MATE664 L02

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Slide 6

$\{\vec{x}_i, \vec{v}_i, \vec{F}_{ij}\}$ can determine system

set of $\{\vec{x}_i, \vec{p}_i\}$ is called phase space

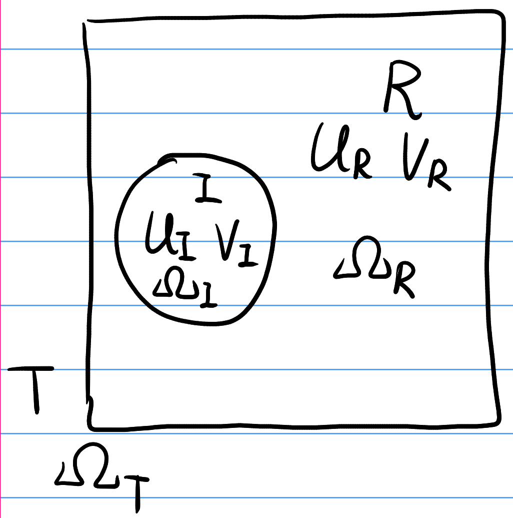
$\vec{p}_i = \vec{v}_i \cdot m_i$

Newtonian dyn.

$$\vec{x}_i(t+\Delta t) = \vec{x}_i(t) + \frac{\vec{p}_i}{m_i}\Delta t$$

$$\frac{\vec{p}_i}{m_i}(t+\Delta t) = \frac{\vec{p}_i}{m_i}(t) + \frac{F\Delta t}{m_i^2}$$

Slide 10 Setup



Internal energy Conservation

$$U_T = U_I + U_R$$

$$dU_I = -dU_R$$

Total entropy / state not conserved

$$\Omega(U_T) = \Omega(U_I) \times \Omega(U_R)$$

Lower U_I $\longrightarrow$ Higher U_R

$\downarrow$ Less Ω_I $\qquad$ $\uparrow$ More Ω_R

At same U_T $\longrightarrow$ many possible Ω_T!

S_T

Slide 11 Boltzmann dist

Lower energy U_I state are more likely

Because we have more reservoir states to exchange energy

$$p(U_I^\circ) \propto \Omega(U_T - U_I^\circ)$$

$$\ln \Omega(U_T - U_I^\circ) \doteq \ln \Omega(U_T) - \left.\frac{\partial \ln \Omega}{\partial U}\right|_{U=U_T} \cdot U_I^\circ$$

Change of states by U

(1^{st} law of thermodyn)

$$\Rightarrow p(U_I^\circ) \propto \Omega(U_T) \exp\left(-\frac{U_I^\circ}{k_B T}\right)$$

OR $$p(U_I^\circ + \Delta U) = p(U_I^\circ) \exp\left(-\frac{\Delta U}{k_B T}\right)$$

How do we know which U_I° to choose?

Change of U_I $\longrightarrow$ maximize total State Ω_T

$$\left(\frac{\partial \ln \Omega_T}{\partial U_I}\right) = 0 \quad \& \quad \left(\frac{\partial^2 \ln \Omega_T}{\partial U_I^2}\right) < 0$$

$\Longrightarrow$ Result $\dfrac{1}{T_I} = \dfrac{1}{T_R} = \dfrac{1}{T_T}$ (equilibrium)