ADVANCED STATISTICAL PHYSICS

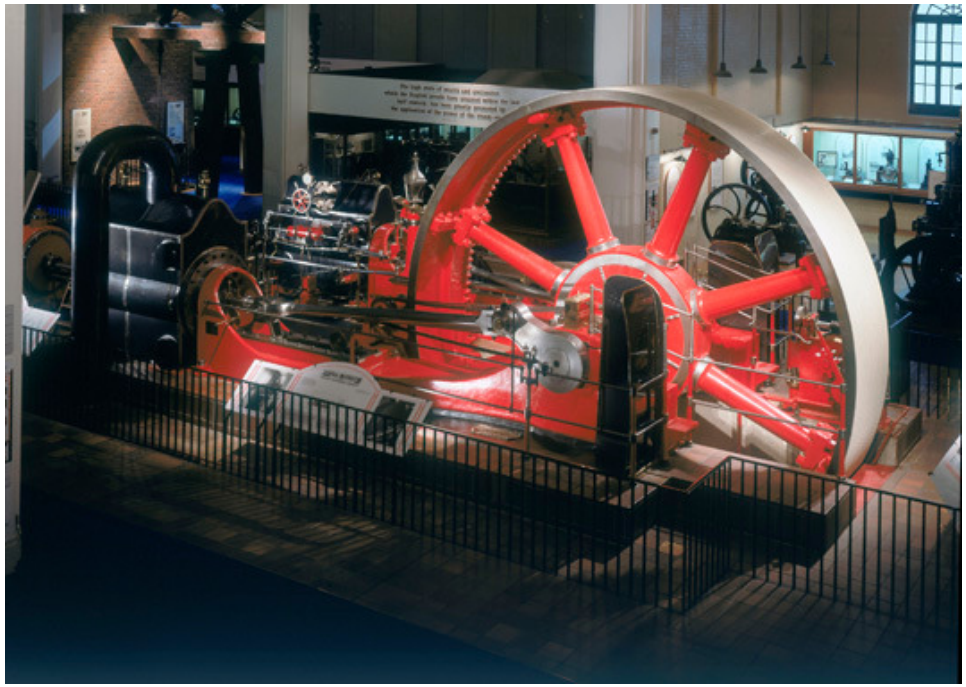
4+2 SWS in SS 24

"Schwerpunkt" and with theory lab course: "Ergänzung"

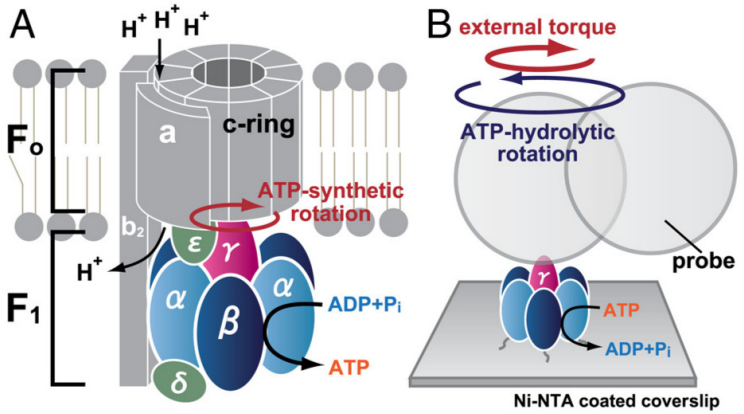
Udo Seifert II. Institut für Theoretische Physik, Universität Stuttgart

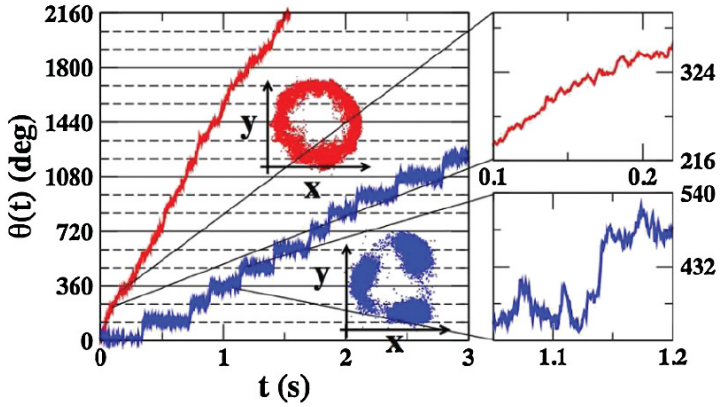
- Foundations of statistical physics
- Brownian motion
  - Langevin equations, Fokker-Planck equations, path integral
- Master equations for non-equilibrium
- Fluctuations beyond the Gaussian regime: Theory of large deviations
- Applications
  - Colloidal particles
  - Molecular motors
  - Active matter
  - Molecular clocks

- From classical th'dynamics to stochastic th'dynamics



19th century steam engine

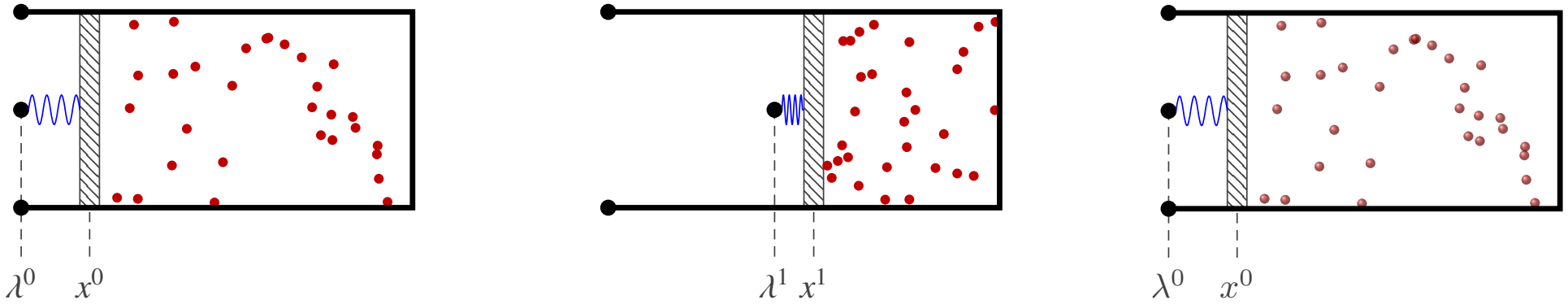




[K. Hayashi, ... H. Noji, PRL 104, 218103 (2010)]

21st century nano-engine: F_1ATP-ase

- Proof and sharpening of the (Kelvin-Planck) second law for a driven, isolated system



[C. Jarzynski, PRL 1997]

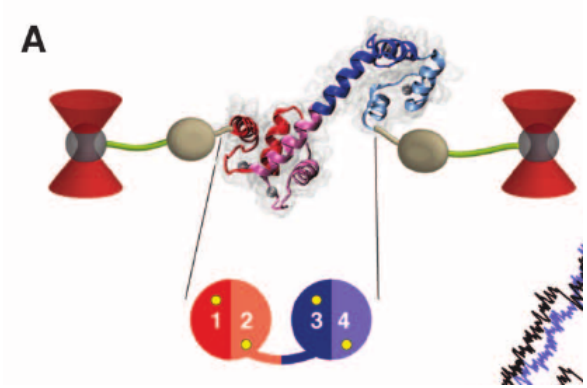
– time-dependent Hamiltonian $H(\xi, \lambda^t)$ along a cyclic path $\lambda^{\mathcal{T}} = \lambda^0$

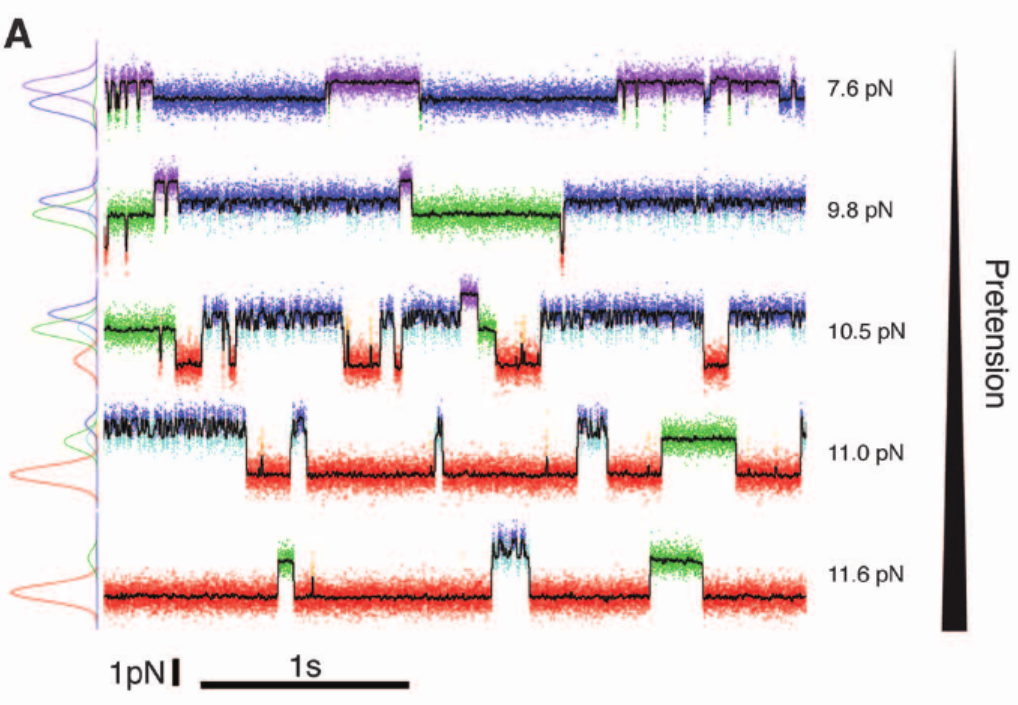
– work $W(\xi^0) \equiv H(\xi^{\mathcal{T}}, \lambda^{\mathcal{T}}) - H(\xi^0, \lambda^0)$ depends on the initial phase point ξ^0

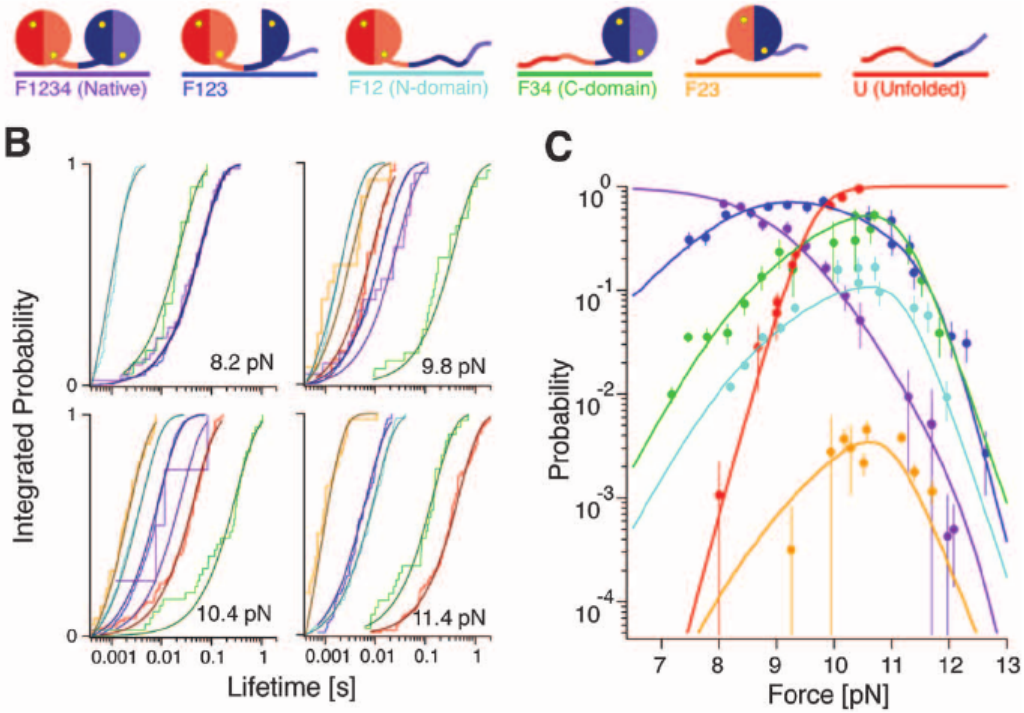
– initial phase point drawn from canonical distribution $\sim \exp[-\beta(H(\xi^0, \lambda^0)] \to p(W)$

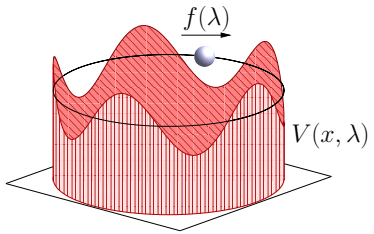
– we will prove $\boxed{\langle W(\xi^0)\rangle \geq 0}$

- Biomolecules in equilibrium: Meso-states of calmodulin [J. Stigler et al, Science **334** 512 (2011)]









- Driven Brownian motion

  - Langevin dynamics $\dot{x} = \mu[-V'(x) + f] + \zeta$ with $\langle \zeta_1 \zeta_2 \rangle = 2\mu T \delta(t_2 - t_1)$

  - first law [(Sekimoto, 1997)]: $\boxed{dw = du + dq}$

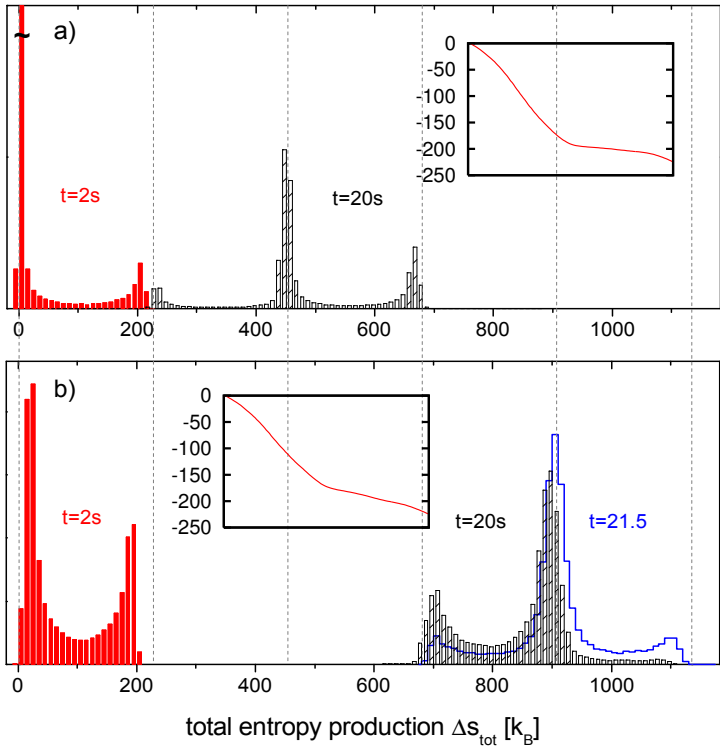
    * applied work: $dw = f\ dx$
    * internal energy : $du = dV$
    * dissipated heat: $dq = dw - du = [-\partial_x V(x) + f]dx = T ds_b$

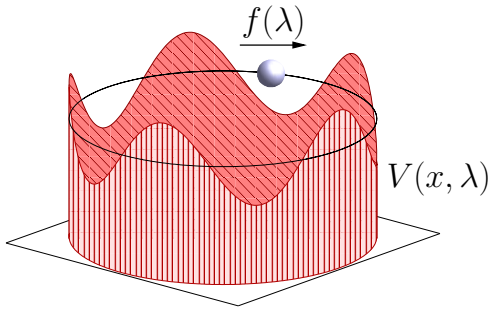
  - total entropy as quantitive measure of broken time reversal symmetry

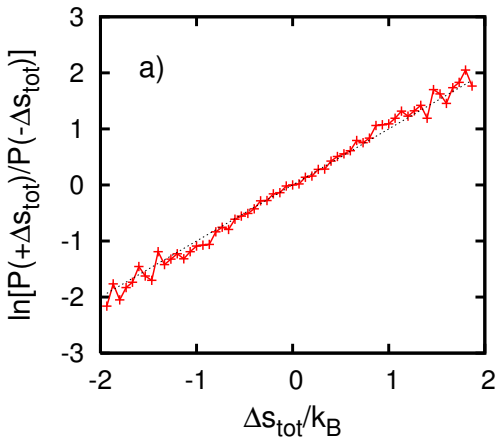
    $x(t) \to \tilde{x}(t) \equiv x(\mathcal{T} - t)$ $\quad \boxed{\Delta s_{\text{tot}}[x(t)] \equiv \ln[p[x(t)]/p[\tilde{x}(t)]] = \Delta[-\ln p^s(x)] + q/T}$

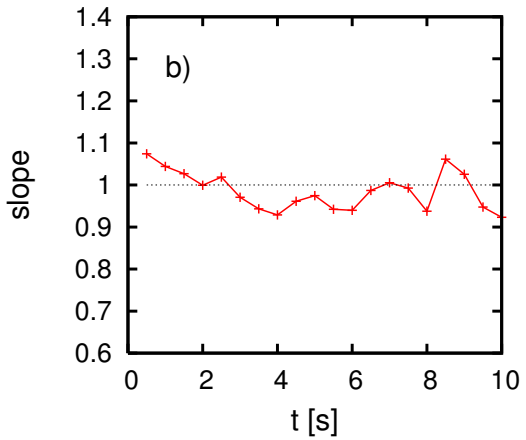
- Fluctuation theorem $\boxed{p(-\Delta s_{\rm tot})/p(\Delta s_{\rm tot}) = \exp(-\Delta s_{\rm tot})}$ in any NESS

- Experimental data [Speck, Blickle, Bechinger, U.S., EPL **79** 30002 (2007)]







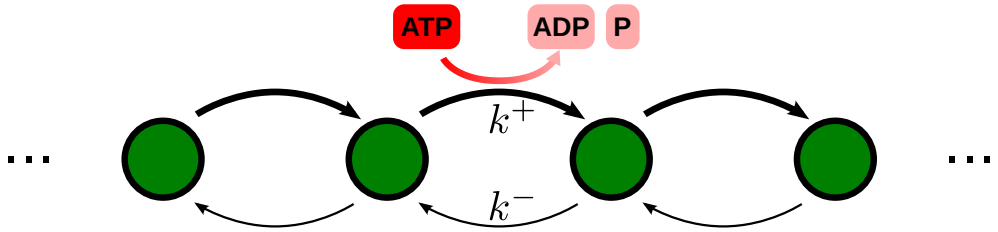


FT-representation

- Temporal precision in a finite temperature environment

at 300 K, a precision of 1 sec/day requires at least 6×10^{-11}J/day

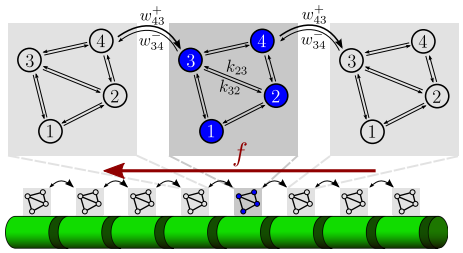
- Cost of running a simple clock: ARW



  - output $n(t)$ with $\langle n \rangle = Jt = (k^+ - k^-)t$
  - variance $\langle (n(t) - \langle n \rangle)^2 \rangle = 2Dt = (k^+ + k^-)t$
  - uncertainty $\epsilon^2 \equiv \text{var}/\text{output}^2 = 2D/J^2 t$
  - th'dyn cost $\mathcal{C} = \sigma t = (k^+ - k^-)\ln(k^+/k^-)t$ with $\sigma \equiv$ rate of entropy production
  - $\boxed{\mathcal{C}\epsilon^2 \geq 2k_B T}$ independent of run time t

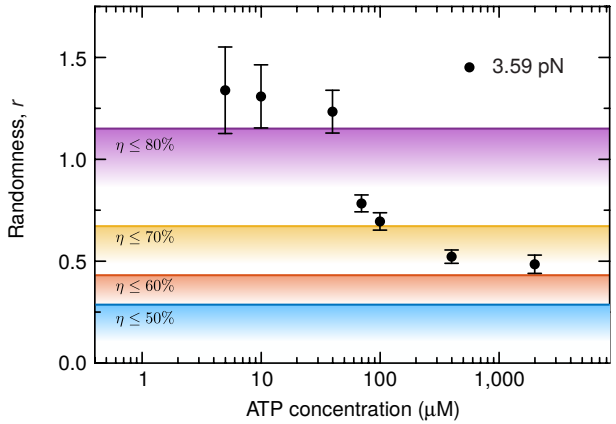
- Thermodynamic inference: Universal bound on the efficiency of molecular machines

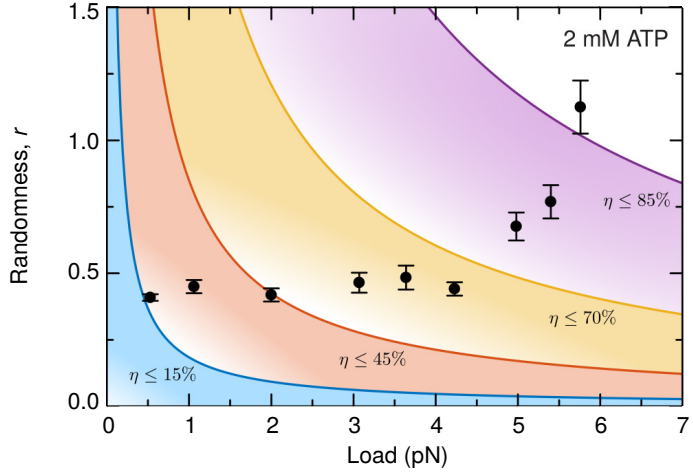
  [P. Pietzonka, AC Barato, U.S., J Stat Mech, 124004, 2016; U.S., Physica A 504, 176, 2018]



  - entropy production rate $\sigma = P^{\text{in}} - P^{\text{out}} = \text{inacc}' \quad \text{chem energy} - fv \geq v^2/D$
  - efficiency

$$\eta \equiv \frac{P^{\text{out}}}{P^{\text{in}}} = \frac{fv}{\text{chem energy}} = \frac{fv}{fv+\sigma} \leq \frac{1}{1+vk_BT/(Df)}$$





  - independent of the specific chemo-mechanical cycles and of $\Delta\mu$