Brownian Motors

Marco Schweizer

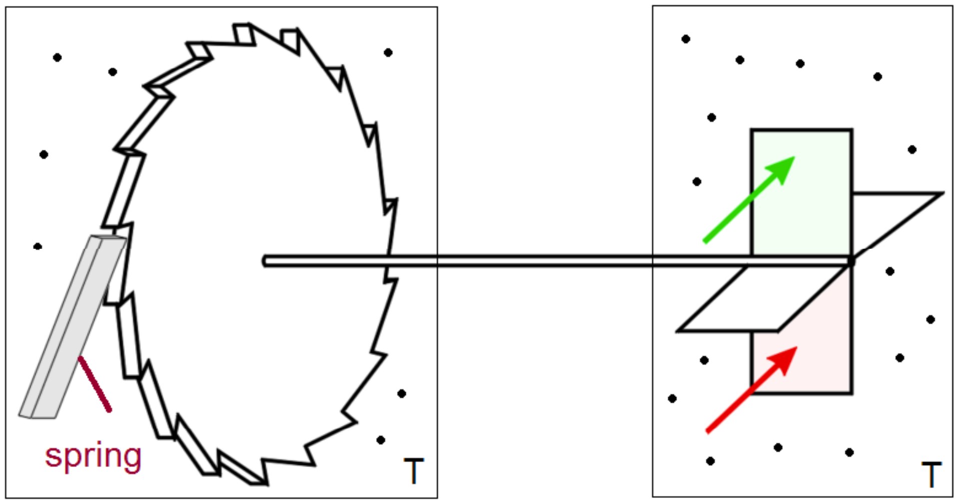
ETH Zürich

April 6, 2009

Feynman ratchet

- Due to collisions of gas atoms with the vane the vane oscillates and jiggles randomly.
- There is a pawl preventing the wheel from moving backwards.
- Therefore, there should be a net motion in the forward direction.

According to the Second Law it is impossible to convert any amount of heat of a thermal bath completely into work in a cyclic process.



Feynman´s resolution

- **The pawl and the wheel also undergo Brownian motion.**

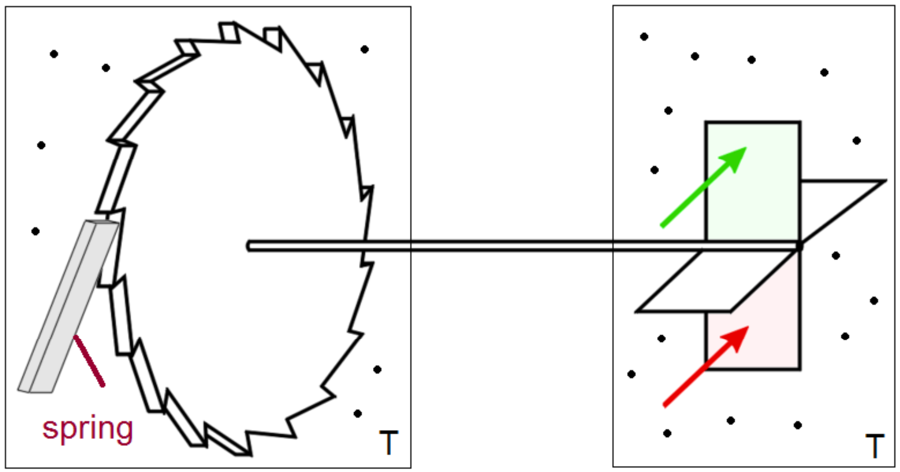
- If the vanes get kicked in forward direction, sometimes there is enough energy to lift the pawl (displace the spring) such that the wheel turns one step forward.

$$P\,(1 \text{ step forward}) \propto \exp\left[-\frac{E}{k_{\mathrm{B}}T}\right]$$

- Sometimes when the wheel tries to run backwards the pawl has already lifted due to its own Brownian motion and the wheel can run one step backward.

$$P\,(1 \text{ step backword}) \propto \exp\left[-\frac{E}{k_{\mathrm{B}}T}\right]$$

- **Remark: The Feynman ratchet tries to use an asymmetry of the system together with Brownian motion (randomness) to generate uniform transport (here: rotation).**



Overview

- Brownian domain
- Construction of a mathematical model to describe Brownian motion
- Different types of Brownian motors in equilibrium and non-equilibrium
- Applications (e.g., motor proteins)

Macro- and microscopic systems

Macroscopic systems

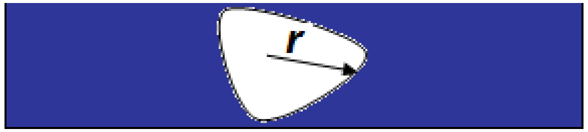
- Energy barriers used to impose constraints and forces are much larger than the thermal energy.
- „Escape times" for jumps (using thermal energy) over these barriers are effectively infinite.
- One does not need to spend energy to impose constraints.
- Brownian motion of large bodies is negligible.

Microscopic systems

- Energy barriers are comparable with the thermal energy.
- „Escape times" are finite.
- Energy needs to be spent constantly.
- Brownian motion is comparable with the size of microscopic particles.

Inertial- and viscous forces

- Consider a macroscopic or a microscopic particle in a fluid (e.g. water):



η, ρ

- The ratio of inertial- and viscous forces can approximately be given as

$$\mathrm{R} := \frac{F_{\text{inertial}}}{F_{\text{viscous}}} \approx \frac{ma}{\eta v} \approx \frac{\rho r^3 v/t}{\eta v} \approx \underbrace{\left(\frac{r\rho}{\eta}\right)}_{1/\nu} rv \approx \frac{rv}{\nu}$$

- Consider a protein ($v \approx 100\mu\mathrm{m/s}$, $r \approx 0.1\mu\mathrm{m}$) and a human ($v \approx 1\mathrm{m/s}$, $r \approx 1\mathrm{m}$) in water ($\nu \approx 1\mathrm{mm^2/s}$), then

$$\mathrm{R}_{\text{human}} \approx 10^6 \qquad\qquad \mathrm{R}_{\text{protein}} \approx 10^{-5}$$

- In the Brownian domain the viscous forces can be much stronger then the inertial forces. **In later steps, the inertial term will therefore be neglected.**

Brownian ratchets

- Brownian ratchets refer to systems with the following properties:

  - Noninteracting Brownian particles (BP) in a fluid at temperature T (thermal bath).

  - The force excerted by the fluid atoms on the BP due to collisions is of stochastic nature.

  - There is a viscuous force slowing the BP down.

  - There is an external periodic potential V with broken parity symmetry (ratchet potential).

  - The ratchet potential and any external forces do not affect the bath properties.

Construction of a mathematical model for Brownian motion

- The motion of a single BP in the fluid is described by the Langevin-eqn.

$$m\frac{d^2x(t)}{dt^2} + \eta\frac{dx(t)}{dt} = F(x(t), t), \quad t \geq 0$$

- The effective force F can be splitted in a deterministic and a (random) stoch. part

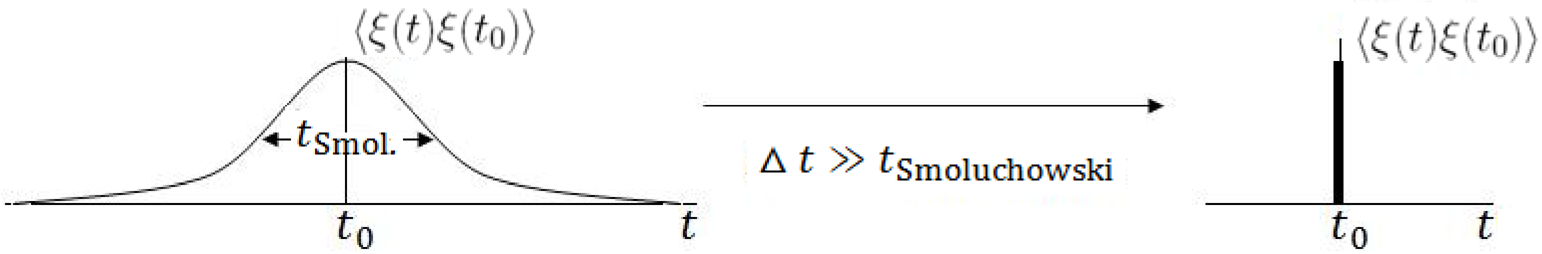
$$F(x(t), t) = F_{\text{det}}(x(t), t) + \xi(t)$$

- To completely determine the Langevin-eqn. the statistics of the stoch. force $\xi(t)$ has to be fixed.

- The fluid collisions shall have no preferential direction and be normal distributed

$$\langle \xi(t) \rangle = 0$$

- Consider the correlation between different times:



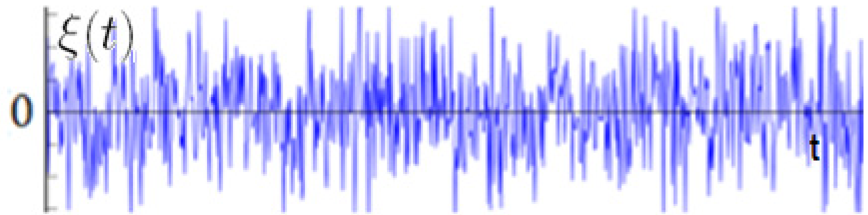
- Working on time scales much larger than the Smoluchowski (interaction) time and assuming stationarity of the stoch. force, implies

$$\langle \xi(t)\xi(t_0) \rangle = q\delta(t - t_0)$$

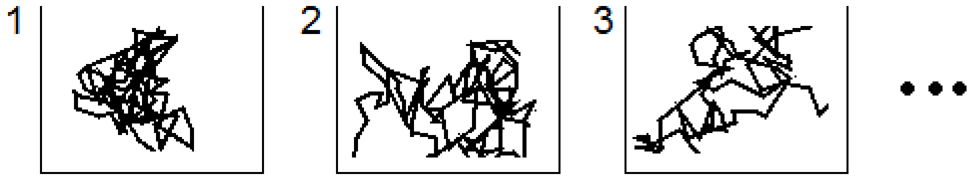
- To satisfy the equipartition principle the fluctuation-dissipation relation has to hold

$$\langle \xi(t)\xi(t_0) \rangle = 2\eta k_{\mathrm{B}} T \delta(t - t_0)$$

- As a result, the stoch. force is totally uncorrelated (white noise):



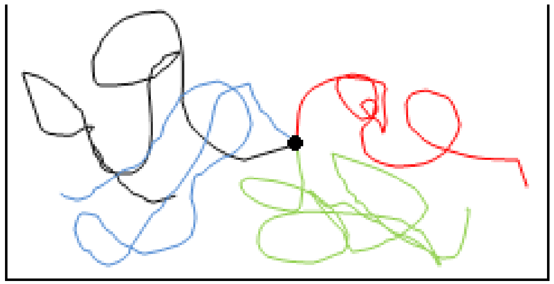
- Consider for example the following series of experiments with $F_{\text{det}} = 0$:



- The path in each experiment depends significantly on the stoch. force $\xi(t)$.

- The probabilistic time evolution of a single BP undergoing Brownian motion is described by a probability density $p(x,t)$ which describes the probability of the BP to be in a region around x at time t . $p(x,t)$ depends on the statistics of $\xi(t)$.

- The same experiment again, but sligtly modified (all BP start at the same time):



- The time evolution of a bunch of BP undergoing Brownian motion is described by the particle density $\rho(x,t)$ which is the particle density of a bunch of BP at position x at time t . $\rho(x,t)$ depends on the statistics of $\xi(t)$.

- It does not matter wheter the Brownian motion of a single BP or a bunch of BP is considered. The two points of view are absolutely identical: $\rho(x,t) = Np(x,t)$

- Consider the overdamped regime, then the Langevin-eqn. is given by

$$\eta\frac{dx(t)}{dt} = F(x(t),t)_{\mathrm{det}} + \xi(t), \quad t \geq 0$$

- Under the constructed type of stochastic force the Langevin-eqn. is connected with a Fokker-Planck-eqn. describing the time evolution of the prob. density of a single BP:

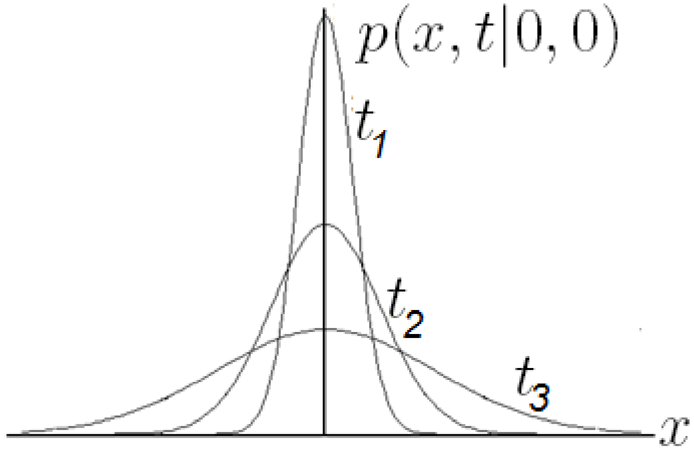
$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial J(x,t)}{\partial x} = -\frac{\partial}{\partial x}\left[\frac{1}{\eta}F(x,t)_{\mathrm{det}}p(x,t) - \frac{\partial}{\partial x}\left(Dp(x,t)\right)\right], \quad t \geq 0$$

Diffusion constant: $D = \frac{k_{\mathrm{B}}T}{\eta}$

- Special case (free diffusion): No external force

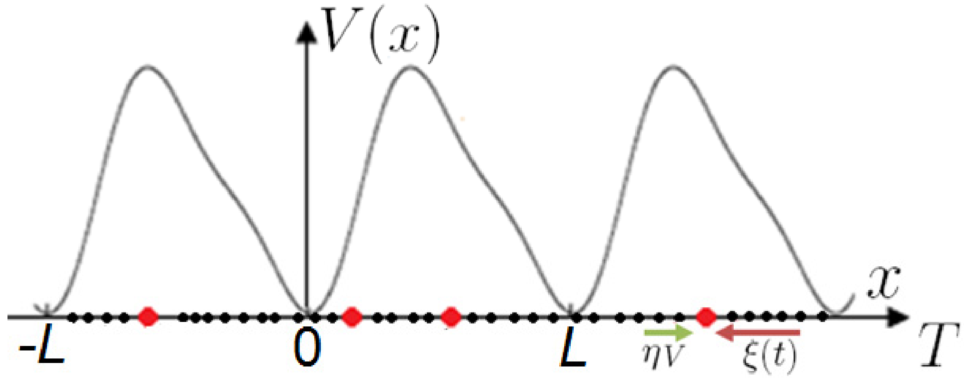
$$p(x,t|0,0) \propto \frac{1}{\sqrt{t}}\exp\left[-\frac{x^2}{4tD}\right]$$

$$\sqrt{\langle x^2\rangle} \propto \sqrt{Dt}$$



Brownian ratchet in equilibrium

- BP in a thermal bath (fluid) and subject to an external time-independent ratchet potential:



$$\frac{\partial p(x,t)}{\partial t} = -\frac{\partial J(x,t)}{\partial x}$$

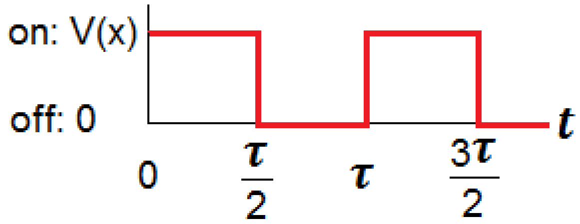
- The Second Law of thermodynamics forbids the BP to have a net average long-time-limit BP (ensemble) transport in a preferential direction.

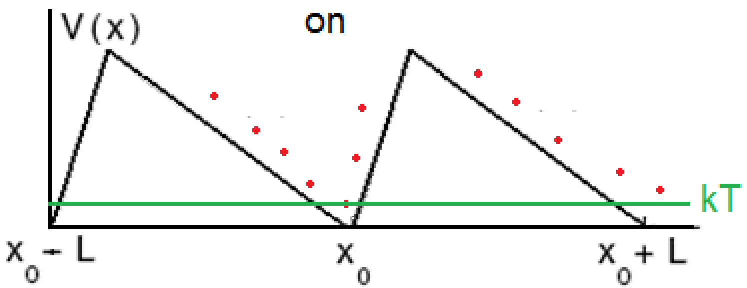
- **Claim: Under the constructed model of Brownian motion (Fokker-Planck-eqn.) and independently of the form of the time-independent ratchet potential, the BP in the thermal bath will not exhibit any long-time-limit ensemble drift.**

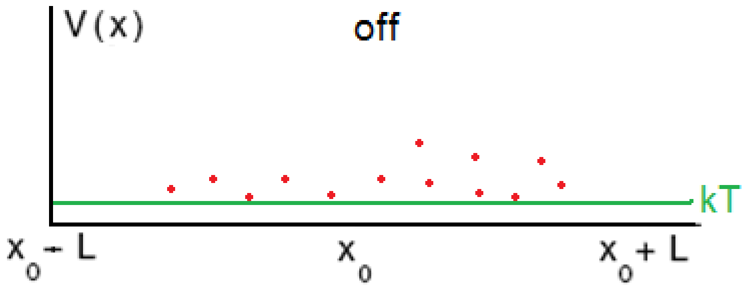
On-off ratchet (non-equilibrium)

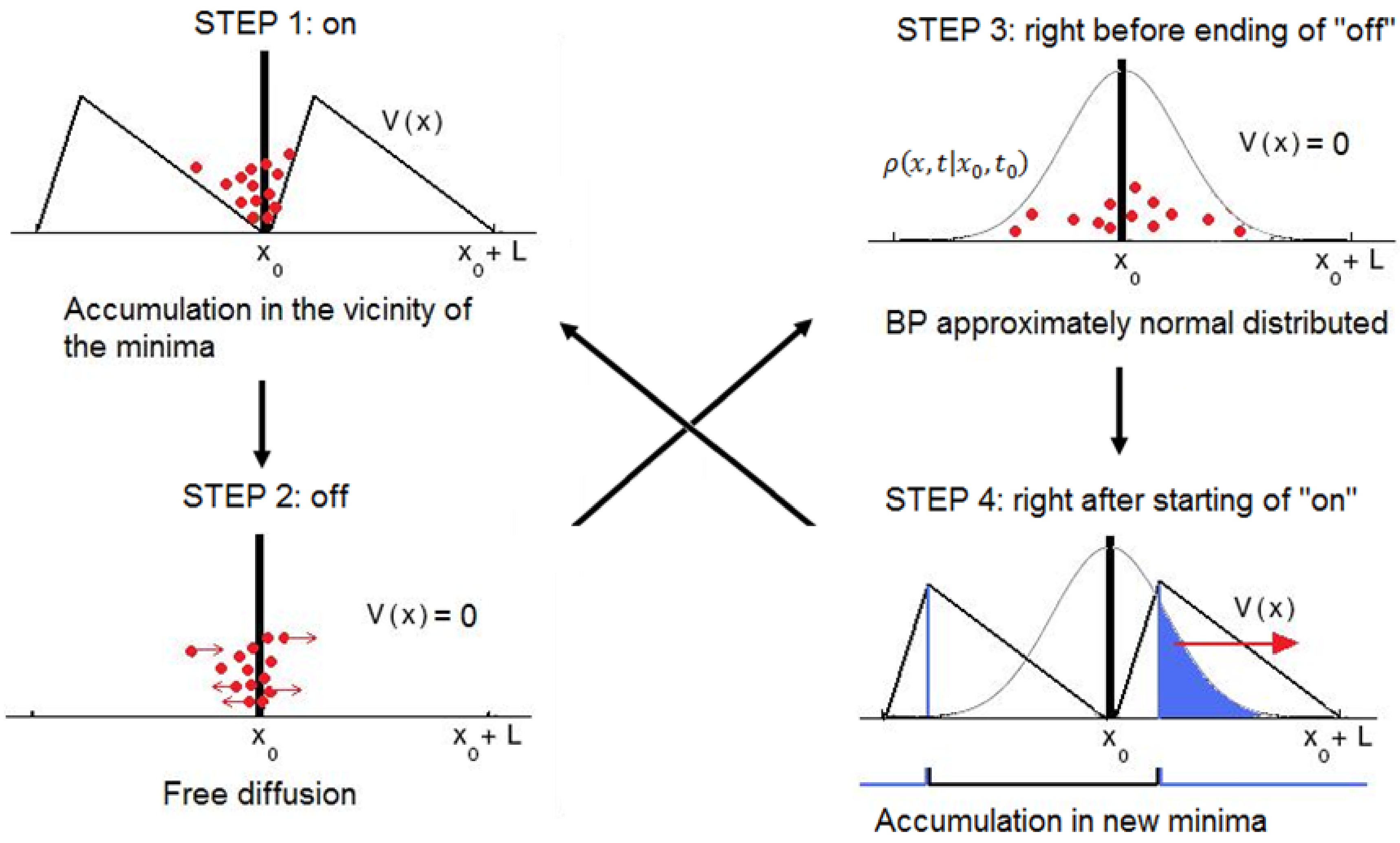
- Consider a ratchet with time-dependent ratchet potential (with sufficiently large time period):

$$V(x,t) = V(x)\mathrm{sign}\left(\sin \frac{2\pi t}{\tau}\right) \qquad k_{\mathrm{B}}T \ll \max V(x)$$









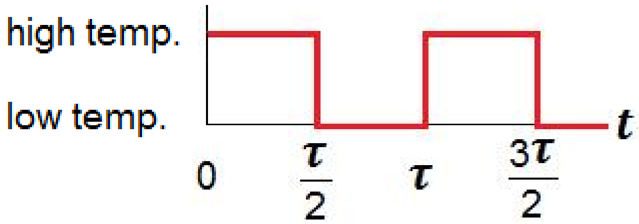
STEP 1: on
V(x)
x_0
x_0 + L
Accumulation in the vicinity of the minima
STEP 2: off
V(x) = 0
x_0
x_0 + L
Free diffusion
STEP 3: right before ending of "off"
$\rho(x,t|x_0,t_0)$
V(x) = 0
x_0
x_0 + L
BP approximately normal distributed
STEP 4: right after starting of "on"
V(x)
x_0
x_0 + L
Accumulation in new minima

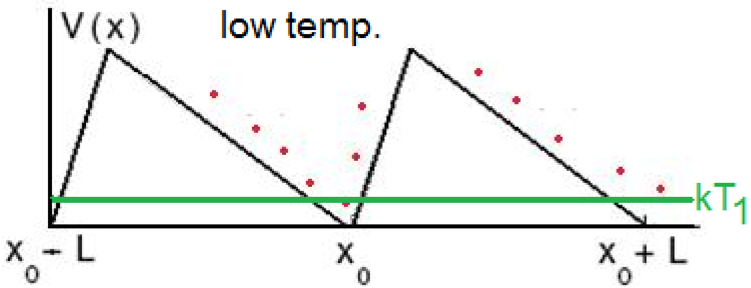
Thermal ratchet (non-equilibrium)

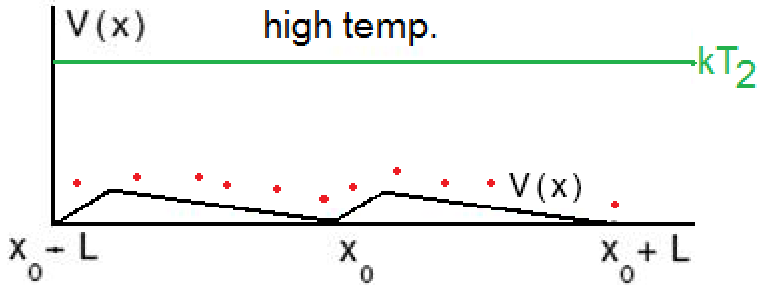
- Consider a ratchet with time-dependent temperature (with sufficiently large time period):

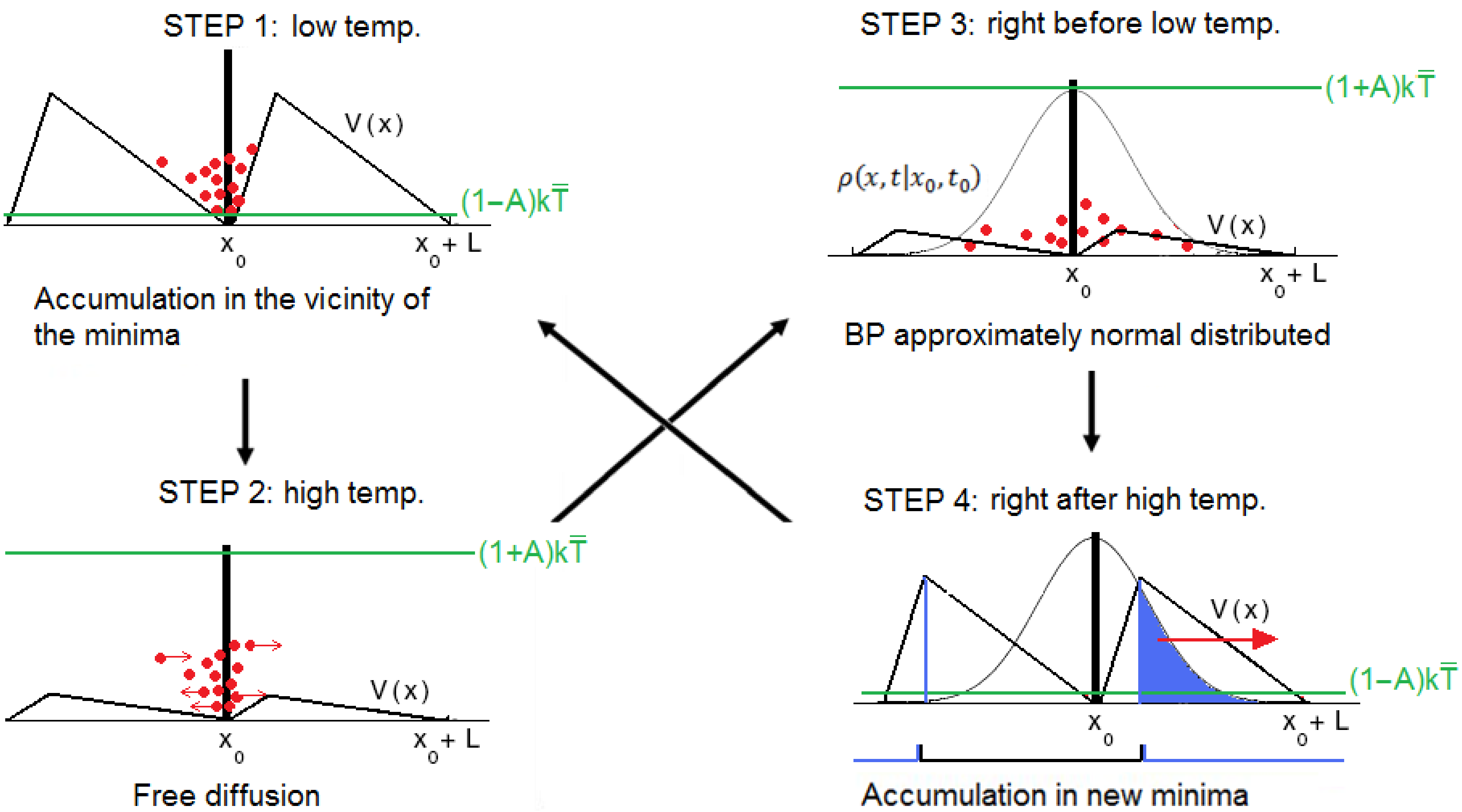
$$T(t) = \bar{T}\left(1 + A\,\mathrm{sign}\left(\sin\left(\frac{2\pi t}{\tau}\right)\right)\right), \quad A \le 1$$

$$k_B\bar{T}(1 - A) \ll \max V(x) \ll k_B\bar{T}(1 + A)$$

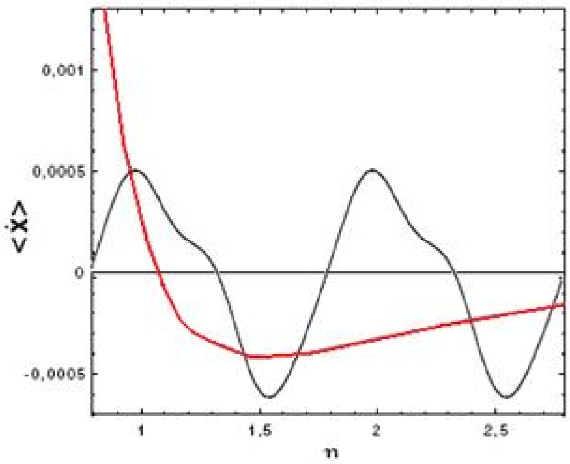






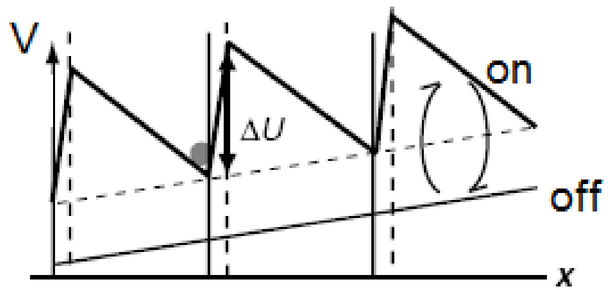

STEP 1: low temp.
V(x)
(1−A)kT̄
x0
x0 + L
Accumulation in the vicinity of the minima
STEP 2: high temp.
(1+A)kT̄
V(x)
x0
x0 + L
Free diffusion
STEP 3: right before low temp.
(1+A)kT̄
ρ(x, t|x0, t0)
V(x)
x0
x0 + L
BP approximately normal distributed
STEP 4: right after high temp.
V(x)
(1−A)kT̄
x0
x0 + L
Accumulation in new minima

- It can be difficult to intuitively understand the direction a ratchet produces transport:



Thermal ratchet $T(t) = \bar{T} \cdot \left(1 + A \cdot \sin\left(\frac{2\pi t}{\tau}\right)\right)^2$

- Through the ratchet mechanism it is possible to have transport against an external force (constant external force → linearly increasing potential):



General comments

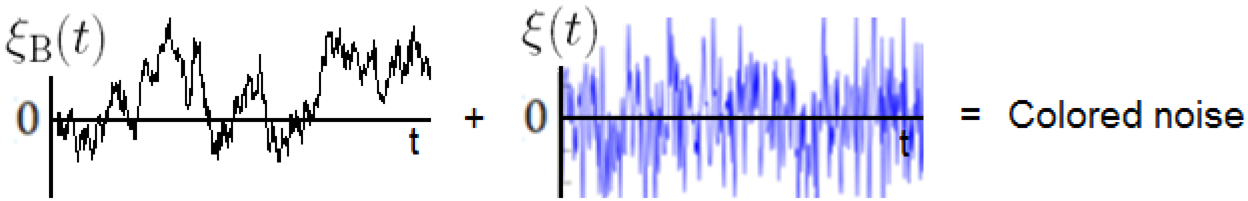
- The **equilibrium ratchet** respects the Second Law of thermodynamics under the constructed model.
- The „**on-off ratchet**“ as constructed respects the Second Law. The energy for the transport is taken from the time-dependent potential.
- The **thermal ratchet** as constructed is similar to a heat engine acting between two temperatures and therefore respects the Second Law.
- In ratchets which act in non-equilibrium the generic case is to have BP transport in a preferential direction. Only under special symmetry conditions and fine-tuned system parameters (friction, ...) there is no transport.
- **White-noise as constructed can only be rectified in non-equilibrium systems.**
- **Question: Can correlated noise be rectified without any other time-dependent forces?**

Stochastic driven ratchet

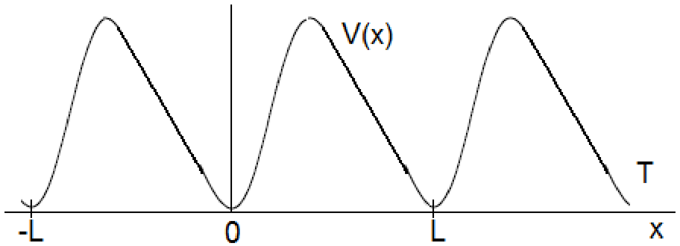
- In all examples, it has been used uncorrelated noise $\langle \xi(t)\xi(t_0)\rangle = 2\eta k_{\mathrm{B}} T \delta(t-t_0)$, that is

$$\langle \xi(t)\xi(t_0)\rangle = 0, \quad t \neq t_0$$

- Take a special “Brown”-noise and add it to the uncorrelated white-noise:



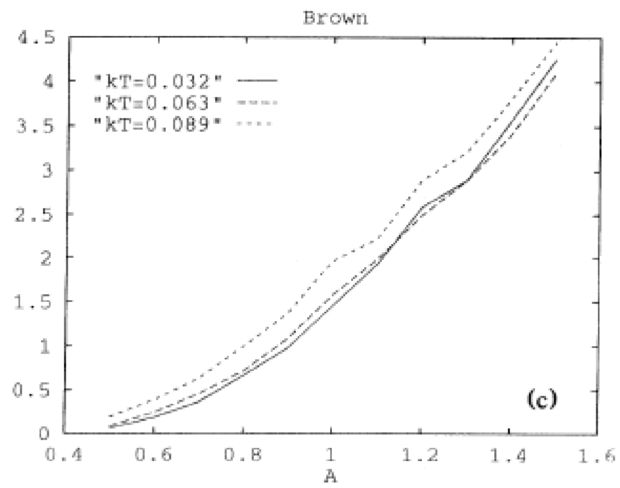
- Take the following ratchet potential and force it with “Brown”-noise:



$$\eta \frac{dx(t)}{dt} = -\frac{\partial V(x(t))}{\partial x} + \left(\xi_{\mathrm{B}}(t) + \xi(t)\right), \quad t \geq 0$$

$$\langle \xi_{\mathrm{B}}(t)\rangle = 0$$

- Numerical result for the long-time-limit:



- Interpretation:

  - It is possible to extract energy out of the time correlated pieces of a stochastic force $\xi_{\rm B}(t) + \xi(t)$ but not out of a source that has white-noise statistics.

  - If the stoch. force $\xi_{\rm B}(t) + \xi(t)$ is excerted in equilibruim by the thermal bath, then the Second Law is violated if the friction-term is as constructed.

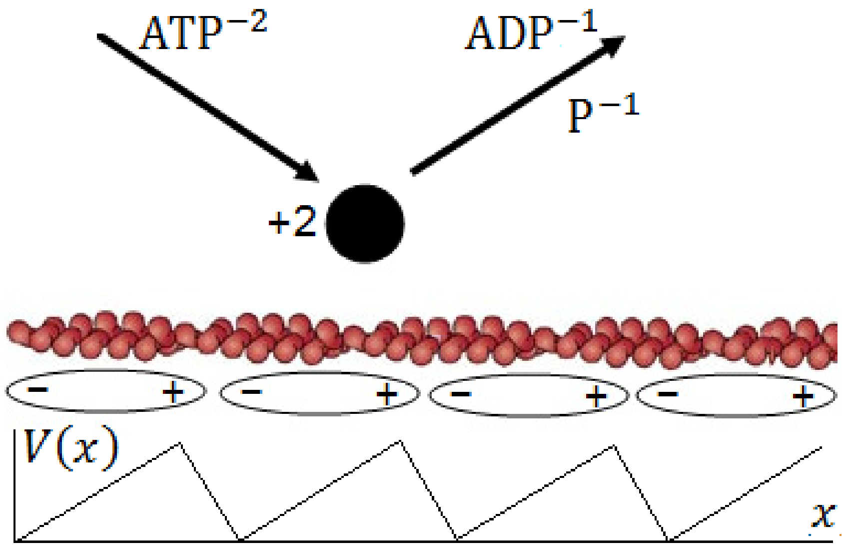
  - Not every combination of friction-term and stochastic force is compatible with the Second Law.

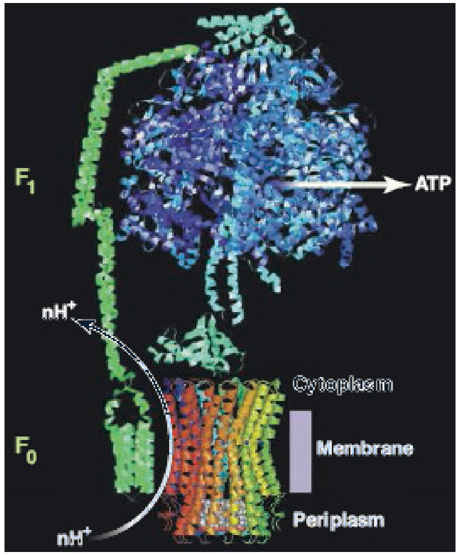
- More general: to ensure the validity of the Second Law, independently of any microscopic details the following "uniqueness-theorem" holds

  For any "linear" thermal bath without external time-dependent-driving force and [...], the form of the dissipation term (if a linear functional of velocity) ***uniquely*** *fixes all statistical properties of the stochastic force term.*

Applications

- The ratchet mechanism is used by motor proteins to bias the Brownian motion:





- Ultimately one can think of modelling nano-machines which are using the ratchet mechanism for specific tasks and operate in non-equilibrium environments.

Conclusion

- **Mathematical models describing Brownian ratchets statistically (Langevin-eqn.) are in accordance with the Second Law iff the statistics of the stochastic force and the viscous force term are chosen appropriately.**

- **Transport in non-equilibrium systems can be achieved using Brownian motion, a potential with broken parity symmetry and time-dependent perturbations (possibly of stochastic nature and possibly with vanishing time-and ensemble-average).**

- **The „ratchet mechanism“ is used in biological systems to bias the Brownian motion.**

References

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