The Sun within

Conference on Frontiers in Statistical Physics, Raman Research Institute, Bangalore

6 December 2023

Christian Maes, KU Leuven

arXiv:2310.14059v2 [cond-mat.stat-mech]: joint work with Faezeh Khodabandehlou

Abstract: some evidence for "hot spots" in biological systems makes us wonder…

What thermal physics for discussing biological power? An engine is not just a bucket of energy…

Making a two-temperature embedding of active matter models (before speaking of work)? Local detailed balance helps…

"An engine is a device that changes the energy from a fuel into mechanical energy, which in turn generates motion."

Reflections on biological engines

Many many references, including

Arya Datta, Patrick Pietzonka, Andre C Barato, Second law for active heat engines. Phys. Rev. X 12, 031034 (2022).

Jae Sung Lee, Jong-Min Park, and Hyunggyu Park, Brownian heat engine with active reservoirs. Phys. Rev. E **102**, 032116 (2020).

Ignacio A. Martınez,a Edgar Roldan, Luis Dinis and Raul A. Rica, Colloidal heat engines: a review. Soft Matter (2017)

Two motivations

1. The conundrum of hot mitochondria: a million-fold discrepancy between experimentally reported temperature measurements and prediction of irreversible thermodynamics.

2. Establishing local detailed balance to start thermal physics of active matter.

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1. The conundrum of hot mitochondria: a million-fold discrepancy between experimentally reported temperature measurements and prediction of irreversible thermodynamics.

2. Establishing local detailed balance to start thermal physics of active matter.

Turns out that they are related

The conundrum of hot mitochondria

Widely discussed experimental paper from 2018 in PLOS Biology,

by D. Chrétien *et al*:

Mitochondria are physiologically maintained at close to 50 C.

Reports temperature measurements identifying hot mitochondria as cellular radiators, with temperature differences of order 10C within a distance of say 10 micrometer.

The conundrum of hot mitochondria

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by D. Chrétien *et al*:

Mitochondria are physiologically maintained at close to 50 C.

Mitochondrion*, membrane-bound organelle found in the cytoplasm of almost all eukaryotic cells (cells with clearly defined nuclei), the primary function of which is to generate large quantities of energy in the form of adenosine triphosphate (ATP). Mitochondria are typically round to oval in shape and range in size from 0.5 to 10 μm. mitochondria share an evolutionary past with prokaryotes (single-celled organisms).*

Still in 2023:

confirms the validity of the initial findings of Chretien et al regarding the hot temperatures at which the mitochondrion is operating

Biochemistry and Chemical Biology, Cell Biology

Mitochondrial temperature homeostasis resists external metabolic stresses

Mügen Terzioglu, Kristo Veeroja, Toni Montonen, Teemu O. Ihalainen, Tiina S. Salminen, Paule Bénit, Pierre Rustin, Young-Tae Chang, Takeharu Nagai, Howard T. Jacobs

Faculty of Medicine and Health Technology, FI-33014 Tampere University, Finland • Université Paris Cité, Inserm, Maladies neurodéveloppementales et neurovasculaires, F-75019 Paris, France • Department of Chemistry, POSTECH, 37673 Pohang, Republic of Korea ... show 2 more

eLife assessment

The study provides **useful** data supporting prior findings that mitochondria in cultured cells maintain a temperature that is at least 15{degree sign}C above the external temperature at which cultured cells are maintained. The evidence supporting the hypothesis is **solid**, although direct measures of temperature in isolated mitochondria or comparison with other cellular compartments would have strengthened the ability to interpret the relevance of the findings. Nevertheless, the bioenergetic implications of the work will be of interest to cell biologists, biochemists, and physiologists.

Paradox?

People appear to "trust" the measurements; checked, redone and the results have remained unchanged.

On the other hand, from a *standard* thermodynamics point of view, it is quite impossible: applying Fourier Law,

$$\kappa \, \Delta T = P / L$$

For cellular power $P = 100$ pW, cell size $L = 10$ µm,
thermal conductivity $\kappa = 0.1 - 1$ W/(mK)

Making a millionfold difference with the measured ΔT …

a steady-state temperature difference in a single cell *cannot* exceed 10^{-5} K.

Hot furnaces inside cells?

Almost everything a cell does that requires energy is sourced by the **hydrolysis of ATP**:

$$\mathrm{ATP} + \mathrm{H_2O} \leftrightharpoons \mathrm{ADP} + \mathrm{P}_i + \mathrm{energy}$$

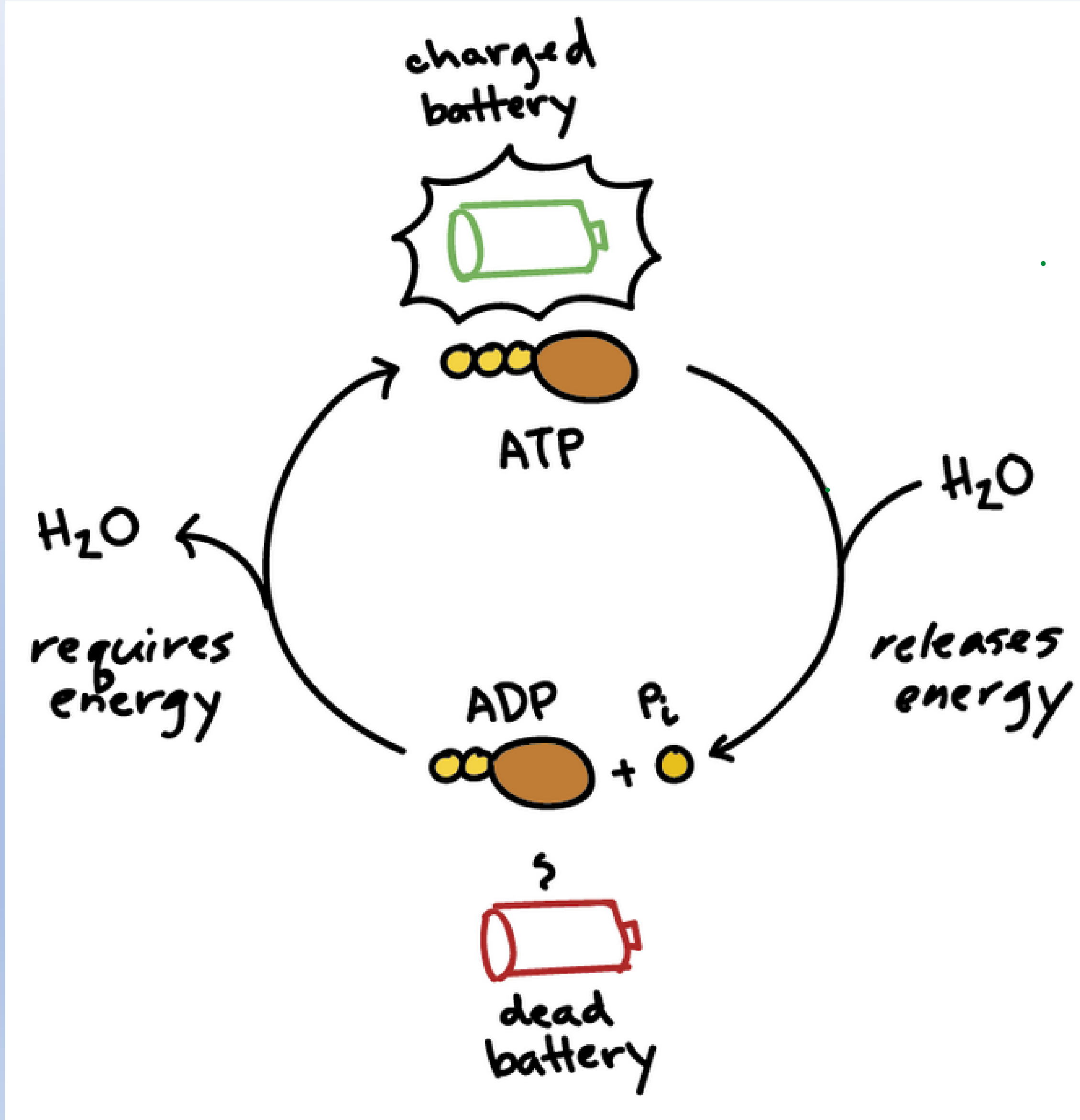
The heat of reaction is 0.43 eV per molecule, which “corresponds” to a temperature **T_{eff} = 5060 K** when stored over two degrees of freedom, **$k_B\, T_{eff}$ = 0.43eV/molecule**.

(Temperature at the surface of the Sun). Quite a ’hot spot’ (molecular size)…

Organisms appear to perform biological work at lower or equal temperatures than environment.

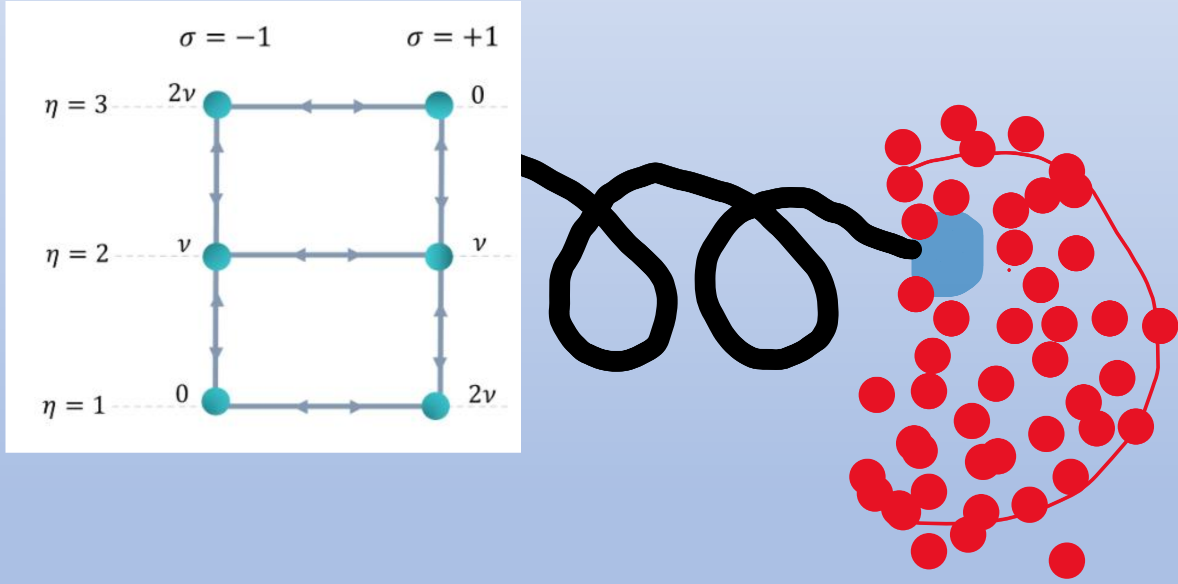
How to argue for Carnot-type efficiency formula ?

Old picture:



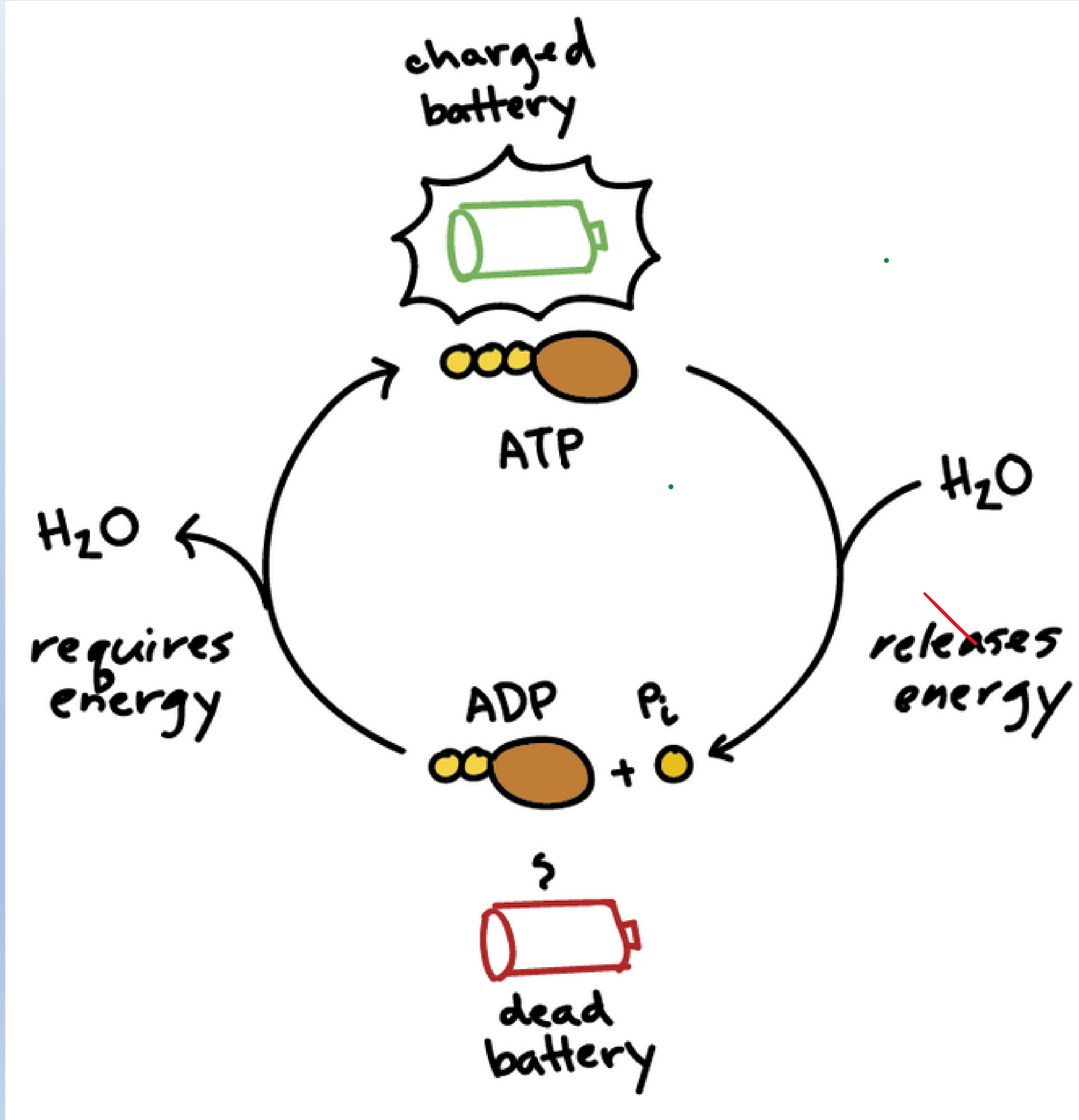
Suggested picture:

Two-temperature modeling of bio-engine with work resulting from energy flow.



The energy (at the hot spot) is used to deliver work (e.g. muscle contraction, locomotion,...), while the waste heat is carried off by the blood stream, water bags etc. which are at 310 K.

Old picture:



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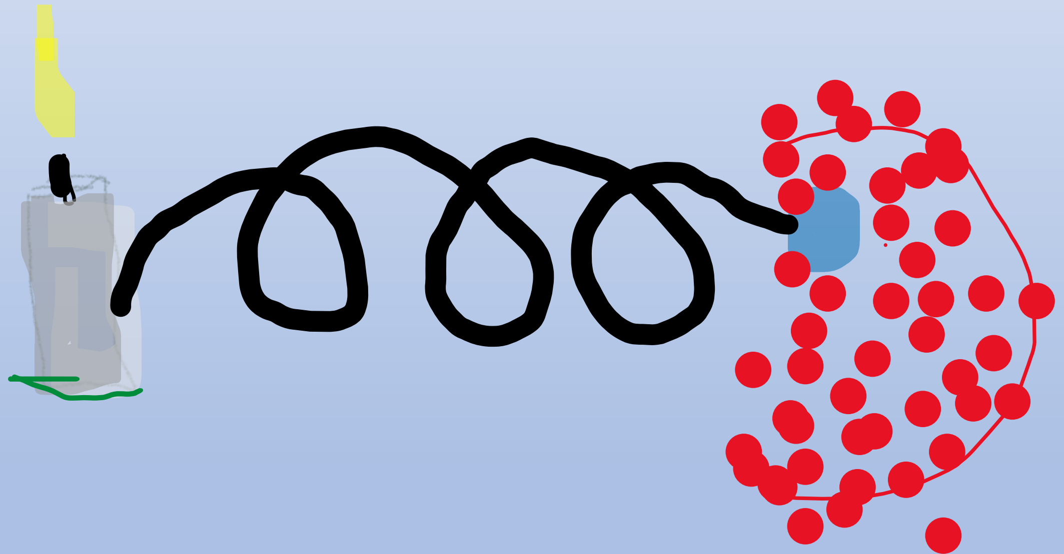

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Summary so far (no math)

To associate tiny hot spots as powerhouses for biological work meets with some evidence, but appears to require novel ideas or perspectives.

Obviously, those hot spots are not the regular textbook heat reservoirs. Our muscles are not Carnot engines:

1) the hot spot needs to resist rapid thermalization while transferring its energy into the (regular) heat reservoir (blood or water), and

2) biological engines are active and far from the reversible limit.

Picture

Bath consisting of many quasi-independent small nonequilibrium systems or active agents. Their corresponding temperature is only (but in some specific sense) effective.

The involved molecules are activated and produced by chemistry, to provide the necessary fuel.

Yet, the activation is not first entirely degraded into heat, after which a Carnot engine is started.

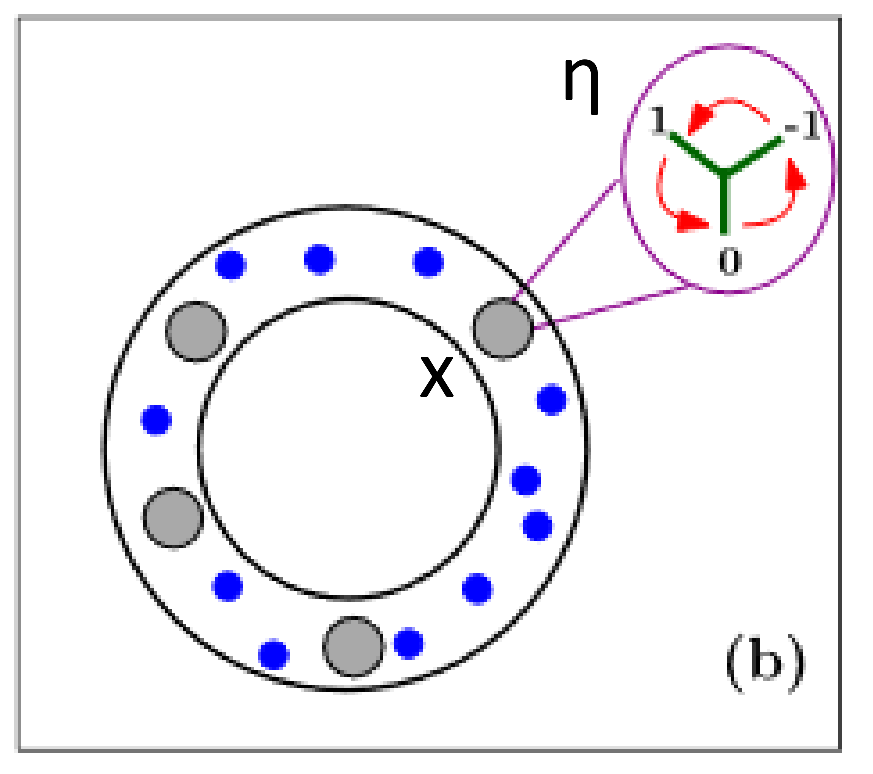
That is why biological processes need to be fast and to have some persistence, exactly to avoid that thermalization.

How to rotate a probe? CM and K.Netocny, Chaos (2019)

CM, Frenesy: Time-symmetric dynamical activity in nonequilibria. Physics Reports (2020).

from $\eta \longrightarrow \eta'$ is

$$k(x,\eta,\eta') = a(x,\{\eta,\eta'\})\exp\left(\frac{\beta}{2}(U(x,\eta) - U(x,\eta') + W(x,\eta,\eta'))\right)$$



$$f(x) = -\langle \nabla_x U(x,\eta)\rangle(x) = -\sum_\eta \nabla_x U(x,\eta)\rho(x,\eta)$$

How to rotate a probe?

from $\eta \longrightarrow \eta'$ is

$$k(x,\eta,\eta') = a(x,\{\eta,\eta'\})\exp\left(\frac{\beta}{2}(U(x,\eta) - U(x,\eta') + W(x,\eta,\eta'))\right)$$

$U(x,1) = \lambda \sin x$ and $U(x,\eta = 2,3) = 0.$

$$a(x,\{1,2\}) = 1 + \lambda b\cos(x+\varphi), \qquad a(x,\{1,3\}) = 1 - \lambda b\cos(x+\varphi)$$

$$a(x,\{2,3\}) = 1$$

$W(x,1,2) = W(x,2,3) = W(x,3,1) = \varepsilon$ along the loop.

$$f(x) = -\langle \nabla_x U(x,\eta)\rangle(x) = -\sum_\eta \nabla_x U(x,\eta)\rho(x,\eta)$$

Bram Lefebvre and CM, [Frenetic steering: nonequilibrium-enabled navigation]. [arXiv:2309.09227v1]

Higher dimensional steering: by applying phase shifts…

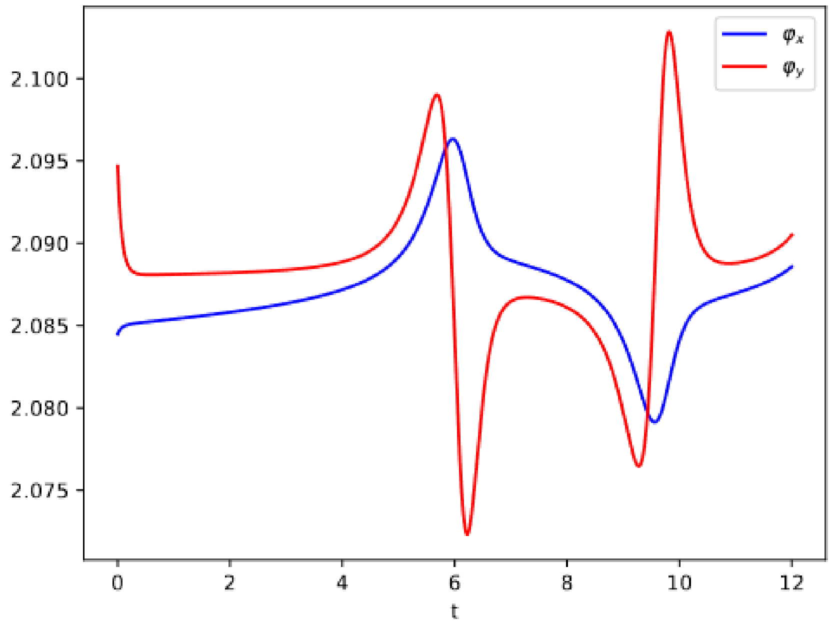


FIG. 6: Phase shifts $\varphi_x(t)$ and $\varphi_y(t)$ for the medium dynamics coupled to the probe that follows the van der Pol oscillator, for $\mu = 1.5$, initial state $x = 3, y = 0$, and time step 0.01.

Bram Lefebvre and CM, Frenetic steering: nonequilibrium-enabled navigation. arXiv:2309.09227v1

Higher dimensional steering: getting van der Pol nonlinear oscillator

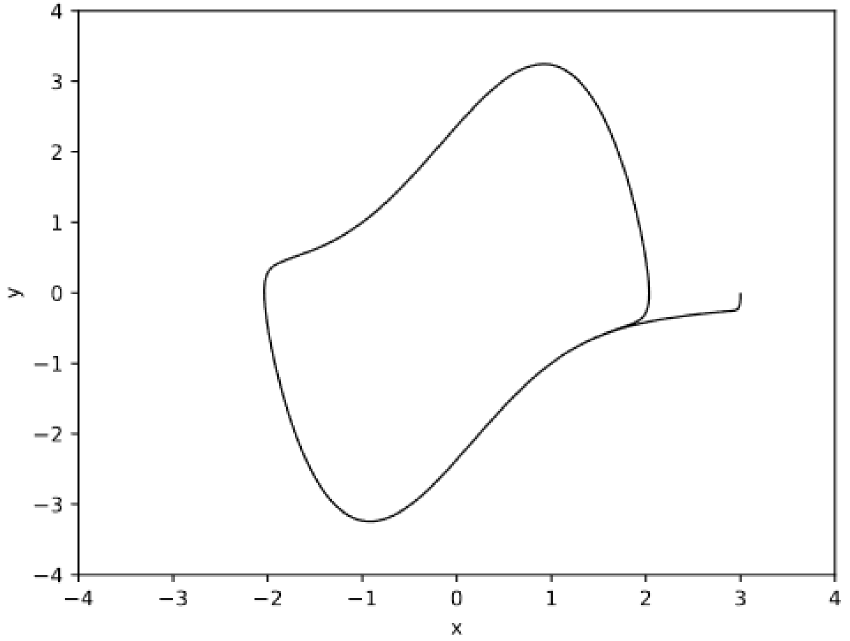
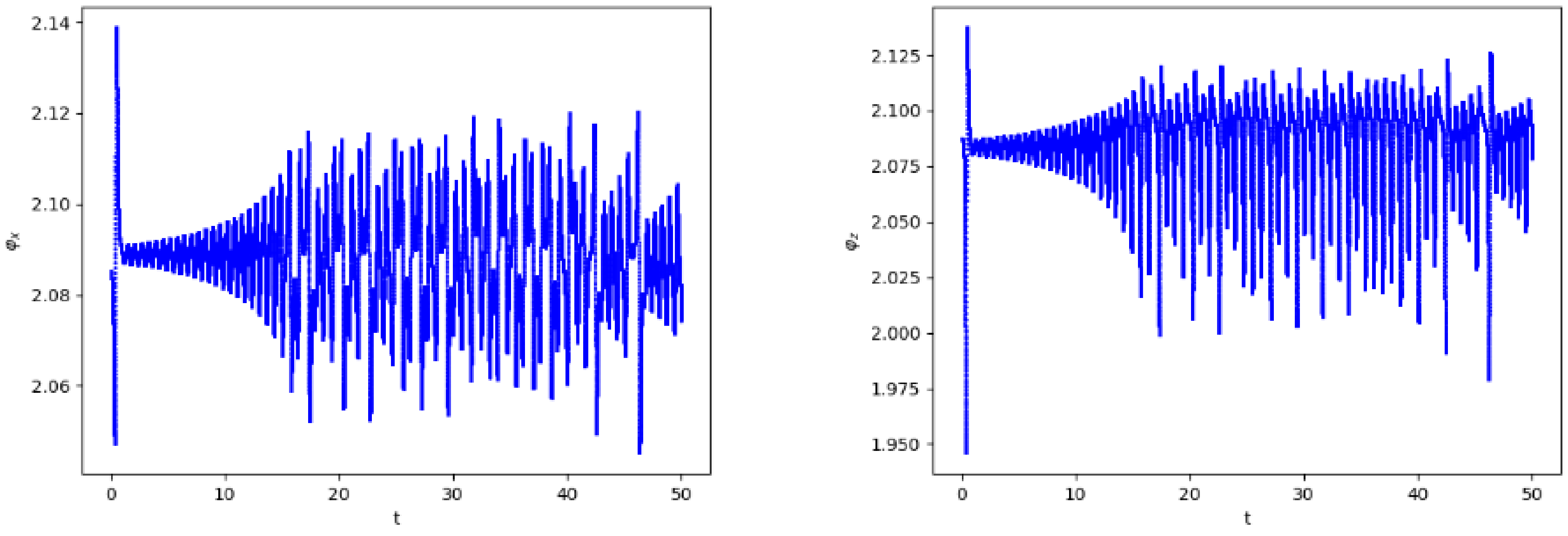


FIG. 5: A trajectory for a probe that approximates the van der Pol oscillator, for damping $\mu = 1.5$, initial state $x = 3, y = 0$, time step 0.01 and duration $T = 12$.

Bram Lefebvre and CM, [Frenetic steering: nonequilibrium-enabled navigation](). [arXiv:2309.09227v1]()

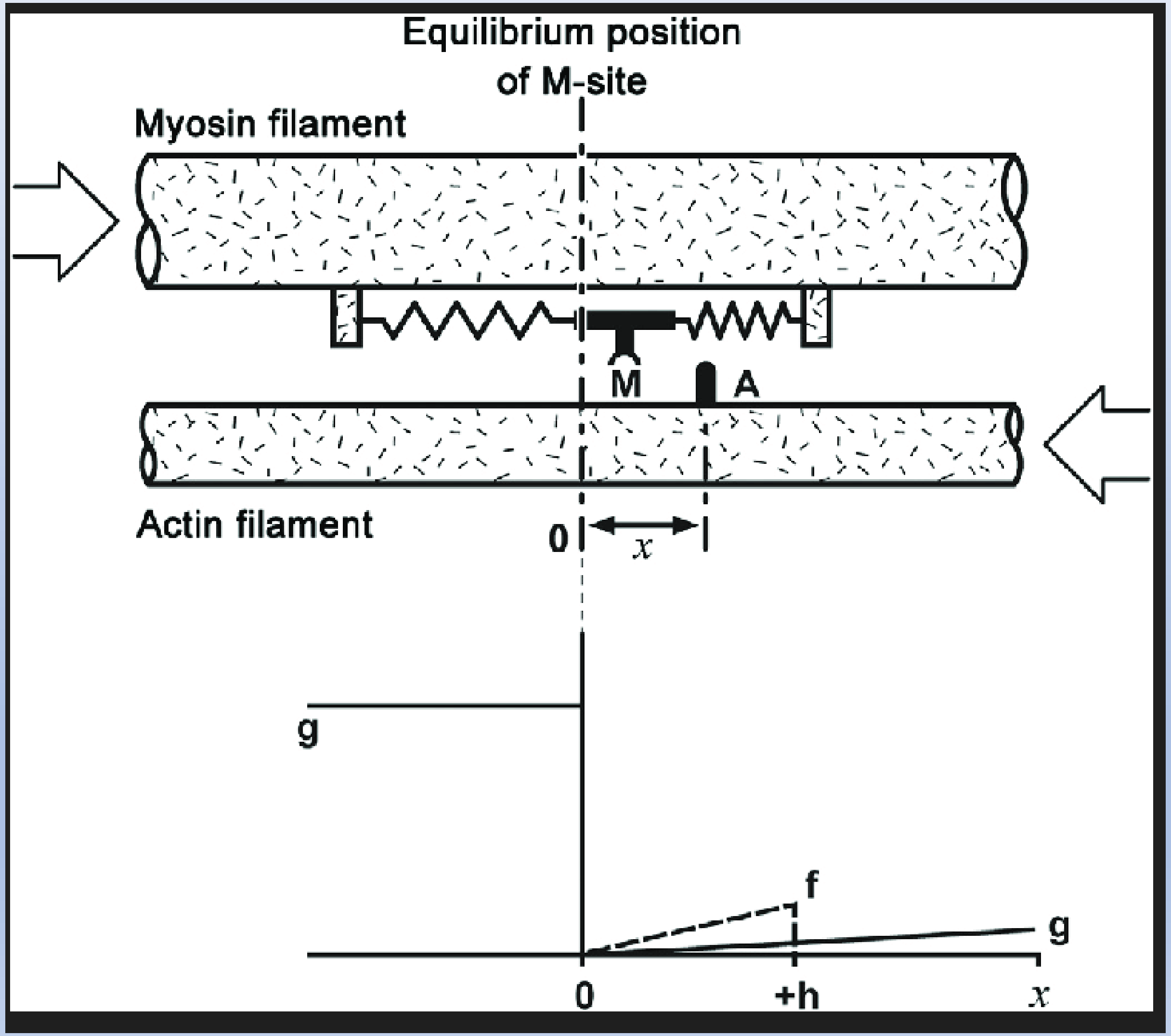
Higher dimensional steering: getting Lorenz dynamics



(a) $\varphi_x(t)$ (b) $\varphi_z(t)$

FIG. 8: $\varphi_x(t)(a)$ and $\varphi_z(t)(b)$ for a dynamics based on our nonequilibrium model that approximates the Lorenz model, for initial state $x = 0, y = 1, z = 0$, time step 0.001 and $T = 50$.

Original cross-bridge model developed by A. F. Huxley (1957)

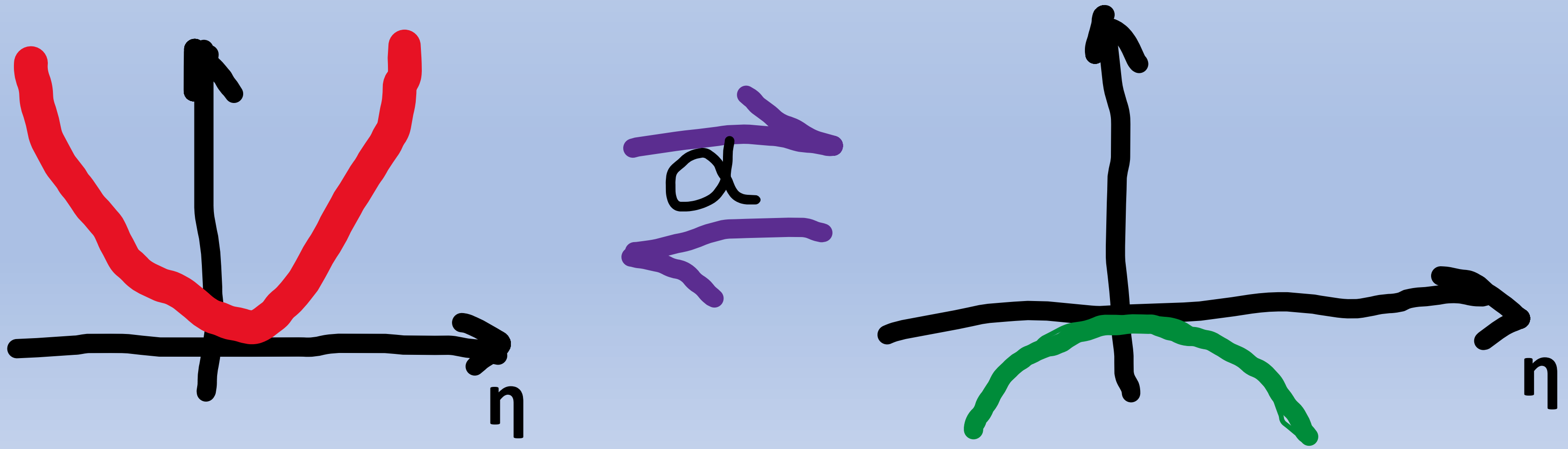


Herzog, Walter
2018/06/01
Why are muscles strong and why do they require little energy in eccentric action?
Journal of Sport and Health Science

A Huxley model for exciting low-energy vibrational mode

$$\Phi(\eta,\sigma) = \frac{\kappa}{2}(1 + w\,\sigma)\eta^2, \qquad \sigma = \pm 1$$

$$\dot{\eta}_t = -\kappa\,(1 + w\,\sigma_t)\,\eta_t + \sqrt{2T}\,\xi_t$$



nonGaussian stationary distribution: but quadratic moments recur

recurrence formulæ

$$a_{2n} = (2n-1)\frac{T}{\kappa} a_{2n-2} - w\, b_{2n}$$

$$b_{2n} = -(2n-1)\frac{T}{\kappa}\,\frac{z(w\, a_{2n-2} - b_{2n-2})}{1 + z(1 - w^2)}$$

in terms of the dimensionless persistence $z = \kappa/\alpha$.

Second moments
(energy measure in vibrational mode)

When $|w| > 1$, there is a critical persistence

$$z_c = \frac{1}{w^2 - 1}$$

$$\langle \eta^2 \rangle^s = a_2 = \frac{1+z}{1+z(1-w^2)} \frac{T}{\kappa}$$

$$\langle \sigma\, \eta^2 \rangle^s = b_2 = -\frac{z\, w}{1+z(1-w^2)} \frac{T}{\kappa}$$

Huxley model for exciting low-energy vibrational mode

For attachment/detachment at rate α:

effective temperature reaches infinite as the flip rate $\alpha \downarrow \alpha_c = \kappa\,(w^2 - 1)$

$$\langle \eta^2 \rangle^s = a_2 = \frac{1+z}{1+z(1-w^2)} \frac{T}{\kappa}$$

$$\langle \sigma\, \eta^2 \rangle^s = b_2 = -\frac{z\, w}{1+z(1-w^2)} \frac{T}{\kappa}$$

$$z = \kappa/\alpha$$

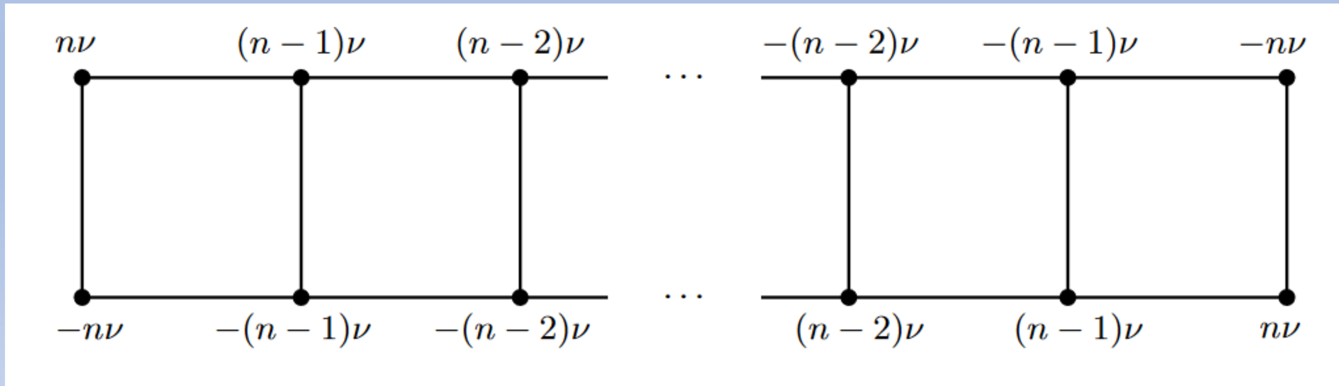
From Huxley model for exciting low-energy vibrational mode

Taking (very) strong coupling between the two oscillators, and 'discretizing' the harmonic oscillator: we move from

We take the "hot spot" $\sigma_t = \pm 1$ flipping at rate α, while we couple $\eta, x \in \mathbb{R}$, as

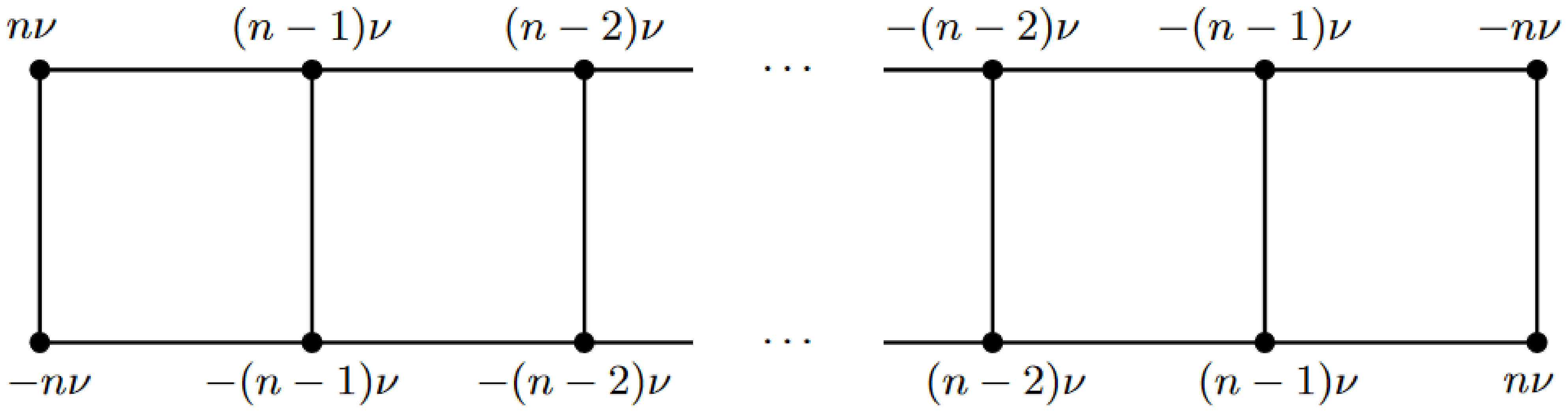
$$\begin{aligned} \dot{\eta}_t &= -\partial_\eta U(x_t - \eta_t) - \kappa\,(1 + w\,\sigma_t)\,\eta_t + \sqrt{2T}\,\xi_t^{(\eta)} \\ m\ddot{x} + \gamma \dot{x}_t &= -\partial_x U(x_t - \eta_t) + F(x) + \sqrt{2m\gamma T}\,\xi_t^{(x)} \end{aligned}$$

to a ladder with equal energy spacing:



Huxley model for exciting low-energy vibrational mode:

exactly solvable lattice version:

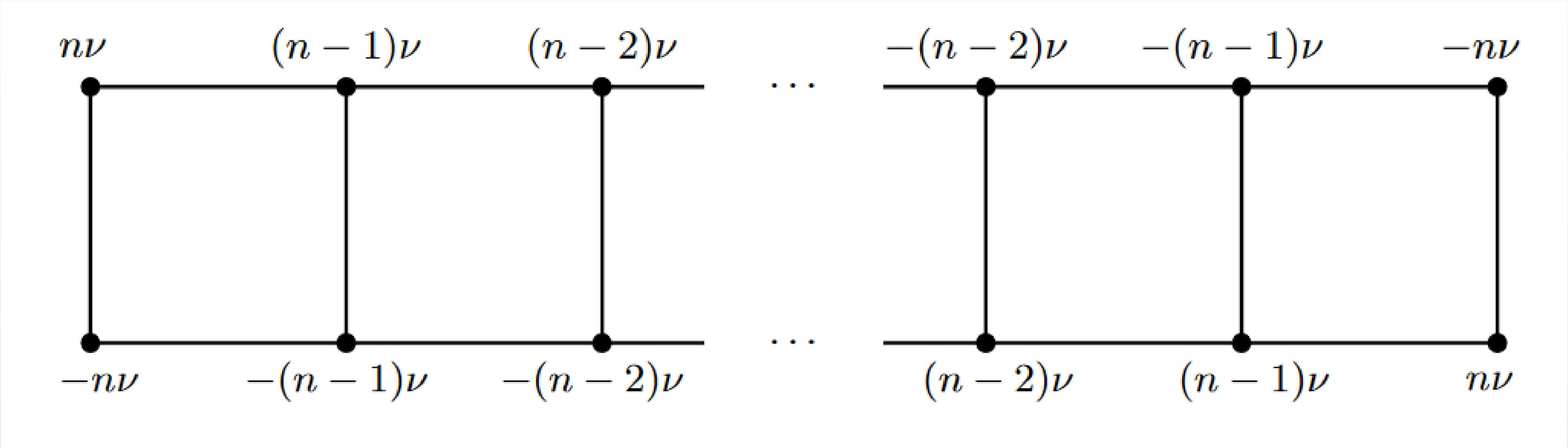


$$k_-(\eta,\eta+1) = k_+(\eta+1,\eta) = \frac{1}{\tau}e^{-\frac{\beta\nu}{2}}$$

$$k_+(\eta,\eta+1) = k_-(\eta+1,\eta) = \frac{1}{\tau}e^{\frac{\beta\nu}{2}}$$

$$k_\eta(\sigma) = \alpha\, e^{\frac{\beta(1-\varepsilon)}{2}(E(\eta,\sigma)-E(\eta,-\sigma))}$$

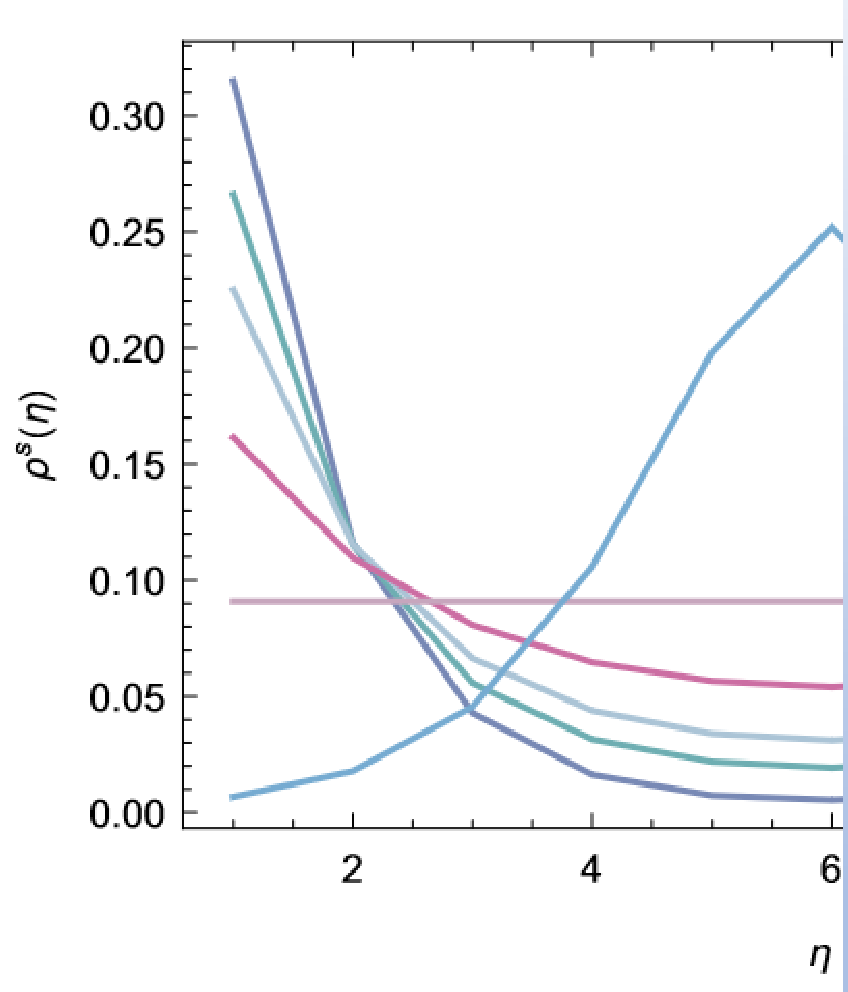
Huxley model for exciting low-energy vibrational mode

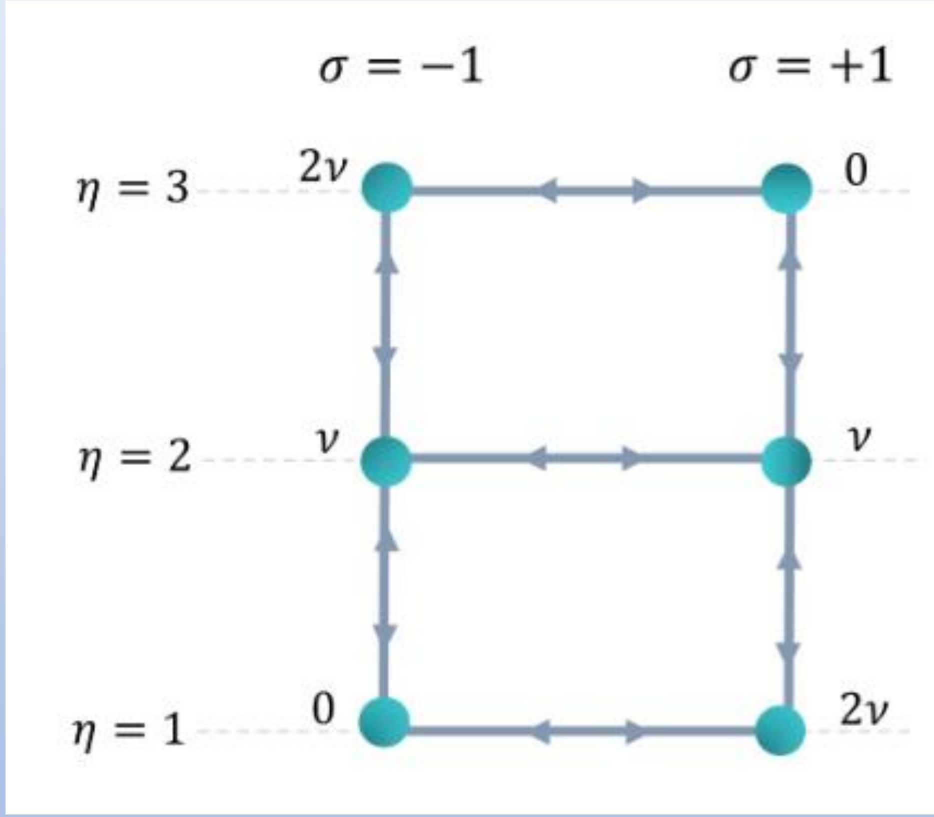


Stationary distribution in large (switching rate) α limit

$$\varrho_{n;\beta,\tilde{\beta}}(x) = \frac{1}{\mathcal{Z}_{n;\beta,\tilde{\beta}}} \prod_{k=0}^{|x|-1} \frac{\cosh\left[\beta\nu + 2k\tilde{\beta}\nu\right] \cosh[2(k+1)\tilde{\beta}\nu]}{\cosh[2k\tilde{\beta}\nu] \cosh\left[\beta\nu - 2(k+1)\tilde{\beta}\nu\right]}$$

Huxley model for exciting low-energy vibrational mode

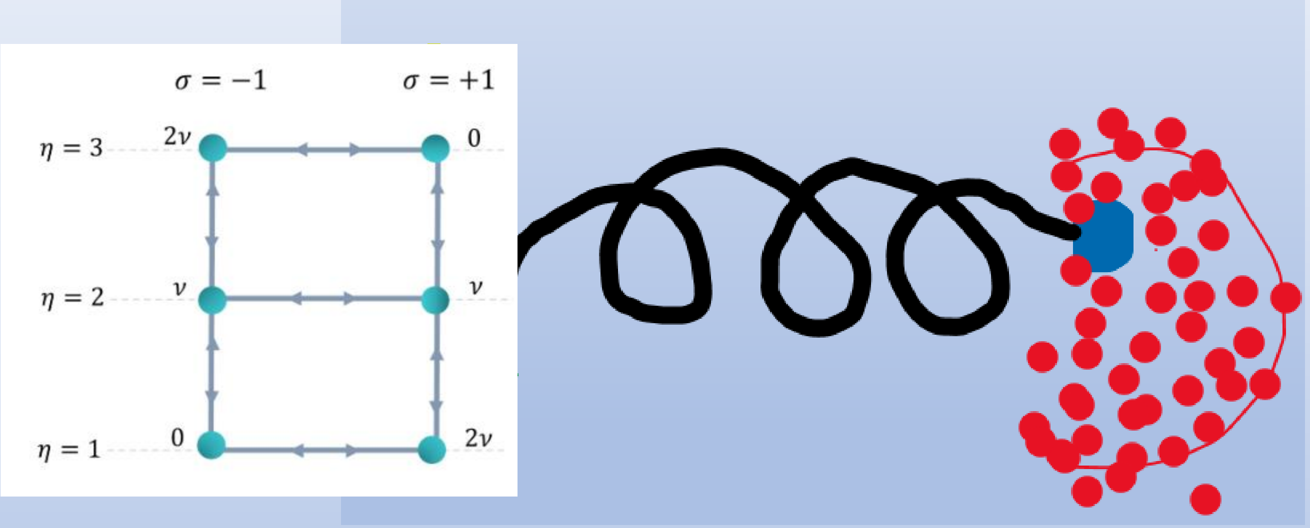




Stationary distribution in large (switching rate) α limit: transfer of effective temperature

Starting from Huxley model for exciting low-energy vibrational mode

Make an engine:



We take the "hot spot" $\sigma_t = \pm 1$ flipping at rate α, while we couple $\eta, x \in \mathbb{R}$, as

$$
\begin{aligned}
\dot{\eta}_t &= -\partial_\eta U(x_t - \eta_t) - \kappa\,(1 + w\,\sigma_t)\,\eta_t + \sqrt{2T}\,\xi_t^{(\eta)} \\
m\ddot{x} + \gamma \dot{x}_t &= -\partial_x U(x_t - \eta_t) + F(x) + \sqrt{2m\gamma T}\,\xi_t^{(x)}
\end{aligned}
$$

Connect active switch with equilibrium system

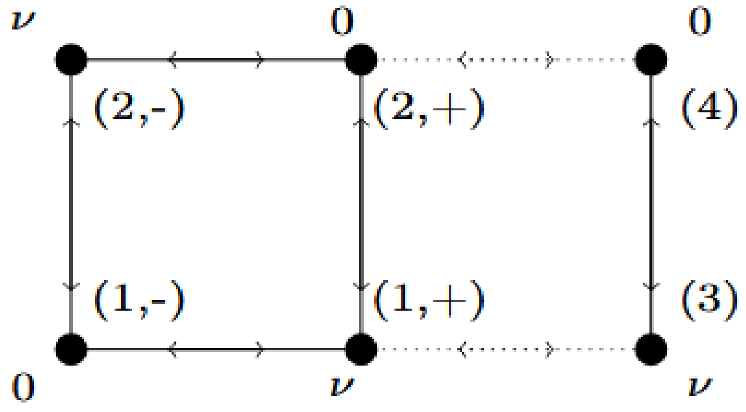


Figure 9: The graph of a two-level switch connected to a two-state equilibrium system.

The transition rates are given by

$$k(1,-;2,-) = k(2,+;1,+) = k(4,3) = \frac{1}{\tau} e^{-\frac{\beta\nu}{2}}$$
$$k(1,+;2,+) = k(2,-;1,-) = k(3,4) = \frac{1}{\tau} e^{\frac{\beta\nu}{2}}$$
$$k(1,-;1,+) = k(2,+;2,-) = \alpha e^{-\frac{\beta\nu(1-\varepsilon)}{2}}$$
$$k(1,+;1,-) = k(2,-;2,+) = \alpha e^{\frac{\beta\nu(1-\varepsilon)}{2}}$$
$$k(2,+;4) = k(4;2,+) = k(1,+;3) = k(3;1,+) = 1$$

Connect active switch with equilibrium system

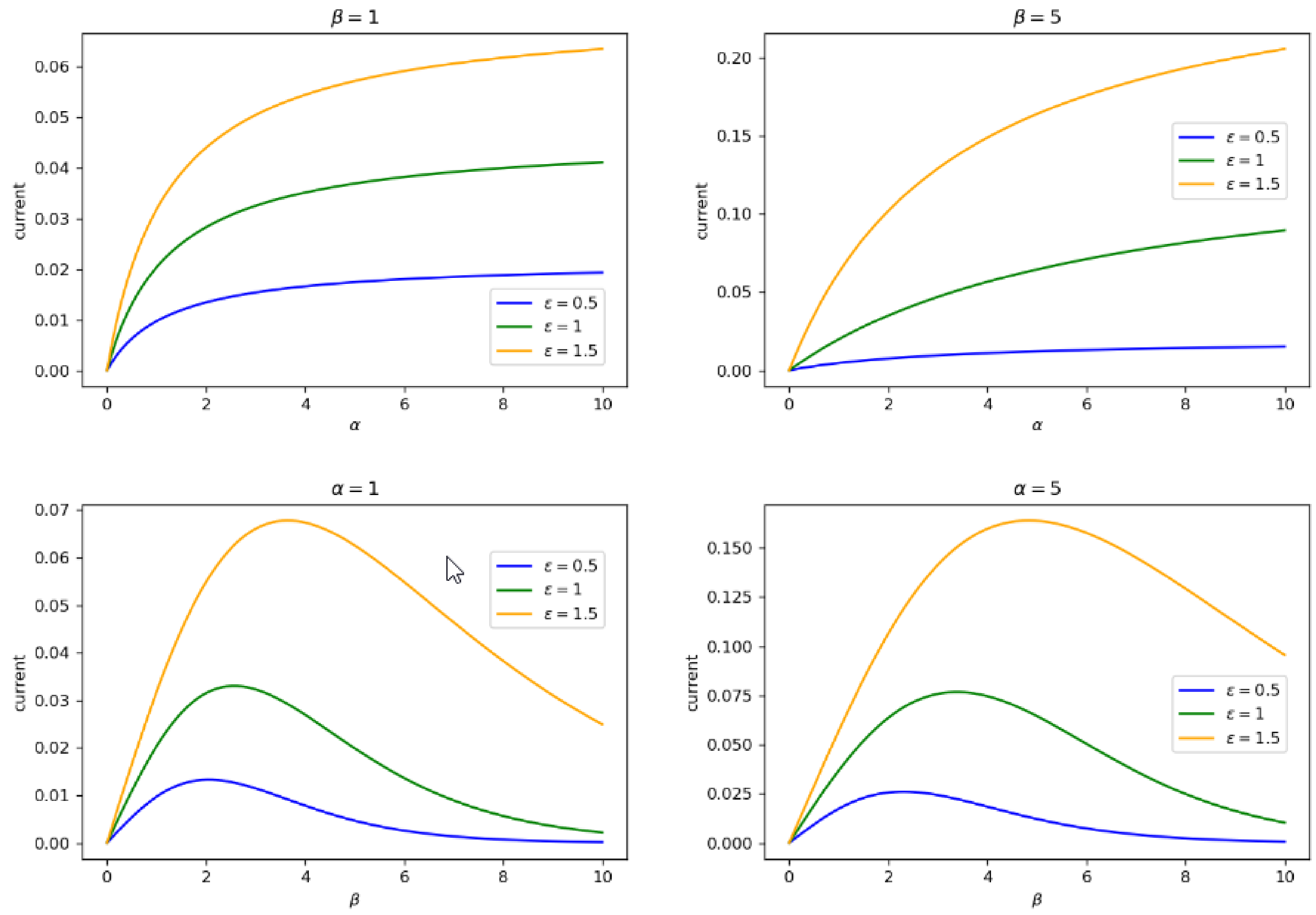


Figure 13: The energy current j_E for $\varepsilon = 0.5$, $\varepsilon = 1$ and $\varepsilon = 1.5$ with $\tau = \nu = 1$ in function of α and β.

Simplifying by identifying eta with x:

The engine becomes a run-and-tumble dynamics (but obviously not interpreting x as the position of bacteria):

We identify x and η, $v = -\kappa w$, to obtain the dynamics

$$\dot{x}_t = v\sigma_t + G(x) + \sqrt{2\gamma T}\,\xi_t$$

with $G(x) = F(x) - V'(x)$. Energy function has become

$$E(x,\sigma) = V(x) - v\sigma\, x, \quad V(x) = U(x) + \frac{\kappa}{2}\,x^2$$

$\sigma \to -\sigma$ with rate $\alpha \exp\{-\beta_{\text{eff}}\, v\, \sigma\, x\}$

For free: interpretation of local detailed balance got possible.

CM, Local detailed balance. SciPost Phys. Lect. Notes (2021).

- allows some consistency in 1st-2nd law prescriptions

- e.g. –allows calorimetry: P.Dolai, CM and K.Netočný, Active Calorimetry, SciPost Phys. (2023).

- e.g. –allows McLennan (close-to-equilibrium) analysis: C.Maes and K.Netočný: Rigorous meaning of McLennan ensembles, Journal of Mathematical Physics **2010.**

- e.g. –allows applying 'usual' response formalism

Other application: extending shape transition

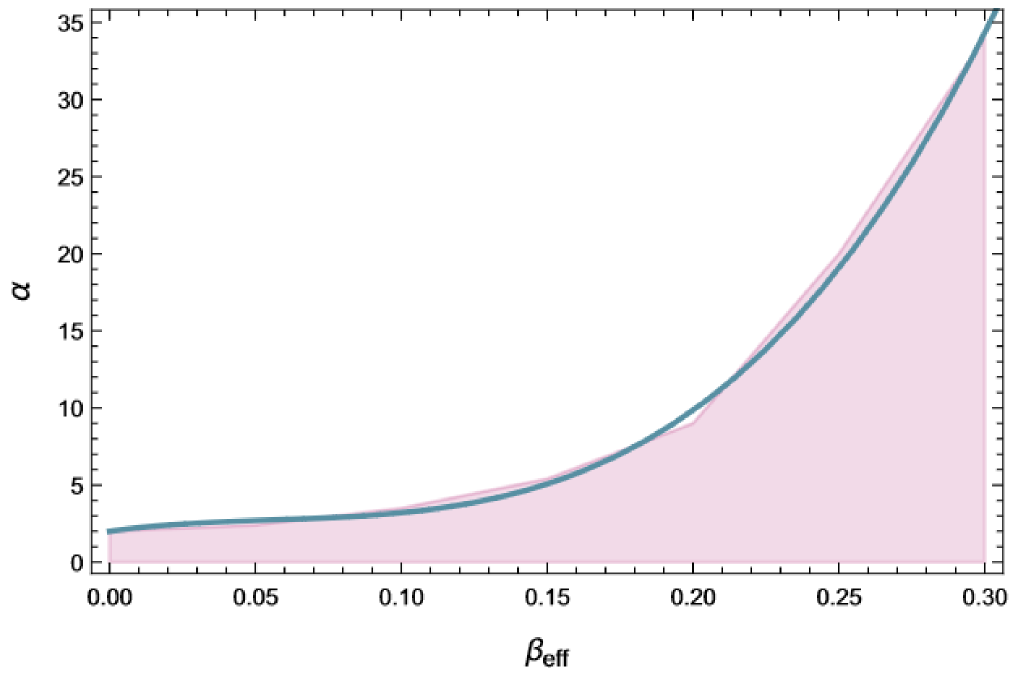
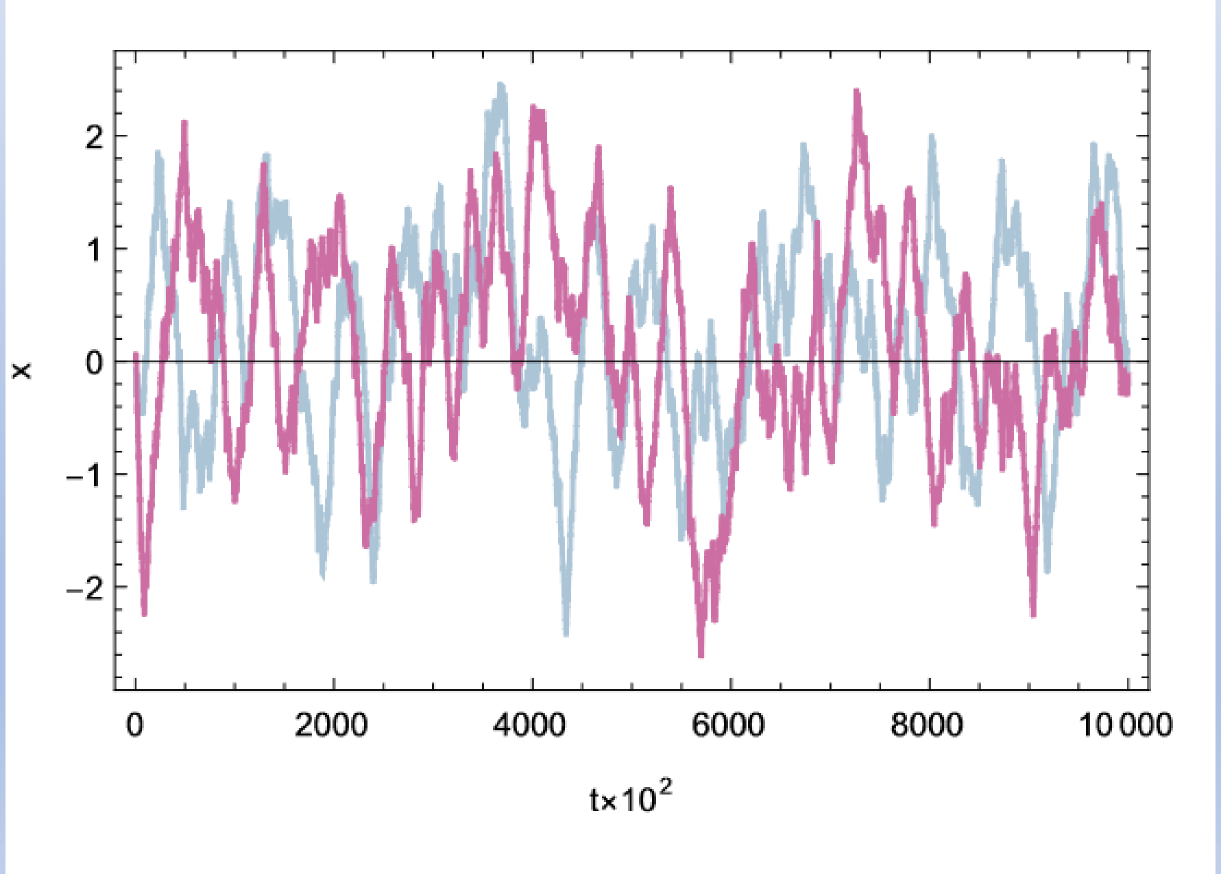
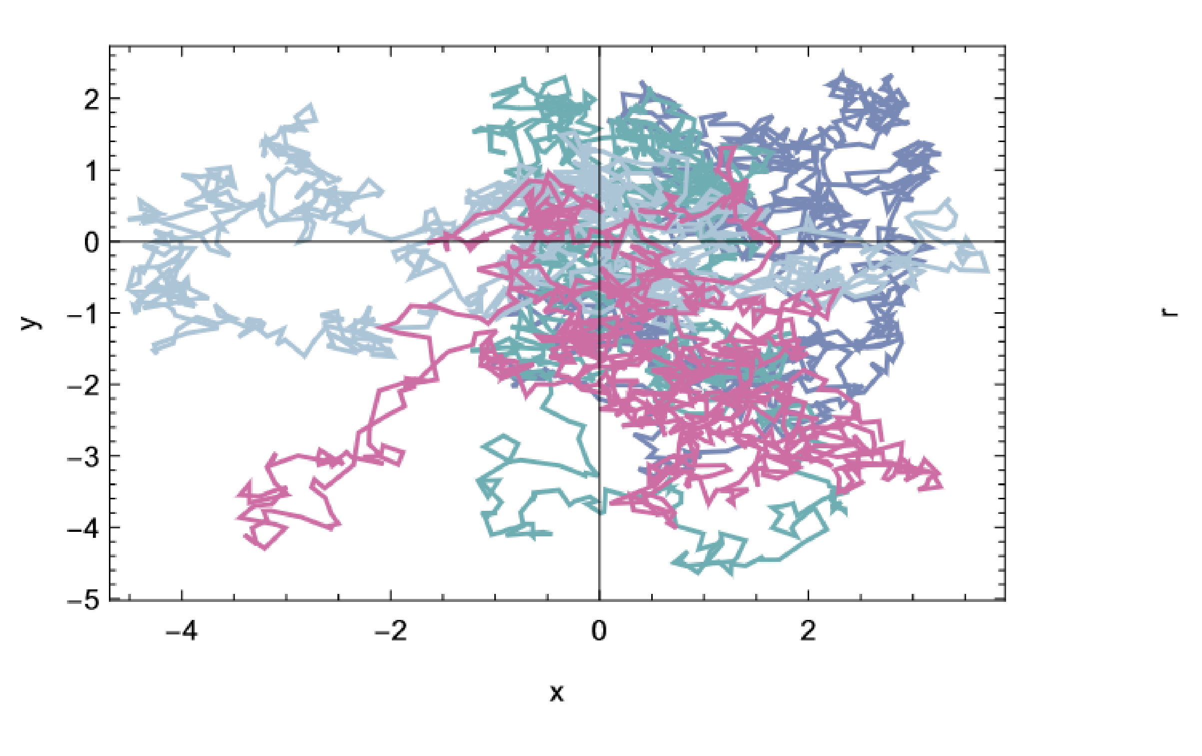


FIG. 4: Shape transition in the $(\beta_{\text{eff}}, \alpha)$-plane for harmonic potential $U(x) = x^2$ at $T = 0$ and with propulsion speed $v = 3$. The colored section represents the edgy regime. For high enough α starts the confined regime, with a sharply increasing transition line, fitting the transition as

Extending shape transition

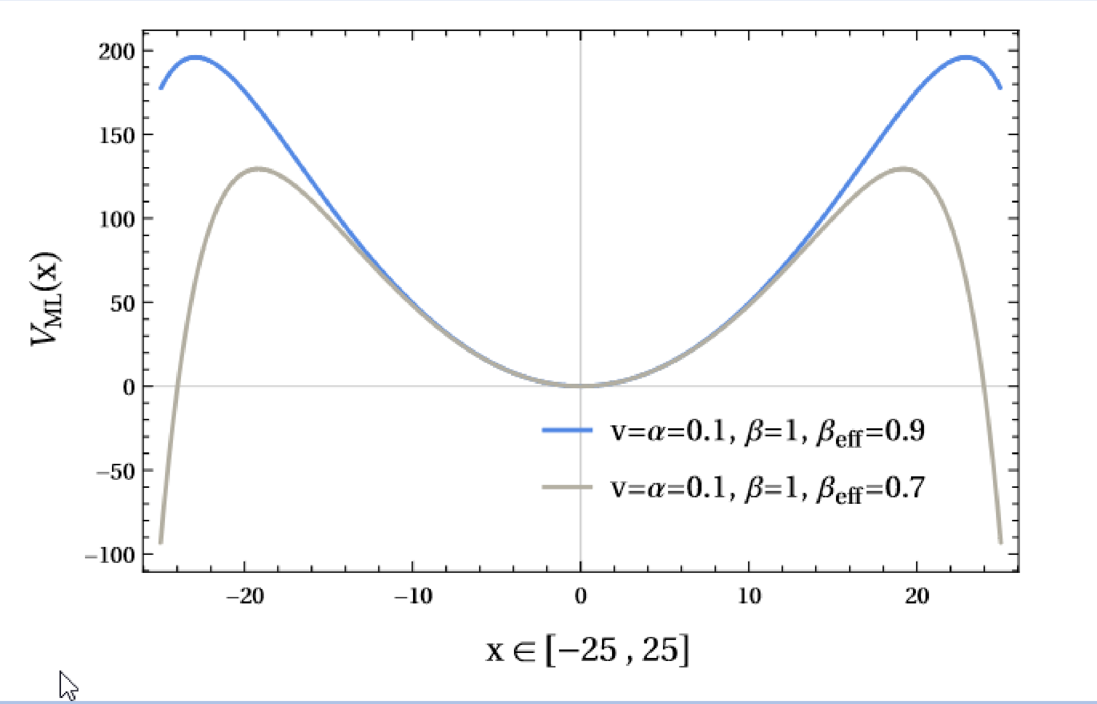
Confinement (without confining potential) at negative effective temperature.





Extending shape transition

Shape transition ‘close-to-equilibrium’



Dirac equation: detailed balance

$$\psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} \qquad \begin{cases} \rho_+ = \psi_+^* \psi_+ \\ \rho_- = \psi_-^* \psi_- \end{cases}$$

$$\boxed{\begin{aligned} \partial_t \rho_+ + \nabla \cdot (\mathbf{v}_+ \rho_+) &= a\rho_- - b\rho_+ \\ \partial_t \rho_- + \nabla \cdot (\mathbf{v}_- \rho_-) &= b\rho_+ - a\rho_- \end{aligned}}$$

$$\mathbf{v}_+ = c \frac{\psi_+^\dagger \boldsymbol{\sigma} \psi_+}{\psi_+^\dagger \psi_+}, \qquad \mathbf{v}_- = -c \frac{\psi_-^\dagger \boldsymbol{\sigma} \psi_-}{\psi_-^\dagger \psi_-}$$

$$a = 2\frac{mc^2}{\hbar} \frac{\left(\mathrm{Im}\, \psi_+^\dagger \psi_-\right)^+}{\psi_-^\dagger \psi_-}, \qquad b = 2\frac{mc^2}{\hbar} \frac{\left(\mathrm{Im}\, \psi_-^\dagger \psi_+\right)^+}{\psi_+^\dagger \psi_+}$$

$$F^+ = \max\{0, F\}$$

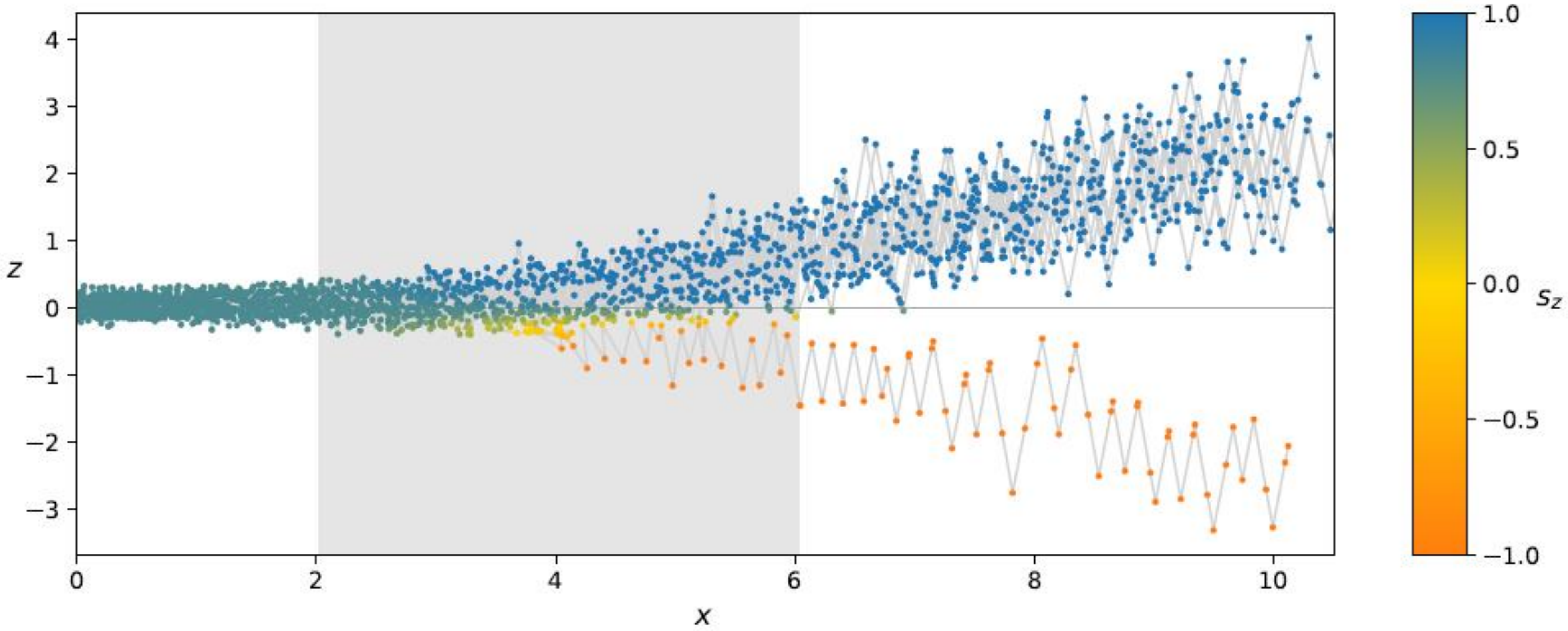


Figure 7: Ten particle trajectories for the spinor $\Psi = \frac{1}{\sqrt{10}}(3\psi_+, i\psi_-)^\mathsf{T}$. As in Fig. 6, the dots represent the locations of the particles at the times of jumps. The color of a dot indicates s_z at the jump event.

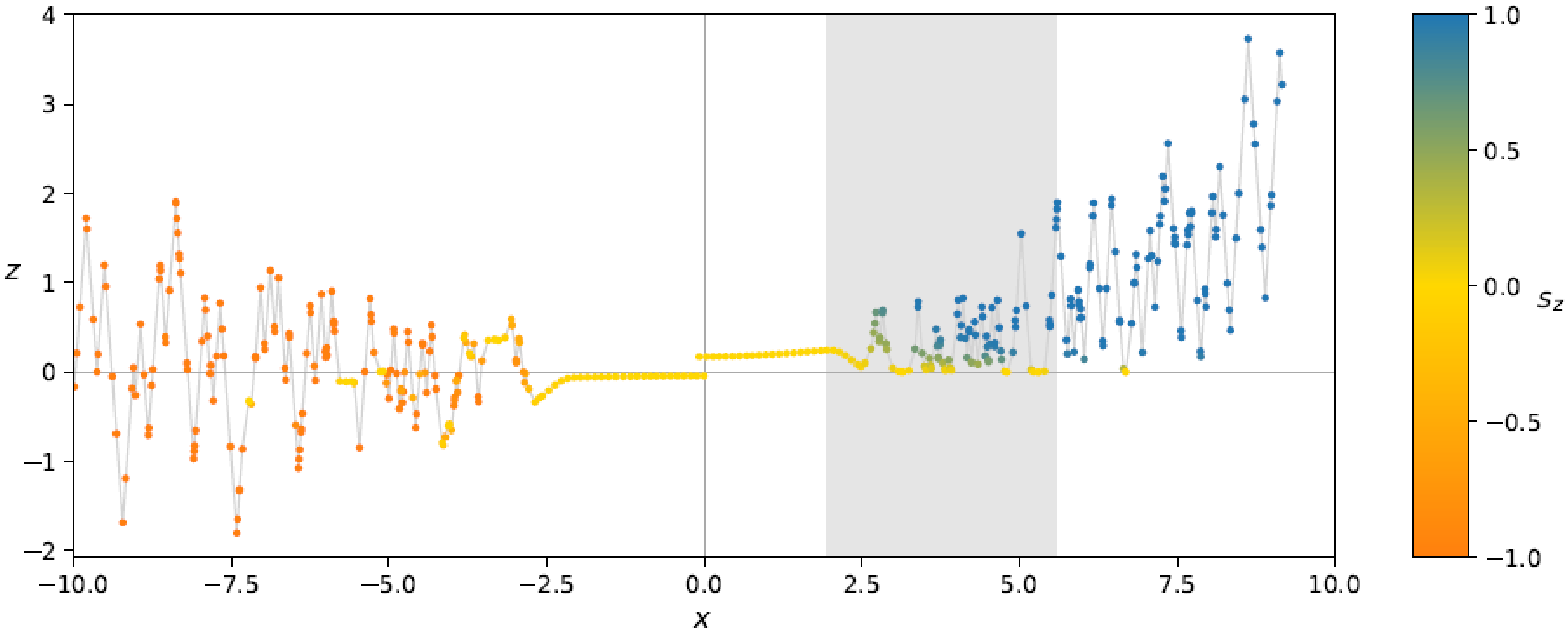


Figure 9: The same trajectories as in Fig. 8, with dots at the location of the chirality jumps and the color indicating the value of s_z.

conclusions

Yes, let us have hot spots, the Sun within.

And make efficiency calculations for energy transport between a thermal reservoir (heat bath) and agitated molecules (those hot spots).

It may be relevant for understanding/modeling biological engines, but it also gives the ‘local detailed balance’ advantage to existing models.