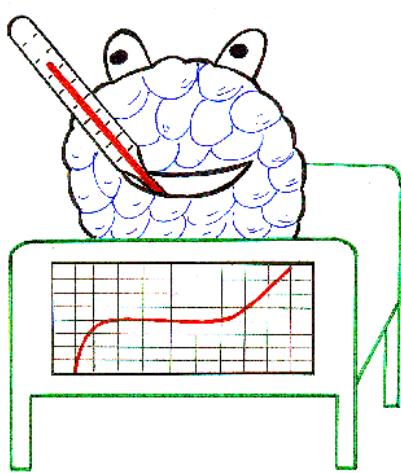
Procedure:

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

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

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

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

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

Caloric Curve
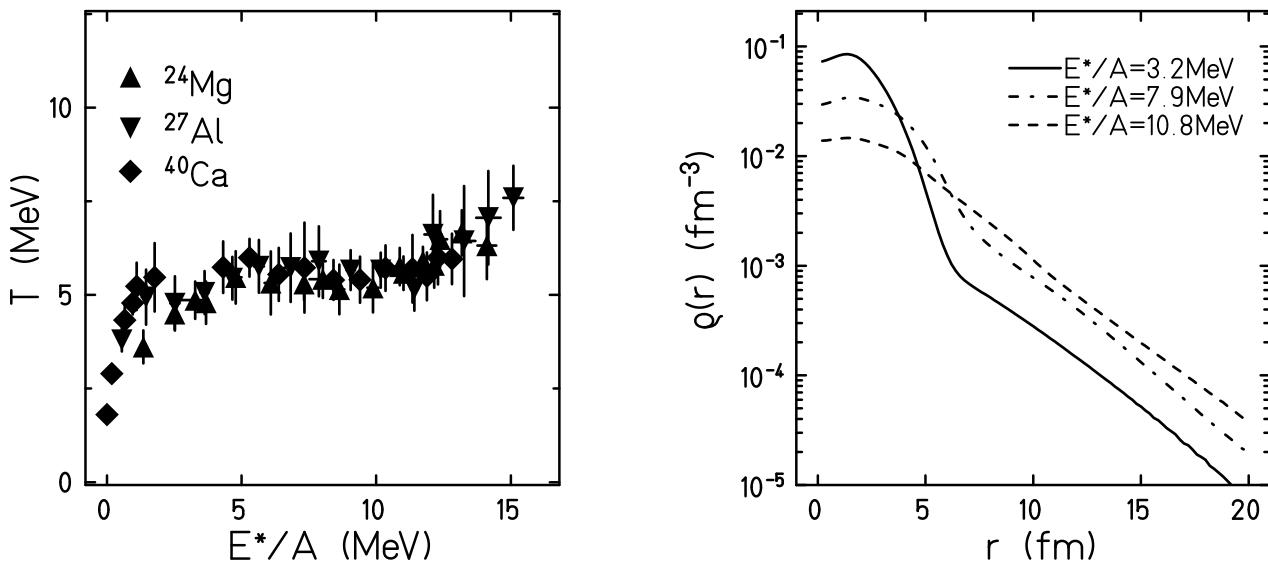
J. Pochodzalla et al., Phys. Rev. Lett. 75 (1995) 1040:
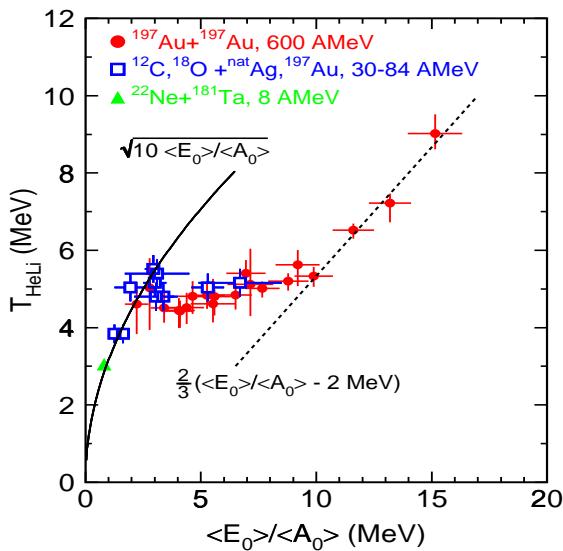
- simulation: equilibrium due to evolution in container over long time, ideal gas thermometer

- experiment: event–ensemble shows equilibrium properties, chemical thermometer

Critical temperature of ^{16}O:
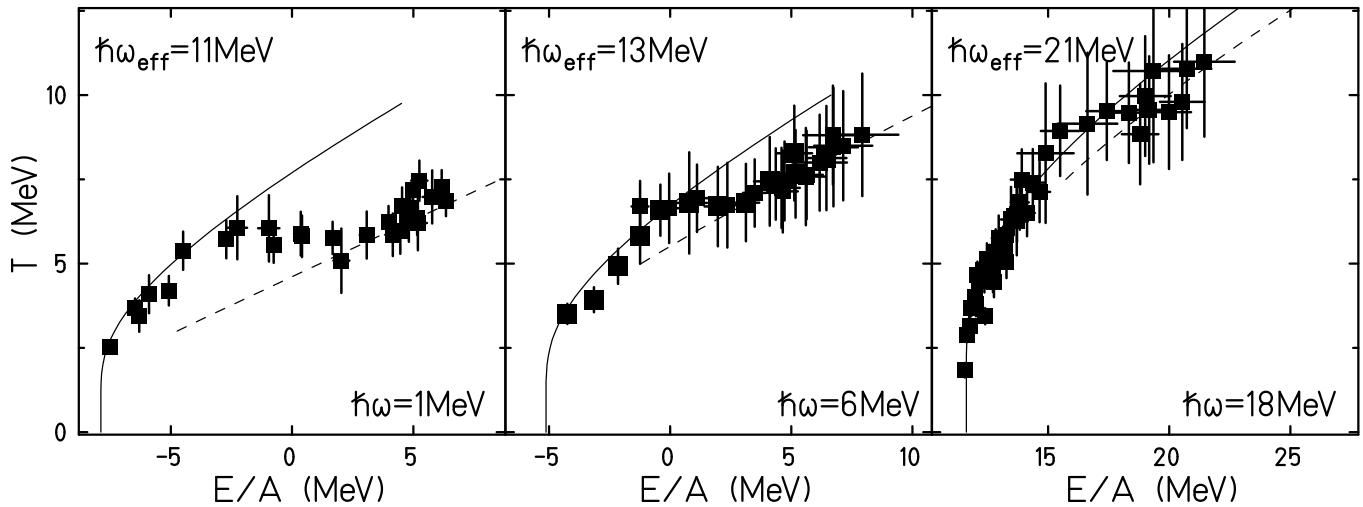
- ω serves as external parameter like volume or pressure
- critical point: latent heat vanishes
- system finite and charged: $T_c = T_c(N, Z)$

Classical Mechanics
Nosé–Hoover–Thermostat

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

$$\frac{d}{dt}\,\vec{r}_i = \frac{\vec{p}_i}{m_i}$$

$$\frac{d}{dt}\,\vec{p}_i = -\frac{\partial V}{\partial \vec{r}_i} - \xi\,\vec{p}_i$$

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

- 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
- one would like to construct a thermostat for a quantum system

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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

Thermostat

Total system:

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

Complex time steps:

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

- T desired temperature

- T_{th} temperature measured by the thermometer

- $d\beta > 0 \ \Rightarrow$ cooling; $\quad d\beta < 0 \ \Rightarrow$ heating
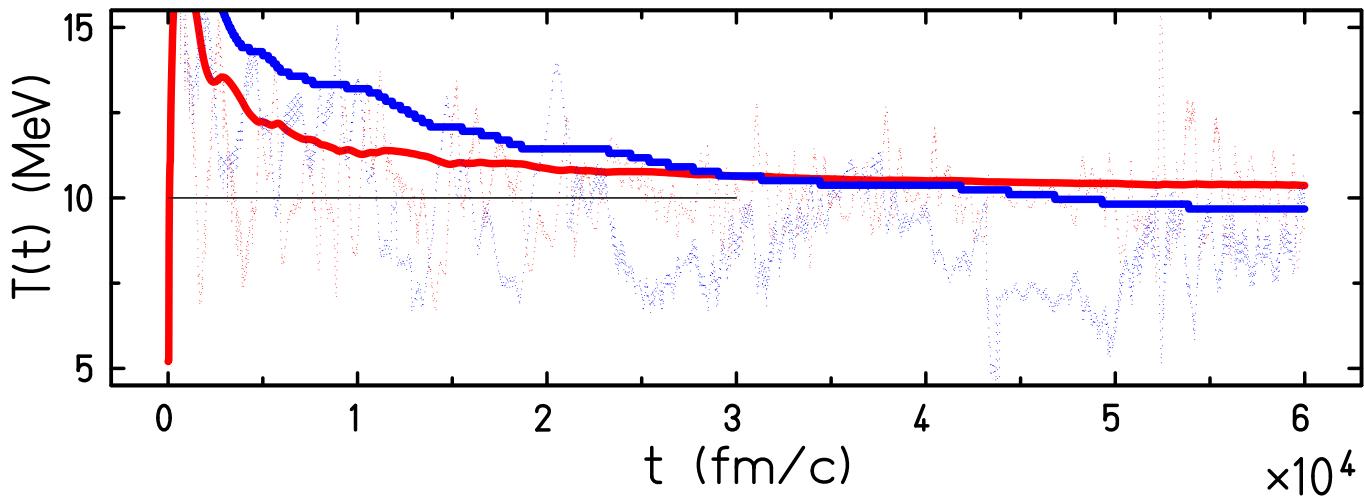
Fermions in a harmonic oscillator:

- actual temperatures – pointed lines

- time averaged temperatures – solid lines

- thermometer – red lines, fermions – blue lines

Summary

- TDVP allows approximate quantum time evolution
- system $(\underset{\sim}{H})$ and observables of interest determine how sophisticated trial state $|Q(t)\rangle$ must be
- Heisenberg uncertainty and Pauli exclusion principle suggest that the system is described by a state instead of classical phase space variables and that the state is anti-symmetric instead of using a Pauli potential
- various models with different sophistication used: CMD, QMD, AMD, FMD
- thermostatic properties depend on resolution of unity
- thermodynamic properties can be extracted from time evolution via thermometer and time averaging
- a thermostat can be defined using a coupled thermometer and complex time steps

Problems to solve
- tunneling, branching
- realistic interactions

Literature

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

2. H. Feldmeier, Nucl. Phys. **A515** (1990) 147

3. H. Feldmeier, K. Bieler, J. Schnack, Nucl. Phys. **A586** (1995) 493

4. H. Feldmeier, J. Schnack, Prog. Part. Nucl. Phys. **39** (1997)

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

6. J. Schnack, H. Feldmeier, Phys. Lett. **B409** (1997) 6

7. H. Feldmeier, J. Schnack, to appear in Rev. Mod. Phys.

8. J. Schnack, Physica **A 259** (1998) 49

9. J. Schnack, Europhysics Letters **45** (1999) 647