Isothermal quantum dynamics: Nosé-Hoover method for coherent states

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The method of Nosé and Hoover, which equilibrates a classical many-body system by means of pseudofriction coefficients, is generalized to a genuine quantum system. We show that for the quantum harmonic oscillator, the equations of motion in terms of coherent states can easily be modified in an analogous manner to mimic the coupling of the system to a thermal bath and create a quantum canonical ensemble. The method can be applied as well to non-interacting Fermi and Bose gases.

http://obelix.physik.uni-osnabrueck.de/~schnack/

Contents

Statement of the problem

Classical partition function:

$$Z_N(\beta) \quad = \quad \int \prod_{i=1}^{N} \mathrm{d}^3 r_i \, \mathrm{d}^3 p_i \; \exp\{-\beta H(\vec{r}_1, \vec{p}_1, \dots)\}$$

- $Z_N(\beta)$ cannot be evaluated directly for interacting particles;
- nevertheless, equations of motion can be solved (numerically) exact;
- goal: determination of canonical ensemble averages as an average over an isothermal time evolution.

Classical Nosé method

Extended set of degrees of freedom[a]**:**

$$H(\vec{r}_1, \vec{p}_1, \dots) \quad \Rightarrow \quad H_{\text{Nosé}} = H(s\vec{r}_1, \frac{\vec{p}_1}{s}, \dots) + \frac{p_s^2}{2M} + k_B T \ln(s)$$

$$Z_{\text{mc}} \quad = \quad \int \prod_{i=1}^{N} \mathrm{d}^3(s r_i) \mathrm{d}^3(\frac{p_i}{s}) \mathrm{d}s \mathrm{d}p_s \; \delta\{H_{\text{Nosé}} - E\}$$

$$\propto \quad \int \prod_{i=1}^{N} \mathrm{d}^3 r_i \; \mathrm{d}^3 p_i \; \mathrm{d}p_s \; \exp\{-\beta H(\vec{r}_1, \vec{p}_1, \dots)\} \exp\left\{-\beta \frac{p_s^2}{2M}\right\}$$

- **ergodic** microcanonical time evolution of the extended system yields canonical distribution of $\vec{r}_i, \vec{p}_i$;
- but microcanonical Nosé time evolution is never ergodic!

[a] S. Nosé, J. Chem. Phys. **81** (1984) 511; S. Nosé, Prog. of Theor. Phys. Suppl. **103** (1991) 1

Classical Nosé–Hoover Thermostat

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

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

- 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;
- this thermostat is also not always ergodic!

[a] W.G. Hoover, Phys. Rev. A **31** (1985) 1685
[b] S. Nosé, Prog. of Theor. Phys. Suppl. **103** (1991) 1

Technical improvements of the classical Nosé–Hoover Thermostat

- chain thermostat method[a]: successive couplings of pseudofriction coefficients in order to equilibrate the first one;
- demon method[b]: nonlinear coupling of several generalized pseudofriction coefficients (demons);
- ergodic time evolution and thus equilibration is guaranteed (to a very high degree).

[a] G. J. Martyna, M. L. Klein, M. Tuckerman, J. Chem. Phys. **97** (1992) 2635
[b] D. Kusnezov, A. Bulgac, W. Bauer, Ann. of Phys. **204** (1990) 155

Quantum Nosé method I

Extended set of degrees of freedom[a]:

$$\underset{\sim}{\vec{x}} \to s\,\underset{\sim}{\vec{x}}\;, \quad \underset{\sim}{\vec{k}} \to \frac{1}{s}\underset{\sim}{\vec{k}}\;, \quad \underset{\sim}{H}_s \;=\; \sum_{i=1}^{N} \frac{\underset{\sim}{\vec{k}}_i^2}{2\,m_i\,s^2} + \underset{\sim}{V}\left(\left\{s\,\underset{\sim}{\vec{x}}_i\right\}\right)$$

$$\begin{aligned} Z_{\text{mc}} &= \int \mathrm{d}s\mathrm{d}p_s\,\mathrm{Tr}\left(\delta\{\underset{\sim}{H}_s + \frac{p_s^2}{2M} + k_B T \ln(s) - E\}\right) \\ &\propto \int \mathrm{d}p_s\,\mathrm{Tr}\left(\exp\left\{-\beta \underset{\sim}{H}\right\}\exp\left\{-\beta\frac{p_s^2}{2M}\right\}\right) \end{aligned}$$

[a]M. Grilli, E. Tosatti, Phys. Rev. Lett. **62** (1989) 2889; F. Mauri, R. Car, E. Tosatti, Europhys. Lett. **24** (1993) 431

Quantum Nosé method II

Equations of motion:

$$i \frac{d}{dt} \mid \Psi(t) \,\rangle \quad = \quad \underset{\sim}{H}_s \mid \Psi(t) \,\rangle \quad ,$$

$$\dot{s} \equiv \frac{d}{dt}\, s = \frac{p_s}{M} \ , \qquad \dot{p_s} \equiv \frac{d}{dt}\, p_s = -\frac{T}{s} - \langle\, \Psi(t) \mid \left(\frac{\partial}{\partial\, s} \underset{\sim}{H}_s \right) \mid \Psi(t) \,\rangle$$

- **ergodic** microcanonical time evolution of the mixed quantum-classical system theoretically yields canonical distribution of $\mid \Psi(t) \,\rangle$ in Hilbert space;
- does not work[a]

[a] J. Schnack, D. Mentrup, H. Feldmeier, in preparation

Quantum Nosé–Hoover thermostat for independent particles in harmonic potentials

Idea[a]**:**

- investigate independent particles in harmonic potentials by means of coherent states;
- introduce pseudofriction coefficients into equations of motion;
- derive equation of motion for the pseudofriction coefficient from generalized Liouville equation;
- built up a chain or BBK thermostat;
- generalize method for indistinguishable particles.

[a] D. Mentrup, J. Schnack, Physica A **297** (2001) 337

Coherent states

Hamilton operator of the 1D quantum harmonic oscillator:

$$\underset{\sim}{H} = \hbar\omega \left(\underset{\sim}{a}^{\dagger} \underset{\sim}{a} + \frac{1}{2} \right)$$

Coherent states:

$$\underset{\sim}{a} \mid z \,\rangle = z \mid z \,\rangle \quad , \qquad z = \sqrt{\frac{m\omega}{2\hbar}}\, r + \frac{i}{\sqrt{2m\hbar\omega}}\, p$$

$$\langle\, x \,|\, z \,\rangle = \langle\, x \,|\, r, p \,\rangle \propto \exp\left\{ -\frac{(\, x - r\,)^2}{2} \frac{m\omega}{\hbar} + \frac{i}{\hbar} p\, x \right\}$$

Important property:

$$\exp(-i\,\omega\, \underset{\sim}{a}^{\dagger} \underset{\sim}{a}\, t) \,|\, z \,\rangle = \,|\exp(-i\omega t) z \,\rangle$$

Time Evolution

Exact time evolution of coherent states:

$$\frac{d}{dt}r = \frac{p}{m} \quad , \qquad \frac{d}{dt}p = -m\omega^2 r$$

Introduction of a pseudofriction coefficient(Nosé-Hoover):

$$\frac{d}{dt}r = \frac{p}{m} \quad , \qquad \frac{d}{dt}p = -m\omega^2 r - p\frac{p_\eta}{Q}$$

- time evolution for p_η determined from the condition that the distribution function $f(\beta; r, p, p_\eta)$ is stationary with regard to the generalized Liouville equation in the phase space $\Gamma = \{r, p, p_\eta\}$.

Pseudofriction coefficient

Generalized Liouville equation[a]**:**

$$\frac{d}{dt} f = -f \cdot \left(\frac{\partial}{\partial \Gamma} \cdot \dot{\Gamma} \right) = -f \cdot \left(\frac{\partial}{\partial r} \dot{r} + \frac{\partial}{\partial p} \dot{p} + \frac{\partial}{\partial p_\eta} \dot{p_\eta} \right)$$

Distribution function:

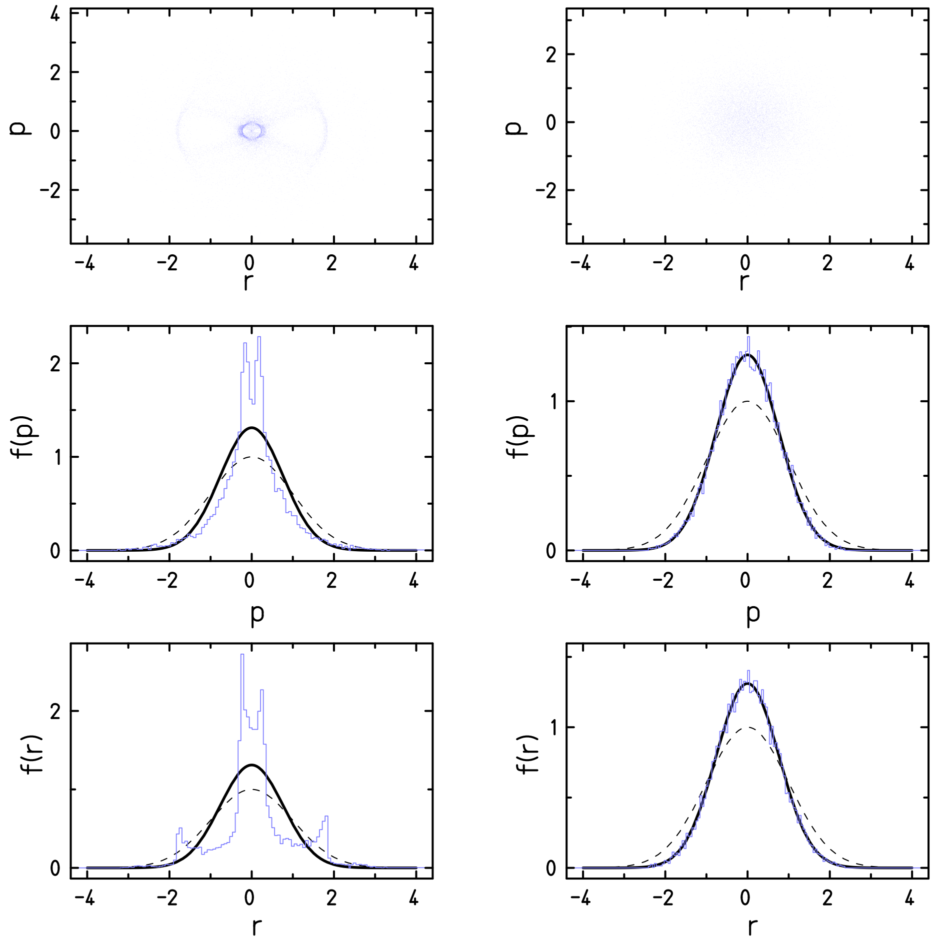
$$\begin{aligned} f(\beta; r, p, p_\eta) &\propto w_{qm}(\beta; r, p) \; \exp(-\beta \frac{p_\eta^2}{2Q}) \\ &\propto \exp\left(-(\frac{p^2}{2m} + \frac{1}{2} m \omega^2 r^2) \frac{e^{\beta \hbar \omega} - 1}{\hbar \omega} - \beta \frac{p_\eta^2}{2Q} \right) \end{aligned}$$

EOM for pseudofriction coefficient:

$$\frac{d}{dt} p_\eta = \frac{1}{\beta} \left(\frac{p^2}{m} \frac{e^{\beta \hbar \omega} - 1}{\hbar \omega} - 1 \right)$$

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

Result for a Single Particle



Left Panel:

Distributions sampled by a simple Nosé-Hoover dynamics,

Right Panel:

Nosé-Hoover chain dynamics

The quantum Nosé-Hoover method for two identical particles

Equations of motion of the wave packet parameters:

$$\frac{d}{dt}\, r_1 = \frac{p_1}{m} \quad , \quad \frac{d}{dt}\, r_2 = \frac{p_2}{m}$$

$$\frac{d}{dt}\, p_1 = -m\omega^2 r_1 - p_1 \frac{p_{\eta_1}}{Q_1} \quad , \quad \frac{d}{dt}\, p_2 = -m\omega^2 r_2 - p_2 \frac{p_{\eta_2}}{Q_2}$$

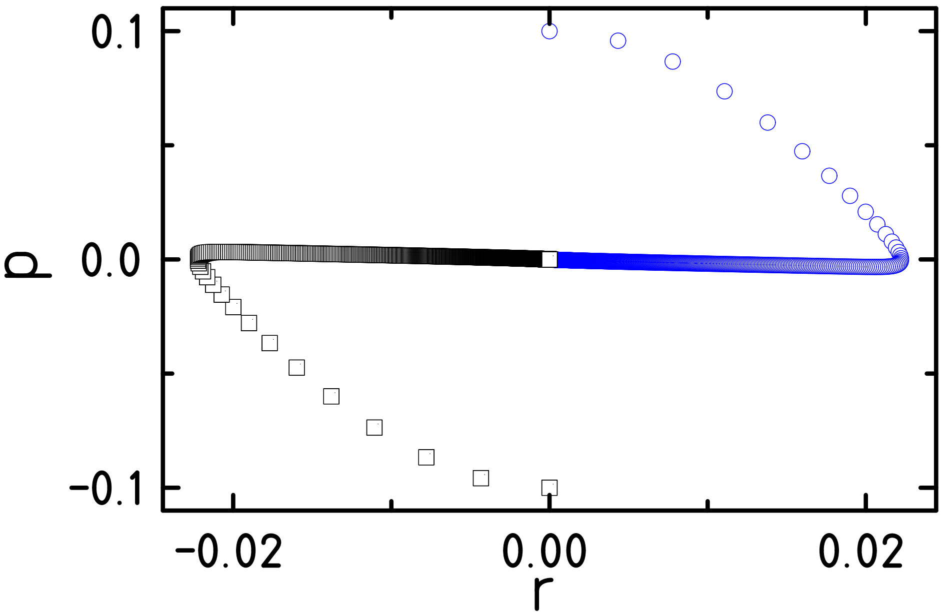
Equations of motion of the pseudofriction coefficients

(+: bosons, −: fermions, $V = |z_1 - z_2|^2$**):**

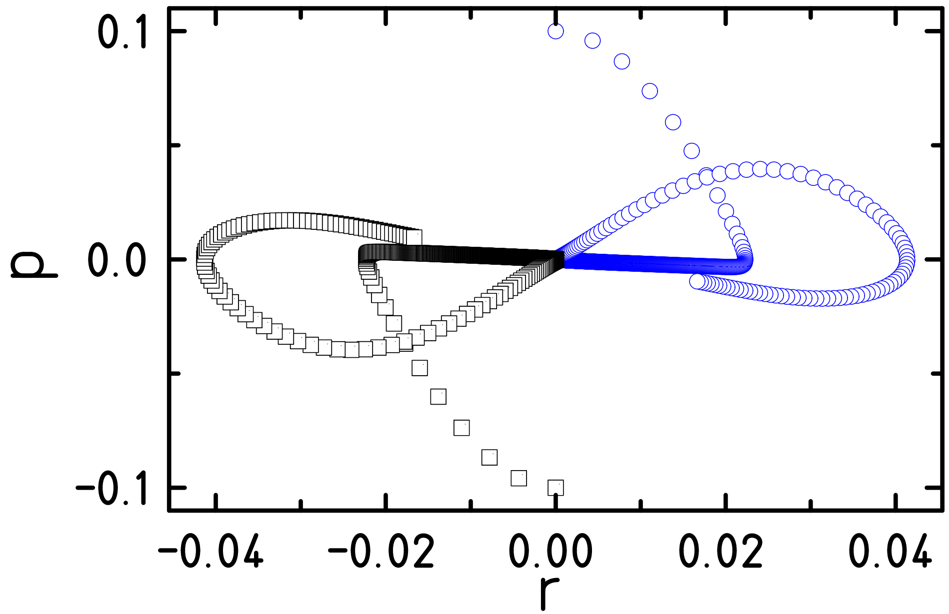
$$\dot{p}_{\eta_1} = \frac{1}{\beta}\left(\frac{p_1^2}{m}\frac{e^{\beta\omega}-1}{\omega} - 1 \pm (p_1^2 - p_1 p_2)\frac{e^{-V}}{m\omega(1 \pm e^{-V})}\right)$$

$$\dot{p}_{\eta_2} = \frac{1}{\beta}\left(\frac{p_2^2}{m}\frac{e^{\beta\omega}-1}{\omega} - 1 \pm (p_2^2 - p_1 p_2)\frac{e^{-V}}{m\omega(1 \pm e^{-V})}\right)$$

Results
"Bose-attraction and Pauli-blocking"



Bosons



Fermions

Summary and Outlook

- N non-interacting fermions can be equilibrated as well;
- Deterministic, but chaotic time-evolution leads to canonical ensemble via time averaging!
- Sign problem for fermions?
- No solution for interacting quantum N-body systems so far, except harmonic interactions, hm ;-)
- Is the quantum Nosé method past remedy?
- Does a generalized Nosé-Hoover thermostat exist? Major problem – a quantum equipartition problem does not exist.
- Approximation: Can a thermalized and weakly coupled particle act as a heat bath to other systems?