Consequences:

- the extended Hamiltonian $H_{Nose}$ is conserved upon evolution according to the extended Hamiltonian equations

  ⇒ microcanonical ensemble for the extended system

- it can be shown that the microcanonical ensemble averages of the extended systems are identical to the canonical ensemble averages of the original Hamiltonian
  (ensured by the choice of $g\, k_B T \ln s$)

- the time evolution of the variable s depends on choice of Q and can be interpreted as a coupling frequency. (bad match, bad scaling)

## §8.3 Velocity Rescaling and Gaussian Thermostat

The earliest idea: just rescale all velocities

$$p_i \rightarrow \sqrt{\frac{T_0}{T}}\, p_i$$

$T$: actual temperature
$T_0$: desired "

⇒ ok, but actual discontinuities in momentum part of phase space trajectory

A bit more formal approach:
constrain the equations of motions to fix $T$

Force added to restrict a particle motion to a constraint hypersurface should be normal to the surface of realistic dynamics.

⤳ add $-\alpha p_i$ to force term of Hamiltonian Eqs.

$$\frac{\partial q_i}{\partial t} = \frac{p_i}{m_i} \quad ; \quad \frac{\partial p_i}{\partial t} = -\frac{\partial V(q)}{\partial q_i} \underbrace{- \alpha p_i}_{\text{friction}}$$

Determine $\alpha$ so that $\frac{dT}{dt} = 0$

$$\frac{g k_B T}{2} = \sum_i \frac{p_i^2}{2 m_i} \quad \Big| \; \frac{\partial}{\partial t}$$

$$\frac{g k_B}{2} \frac{\partial T}{\partial t} = \sum_i \frac{p_i}{m_i} \frac{\partial p_i}{\partial t} \overset{!}{=} 0$$

insert from above

$$\sum_i \frac{p_i}{m_i} \left( - \frac{\partial V(q)}{\partial q_i} - \alpha p_i \right) = 0$$

$$-\sum_i \frac{\partial V(q)}{\partial q_i} \frac{p_i}{m_i} = \alpha \sum_i \frac{p_i^2}{m_i}$$

$$\Rightarrow \alpha = - \frac{\sum \frac{\partial V(q)}{\partial q_i} \frac{p_i}{m_i}}{\sum_i \frac{p_i^2}{m_i}}$$

Conserves canonical distribution in coordinate space.

## § 8.4 Proportional Timescaling: Berendsen thermostat

Velocity rescaling works too well. Temperature is really fixed, while in the canonical ensemble, the avoge energy is fixed and allowed fluctuations also translate into fluctuations of the instantaneous temperature.

Idea: Use a weaker coupling and try to drive the system dynamics towards the desired $T_0$

How? Velocities are scaled at each time-step in such a way that the rate of change of temperature is proportional to the difference in temperature:

$$\frac{dT}{dt} = \frac{1}{\tau}(T_0 - T) \qquad (*)$$

$\tau$: coupling parameter

$$\Rightarrow \quad T = T_0 - C_1 e^{-t/\tau}$$

exponential decay of $T$ to $T_0$.

$(*)$ in discrete version:

$$\Delta T = \frac{\Delta t}{\tau}(T_0 - T)$$

and modification of momenta

$$p_i \to \lambda p_i$$

with $$\lambda^2 = 1 + \frac{\Delta t}{\tau}\left(\frac{T_0}{T} - 1\right)$$