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BROKEN DETAILED BALANCE

Understanding non-equilibrium phenomena and internally driven systems by studying "Active Brownian Particles"

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Workshop

Idea!

epl A LETTERS JOURNAL EXPLORING THE FRONTIERS OF PHYSICS

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Instances of

ACTIVE MOTION

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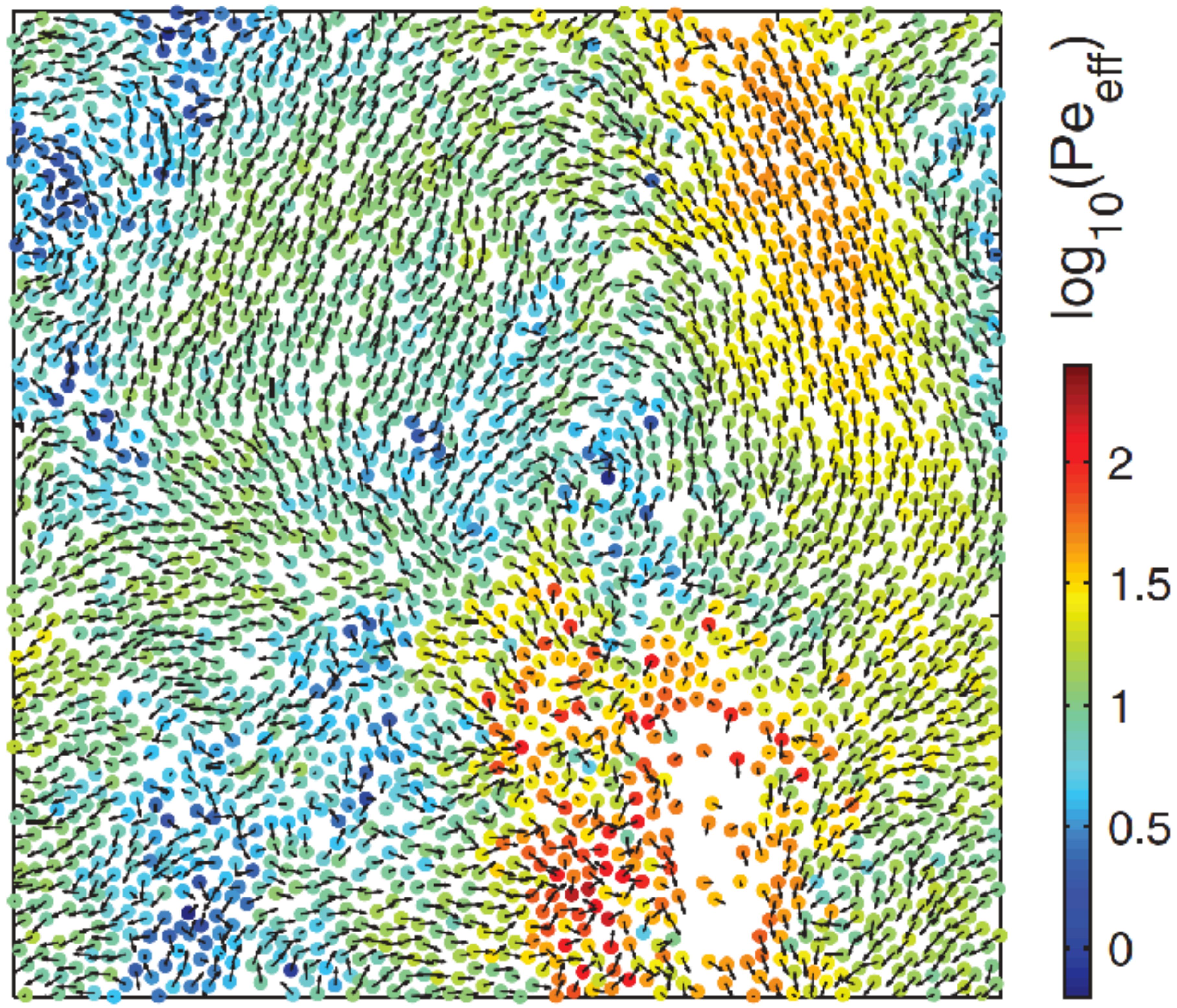
Cooperative motion of active Brownian spheres in three-dimensional dense suspensions

ADAM WYSOCKI, ROLAND G. WINKLER and GERHARD GOMPPER

- Self-propelled Brownian particles in three spatial dimensions
- Phase separation into dilute and dense phase
- Long-lived cooperative motion of particles, without any intrinsic alignment mechanism



Instances of

ACTIVE MOTION

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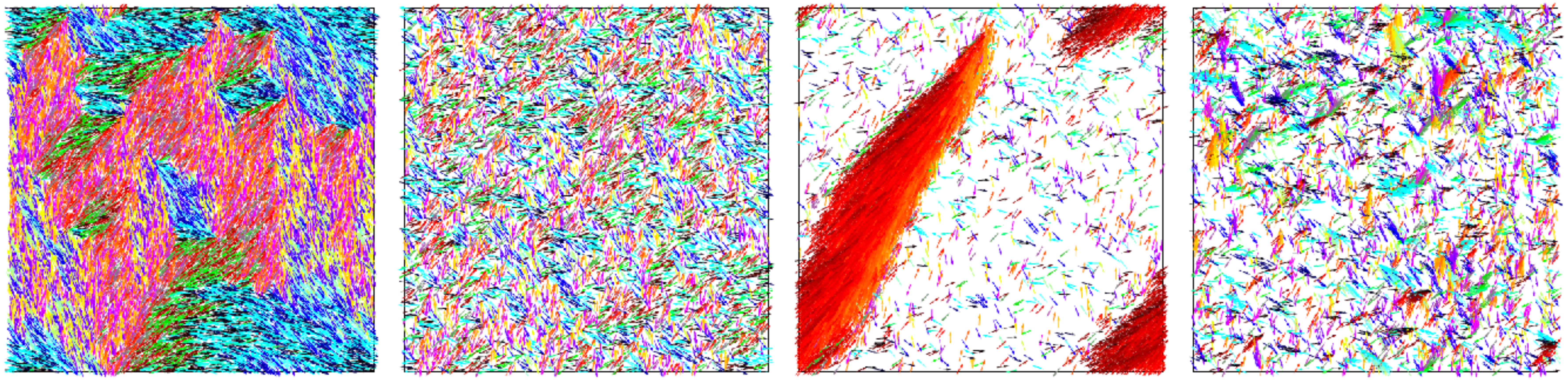
PHYSICAL REVIEW E **88**, 062314 (2013)

Collective behavior of penetrable self-propelled rods in two dimensions

Masoud Abkenar, Kristian Marx, Thorsten Auth, and Gerhard Gompper



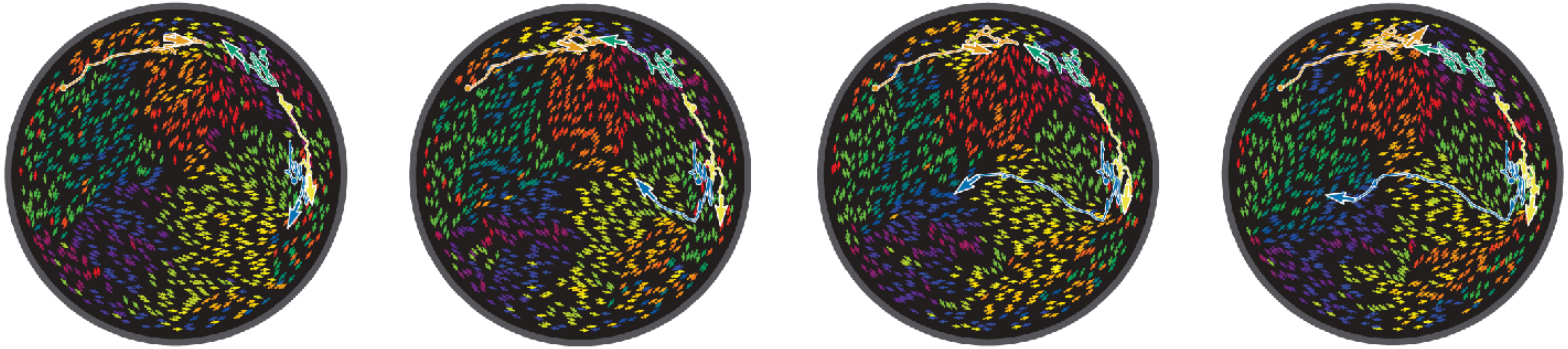
(a) $\mathrm{Pe} = 0,\ \rho L_{\mathrm{rod}}^2 = 10.2$ (b) $\mathrm{Pe} = 0,\ \rho L_{\mathrm{rod}}^2 = 5.1$ (c) $\mathrm{Pe} = 20,\ \rho L_{\mathrm{rod}}^2 = 5.1$ (d) $\mathrm{Pe} = 100,\ \rho L_{\mathrm{rod}}^2 = 5.1$

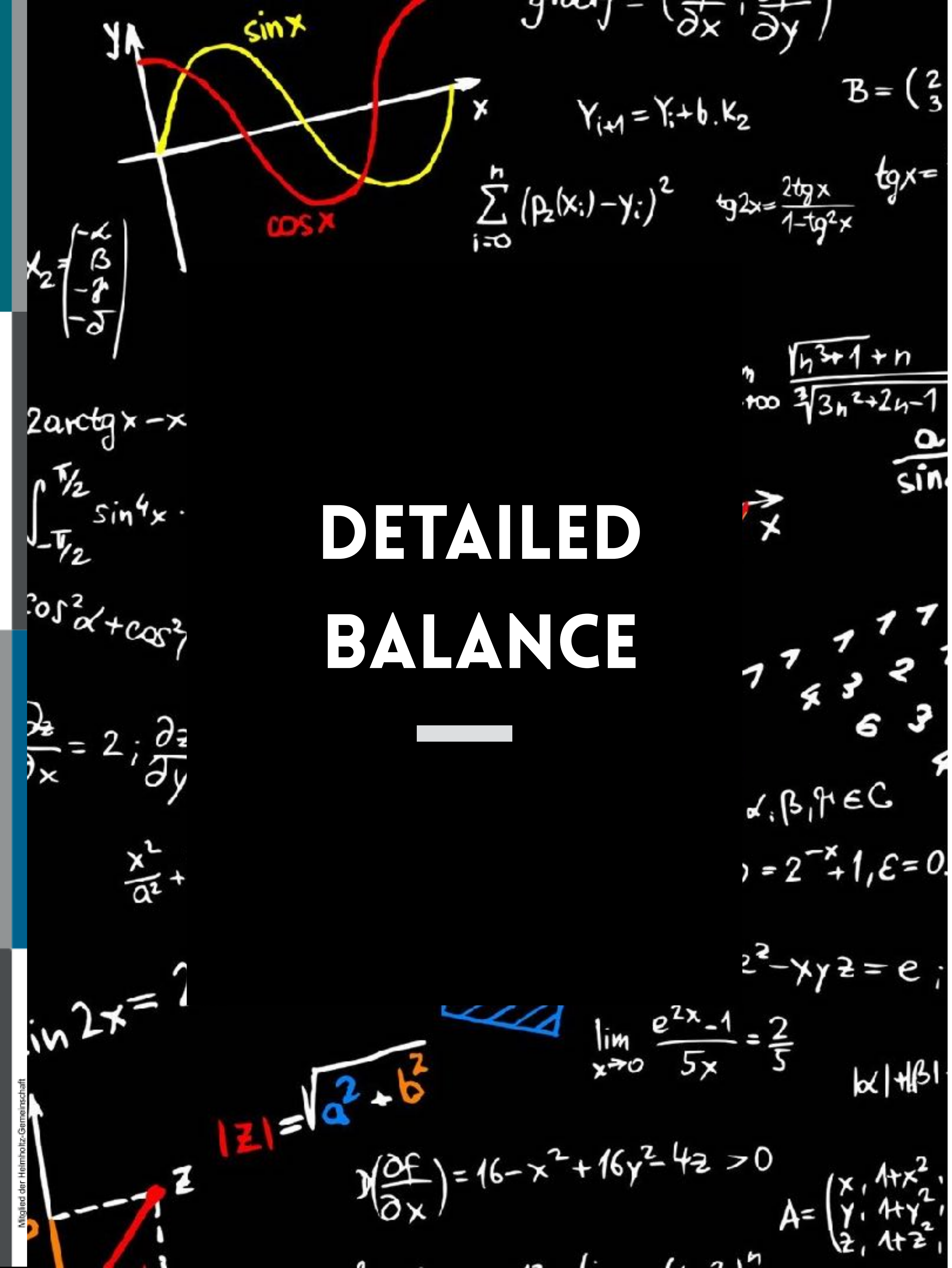
Instances of

ACTIVE MOTION

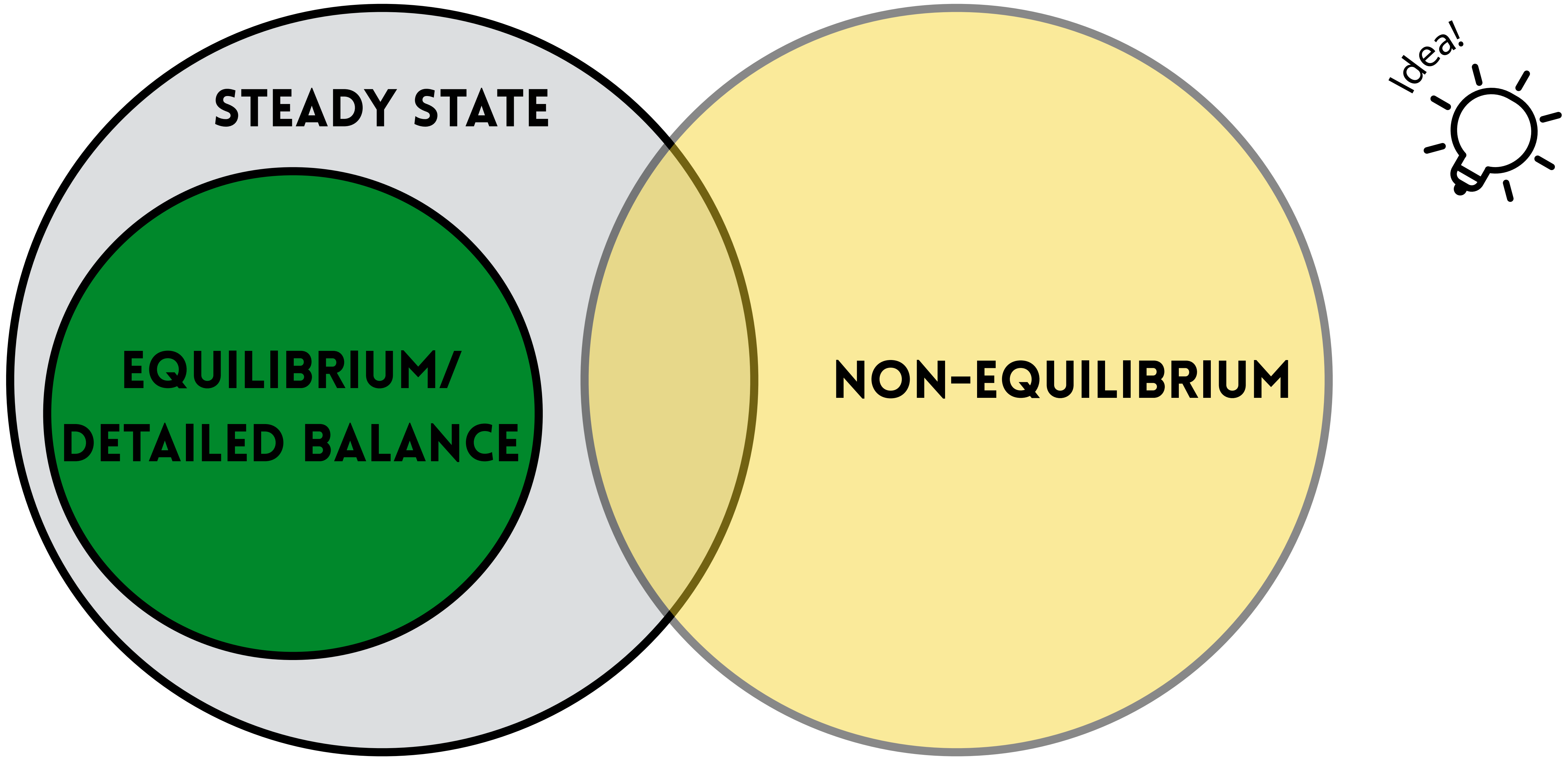
Enhanced Dynamics of Confined Cytoskeletal Filaments Driven by Asymmetric Motors

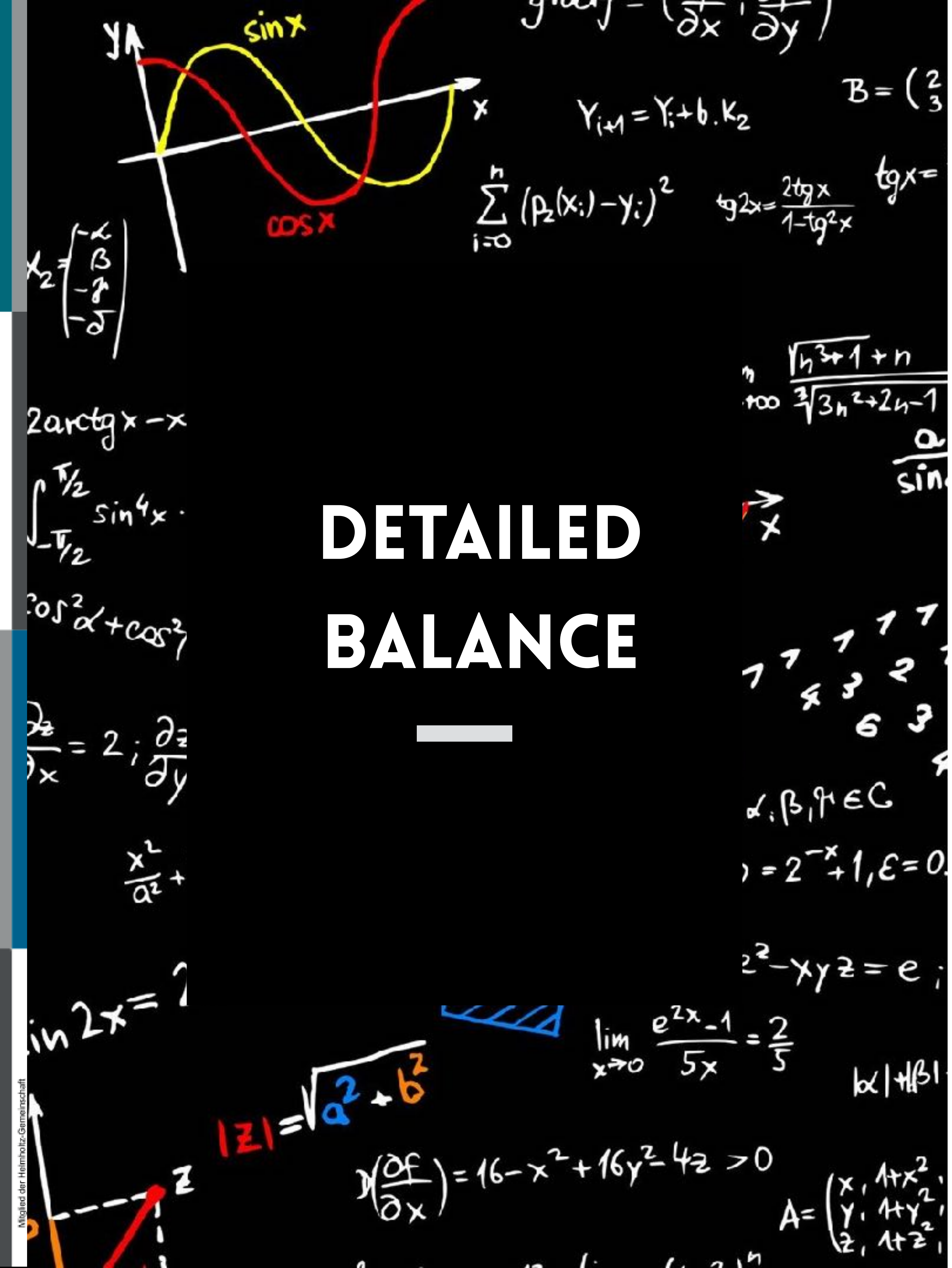
A. Ravichandran, G. A. Vliegenthart, G. Saggiorato, T. Auth, and G. Gompper





DETAILED BALANCE

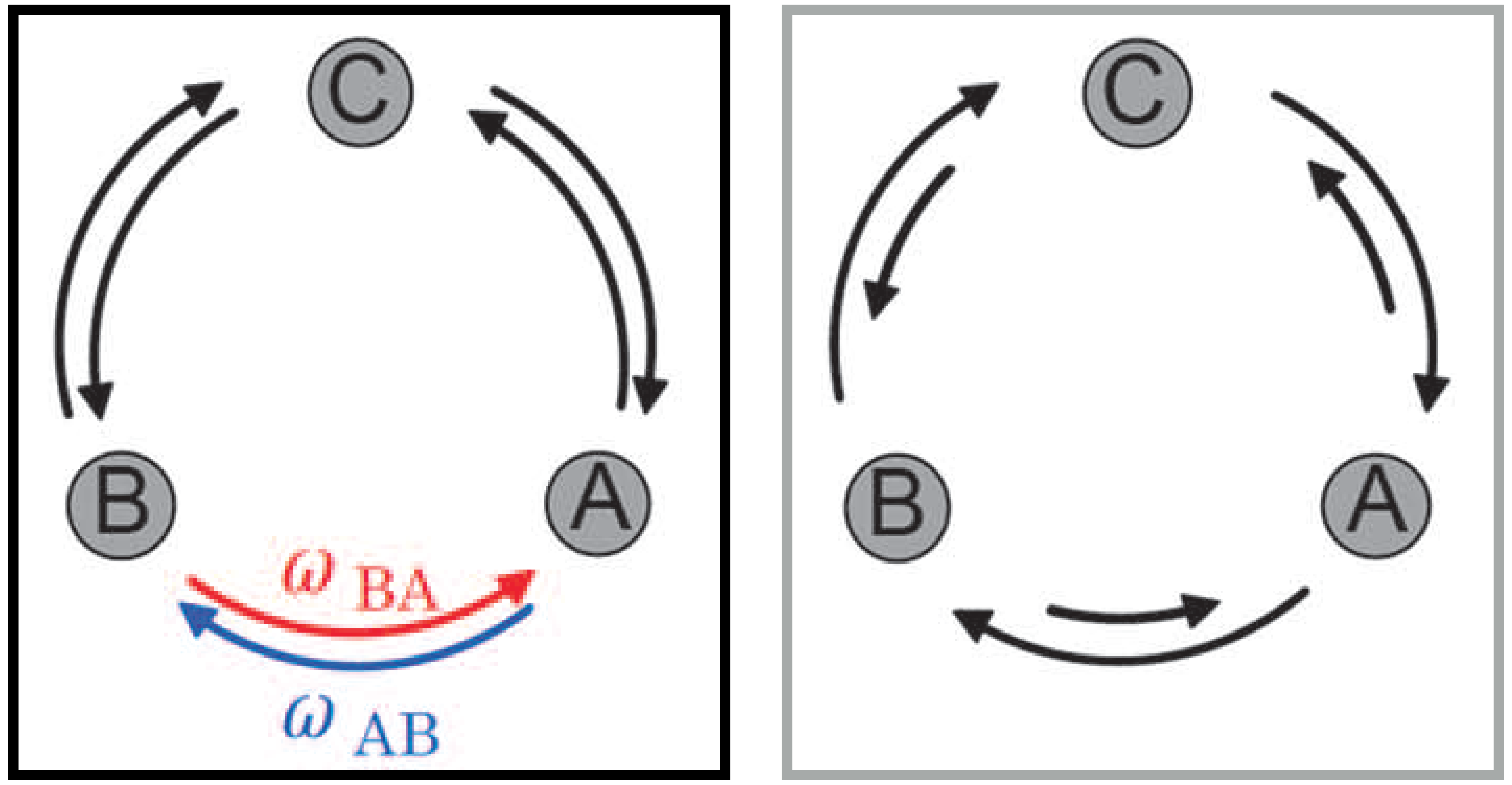


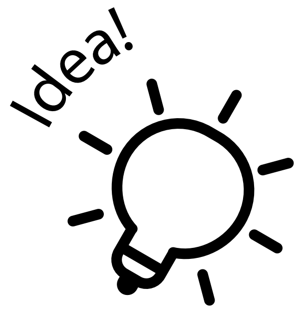


DETAILED BALANCE

DETAILED BALANCE

DETAILED BALANCE BROKEN





Transition rates between *any pair of* microstates is balanced

BROWNIAN MOTION

We can see diffusion when someone sprays deodorant in a corner of the room, or when we put a tea bag in water. Particles move because they have thermal energy due to their temperature. Their thermal energy is converted into kinetic energy $k_B T \sim 1/2\ mv^2$.

RANDOM WALKS

- Random walks are *Markovian*
  i.e. the next step is independent of the previous step.
- Random walk of N steps each of length a taking a time Δt.

- The position at time, $t = N\Delta t$ is given by,

$$\mathbf{X} = \sum_{i=1}^{N} \mathbf{a}_i$$

- Since each successive step, $\mathbf{a}_i$ is in a different direction, these vectors average to zero, $\langle \mathbf{a}_i \rangle = 0$ (isotropic). Which means,

$$\langle \mathbf{X} \rangle = 0$$

- On average, the random walker goes nowhere, but the spreading behaviour comes from the variance: $\langle X^2 \rangle = Na^2$

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RANDOM WALKS

- Random walks are *Markovian*
  i.e. the next step is independent of the previous step.
- Random walk of N steps each of length a taking a time Δt.

- By defining the diffusion coefficient,

$$D = \frac{a^2}{2\Delta t}$$

- We can write, in *d* dimensions:

$$\langle X^2 \rangle = 2dDt$$

Idea!

- Note that the variance of X is proportional to t
- The standard deviation grows with $\sqrt{t}$.

DISTRIBUTION OF POSITIONS

- Consider a 1-D random walk, where each step can either be in the positive or negative direction.
- We end up with *P(X)*, the probability of being at position *X* after *N* steps.

- This can be given by the Binomial Distribution:

$$P(X) = \frac{1}{2^N}\binom{N}{N+}$$

- When $N \gg 1$ and, it can be shown that the Binomial Distribution can be written as:

$$P(X) = \frac{1}{\sqrt{4\pi Dt}} e^{\frac{-x^2}{4Dt}}$$

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DISTRIBUTION OF POSITIONS

- Consider a 1-D random walk, where each step can either be in the positive or negative direction.
- We end up with *P(X)*, the probability of being at position *X* after *N* steps.

what will happen when N^+ is not equal to N^-

- do we satisfy equilibrium conditions?
- is detailed balance broken?

Workshop

COUPLED OSCILLATORS

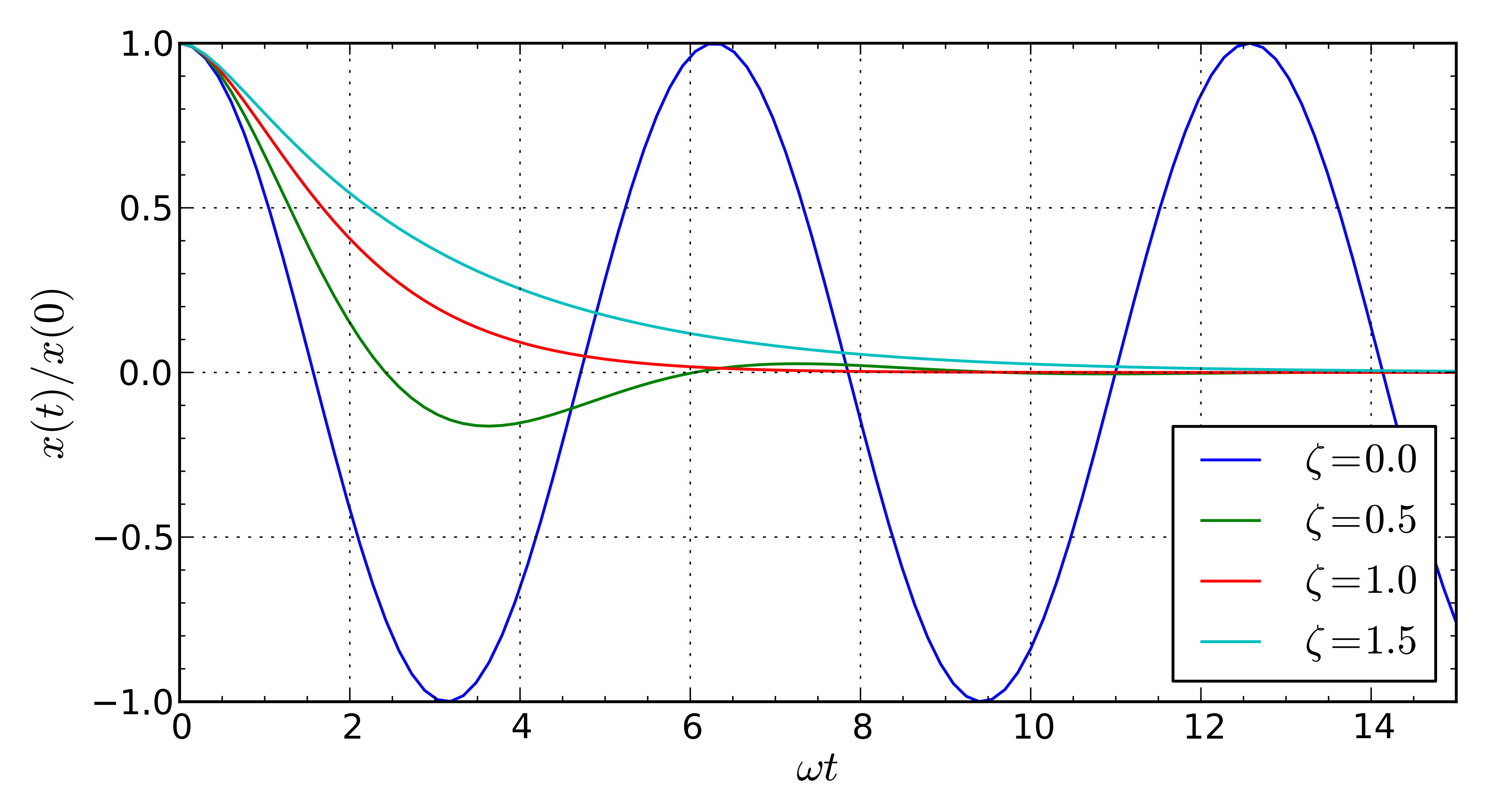
OVERDAMPED (BROWNIAN DYNAMICS)

$$F = F_{\text{ext}} - kx - c\frac{\mathrm{d}x}{\mathrm{d}t} = m\frac{\mathrm{d}^2x}{\mathrm{d}t^2}$$

$$\omega_0 = \sqrt{k/m}$$

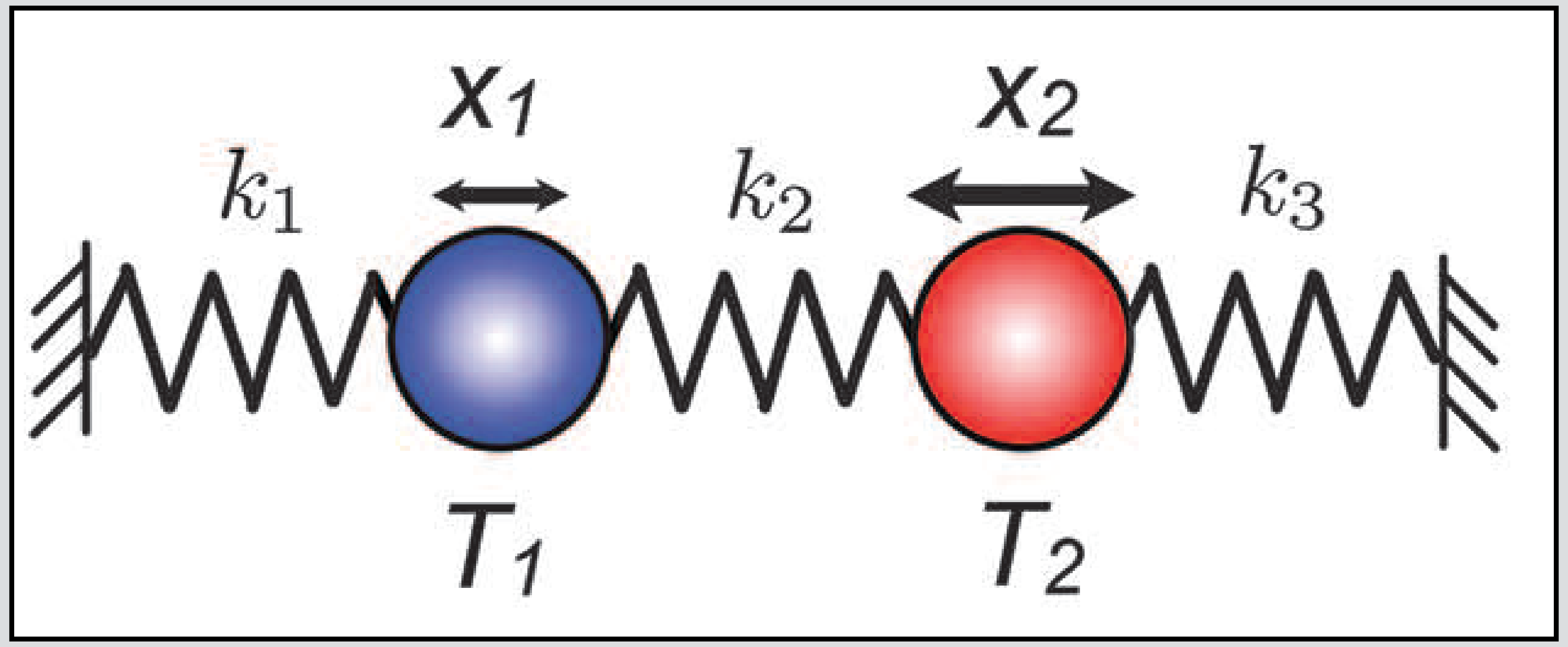
$$\frac{\mathrm{d}^2x}{\mathrm{d}t^2} + 2\zeta\omega_0\frac{\mathrm{d}x}{\mathrm{d}t} + \omega_0^2 x = 0$$

$$\zeta = \frac{c}{2\sqrt{mk}}$$



$\zeta > 1;$ overdamped
$\zeta = 1;$ criticallydamped
$\zeta < 1;$ underdamped

COUPLED OSCILLATORS

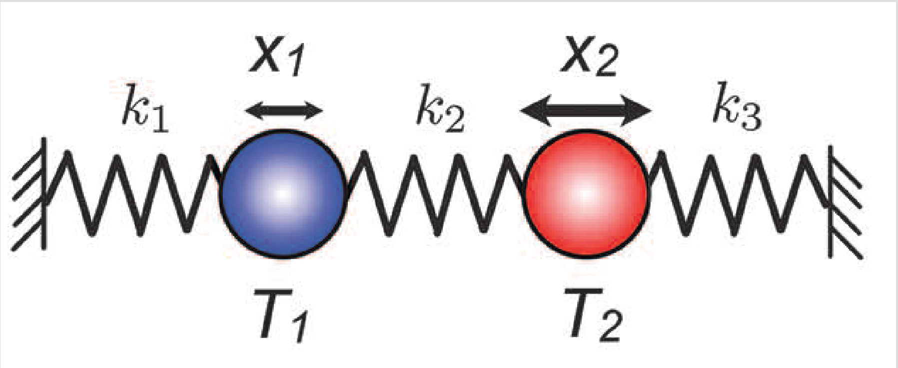


$$\zeta \frac{dx_1(t)}{dt} = k\,(x_2(t) - 2x_1(t)) + \xi_1(t), \qquad \text{and}$$

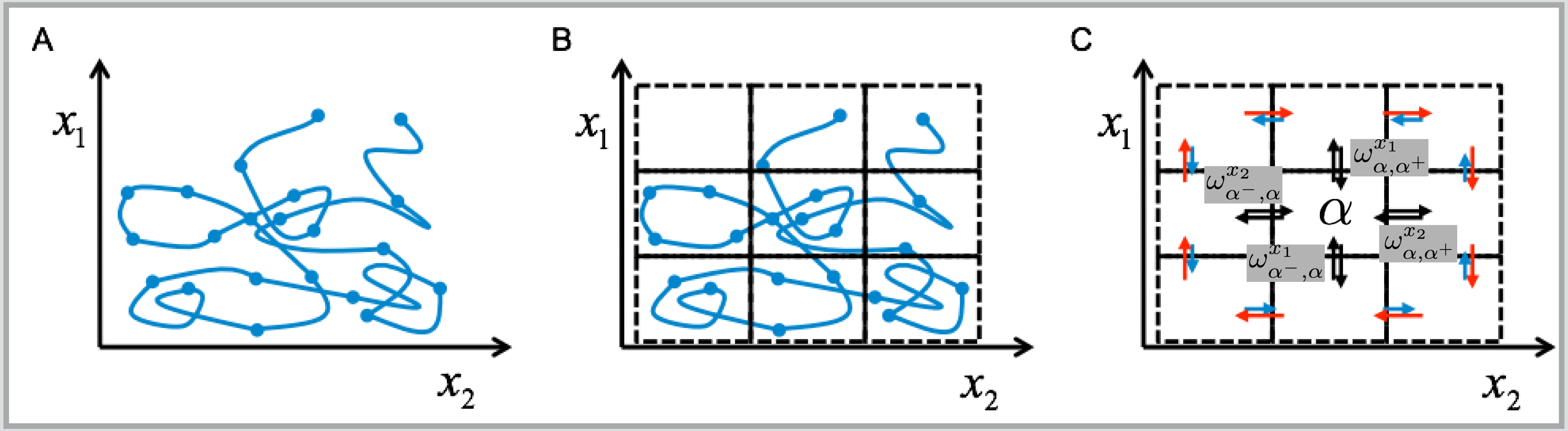
$$\zeta \frac{dx_2(t)}{dt} = k\,(x_1(t) - 2x_2(t)) + \xi_2(t),$$

Signatures of Non-Equilibrium

COUPLED OSCILLATORS

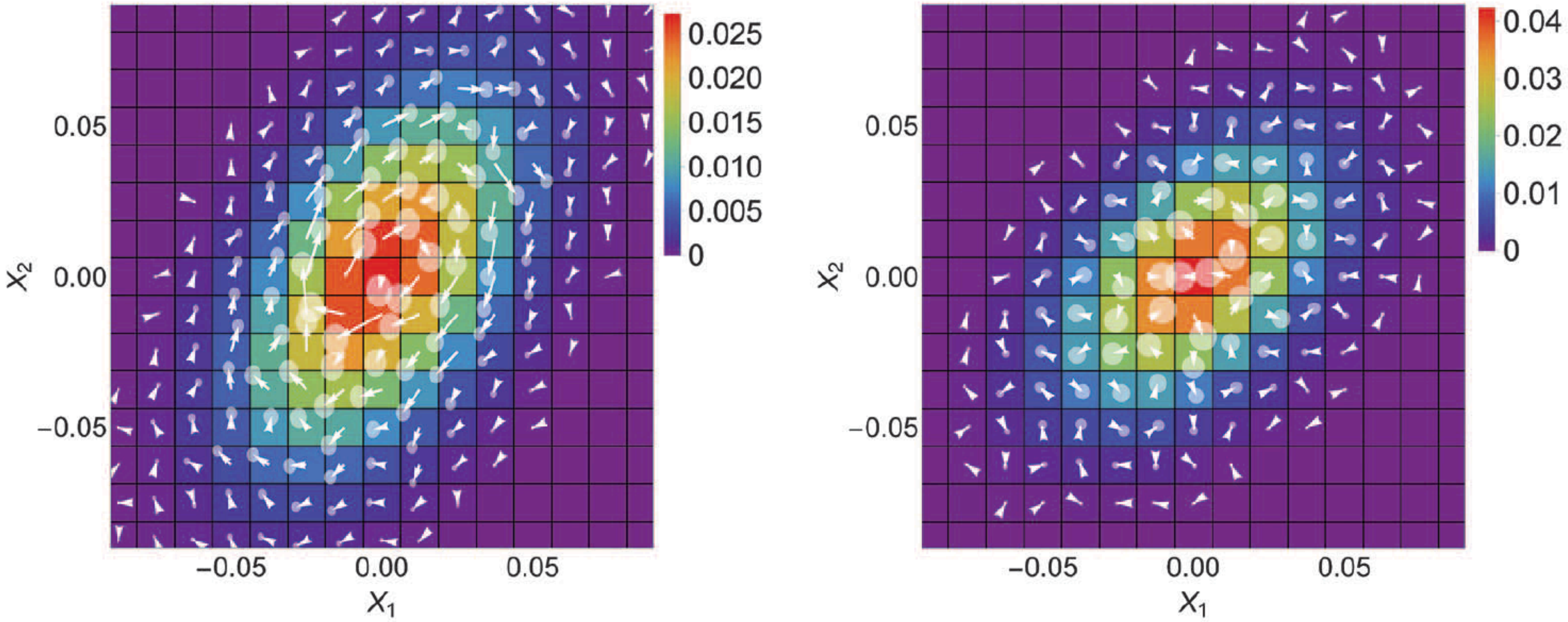


COARSE GRAINED PHASE SPACE (PROBABILITY FLUX ANALYSIS)



Signatures of Non-Equilibrium

PROBABILITY FLUX



ON TO THE EXERCISES!

SUPPLEMENTARY SLIDES

TWO ISSUES WITH DIFFUSION

1. Colloid particles are too massive to be kicked about by thermal forces.

Idea!

2. Water molecules collide with colloids far too frequently for observation.

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COLLOID PARTICLES TOO LARGE

- Atoms are four orders of magnitude smaller than colloids.
- Water molecules can “kick” the colloid, but these kicks will be too small.
- It is too small to see in the microscope.

THERMAL “KICKS” ARE FREQUENT

- How fast do water molecules move:

$$mv^2 \sim k_\mathrm{B}T$$

$$v \sim \sqrt{\frac{k_\mathrm{B}T}{m}}$$

$$\sim \sqrt{\frac{10^{-21}\mathrm{J}}{10^{-26}\mathrm{kg}}} \sim 500\mathrm{ms}^{-1} \sim \boxed{100\mathrm{kph}}$$

- Water molecules move as fast as a fast car!

COLLOID PARTICLES TOO LARGE

- Atoms are four orders of magnitude smaller than colloids.
- Water molecules can "kick" the colloid, but these kicks will be too small.
- It is too small to see in the microscope.

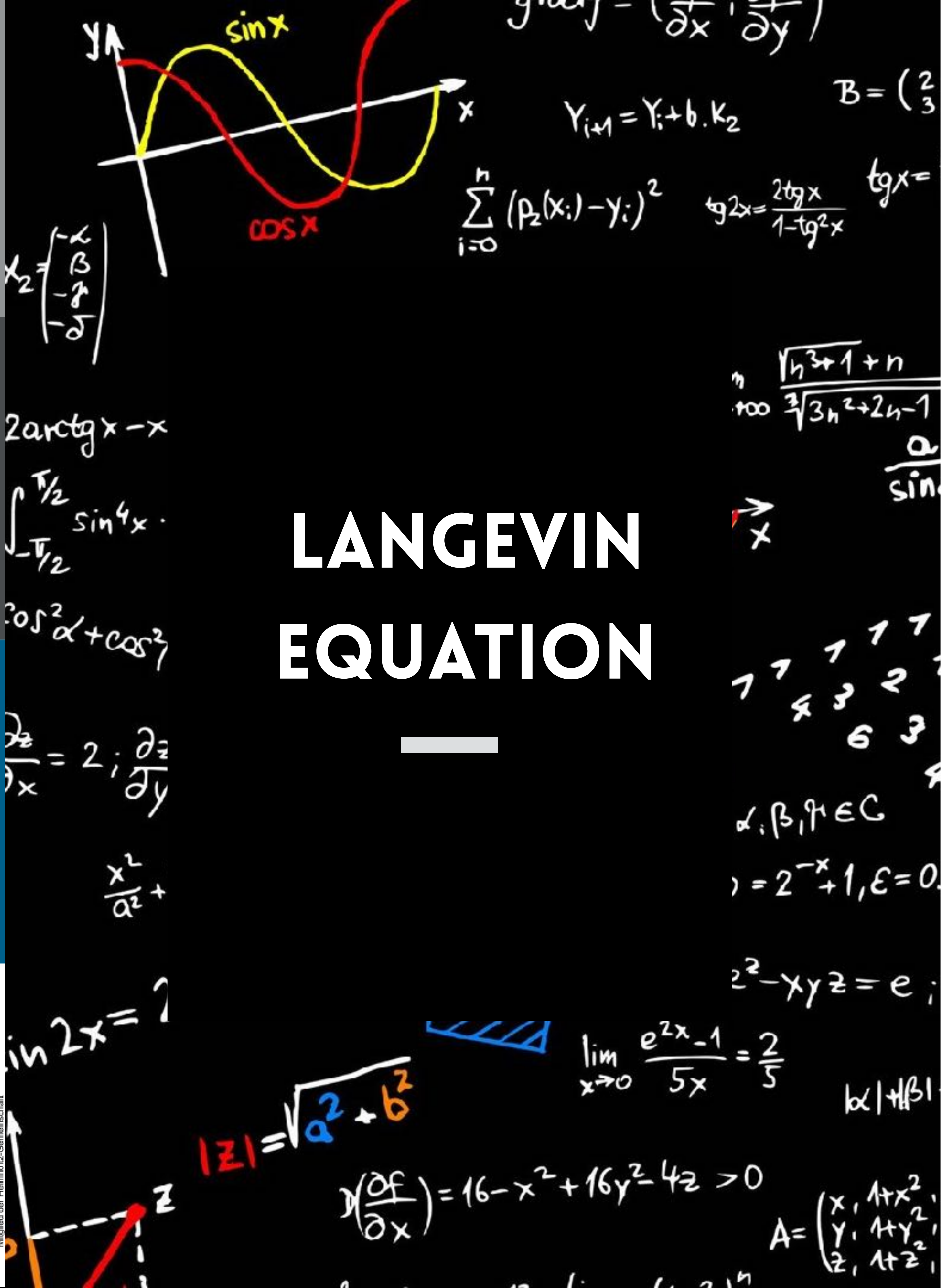
THERMAL "KICKS" ARE TOO FREQUENT

- Collision rate is speed divided by distance moved before hitting another colloid (~ 1 nm).
- Frequency of collision:

$$10^3/10^{-9} \sim 10^{12} s^{-1}$$

- Far too frequent for observation!

Idea!



LANGEVIN EQUATION

- Langevin Equation is simply Newton's second law:

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$$m\frac{d\mathbf{v}}{dt} = -\xi\mathbf{v} + \mathbf{f}_s(t)$$

Idea!

dissipative force

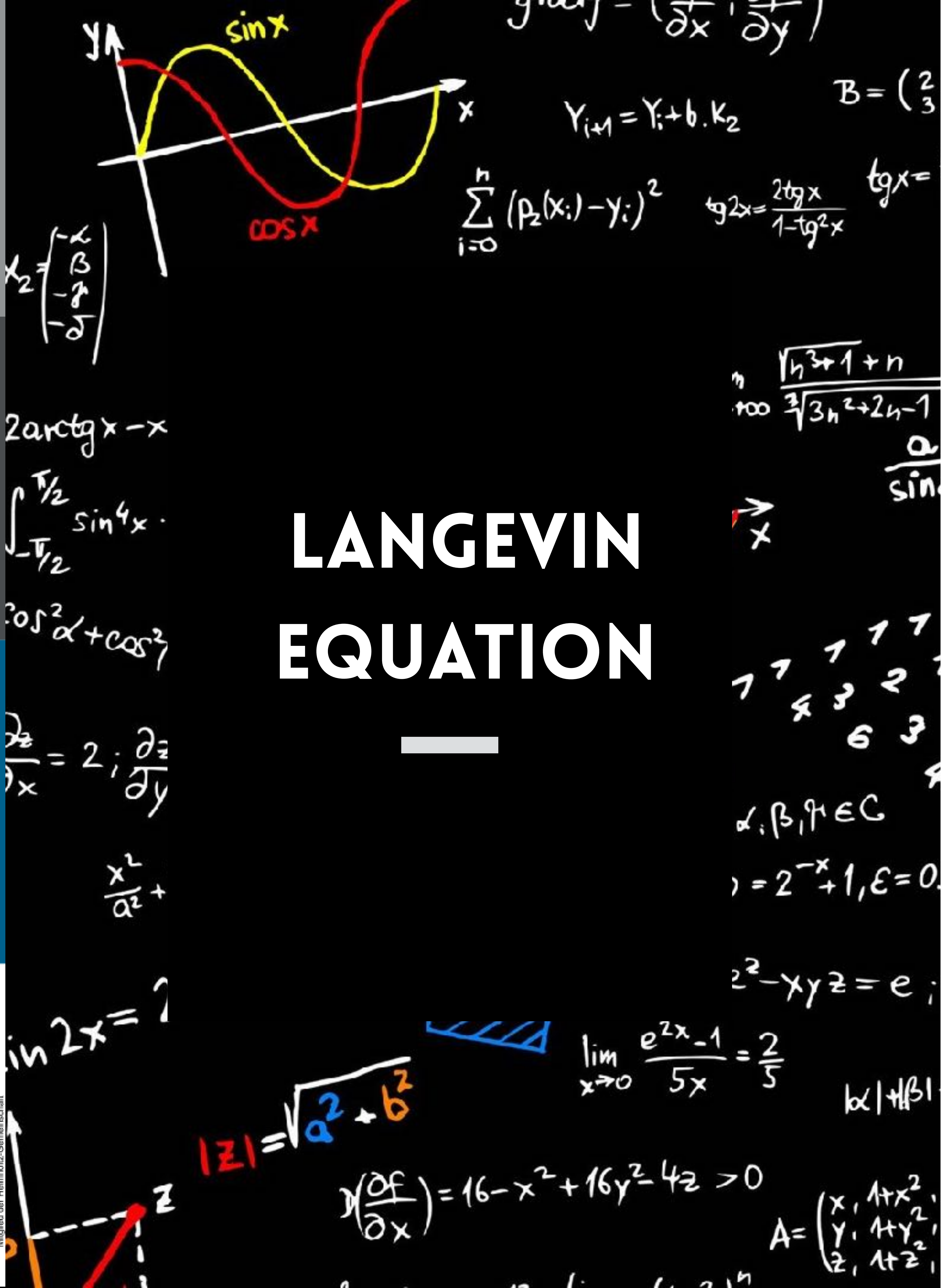
$$\langle \mathbf{v}^2(t) \rangle = k_\mathrm{B}T/m$$

stochastic force

$$\langle \mathbf{f}_s(t) \rangle = 0$$

$$\langle \mathbf{f}_s(t)\mathbf{f}_s(t') \rangle = 2B\delta(t-t')$$

Two moments of stochastic force



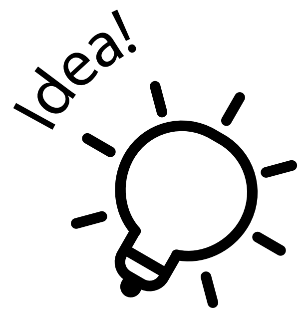
LANGEVIN EQUATION

- Langevin Equation is simply Newton's second law:

$$m\frac{d\mathbf{v}}{dt} = -\xi\mathbf{v} + \mathbf{f}_s(t)$$

- Since on average, the stochastic force = 0, average velocity is,

$$\langle \mathbf{v}(t) \rangle = \mathbf{v}_1 e^{-t/\tau}$$



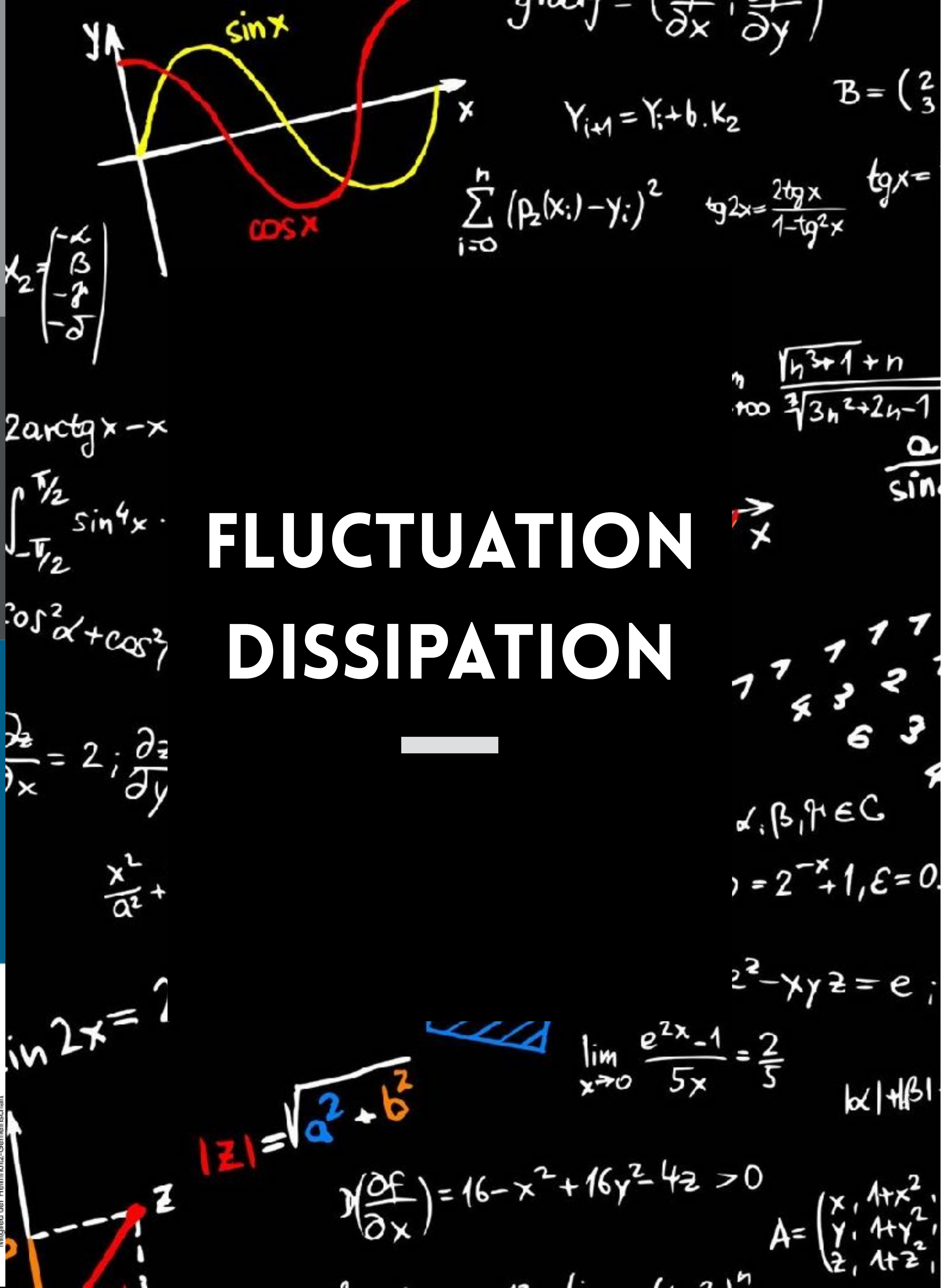
- The initial velocity decays to zero over the time τ
- At long times, $t \gg \tau$, where $\tau = m/\xi$,

$$\langle \mathbf{v}(t) \rangle = 0$$

- The variance in velocity can be shown to be:

$$\langle \mathbf{v}^2(t) \rangle = e^{-2t/\tau} v_1^2 + \frac{B}{\tau\xi^2}(1 - e^{-2t/\tau})$$

FLUCTUATION DISSIPATION



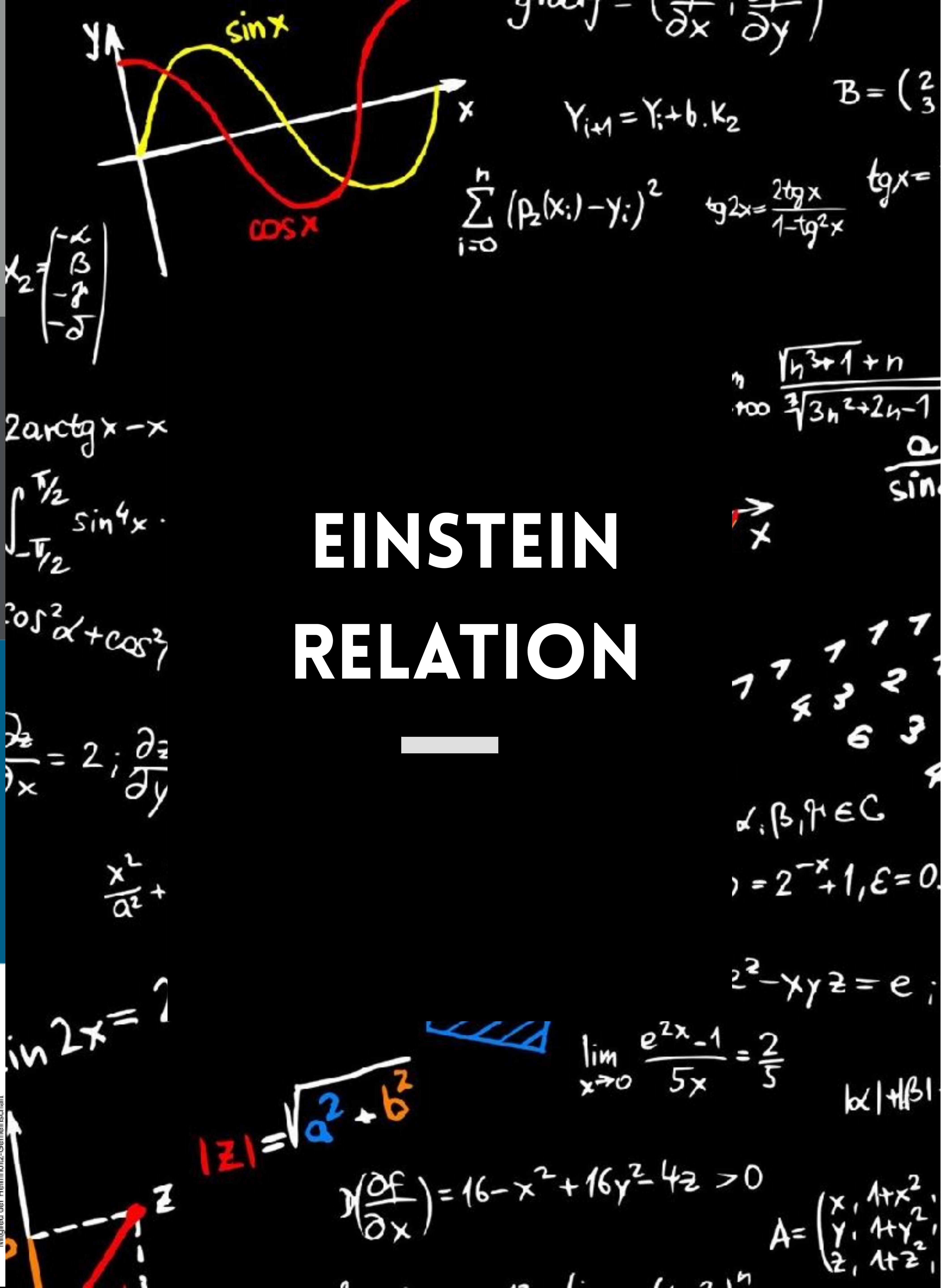
$$\langle \mathbf{v}^2(t) \rangle = e^{-2t/\tau} v_1^2 + \frac{B}{\tau \xi^2}(1 - e^{-2t/\tau})$$

At long times …

$$\langle \mathbf{v}^2(t) \rangle \to \frac{B}{\tau \xi^2} = k_\mathrm{B} T / m$$

$$\boxed{B = \xi k_\mathrm{B} T}$$

Strength of the random noise relates to the magnitude of the friction or dissipation.



EINSTEIN RELATION

- For a particle at $r = 0$, at time $t = 0$, diffusing in 3-D we know that its long time average displacement is $\langle r \rangle = 0$ and $\langle r^2 \rangle = 6Dt$. We can use these results, and the result from the Langevin equation to derive:

$$\left\langle \mathbf{r}^2(t) \right\rangle = \frac{6k_BT}{m} t\tau = 6Dt$$

- And the Einstein relation:

$$D = \frac{k_BT}{\xi}$$