

Dissipation-based uncertainty bounds for currents

Todd Gingrich

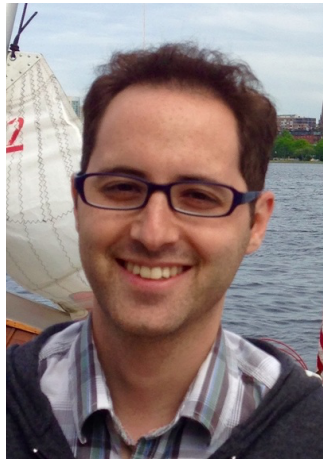
Physics of Living Systems Fellow, MIT

Large deviation theory in statistical physics:

Recent advances and future challenges

September 14, 2017

ICTS, Bangalore



Jordan Horowitz
(MIT)



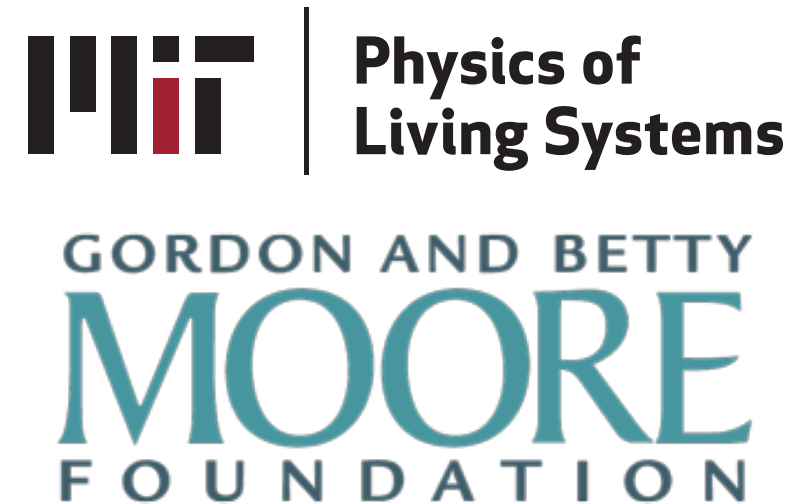
Nikolay Perunov
(formerly MIT)



Jeremy England
(MIT)



Grant Rotskoff
(NYU)



T.R. Gingrich, J.M. Horowitz, N. Perunov, J.L. England, *PRL*, 116, 120601, 2016.

T.R. Gingrich, G.M. Rotskoff, J.M. Horowitz, *J Phys A*, 50, 184004, 2017.

J.M. Horowitz and T.R. Gingrich, *PRE*, 96, 020103(R), 2017.

T.R. Gingrich and J.M. Horowitz, arXiv:1706.09027, 2017

See also:

A.C. Barato and U. Seifert, *PRL*, 114, 158101, 2015.

P. Pietzonka, A.C. Barato, U. Seifert, *PRE*, 93, 052145, 2016.

M. Polettini, A. Lazarescu, M. Esposito, *PRE*, 94, 052104, 2016.

P. Pietzonka, A.C. Barato, U. Seifert, *J Phys A*, 49, 34LT01, 2016.

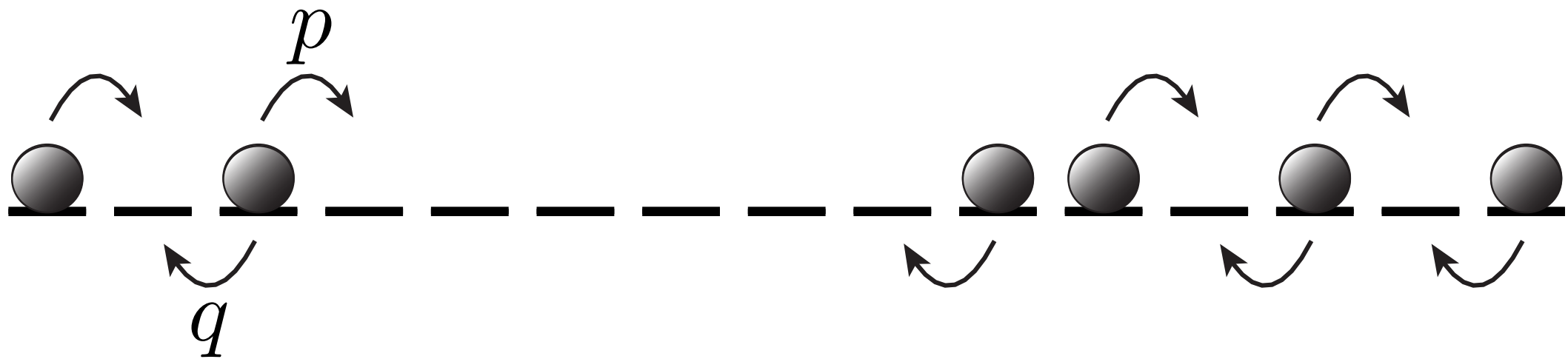
P. Pietzonka, F. Ritort, U. Seifert, *PRE*, 96, 012101, 2017.

J.P. Garrahan, *PRE*, 95, 032134, 2017.

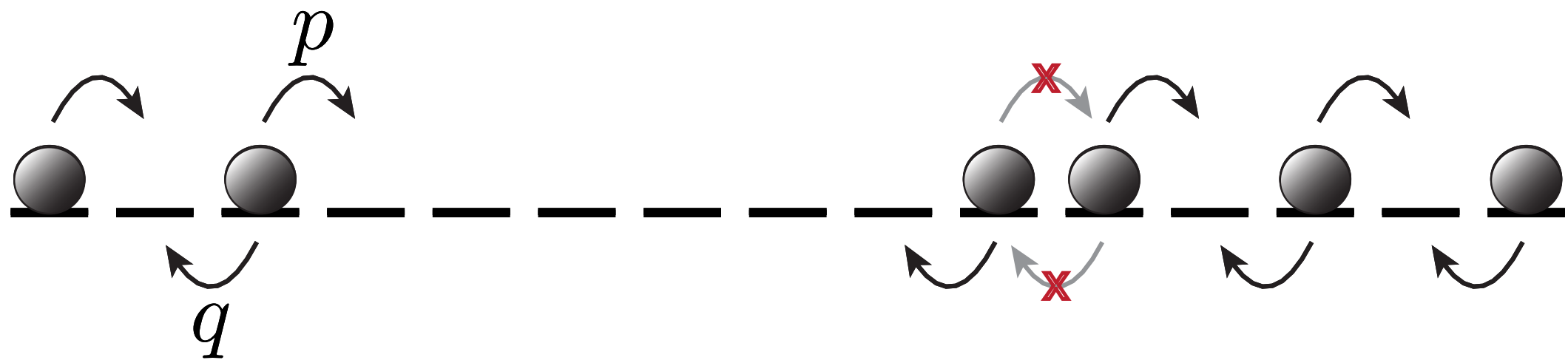
ASEP as a motivating example



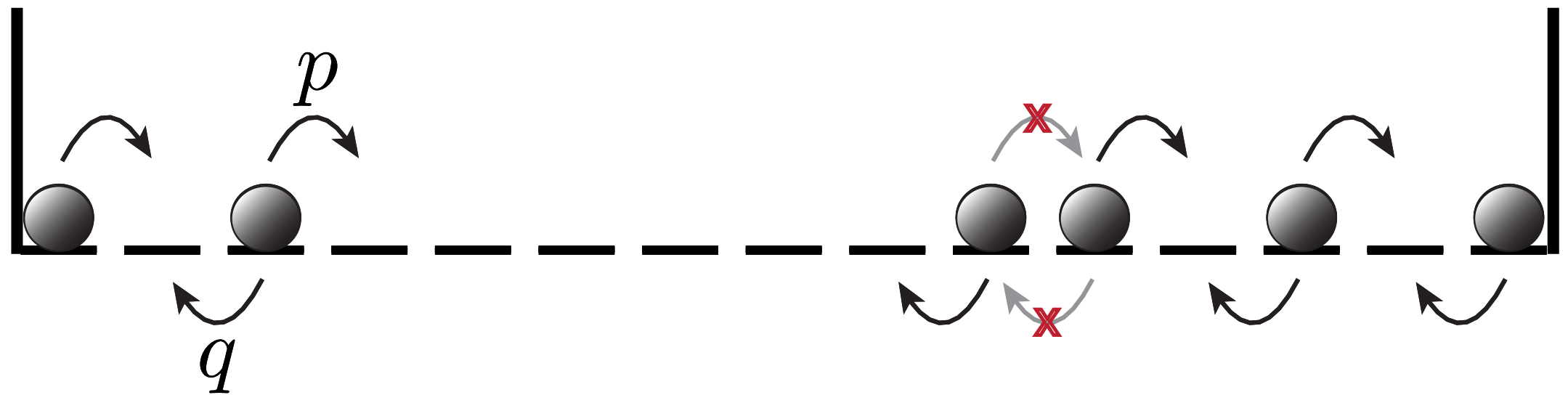
ASEP as a motivating example



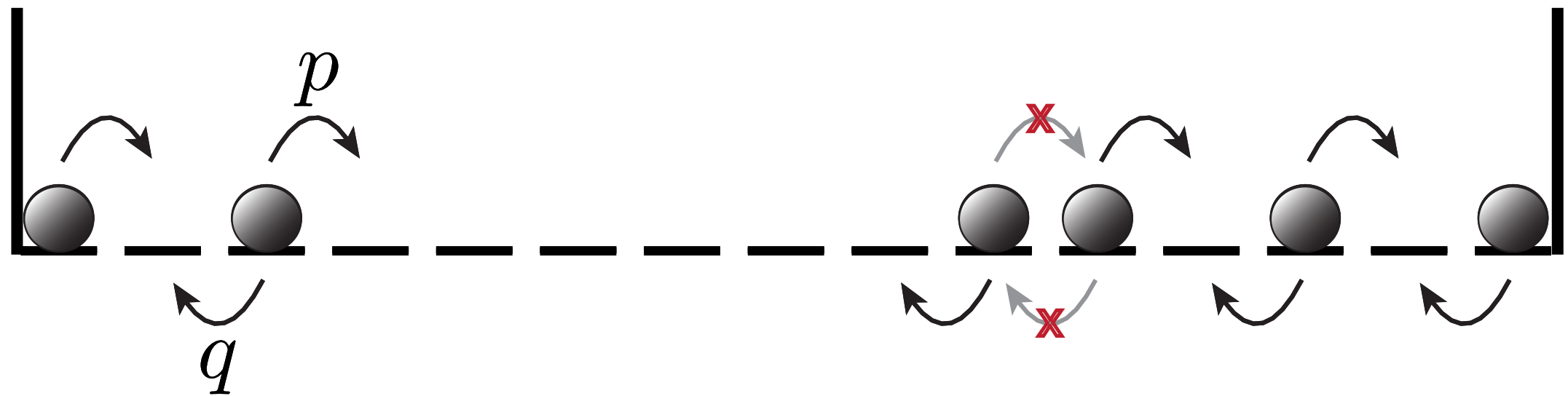
ASEP as a motivating example



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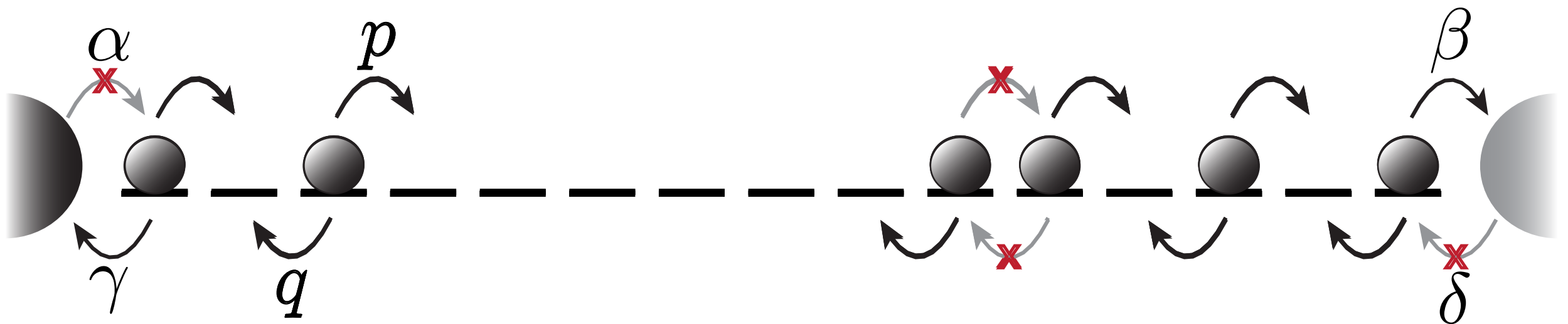


ASEP as a motivating example



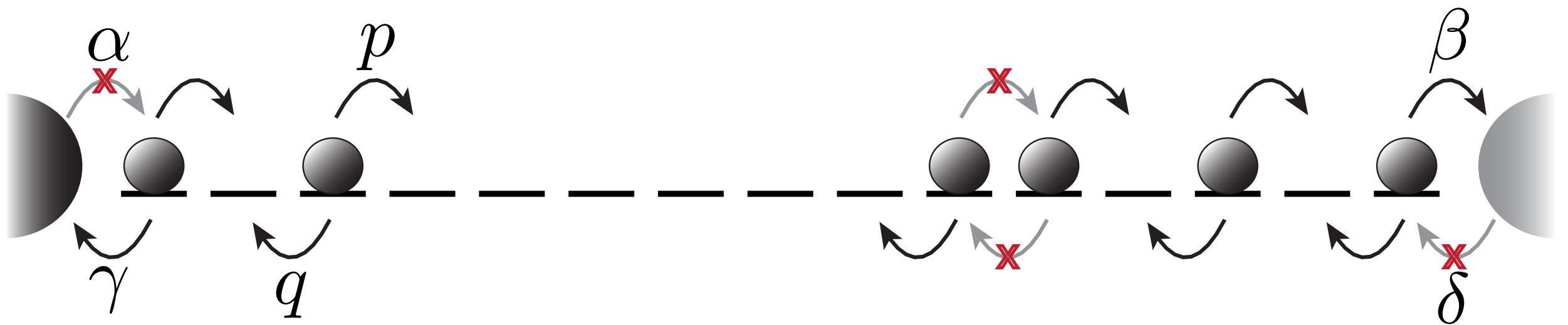
Equilibrium steady-state distribution supports a density gradient but no average particle current

ASEP as a motivating example

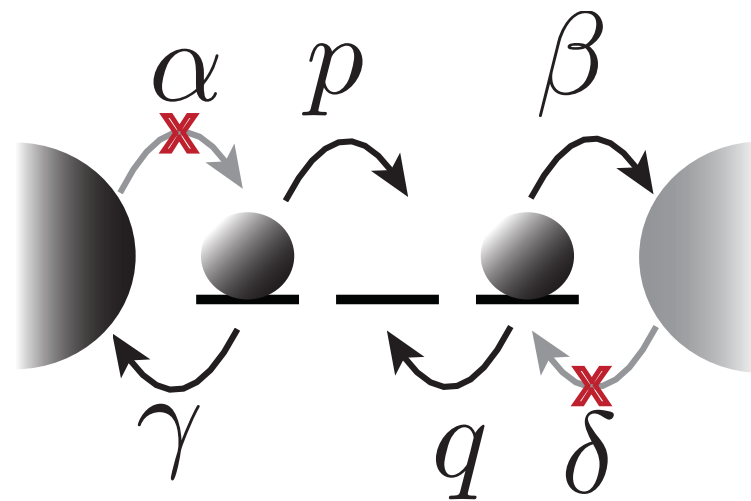


By coupling to multiple reservoirs, the nonequilibrium steady-state distribution can support currents

The exclusion process is an example of a Markov jump process

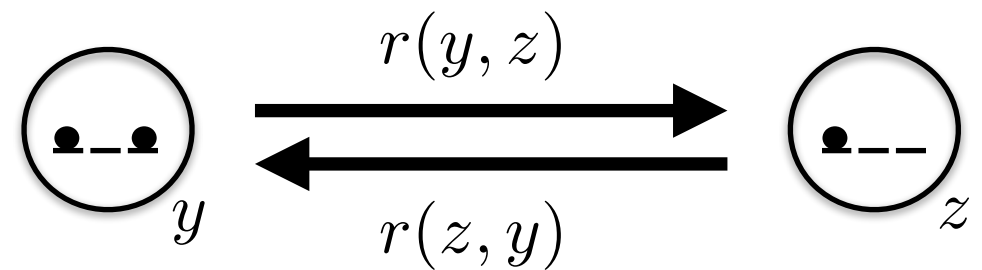
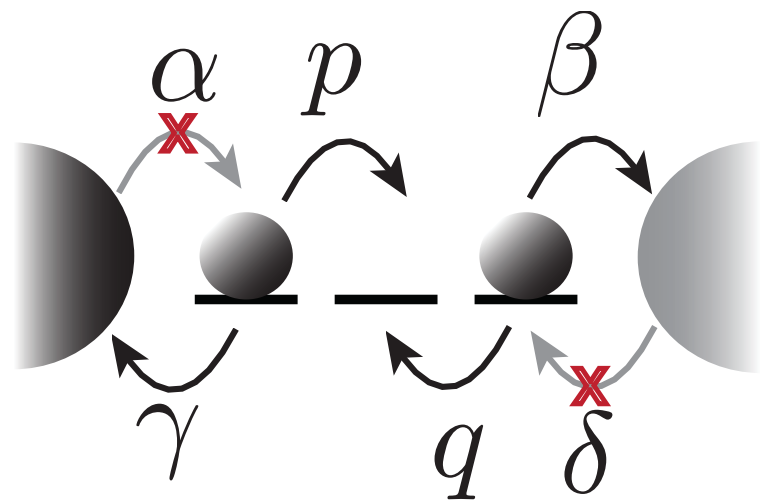


The exclusion process is an example of a Markov jump process

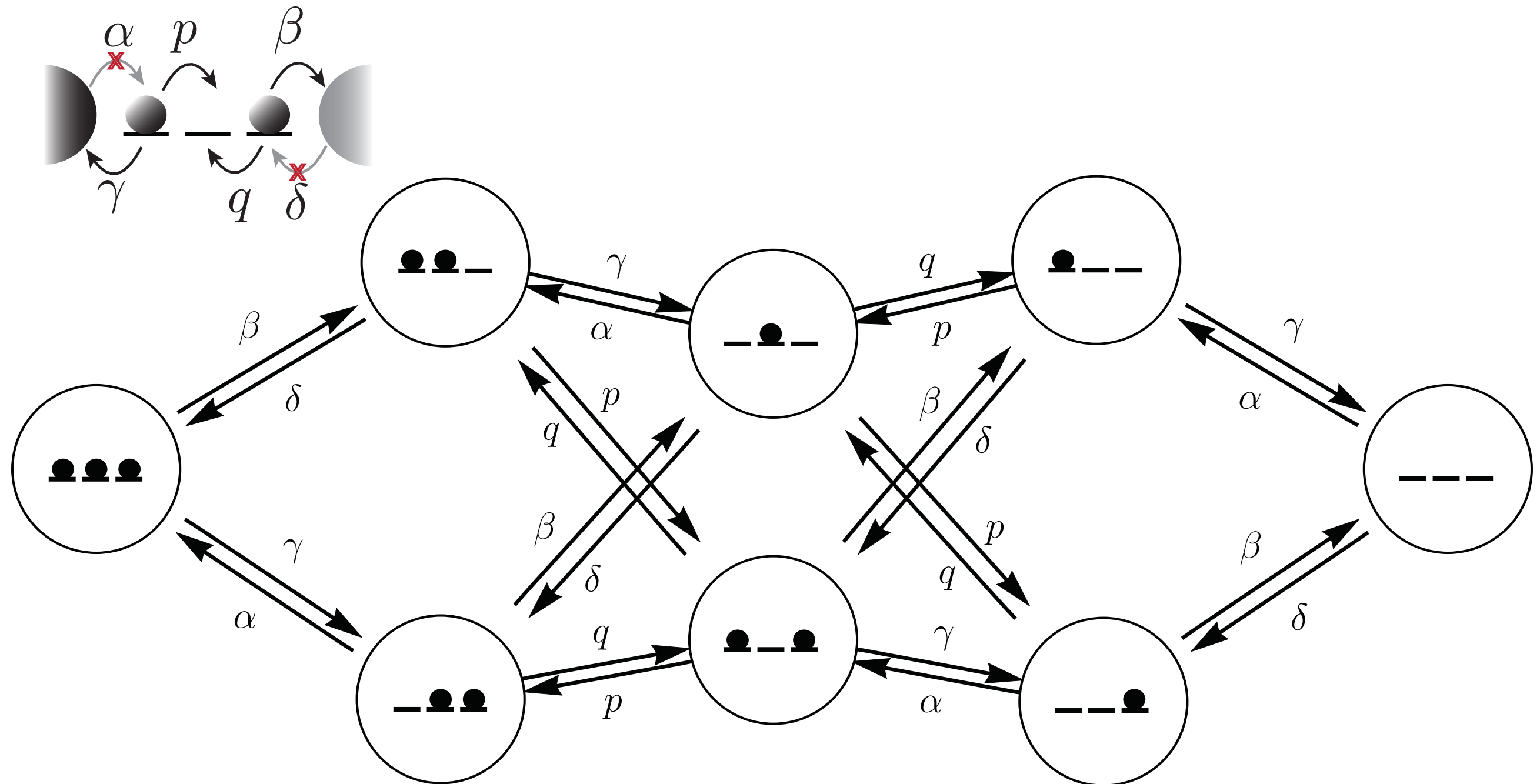


Three sites for simplicity

The exclusion process is an example of a Markov jump process

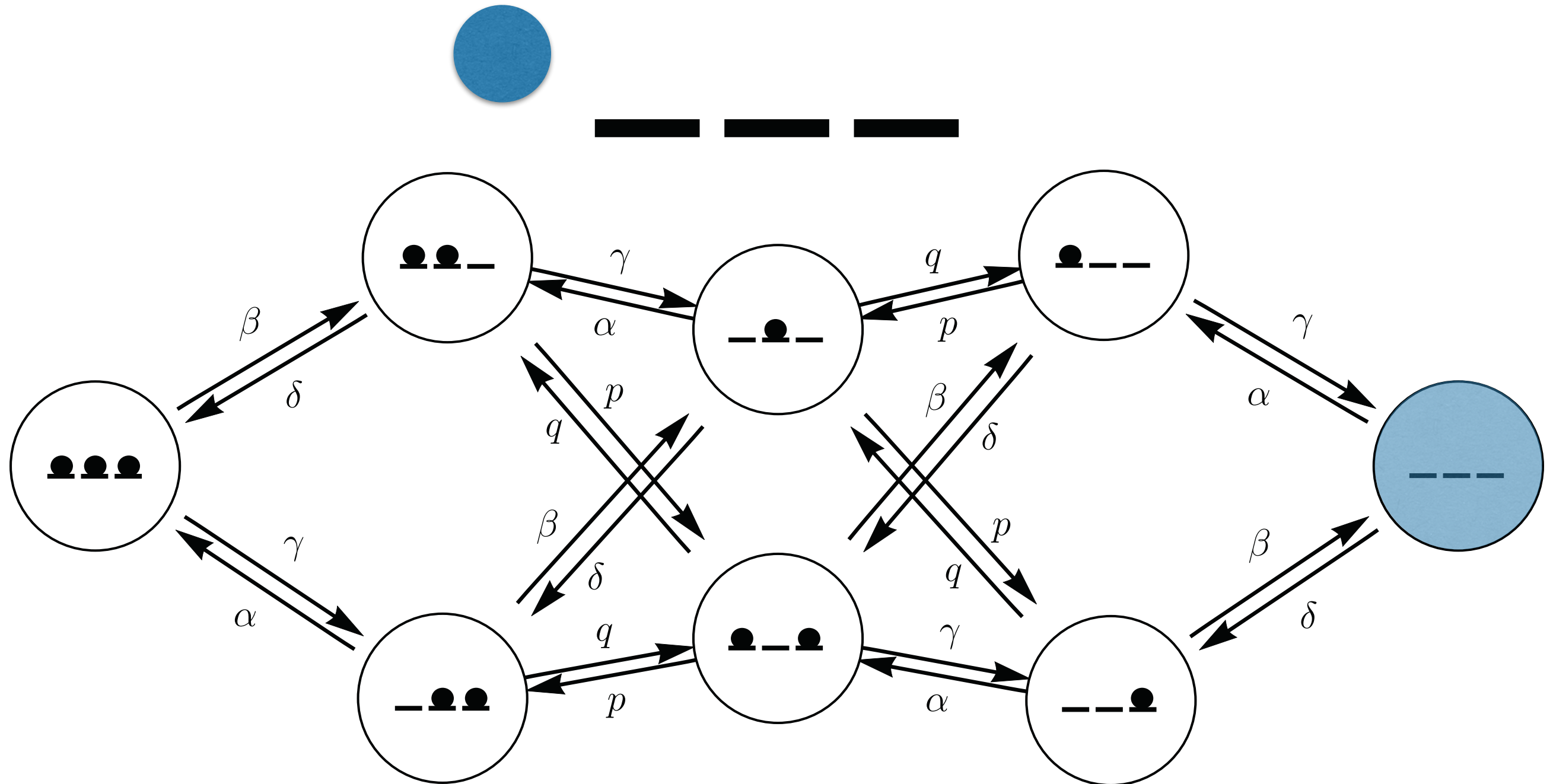


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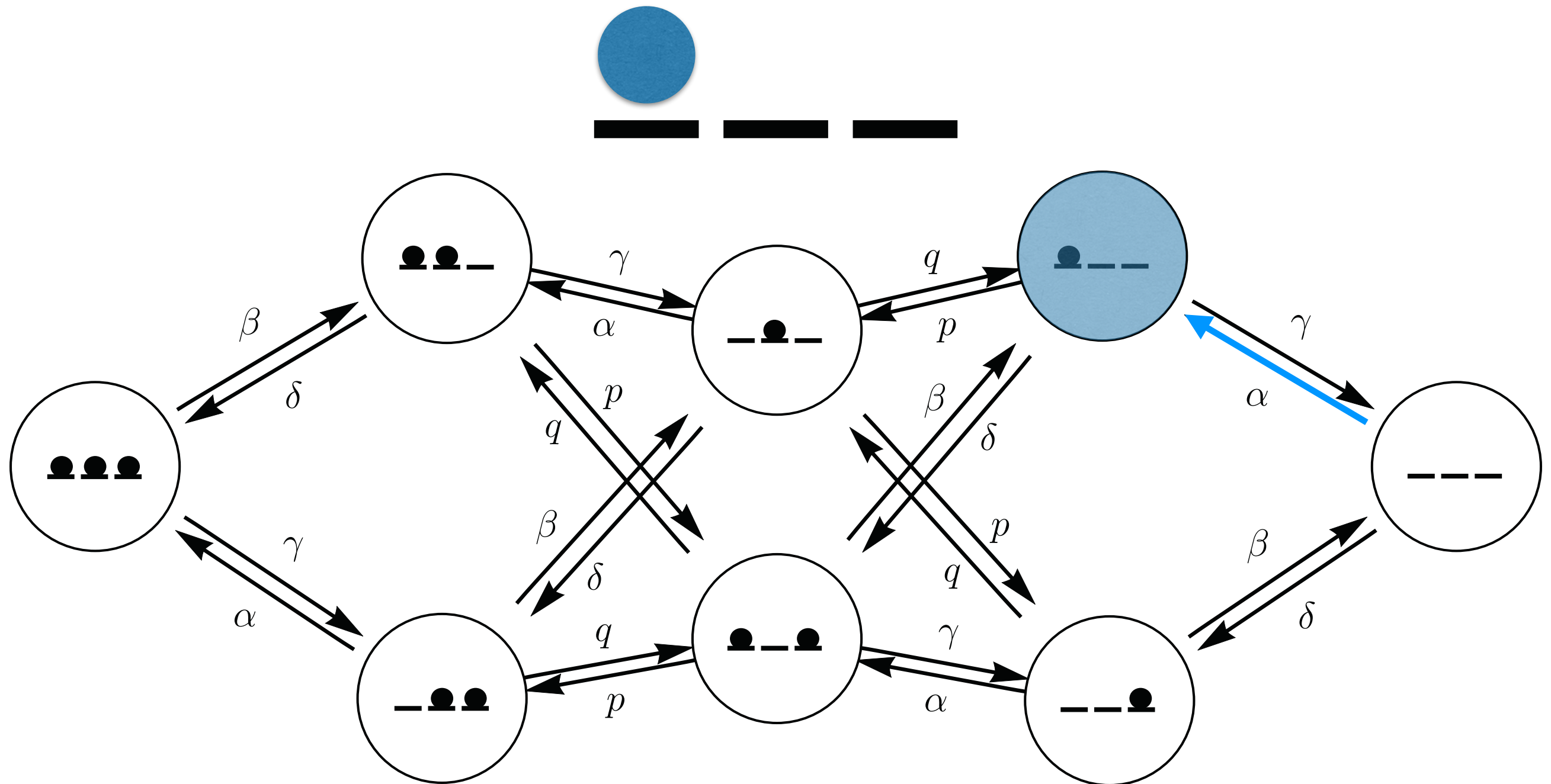
The reservoirs break detailed balance

Particle transported from left to right:



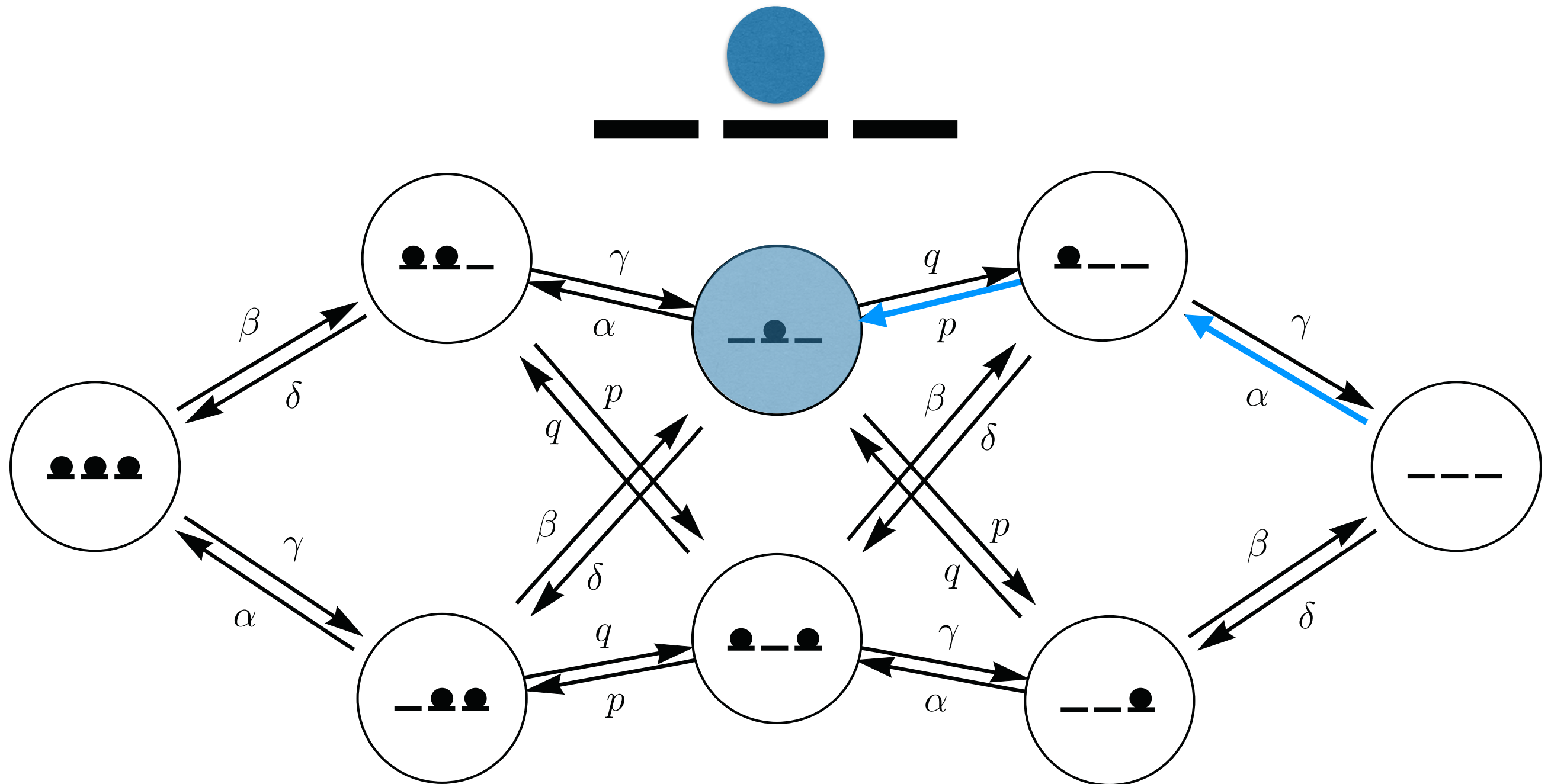
The reservoirs break detailed balance

Particle transported from left to right: α



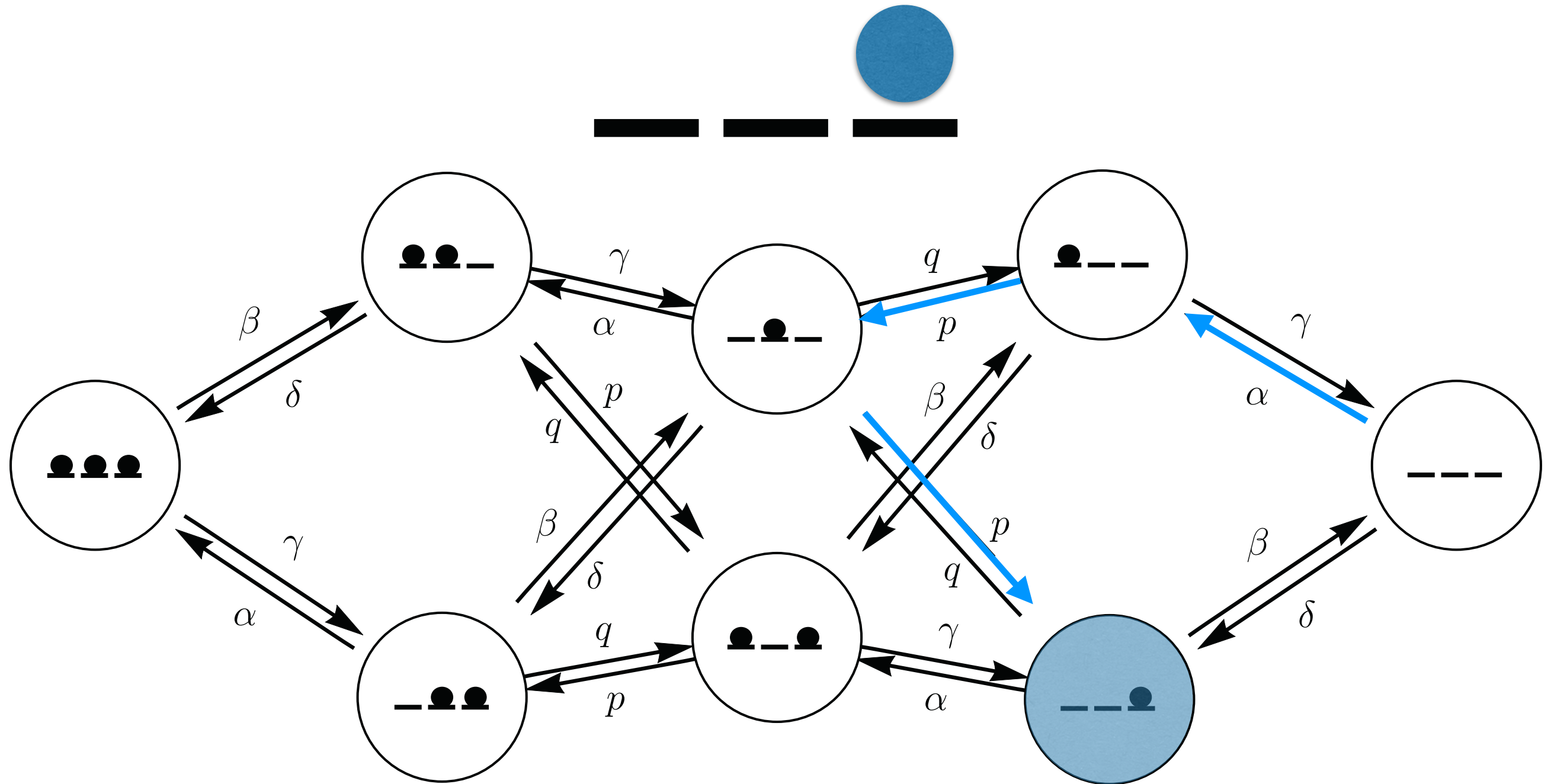
The reservoirs break detailed balance

Particle transported from left to right: α p



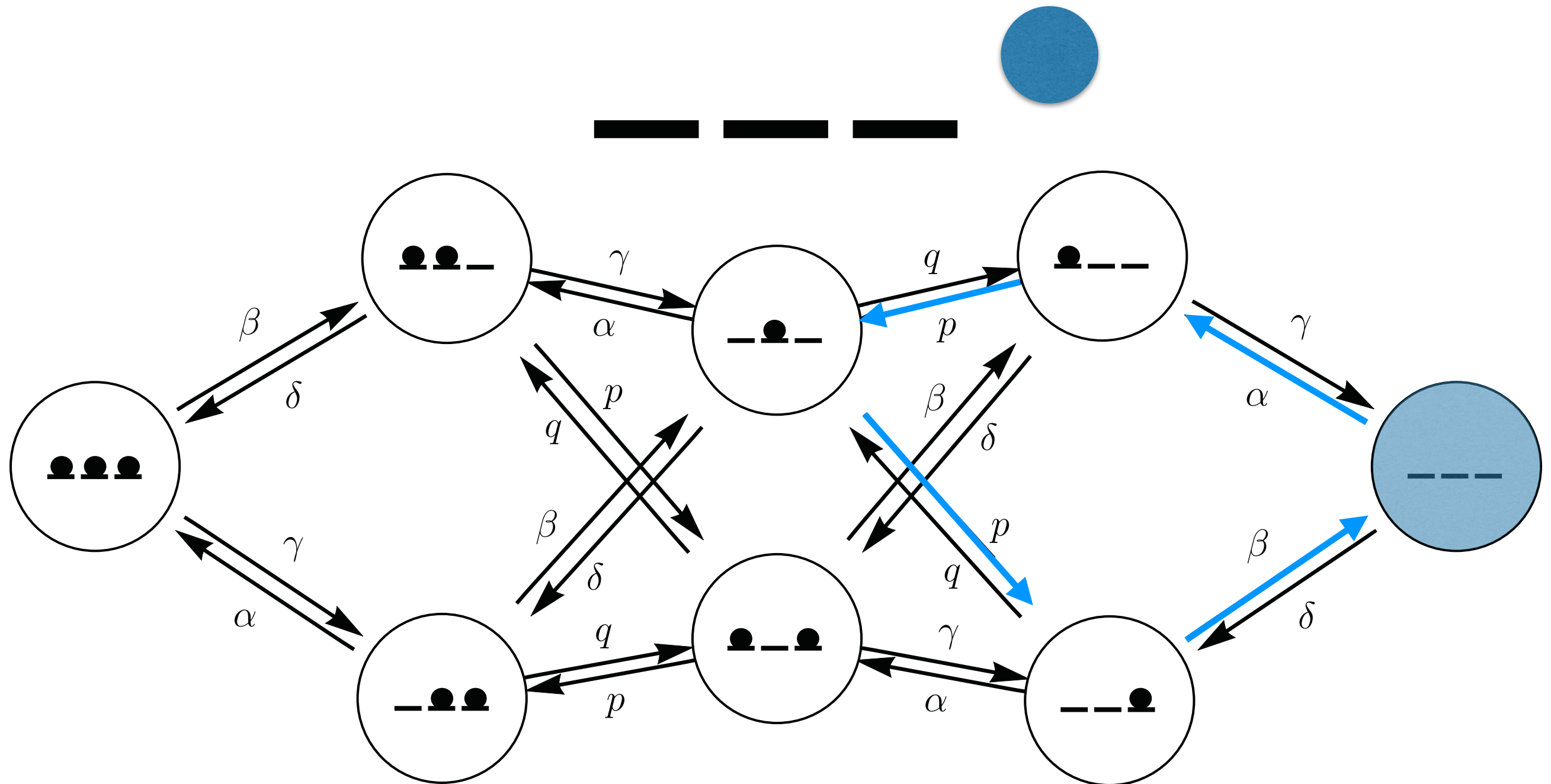
The reservoirs break detailed balance

Particle transported from left to right: α p p



The reservoirs break detailed balance

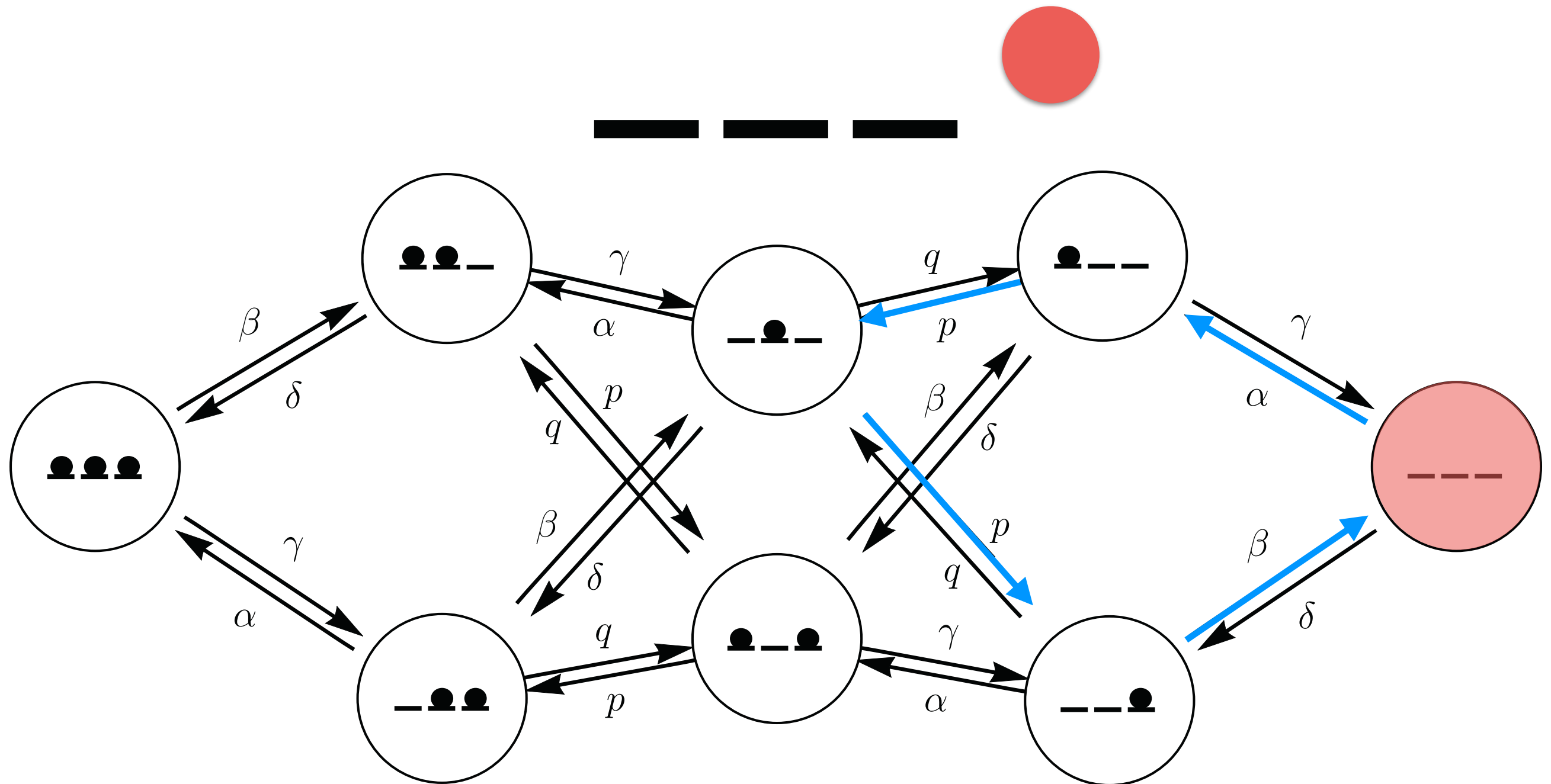
Particle transported from left to right: α p p β



The reservoirs break detailed balance

Particle transported from left to right: α p p β

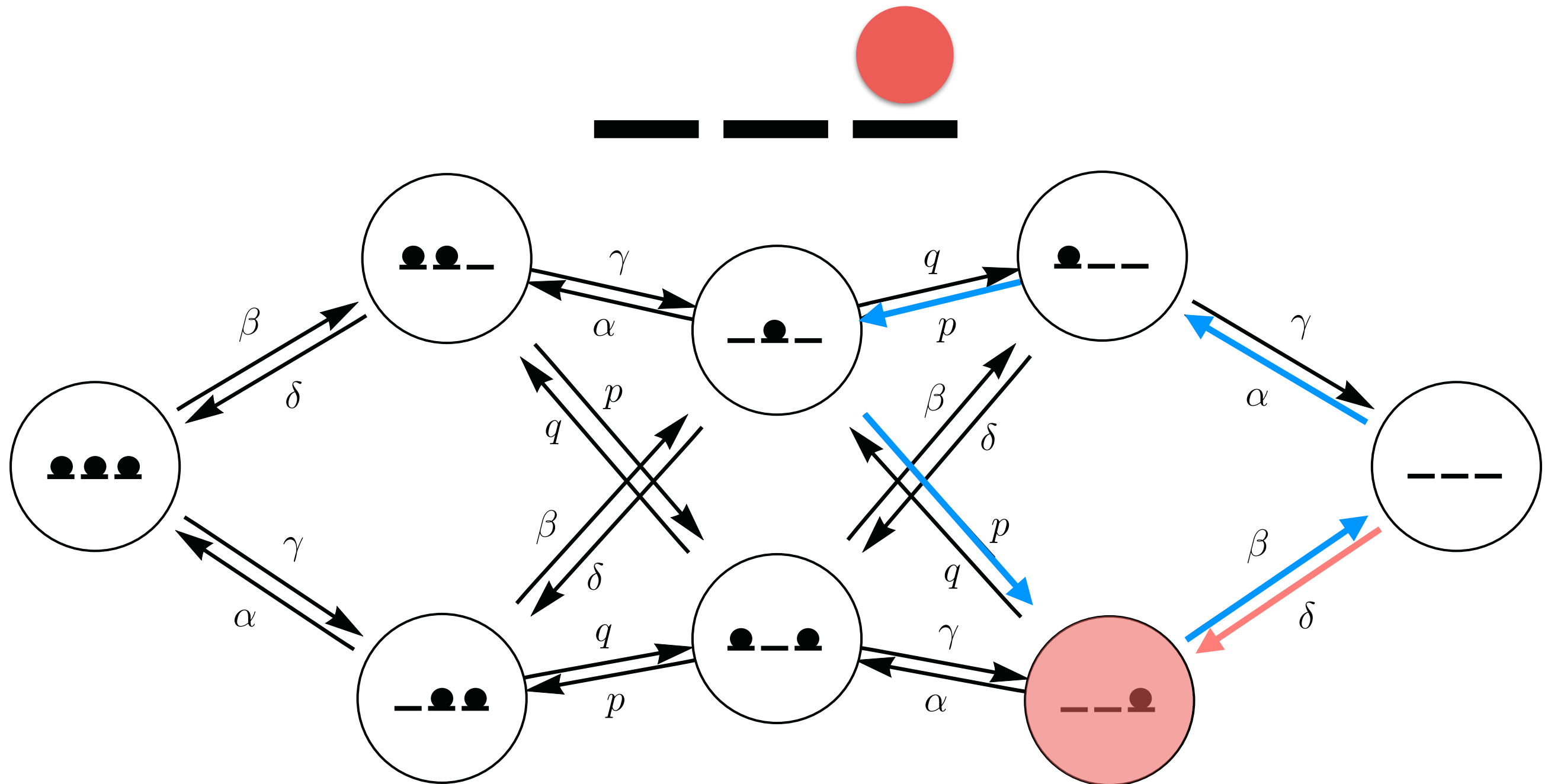
Particle transported from right to left:



The reservoirs break detailed balance

Particle transported from left to right: α p p β

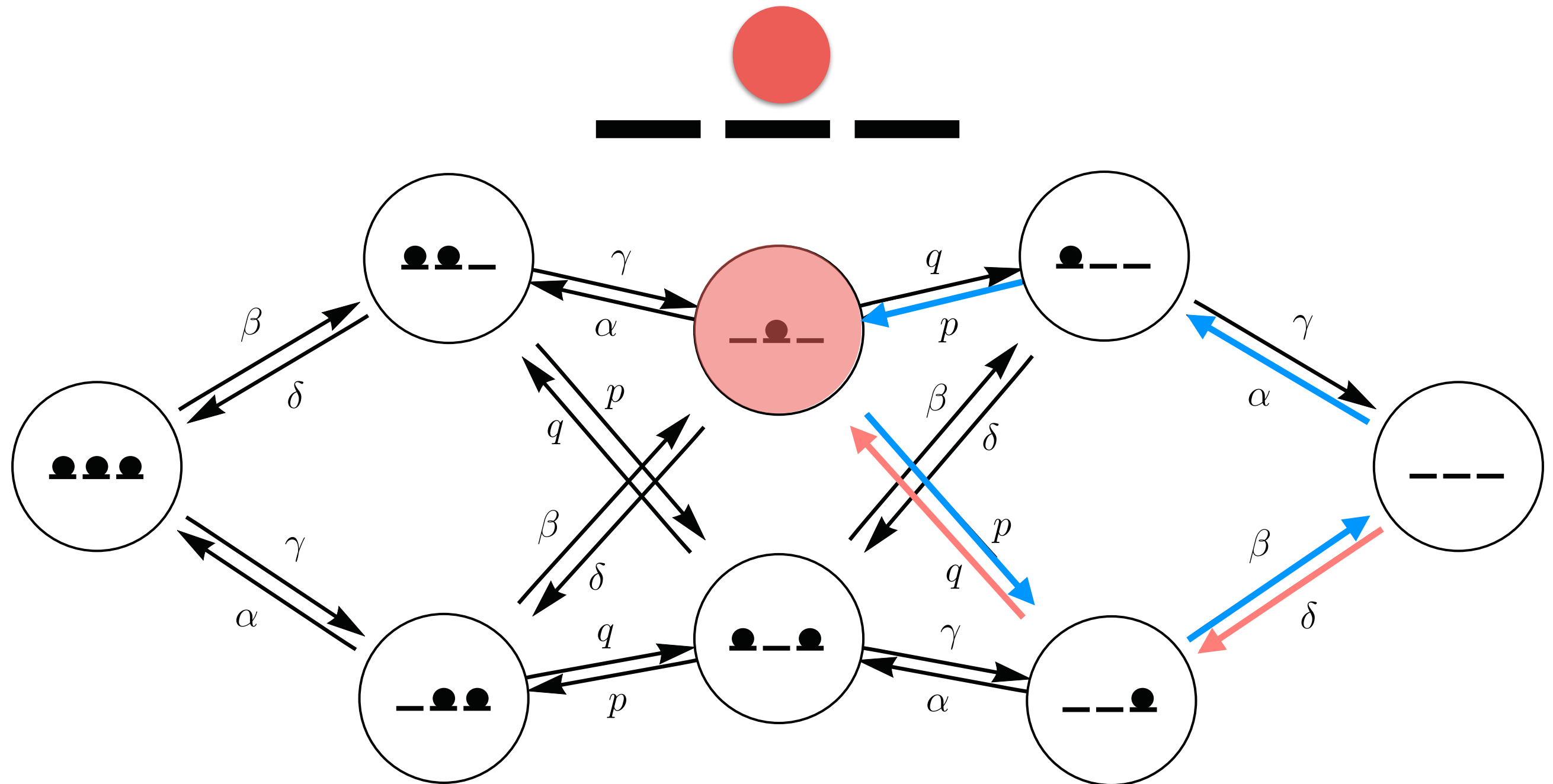
Particle transported from right to left: δ



The reservoirs break detailed balance

Particle transported from left to right: α p p β

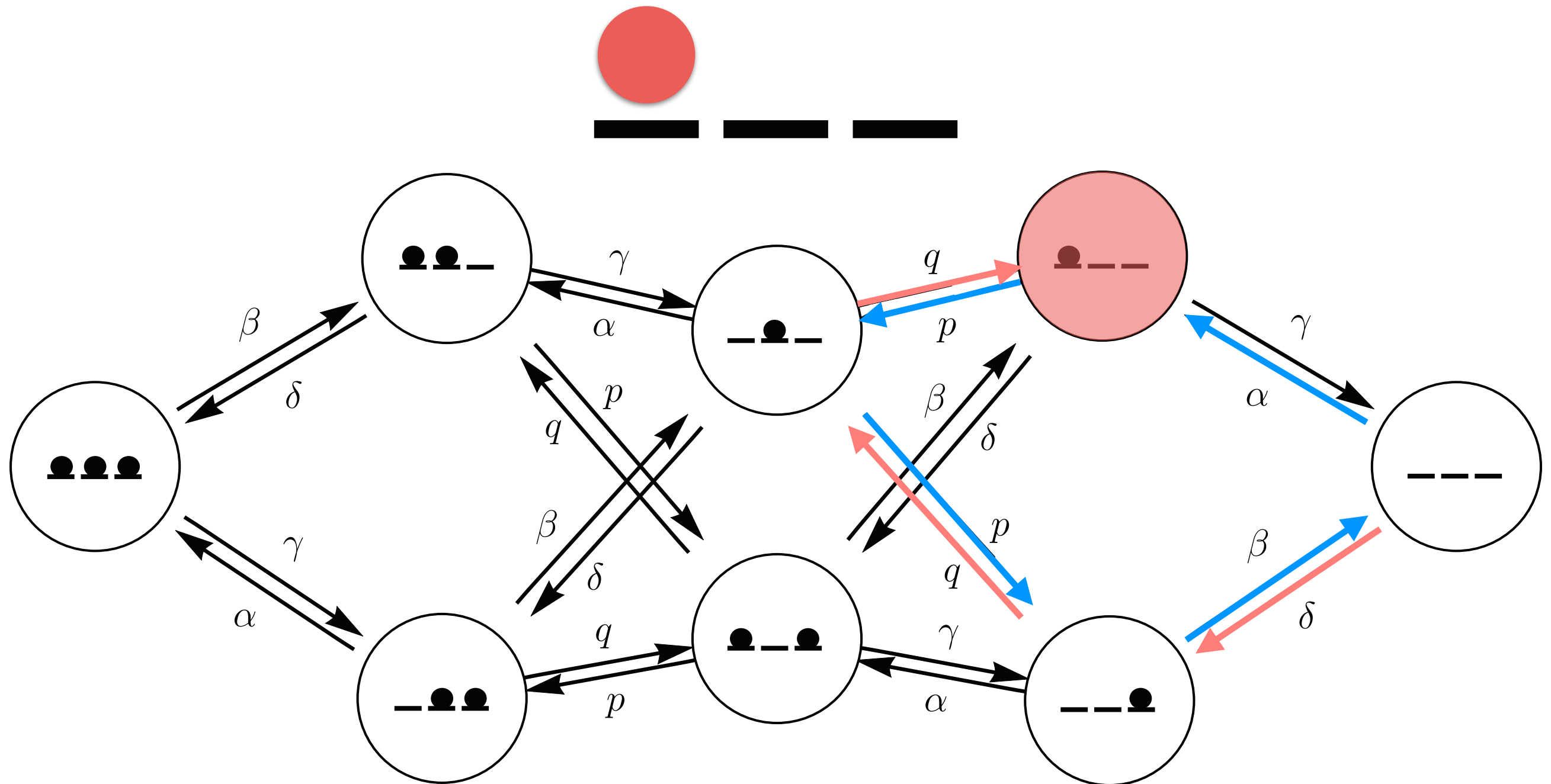
Particle transported from right to left: δ q



The reservoirs break detailed balance

Particle transported from left to right: α p p β

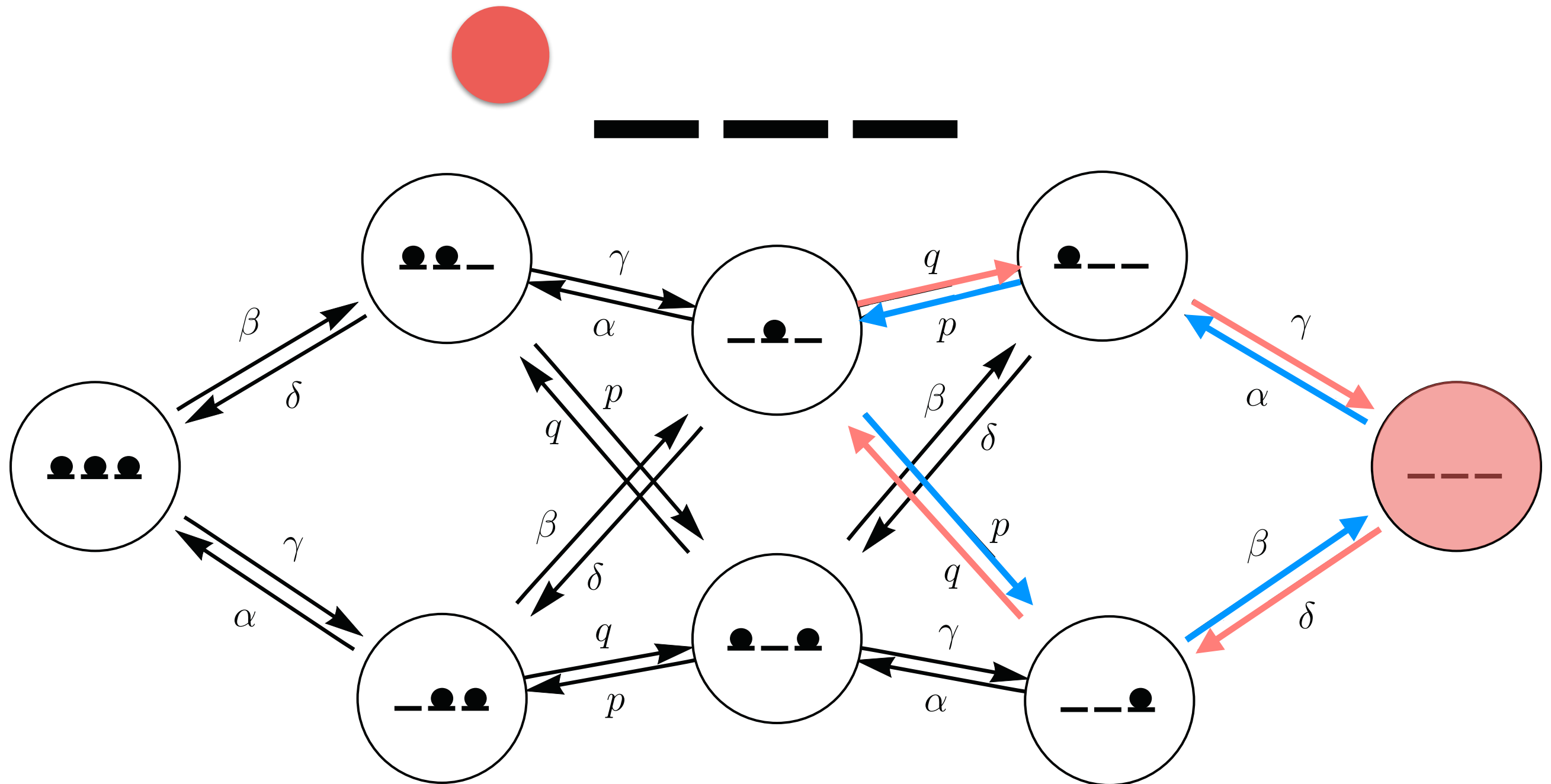
Particle transported from right to left: δ q q



The reservoirs break detailed balance

Particle transported from left to right: α p p β

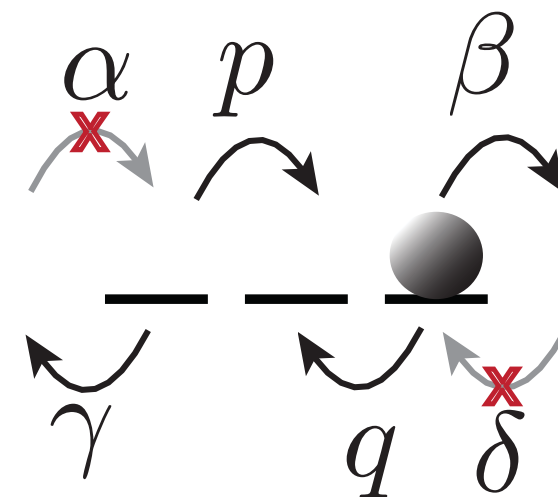
Particle transported from right to left: δ q q γ



Kinetics of the cycles reports on the thermodynamic cost paid by the reservoirs

Thermodynamic
cost (reservoirs)

Cycle kinetics
(system)

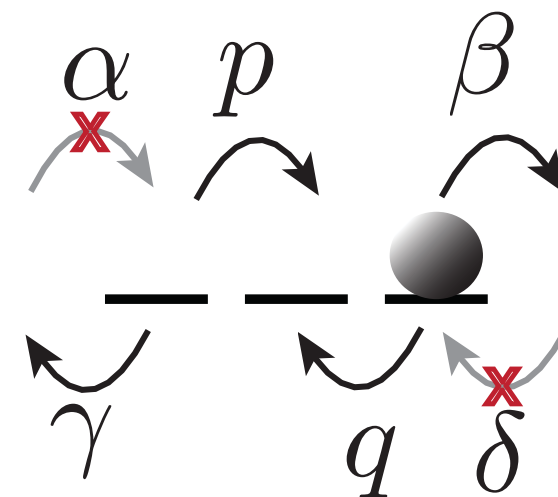


$$\frac{\Delta\mu}{k_B T} = \ln \frac{P_{\text{counterclockwise}}}{P_{\text{clockwise}}} = \ln \frac{\alpha p^2 \beta}{\delta q^2 \gamma}$$

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Cost for one particle

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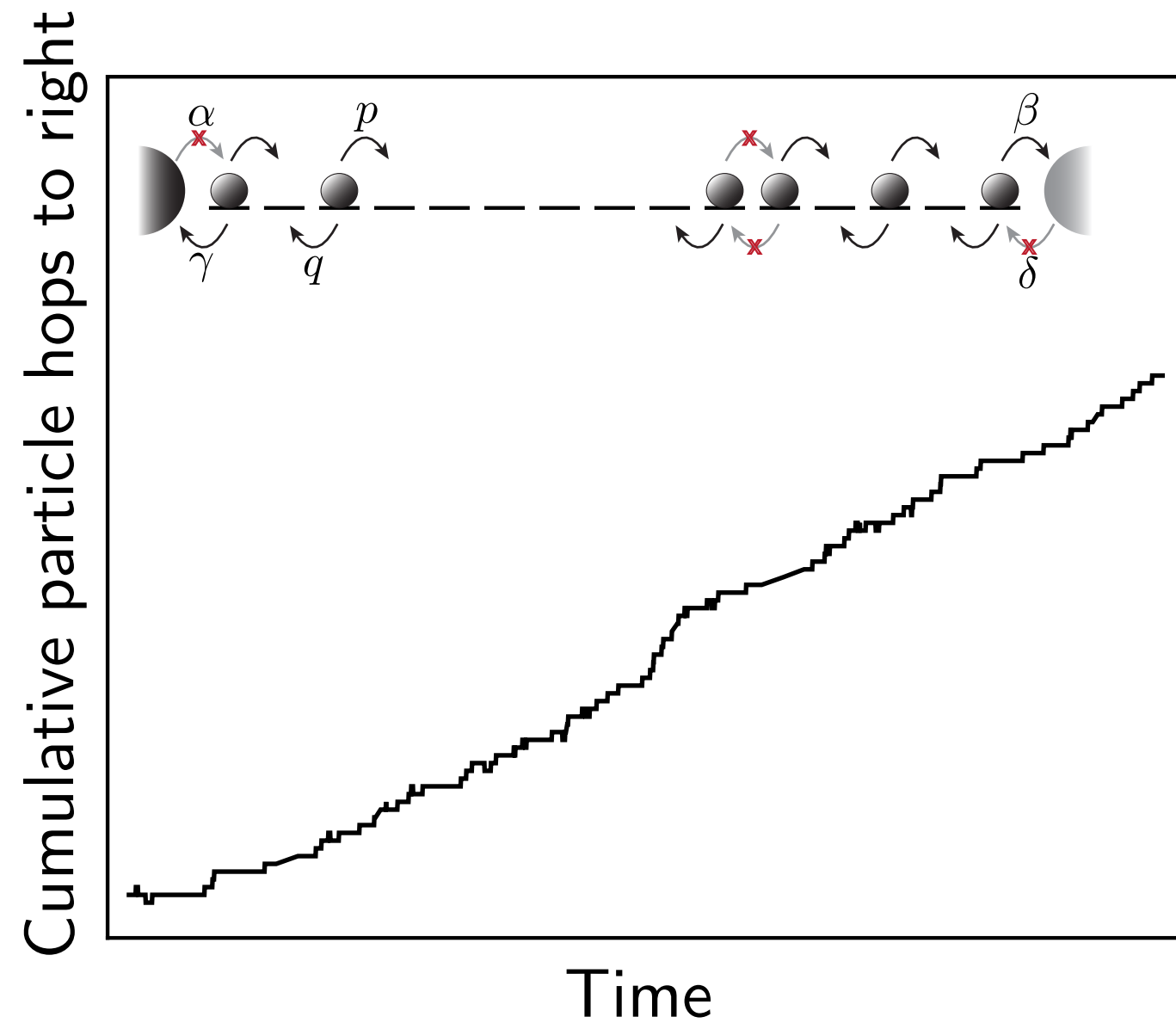
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Cost for one particle

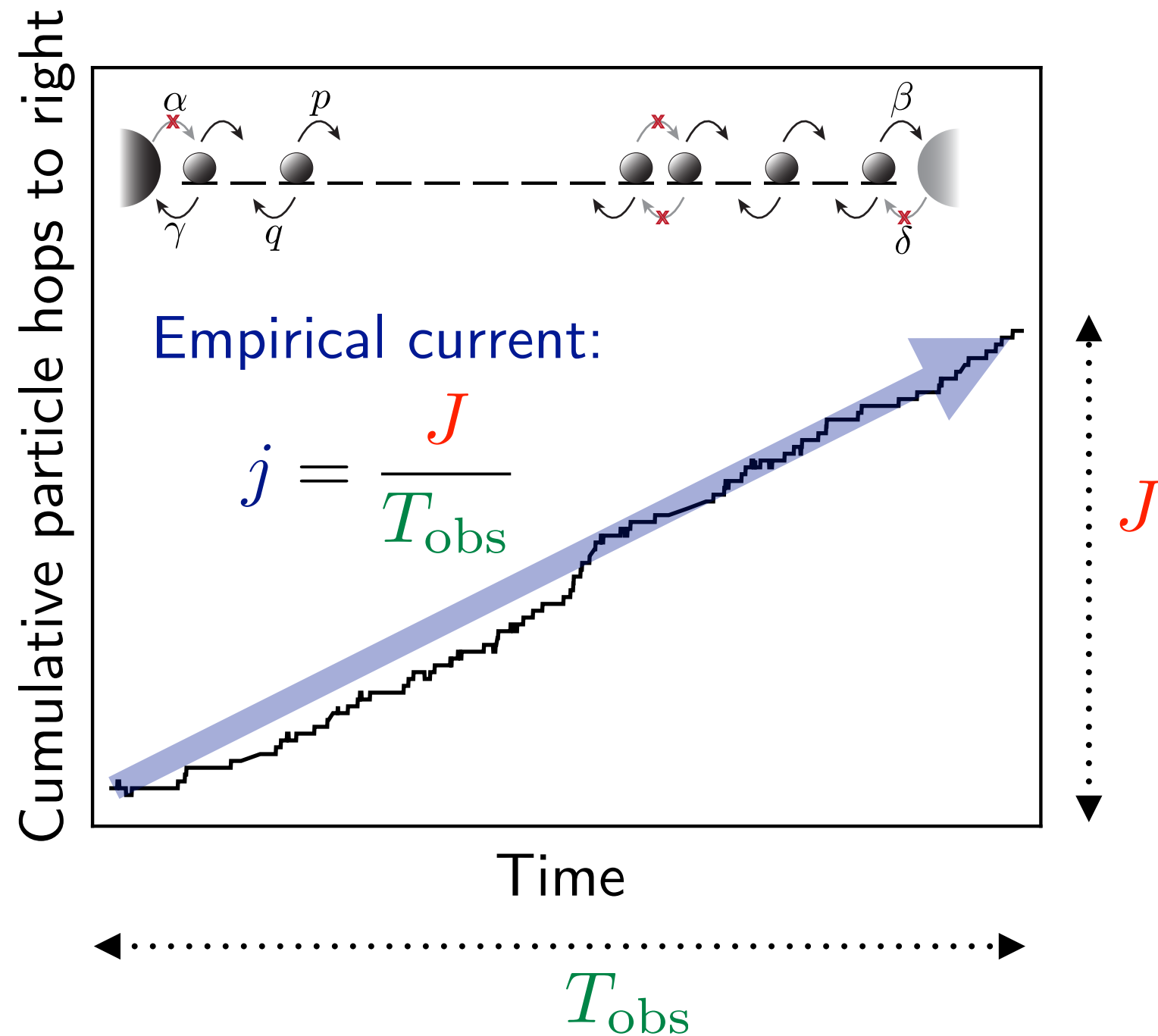
$$\text{Steady-state Dissipation Rate} = \text{Thermodynamic force (cost per particle)} \times \text{Flux (particle current)}$$

$$\langle \Sigma \rangle = \ln \frac{\alpha p^2 \beta}{\delta q^2 \gamma} \times \langle j \rangle$$

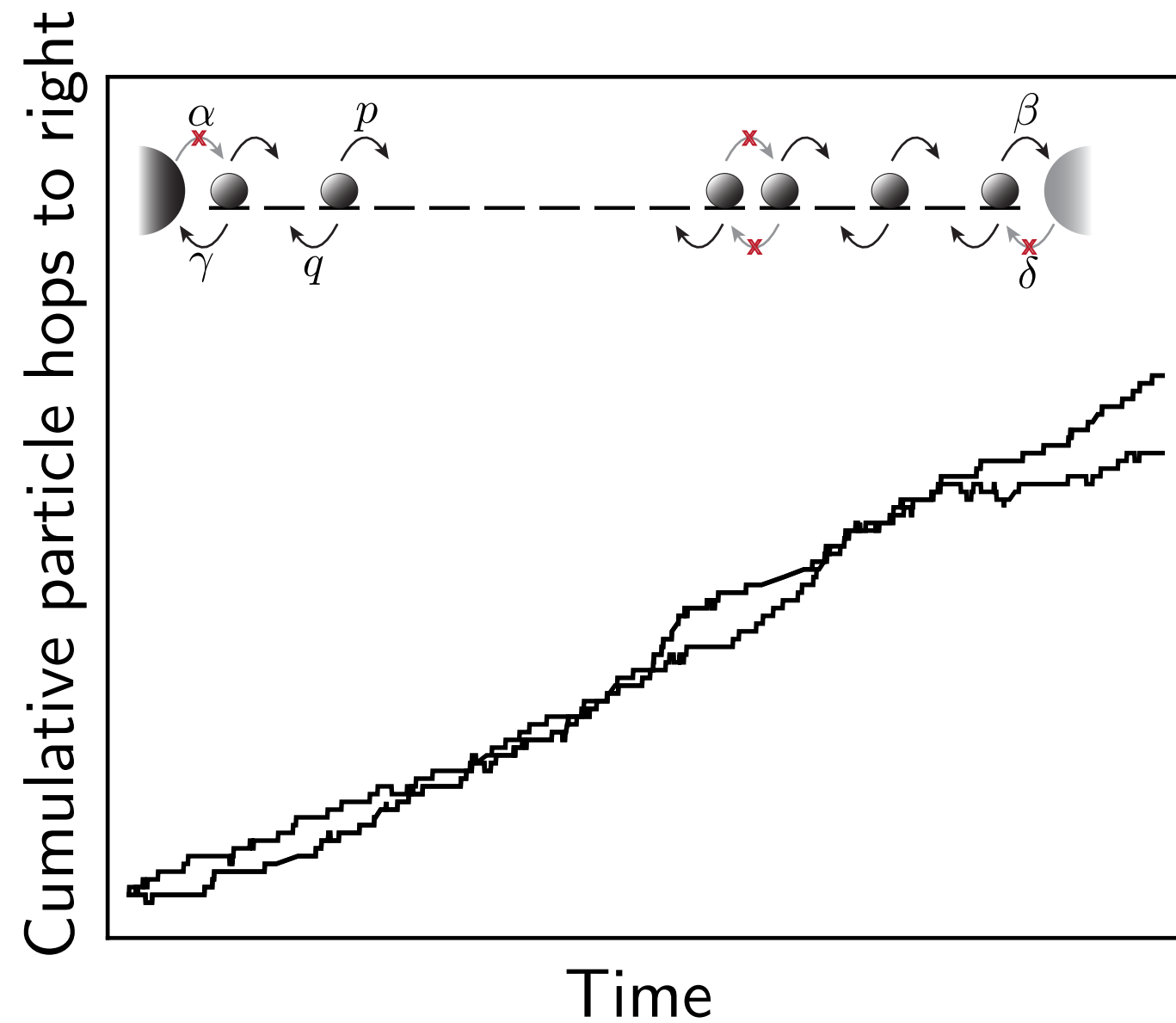
The empirical current fluctuates



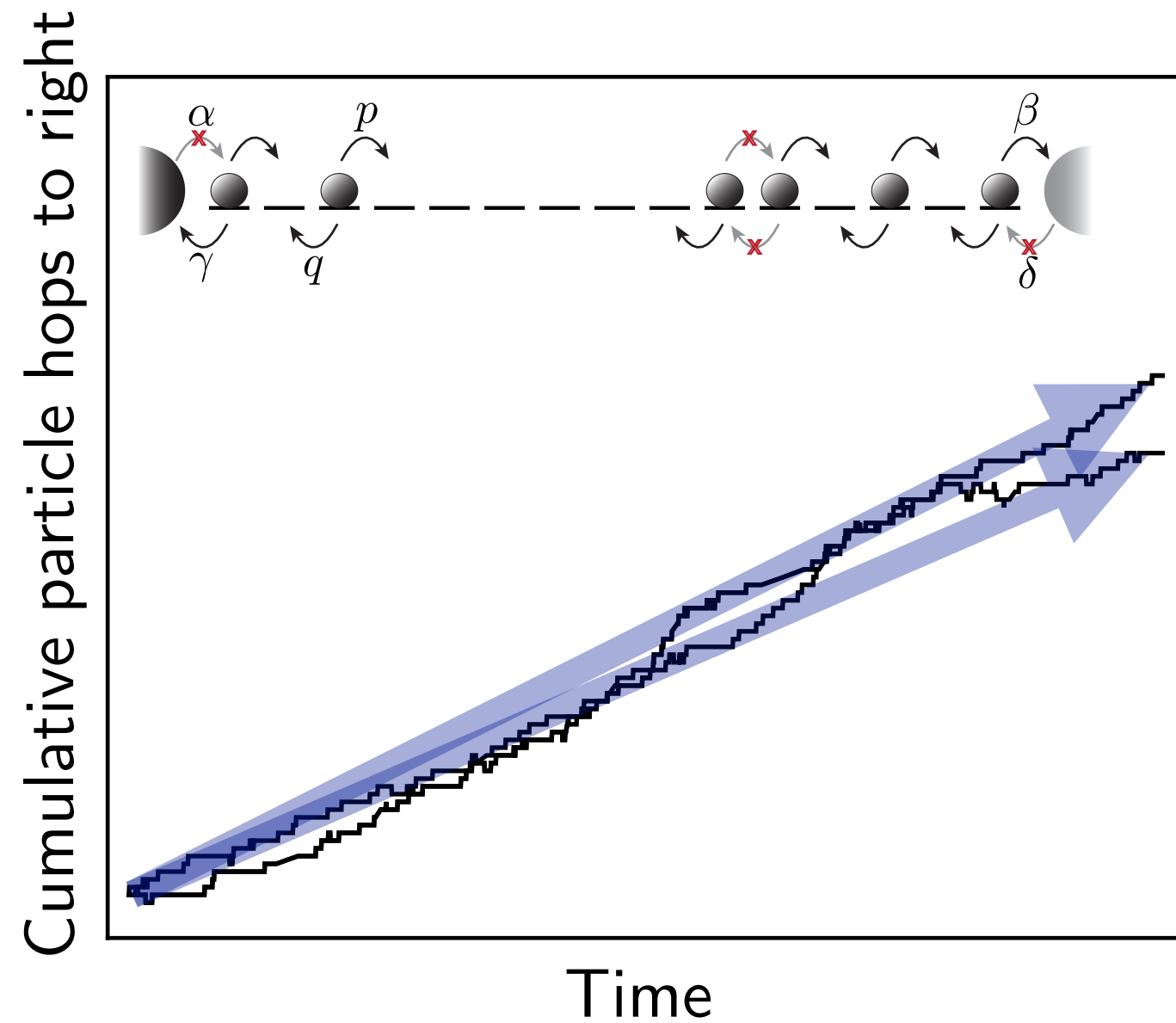
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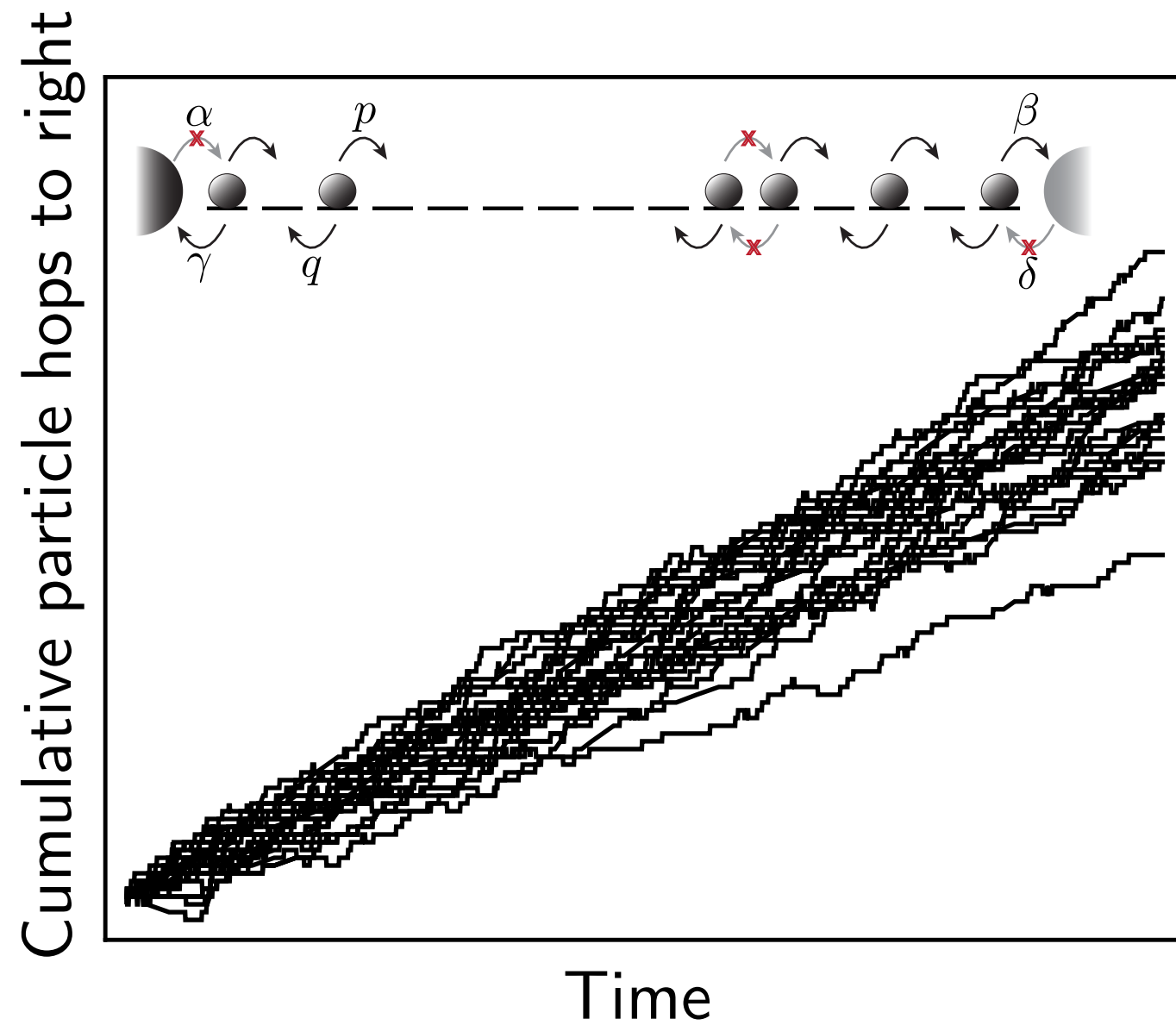
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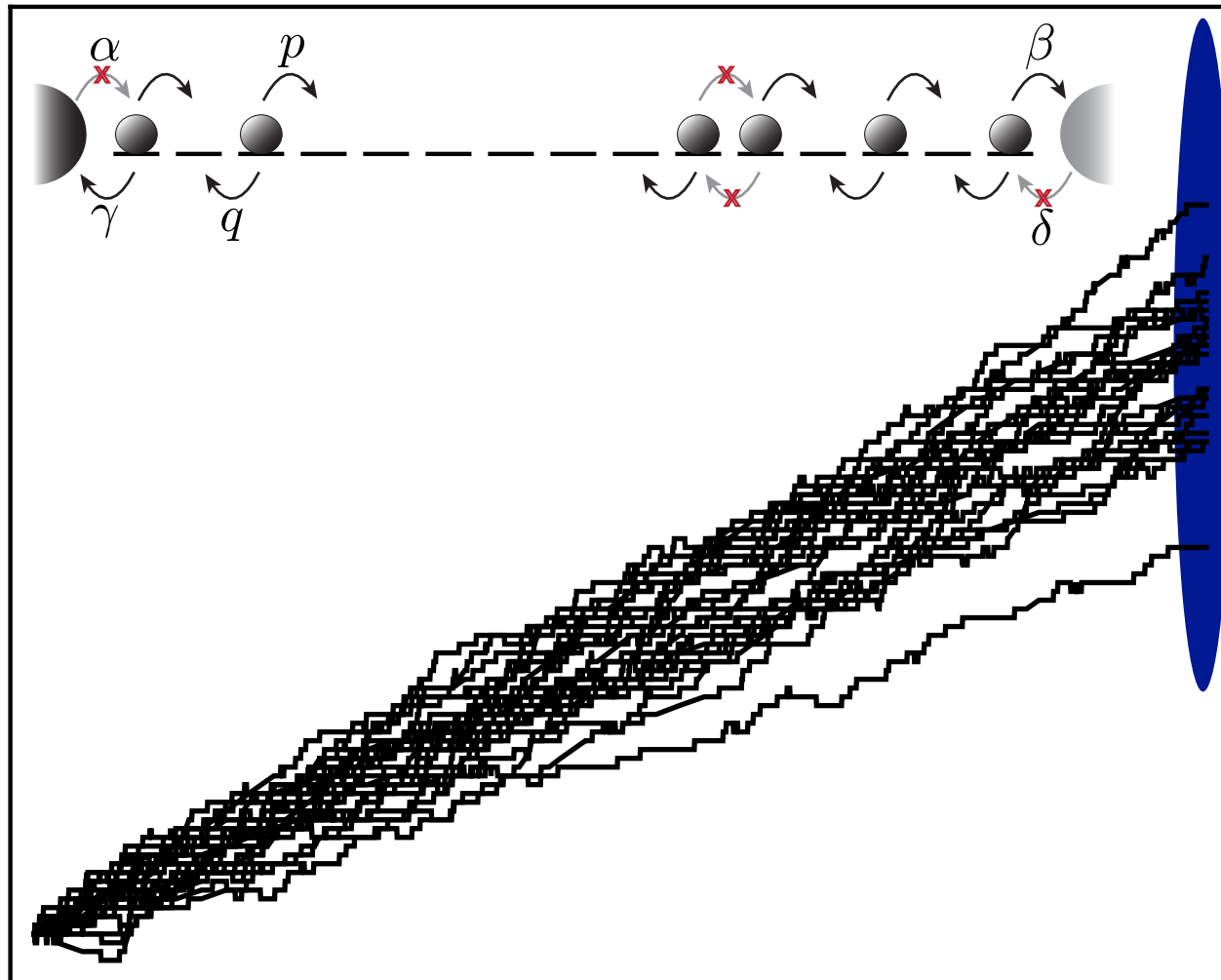


The empirical current fluctuates



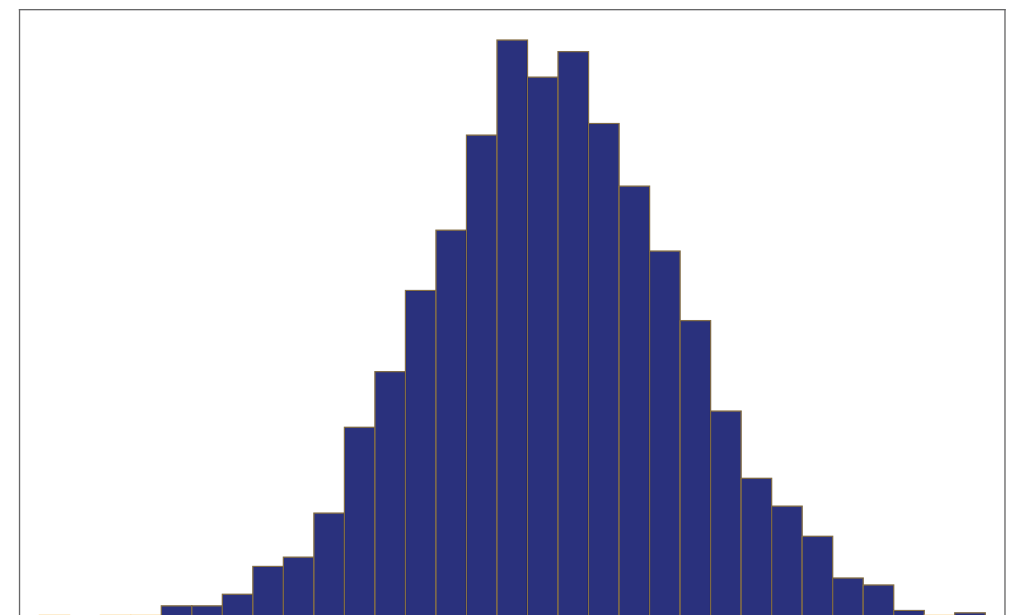
The empirical current fluctuates

Cumulative particle hops to right



Time

Probability

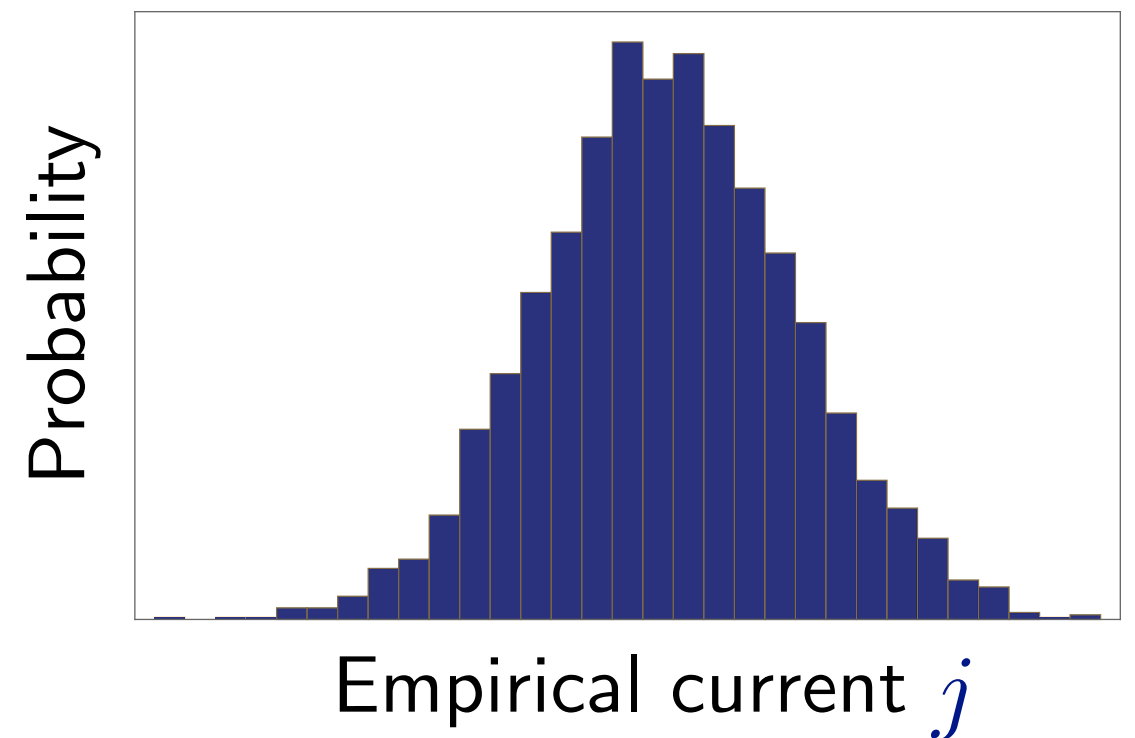


Empirical current j

Under certain conditions, the current distribution obeys an *uncertainty principle*

$$\frac{\text{Variance}}{\text{Mean}^2} \geq \frac{2}{\text{Dissipation}}$$

$$\frac{\langle (J - \langle J \rangle)^2 \rangle}{\langle J \rangle^2} \geq \frac{2}{\langle \Sigma \rangle T_{\text{obs}}}$$

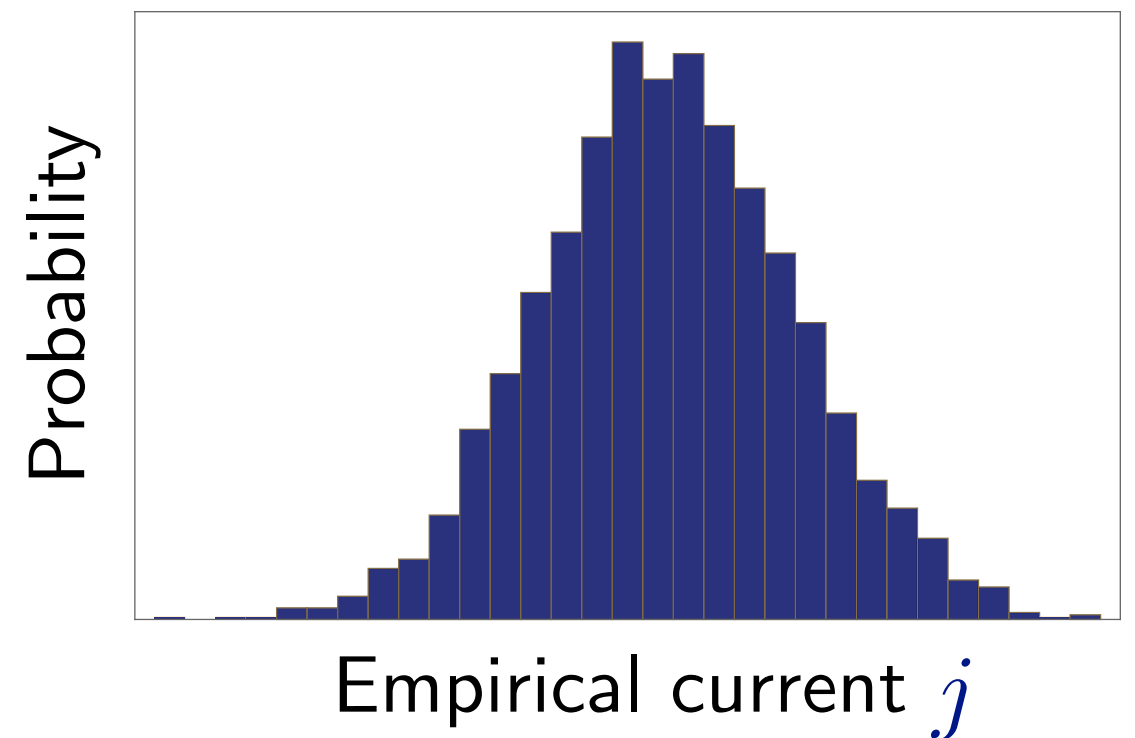


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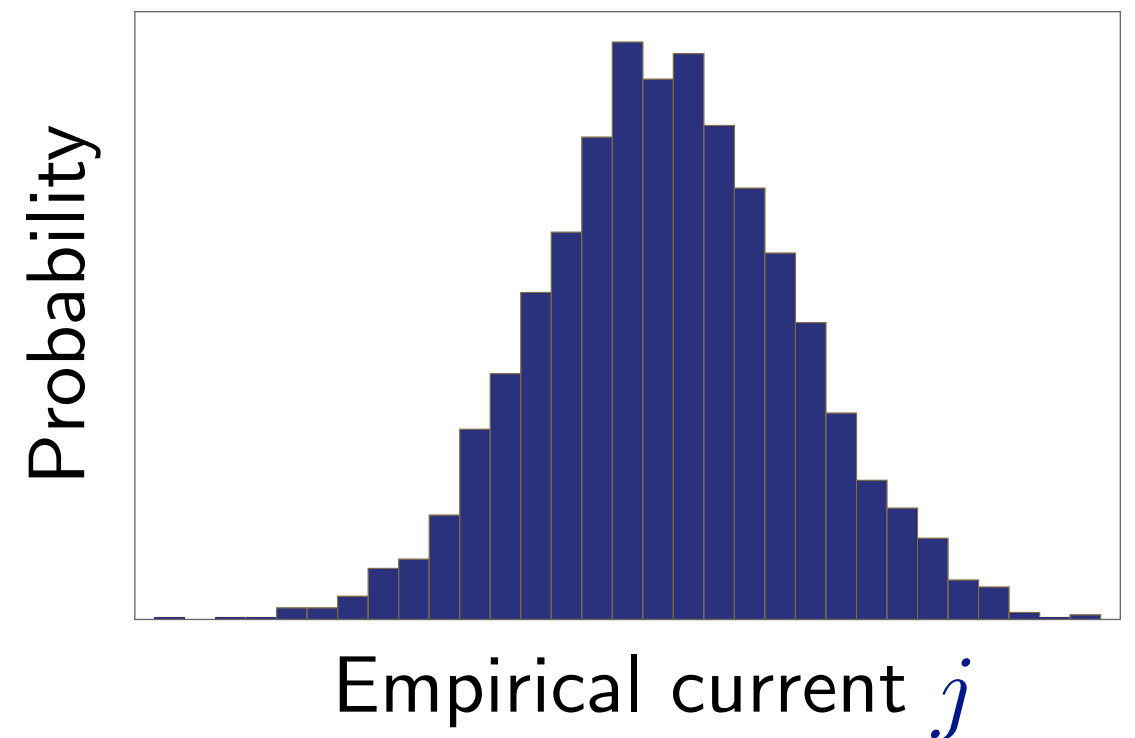
Cost borne by reservoirs, e.g., ATP or proton baths



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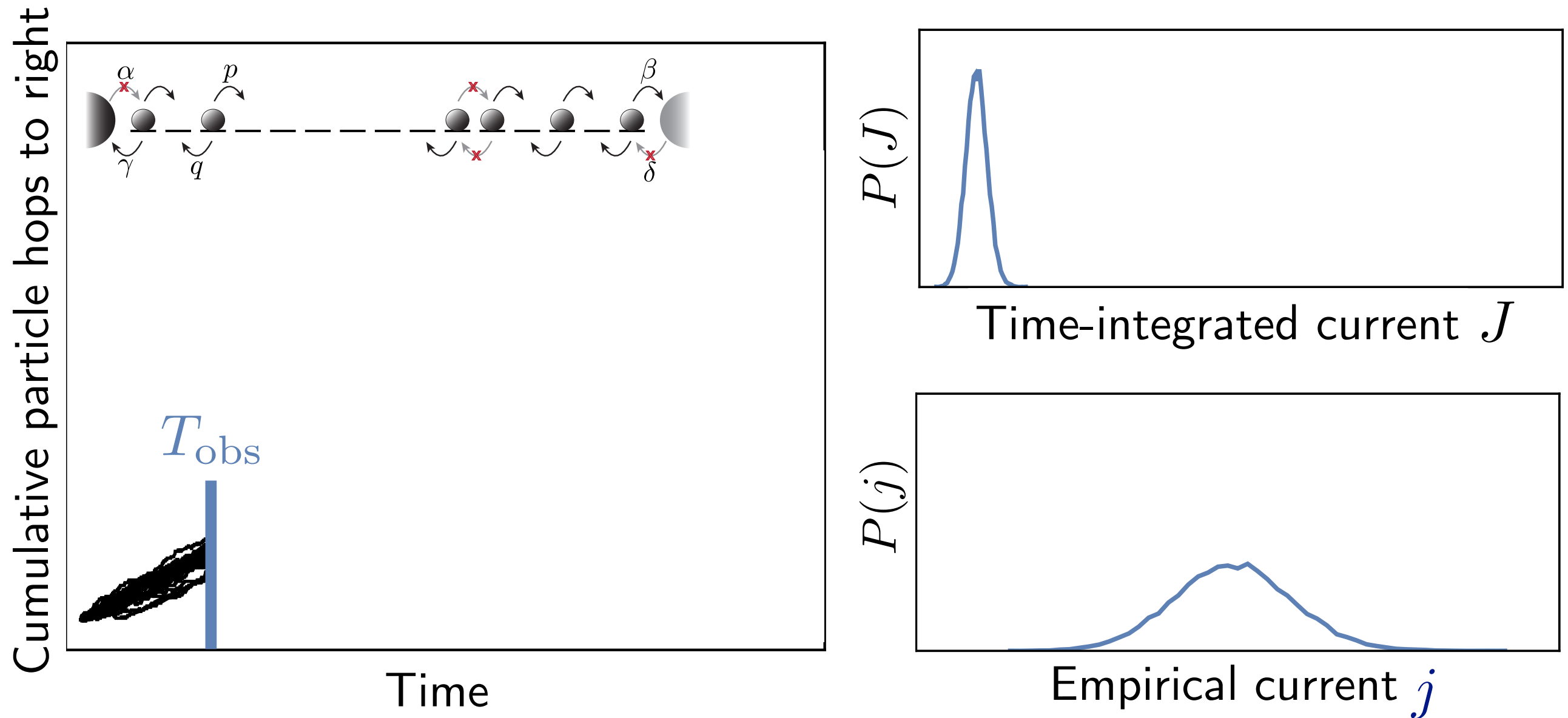
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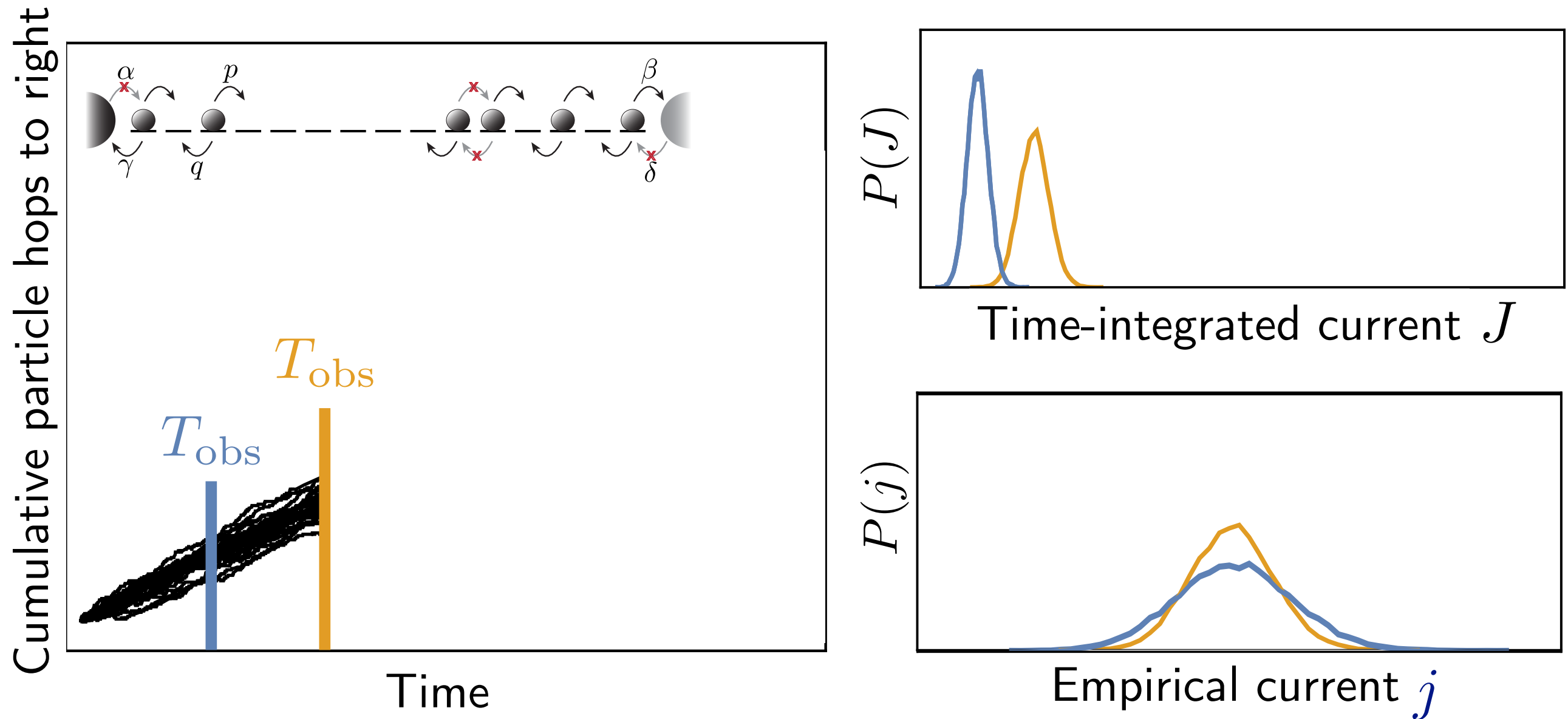


Reliable currents require more dissipation!

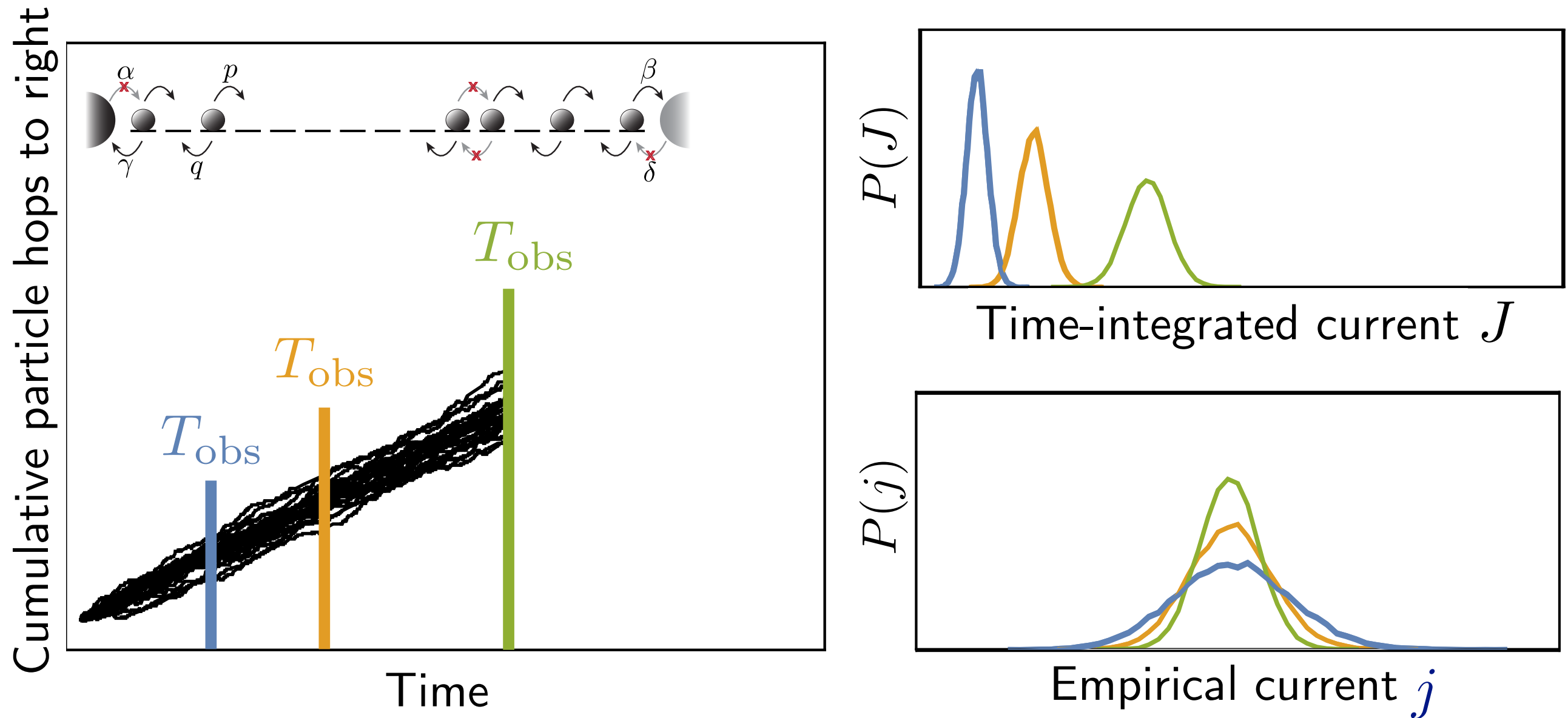
At long (but finite) times, current fluctuations are described using *large deviation theory*



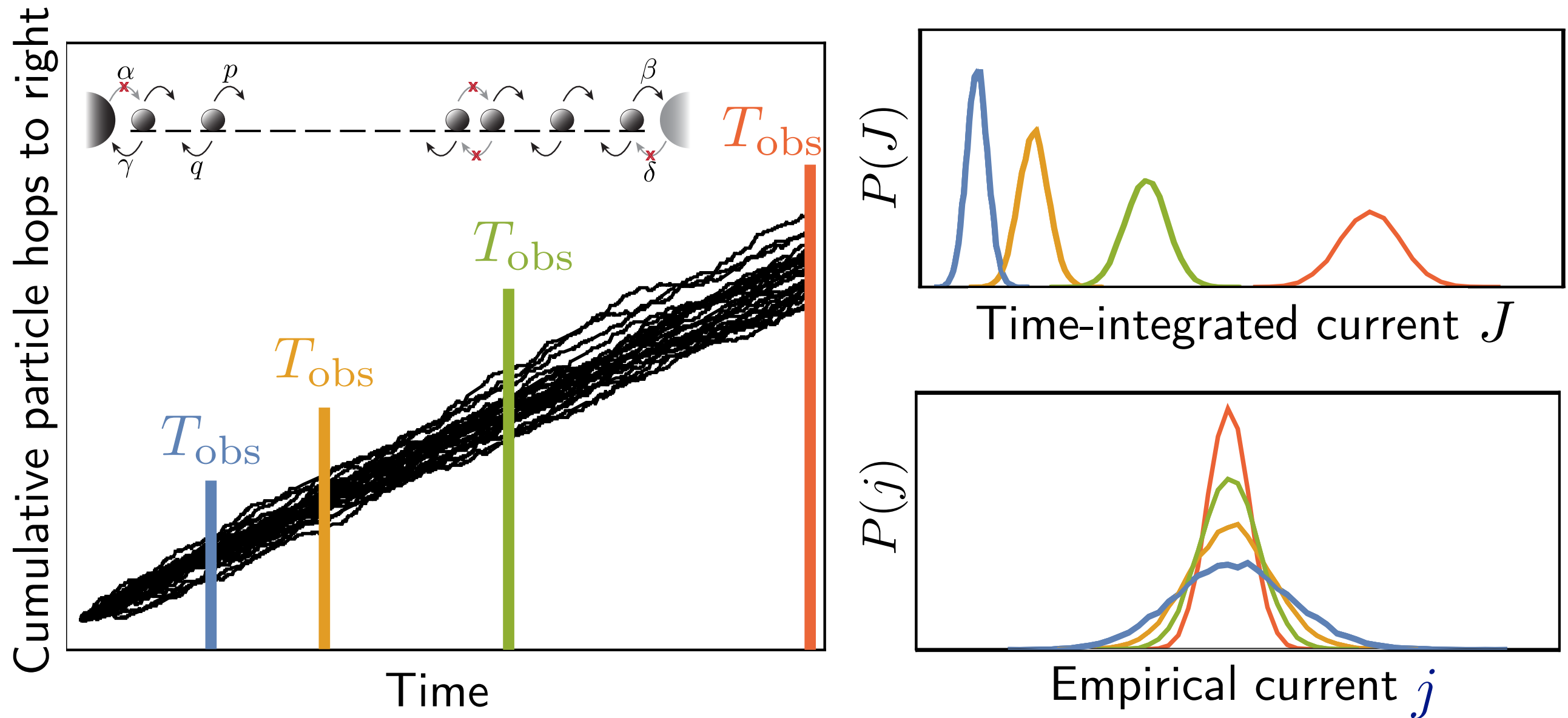
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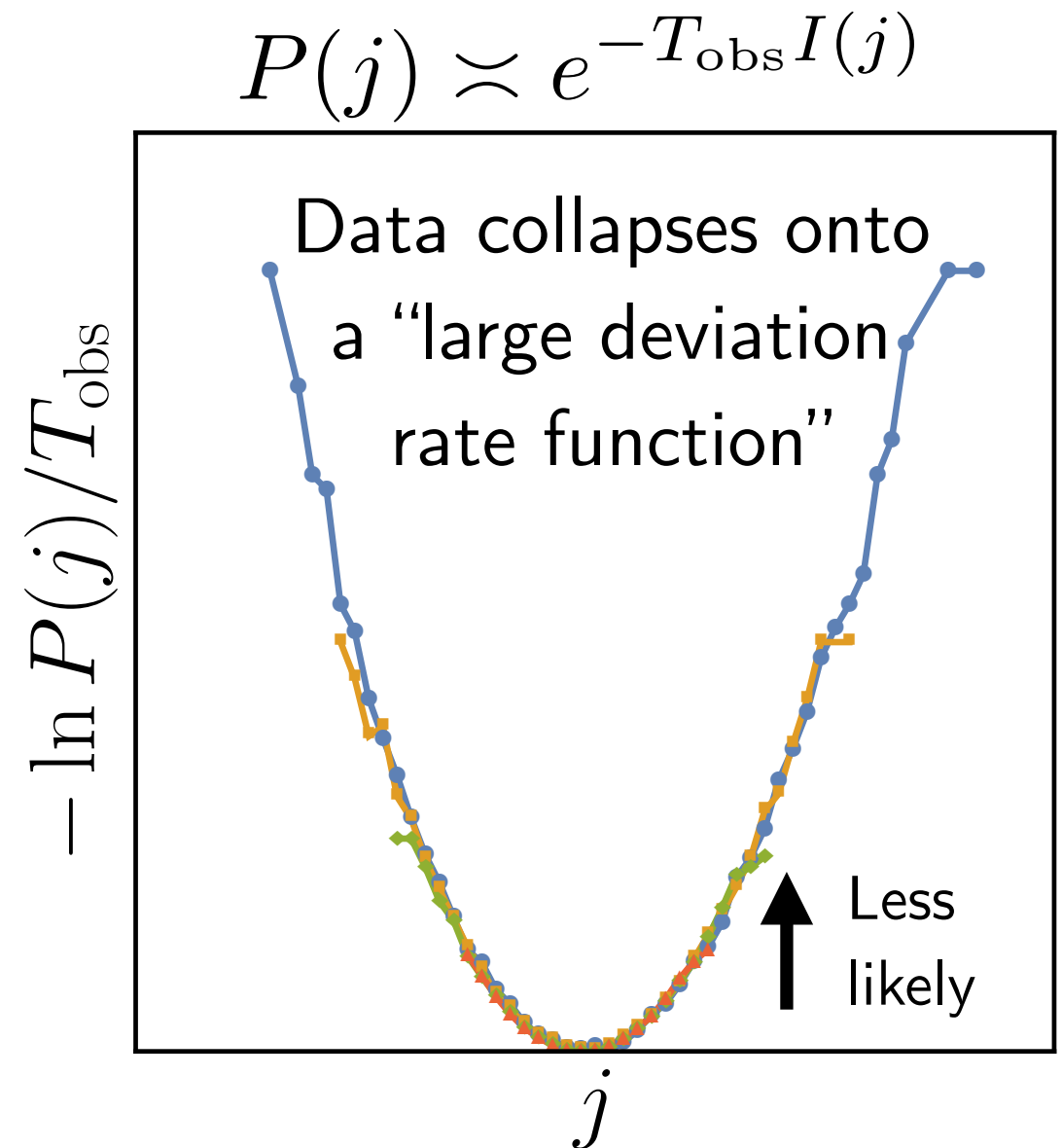
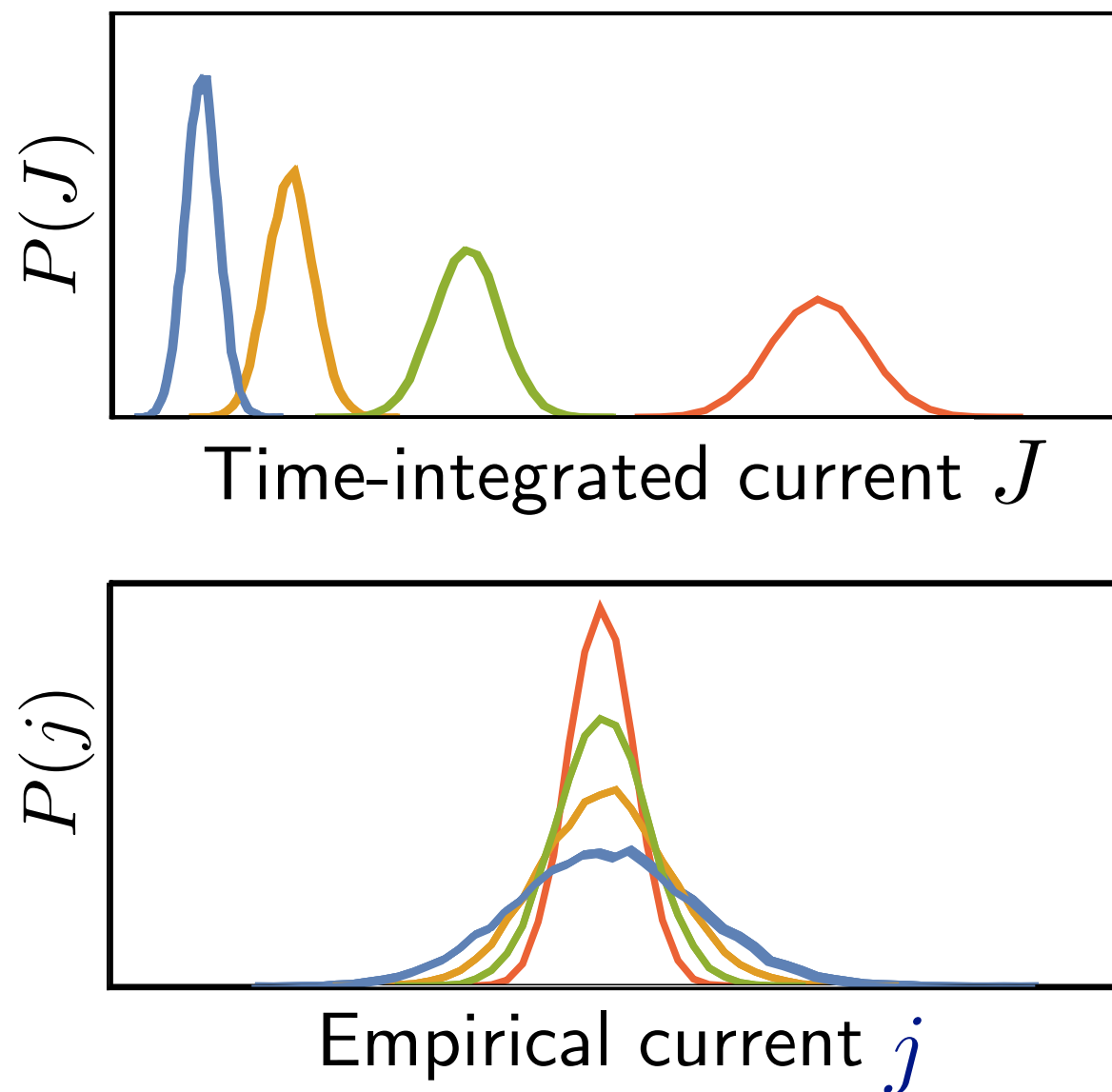
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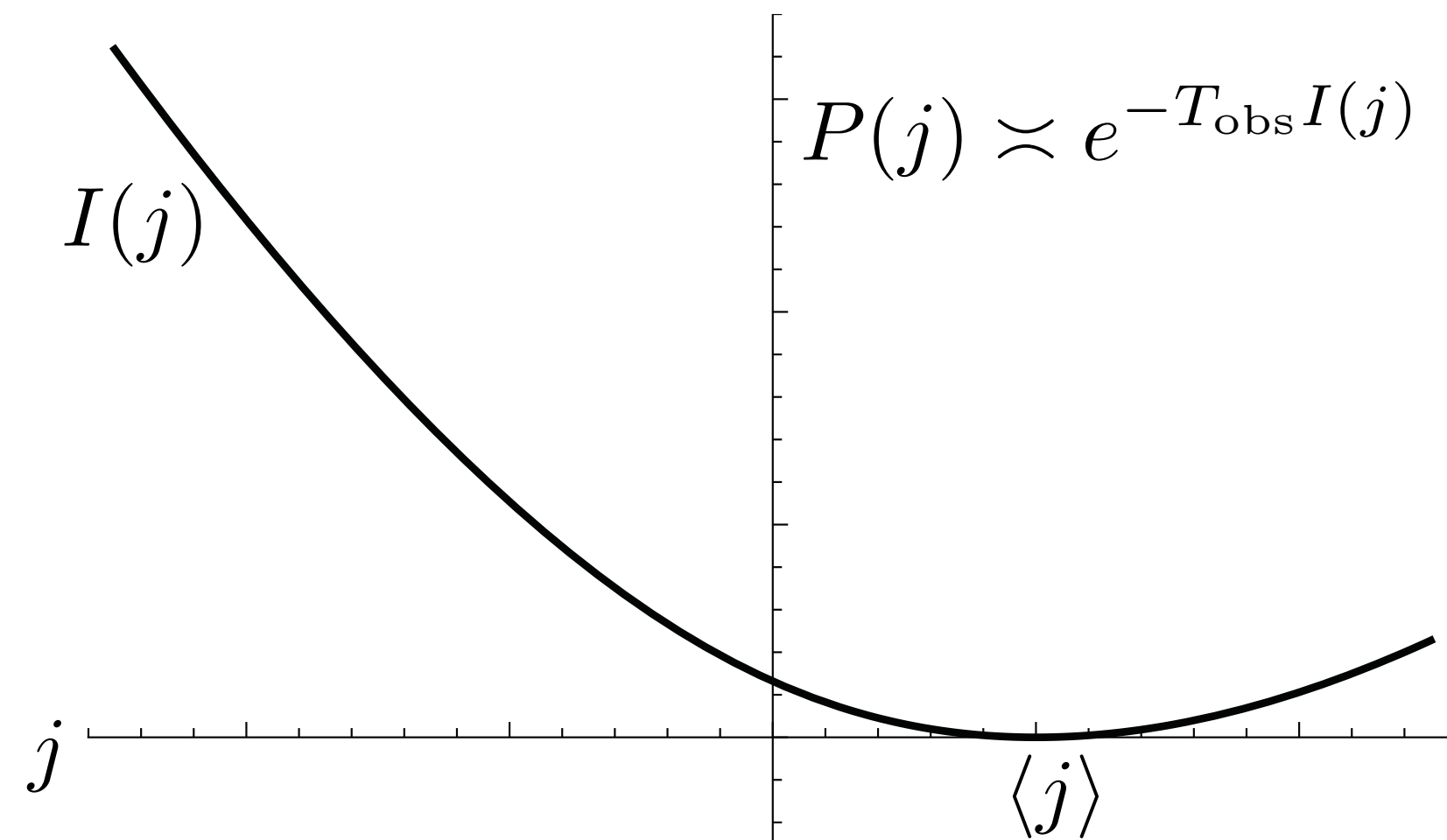
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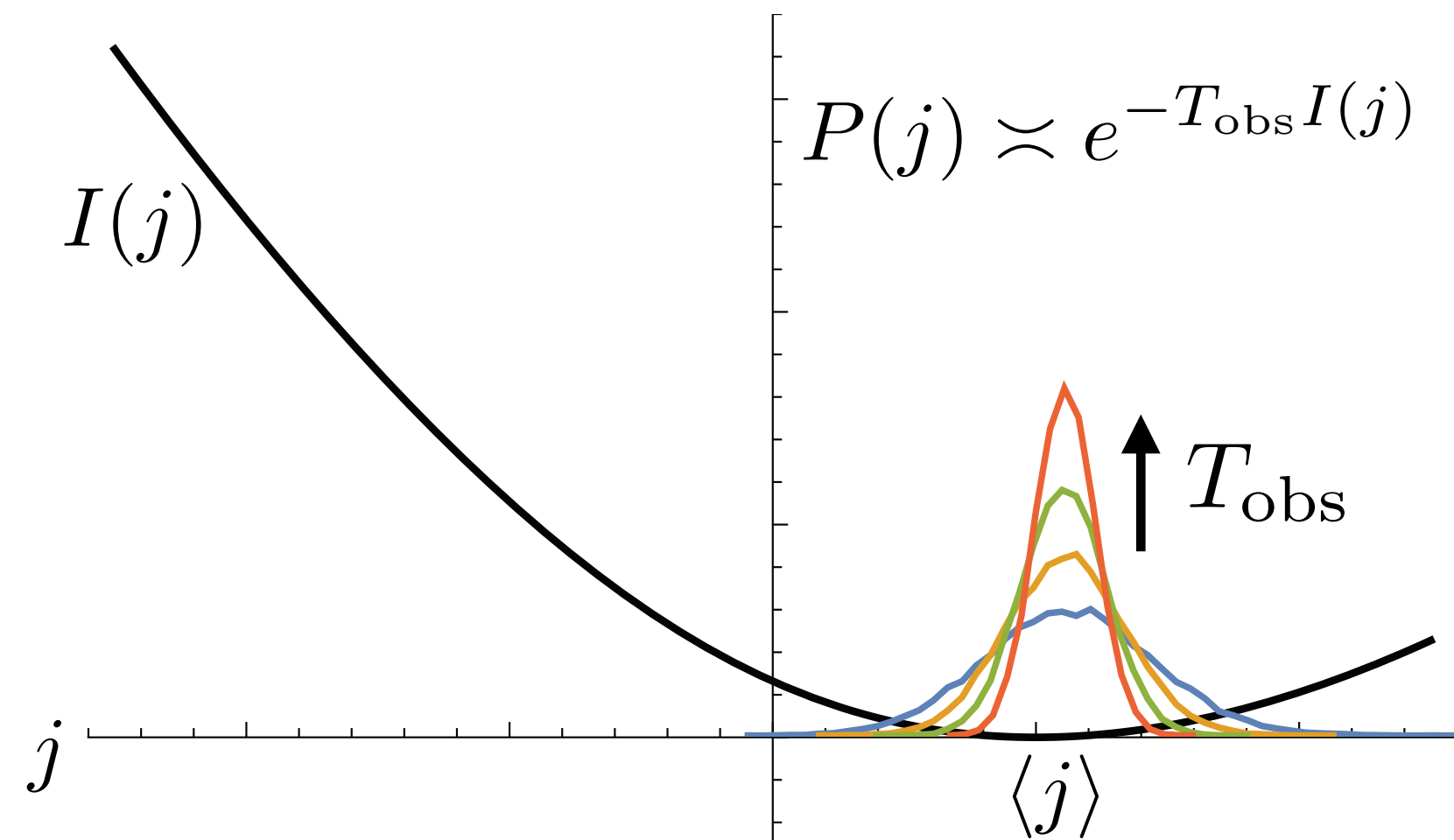


The rate function, $I(j)$, describes the rate of convergence to the mean



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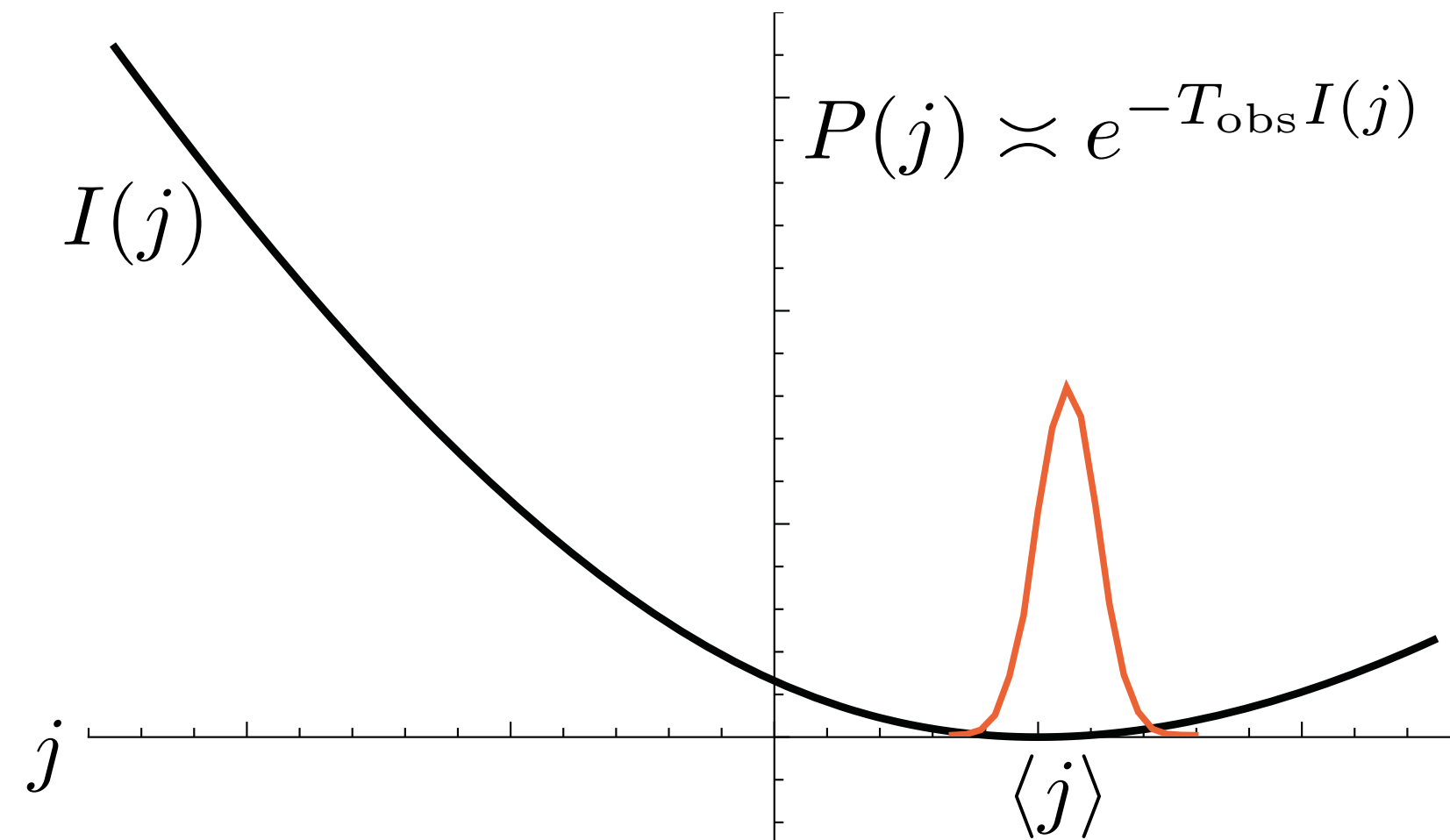
1. Minimum at the steady-state current
(Law of Large Numbers)



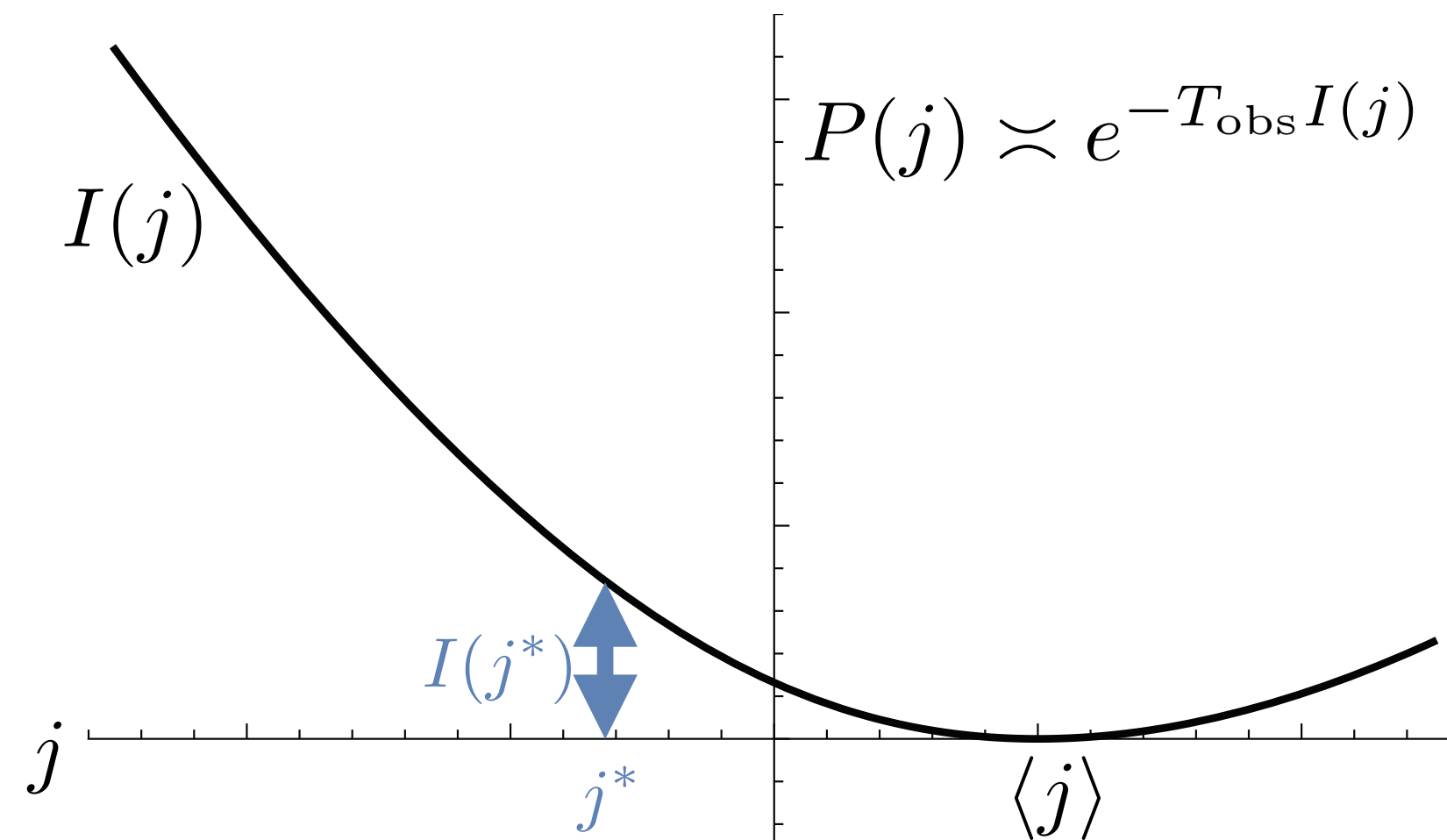
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1. Minimum at the steady-state current
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2. The *locally quadratic* minimum determines long-time *Gaussian current fluctuations*
(Central Limit Theorem)

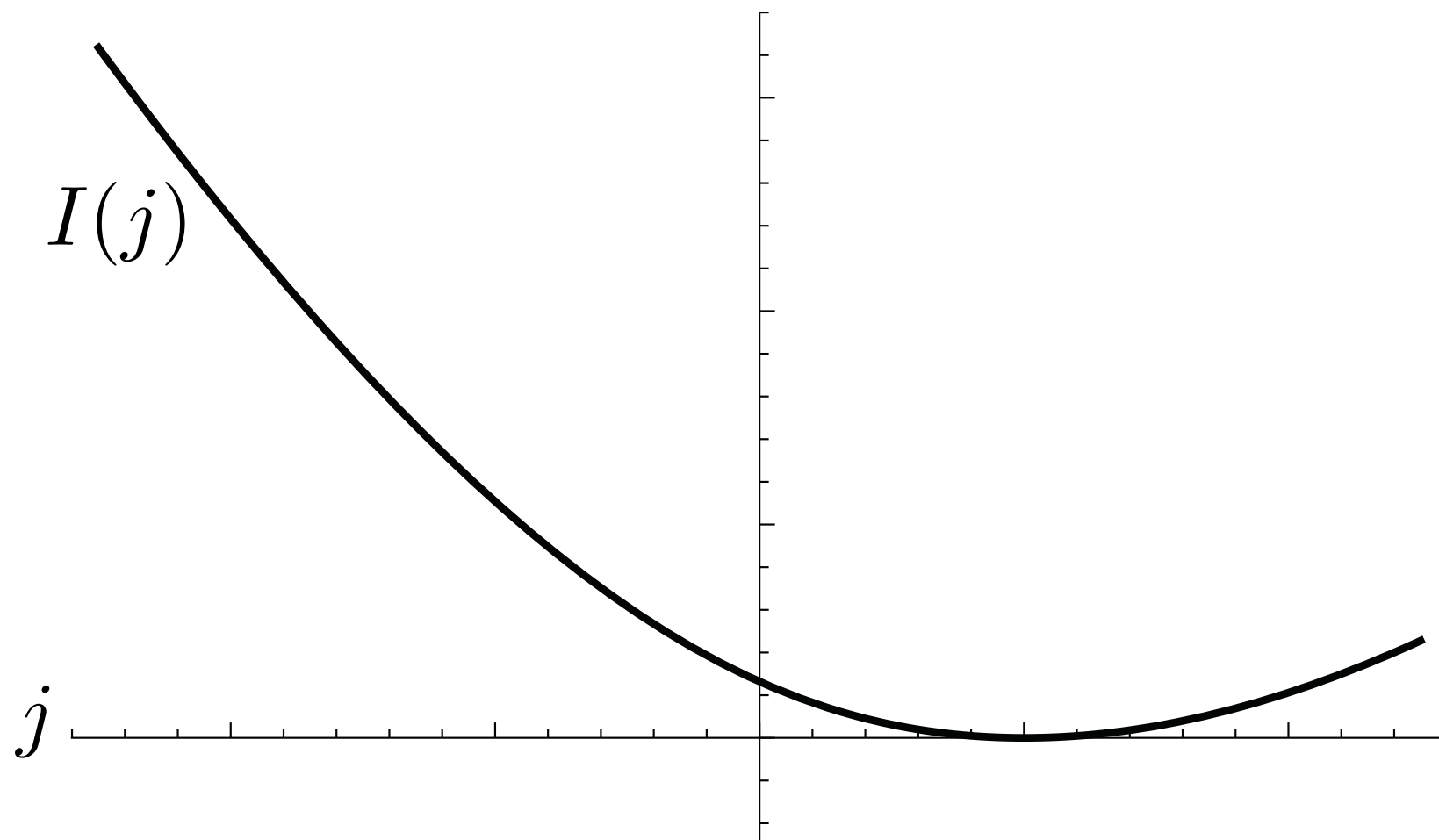


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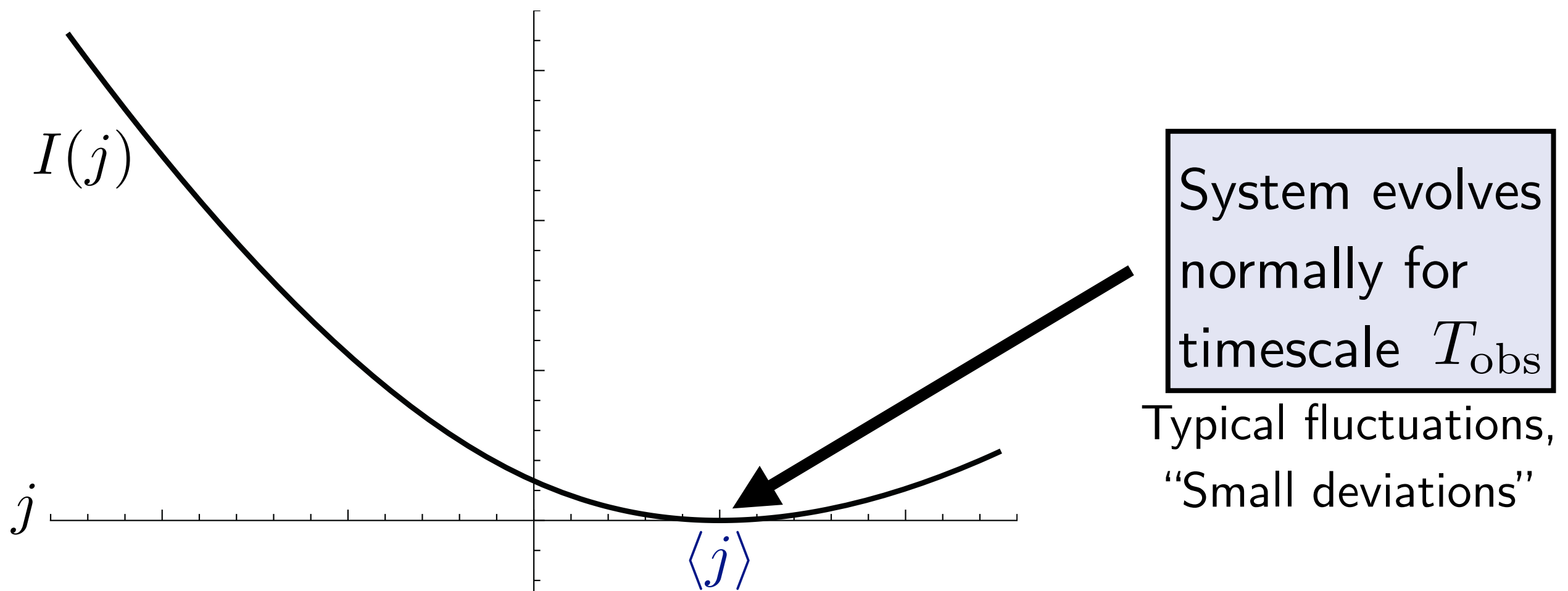


1. Minimum at the steady-state current
(Law of Large Numbers)
2. The *locally quadratic* minimum determines long-time *Gaussian current fluctuations*
(Central Limit Theorem)
3. $I(j^*)$ measures — on an exponential scale — the probability of measuring empirical current j^*

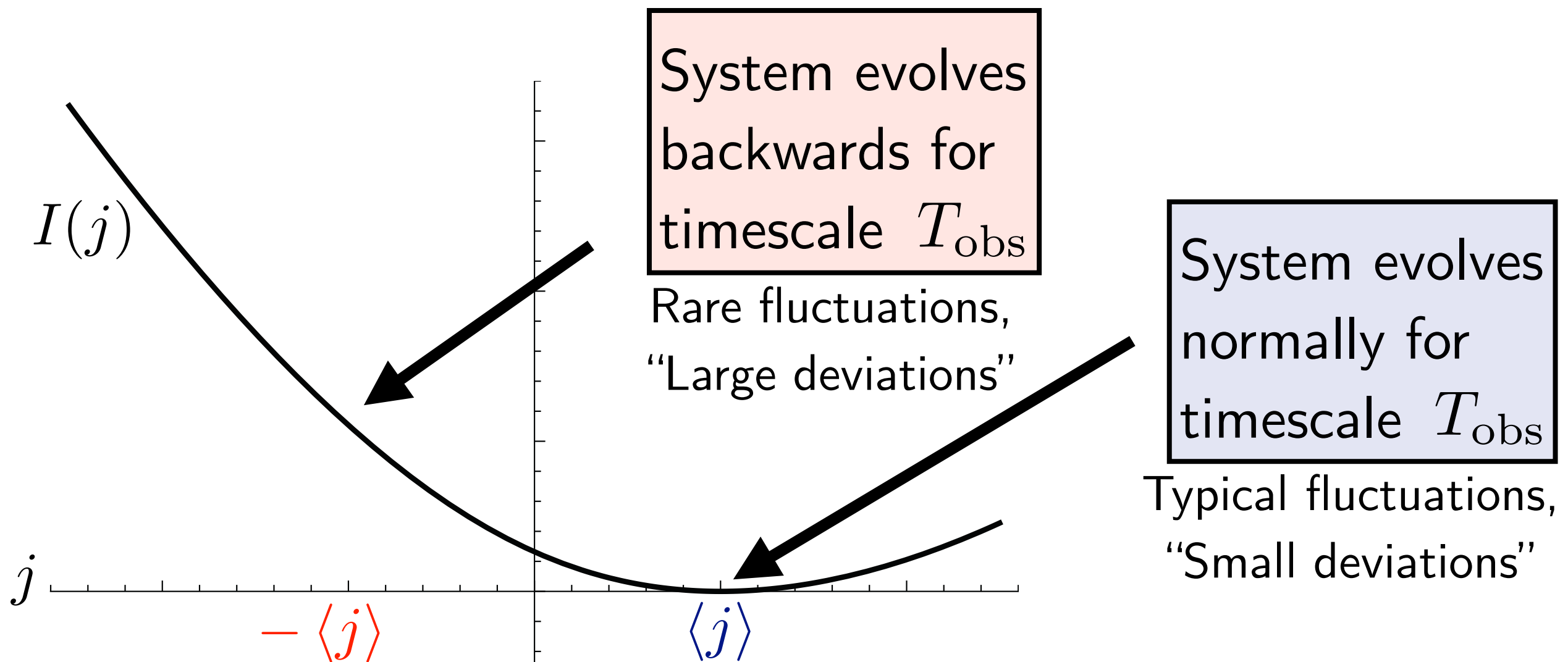
How probable is a forward versus a reversed current?



How probable is a forward versus a reversed current?

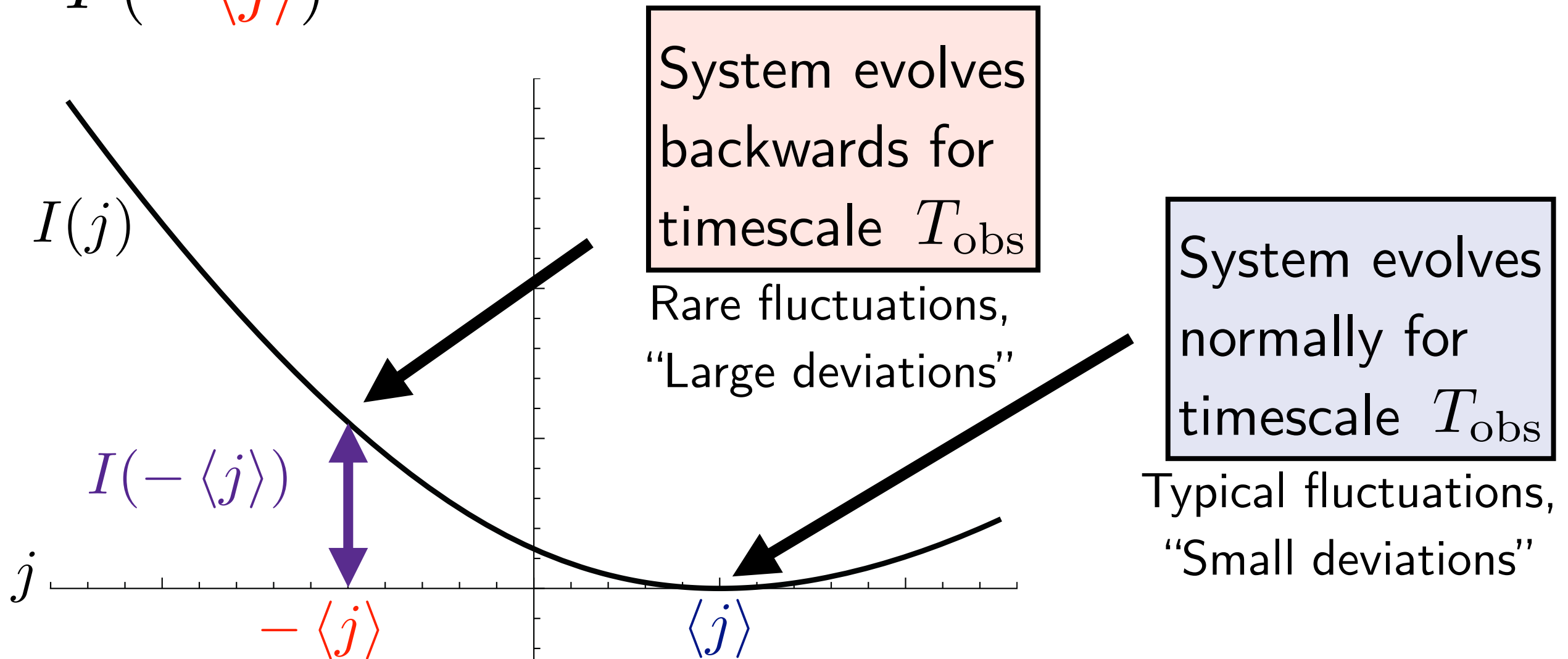


How probable is a forward versus a reversed current?



How probable is a forward versus a reversed current?

$$\frac{P(\langle j \rangle)}{P(-\langle j \rangle)} \asymp e^{T_{\text{obs}} I(-\langle j \rangle)}$$



Comparing forward and reversed probabilities has
the flavor of the Crooks Fluctuation Theorem

$$\frac{\text{Probability of forward trajectory}}{\text{Probability of time-reversed trajectory}} = e^{\text{Dissipation}}$$

G.E.Crooks, *PRE*, 60(3), 2721, 1999.

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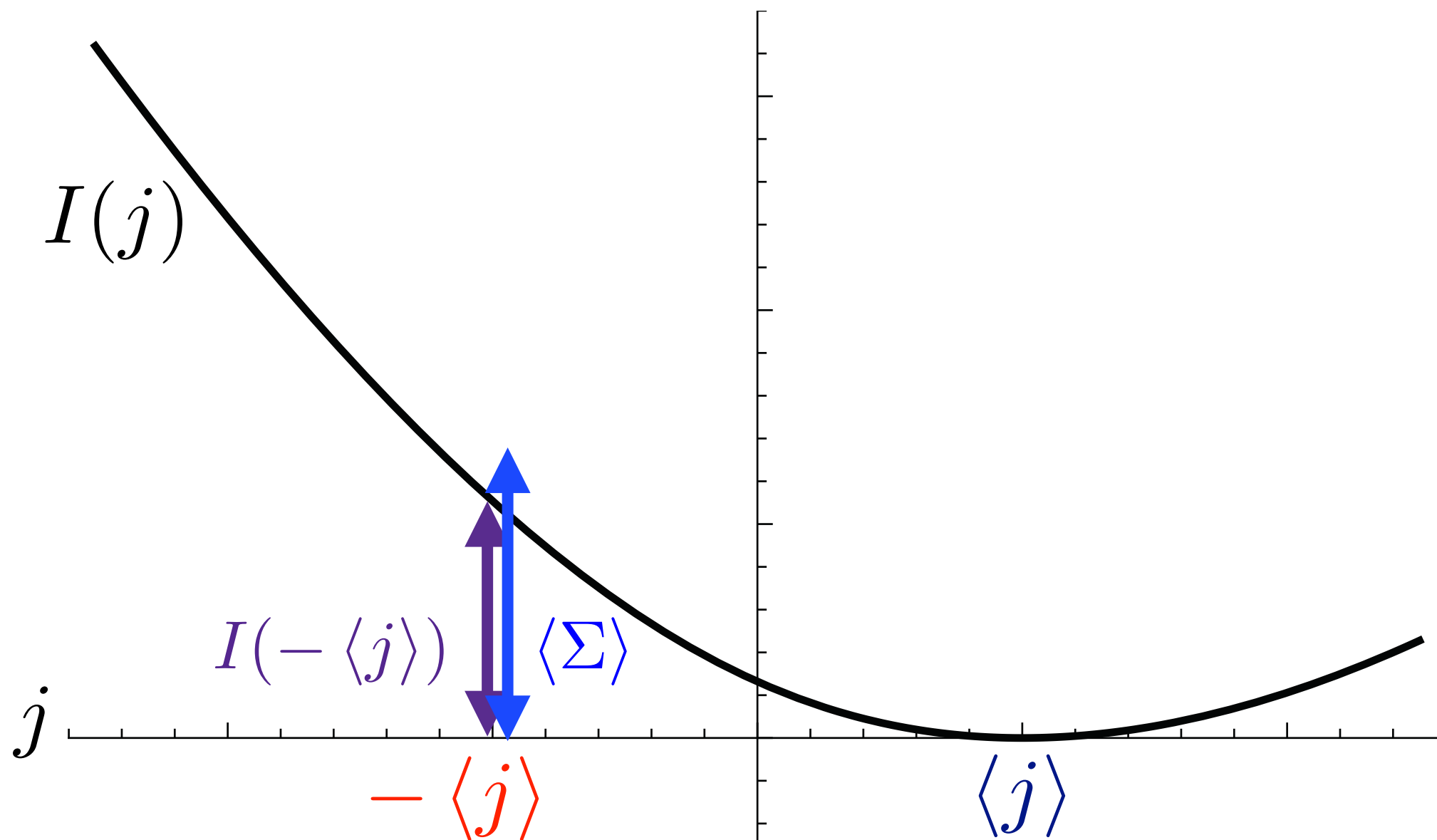
G.E.Crooks, *PRE*, 60(3), 2721, 1999.

Dissipation also plays a prominent role for the currents:

$$\frac{P(\langle j \rangle)}{P(-\langle j \rangle)} \asymp e^{T_{\text{obs}} I(-\langle j \rangle)}$$

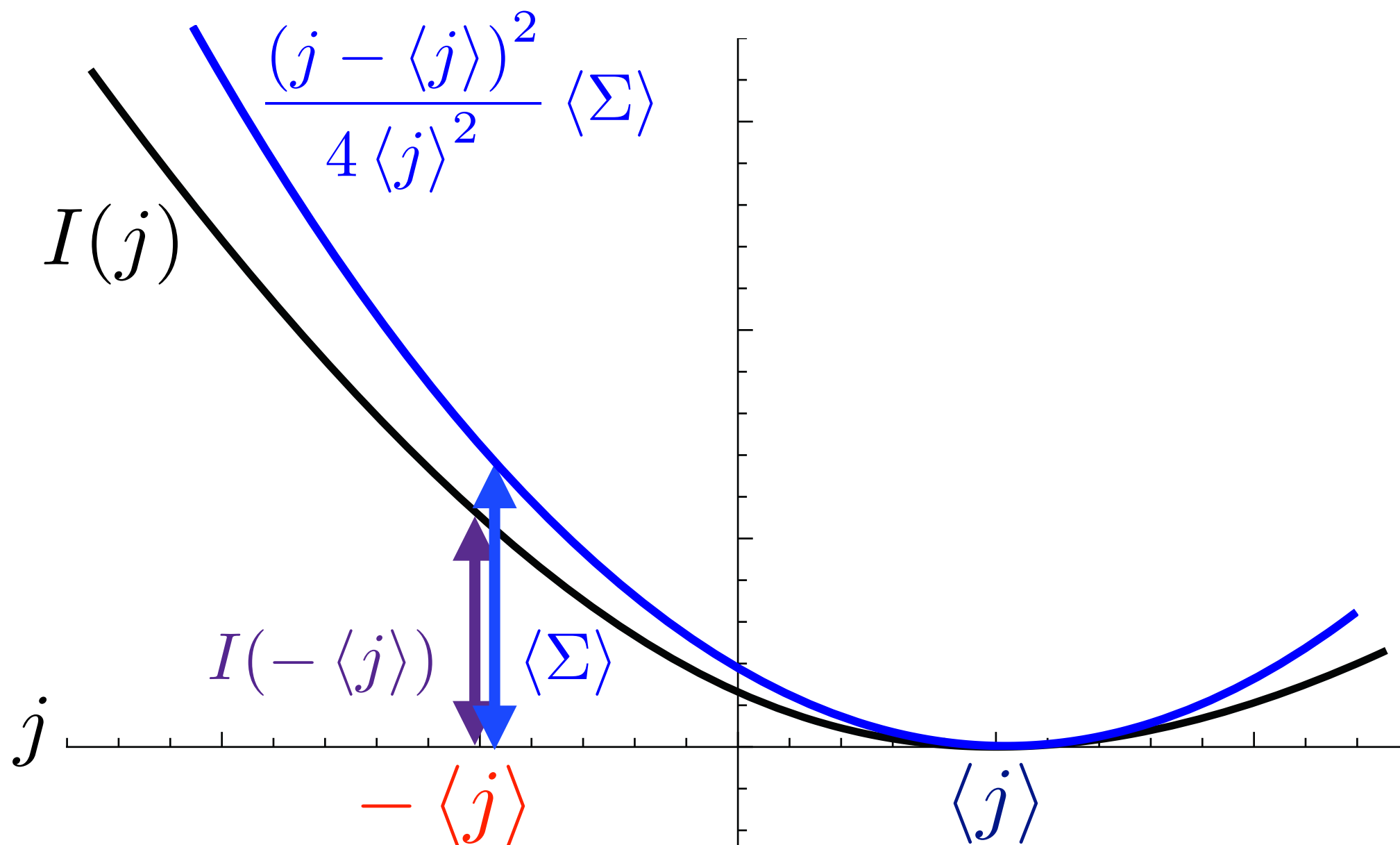
$$I(-\langle j \rangle) \leq \text{Dissipation rate}$$

Our result: Dissipation constrains all current fluctuations — small and large



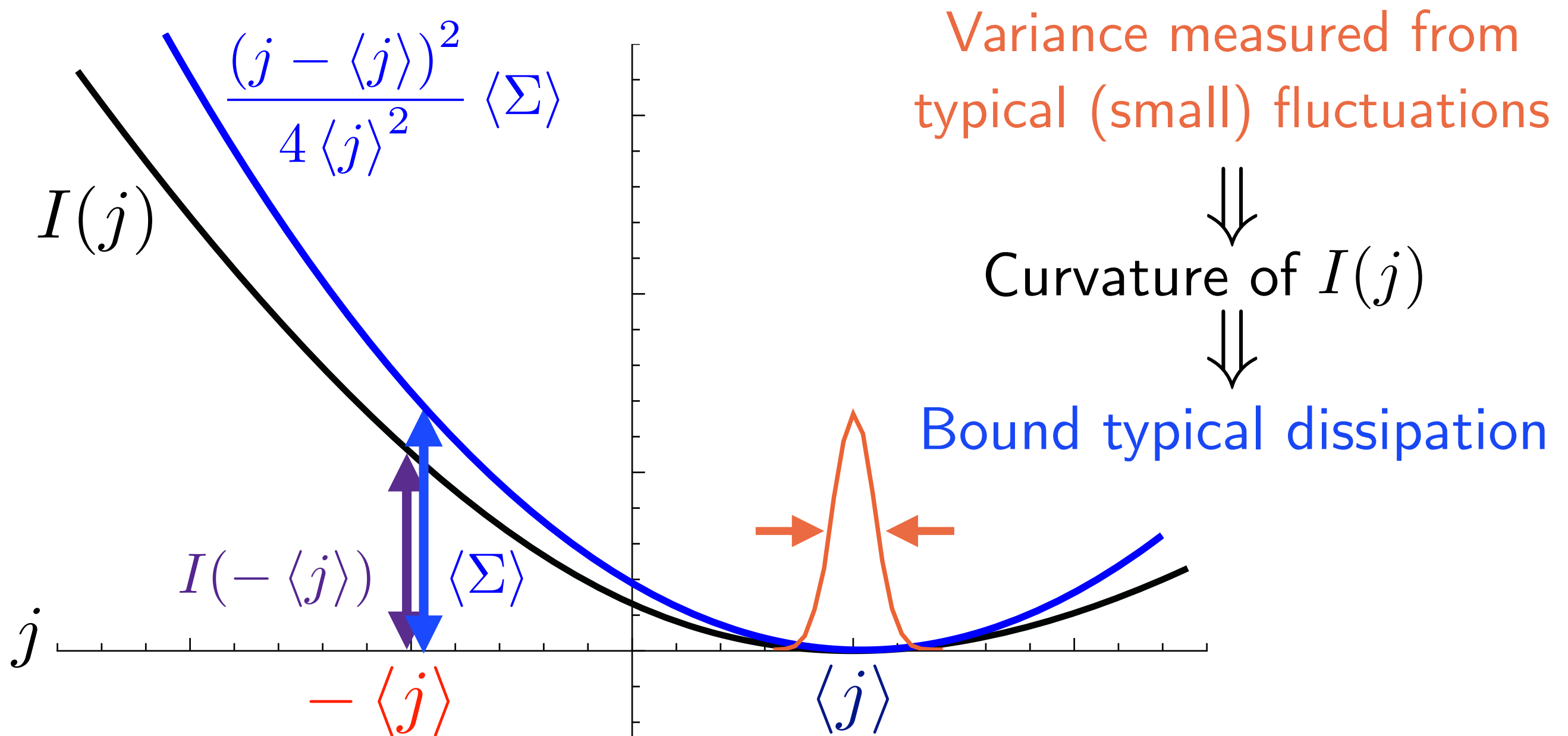
14 $I(-\langle j \rangle) \leq \text{Dissipation rate}$

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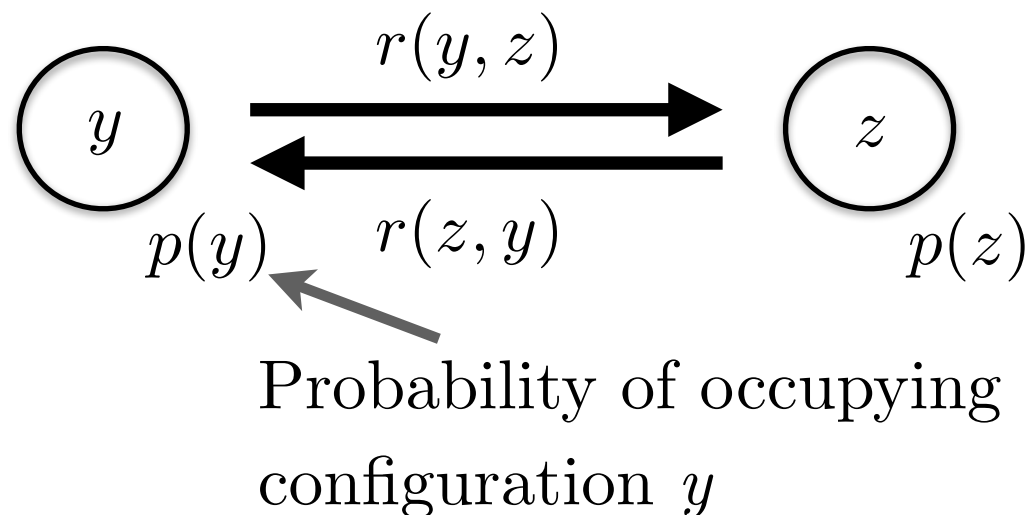
Sketch of a Derivation

Continuous time jump process

Dynamics:

Master equation: $\frac{\partial}{\partial t} \vec{p} = \mathbb{W} \vec{p}$

Current from y to z : $j(y, z) = p(y)r(y, z) - p(z)r(z, y)$



Rate Matrix:

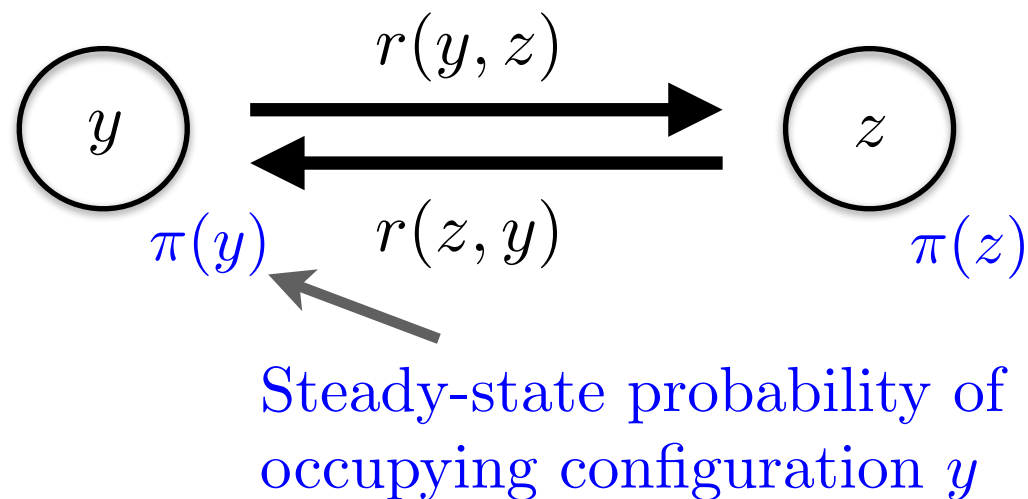
$$\mathbb{W} = \begin{pmatrix} -\sum_{i \neq 1} r(i, 1) & r(1, 2) \dots & \\ r(2, 1) & -\sum_{i \neq 2} r(i, 2) & \dots \\ \vdots & \vdots & \ddots \end{pmatrix}$$

Continuous time jump process

Steady State:

Master equation: $\frac{\partial}{\partial t} \vec{\pi} = \mathbb{W} \vec{\pi} = 0$

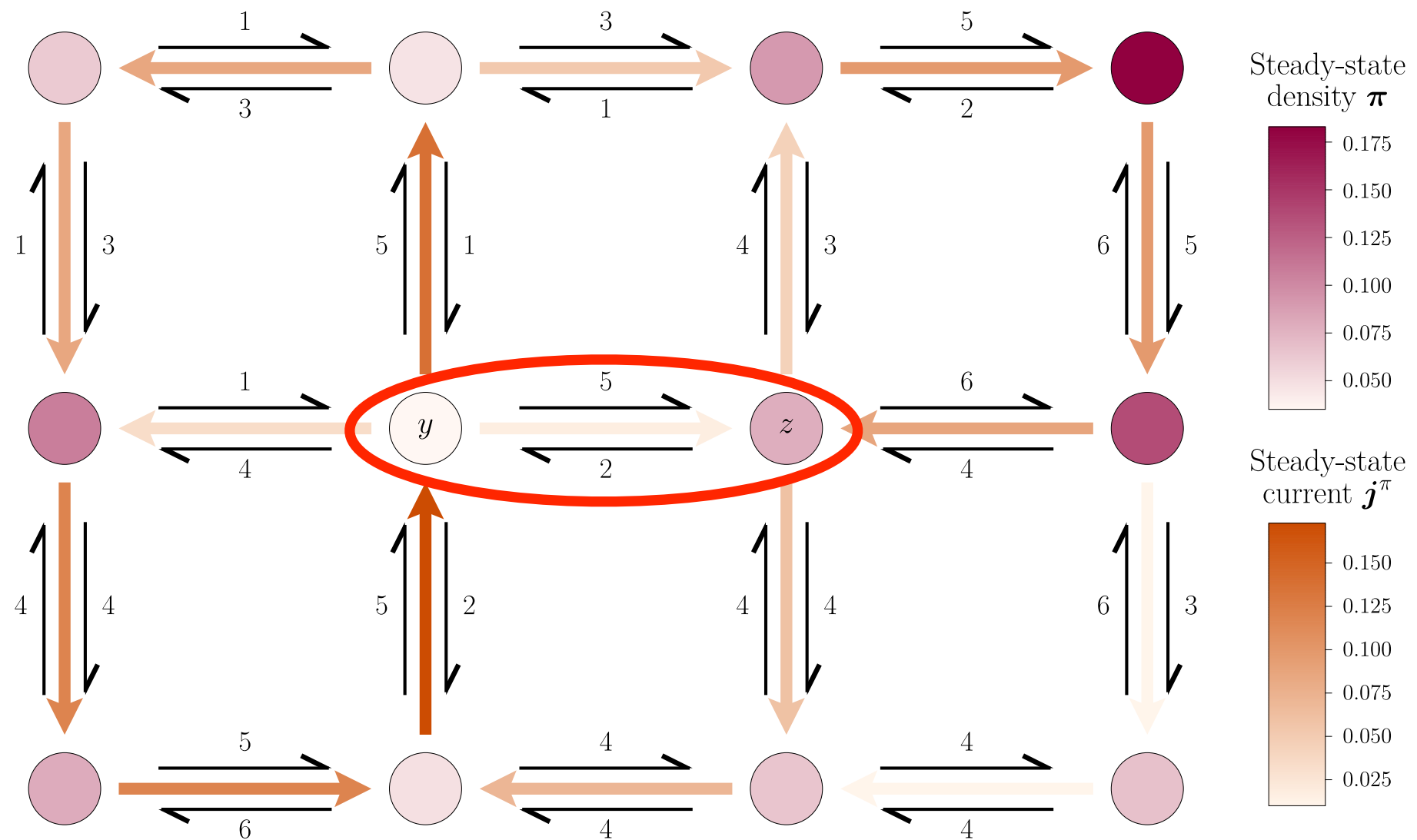
Current from y to z : $j^\pi(y, z) = p^\pi(y)r(y, z) - p^\pi(z)r(z, y)$



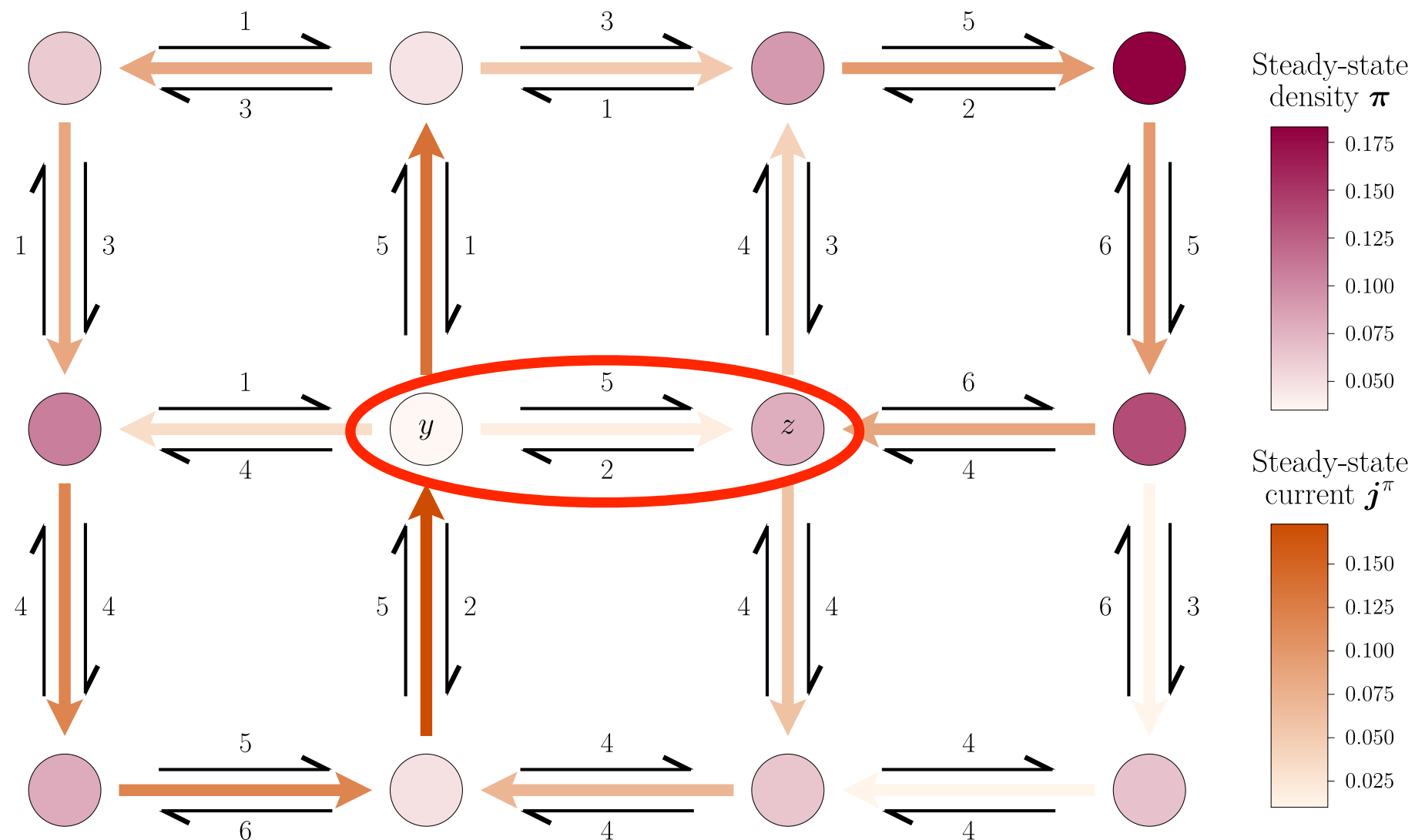
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An example network of states



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Of course any realization of the process has densities and currents which differ from the steady-state values

Level 2.5

Consider a jump trajectory $x(t) \dots$

Empirical density:

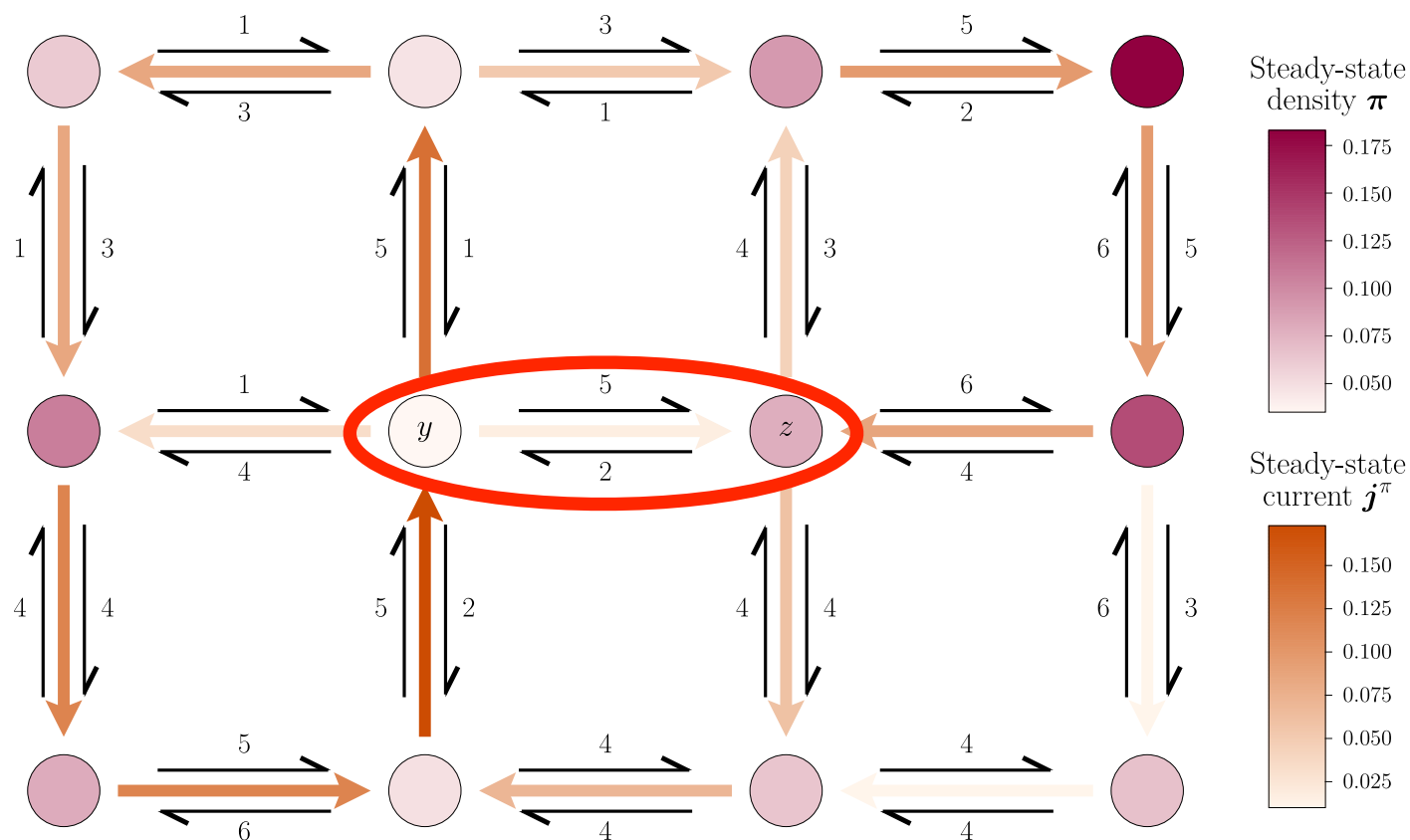
$$p(y) = \frac{1}{T} \int_0^T dt \delta_{x(t),y}$$

Empirical flow:

$$q(y, z) = \frac{1}{T} \int_0^T dt \delta_{x(t^-),y} \delta_{x(t^+),z}$$

Empirical current:

$$j(y, z) = q(y, z) - q(z, y)$$



$$P(\mathbf{p}, \mathbf{q}) \asymp e^{-TI(\mathbf{p}, \mathbf{q})}$$

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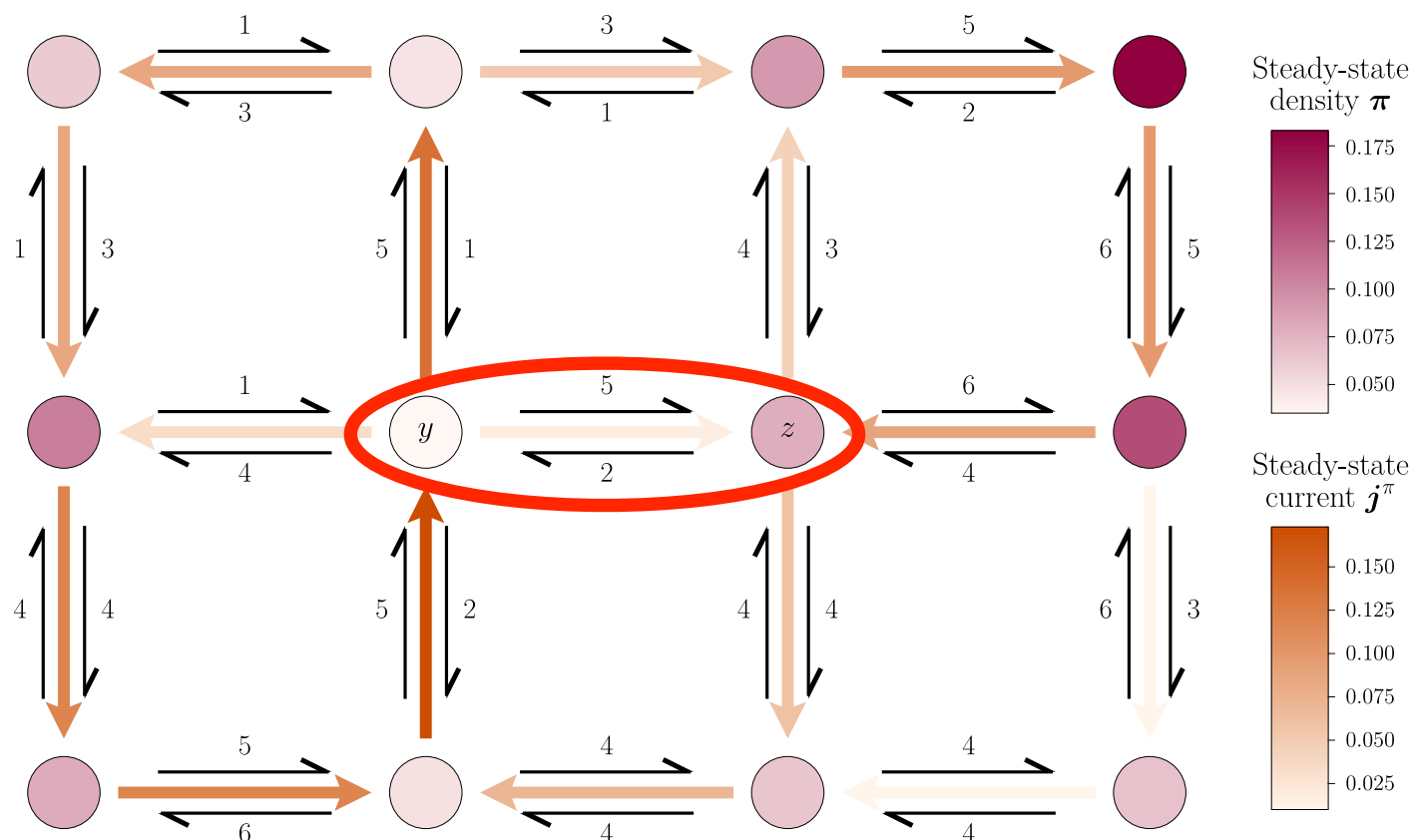
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Empirical current:

$$j(y, z) = q(y, z) - q(z, y)$$



Rate functions $I(\mathbf{p}, \mathbf{q})$ and $I(\mathbf{p}, \mathbf{j})$ are explicit

$$P(\mathbf{p}, \mathbf{q}) \asymp e^{-TI(\mathbf{p}, \mathbf{q})}$$

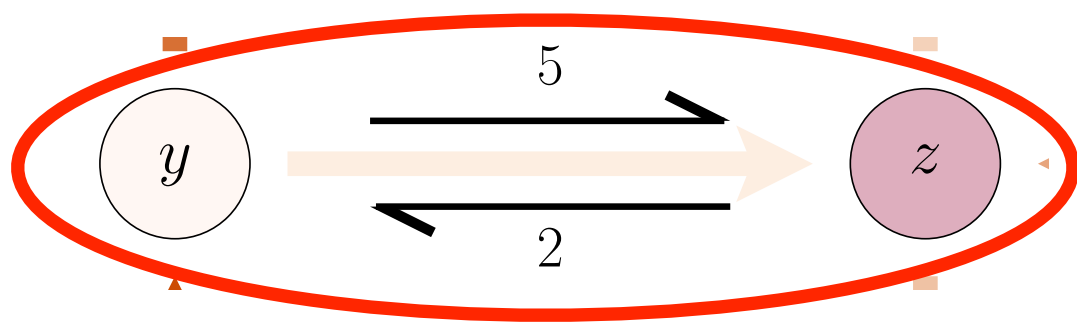
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C. Maes and K. Netocný, EPL (Europhysics Letters) 82, 30003 (2008)

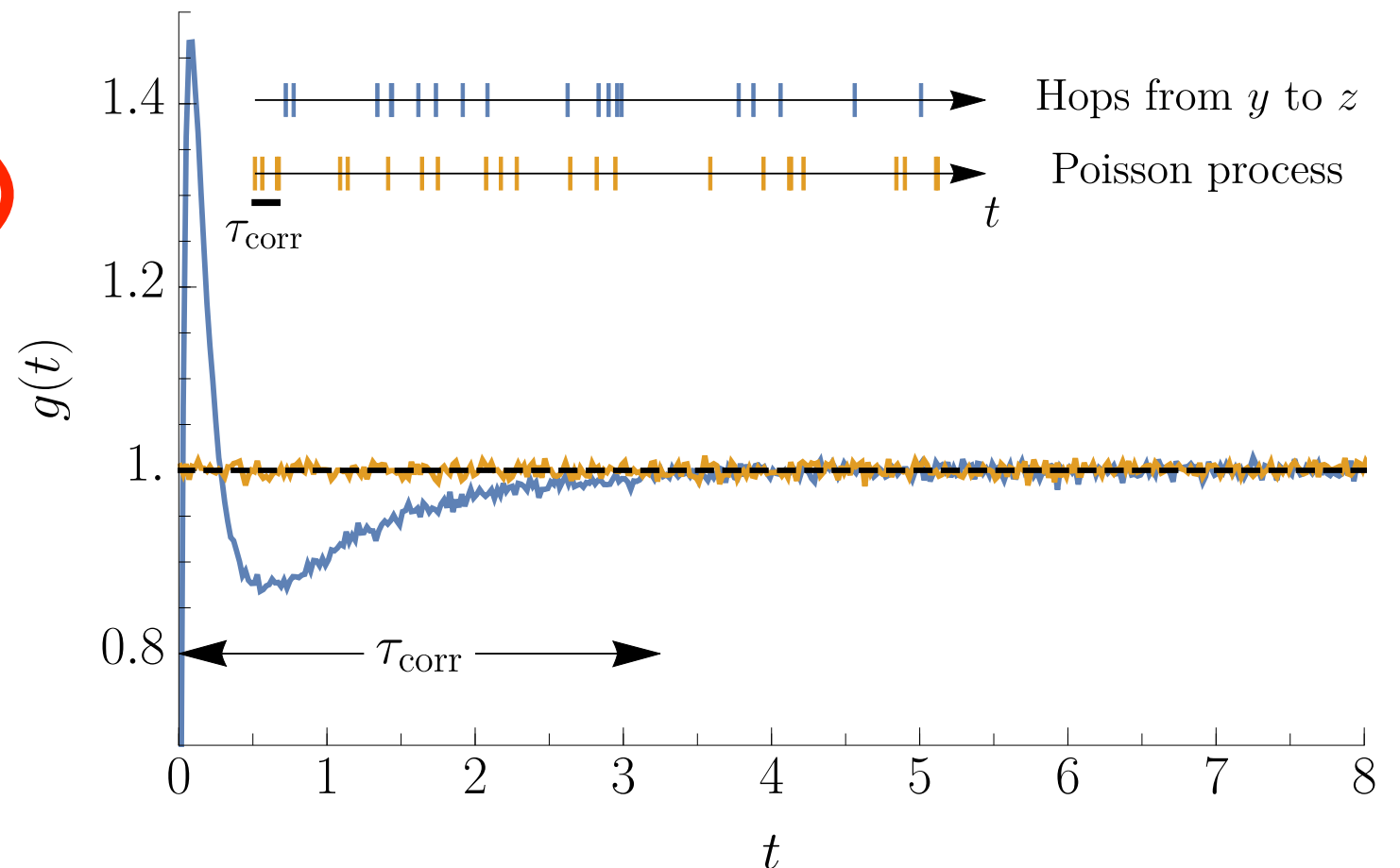
L. Bertini, A. Faggionato, and D. Gabrielli, Stochastic Processes and their Applications 125, 2786 (2015).

L. Bertini, A. Faggionato, and D. Gabrielli, Annales de l'Institut Henri Poincaré. Section B, Probabilités et Statistiques 51, 867 (2015).

Handwaving argument for the explicit level 2.5 form



Focus on a single directed edge of the graph



Asymptotically like a Poisson clock for each directed edge, with a Poisson point process rate $p(y)r(y, z)$.

Handwaving argument for the explicit level 2.5 form

$$P_{\text{ind}}(p(y), q(y, z)) \asymp \frac{(Tp(y)r(y, z))^{Tq(y, z)} e^{-Tp(y)r(y, z)}}{(Tq(y, z))!}$$

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Treat the directed edge from y to z as though it is independent

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$$P_{\text{ind}}(p(y), q(y, z)) \asymp e^{-TI_{\text{ind}}(p(y), q(y, z))}$$

$$\Rightarrow I_{\text{ind}}(p(y), q(y, z)) = p(y)r(y, z) - q(y, z) + q(y, z) \ln \frac{q(y, z)}{p(y)r(y, z)}$$

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$$I(\mathbf{p}, \mathbf{q}) = \begin{cases} \sum_{y \neq z} I_{\text{ind}}(p(y), q(y, z)), & \mathbf{q} \text{ conserves probability} \\ \infty, & \text{otherwise} \end{cases}$$

Handwaving argument for the explicit level 2.5 form

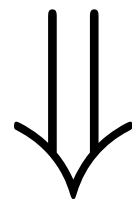
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Integrate out $q(y, z)$ and $q(z, y)$ subject to the constraint $j(y, z) = q(y, z) - q(z, y)$

Handwaving argument for the explicit level 2.5 form

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$$I(\mathbf{p}, \mathbf{j}) = \begin{cases} \sum_{y < z} \Psi(p(y), p(z), j(y, z)), & \mathbf{j} \text{ conservative} \\ \infty, & \text{otherwise} \end{cases}$$

$$\Psi(p(y), p(z), j(y, z)) = \inf_{q(y, z)} I_{\text{ind}}(p(y), q(y, z)) + I_{\text{ind}}(p(z), q(y, z) - j(y, z))$$

Handwaving argument for the explicit level 2.5 form

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$$\begin{aligned}\text{Minimizer: } q_{\star}(y, z) &= \frac{1}{2} \left(j(y, z) + \sqrt{j(y, z)^2 + a^p(y, z)^2} \right) \\ &\quad \left(a^p(y, z) \equiv 2\sqrt{p(y)p(z)r(y, z)r(z, y)} \right)\end{aligned}$$

Handwaving argument for the explicit level 2.5 form

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$$\left(a^p(y, z) \equiv 2\sqrt{p(y)p(z)r(y, z)r(z, y)}; \quad j^p(y, z) \equiv p(y)r(y, z) - p(z)r(z, y) \right)$$

Re-express in terms of thermodynamic forces

$$\begin{aligned} \Psi(j(y, z), j^p(y, z), a^p(y, z)) = & \sqrt{j(y, z)^2 + a^p(y, z)^2} + \sqrt{j^p(y, z)^2 + a^p(y, z)^2} \\ & + j(y, z) \left(\operatorname{arcsinh} \frac{j(y, z)}{a^p(y, z)} - \operatorname{arcsinh} \frac{j^p(y, z)}{a^p(y, z)} \right) \end{aligned}$$

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For small force...

$$\Psi = j^p \left[\frac{(\bar{j} - 1)^2 F^p}{4} - \frac{(\bar{j}^2 - 1)^2 (F^p)^3}{192} + \frac{(\bar{j}^2 - 1)^2 (3\bar{j}^2 + 1) (F^p)^5}{7680} + \mathcal{O}((F^p)^7) \right]$$

The first term gives a quadratic bound

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Pf.
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$$\text{Let } \Delta \equiv \Psi_{\text{quad}} - \Psi \Rightarrow \Delta = 0 \text{ for } \bar{j} = \pm 1$$

$$\frac{\partial \Delta}{\partial \bar{j}} = j^p \left[\operatorname{arcsinh} \left(\bar{j} \sinh \frac{F^p}{2} \right) - \frac{\bar{j} F^p}{2} \right]$$

Inspect signs.

Jump process level 2.5

$$I(\mathbf{p}, \mathbf{j}) = \begin{cases} \sum_{y < z} \Psi(p(y), p(z), j(y, z)), & \mathbf{j} \text{ conservative} \\ \infty, & \text{otherwise} \end{cases}$$

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A quadratic upper bound

$$I(\mathbf{p}, \mathbf{j}) \leq \begin{cases} \sum_{y < z} \frac{(j(y, z) - j^p(y, z))^2 \sigma^p(y, z)}{4j^p(y, z)^2}, & \mathbf{j} \text{ conservative} \\ \infty, & \text{otherwise} \end{cases}$$

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What if we are only interested in the statistics of some scalar current...

$$j_d \equiv \sum_{y < z} d(y, z) j(y, z)$$

$$I(j_d) = \inf_{\mathbf{p}, \mathbf{j} | \mathbf{j} \cdot \mathbf{d} = j_d} I(\mathbf{p}, \mathbf{j})$$

Scalar current upper bound

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LDF bound:

$$I(j_d) \leq I\left(\boldsymbol{\pi}, \frac{j_d}{j_d^\pi} \mathbf{j}^\pi\right) \leq \frac{1}{4} \left(\frac{j_d}{j_d^\pi} - 1\right)^2 \sum_{y < z} \sigma^\pi(y, z) = \frac{(j_d - j_d^\pi)^2 \Sigma^\pi}{4(j_d^\pi)^2}$$

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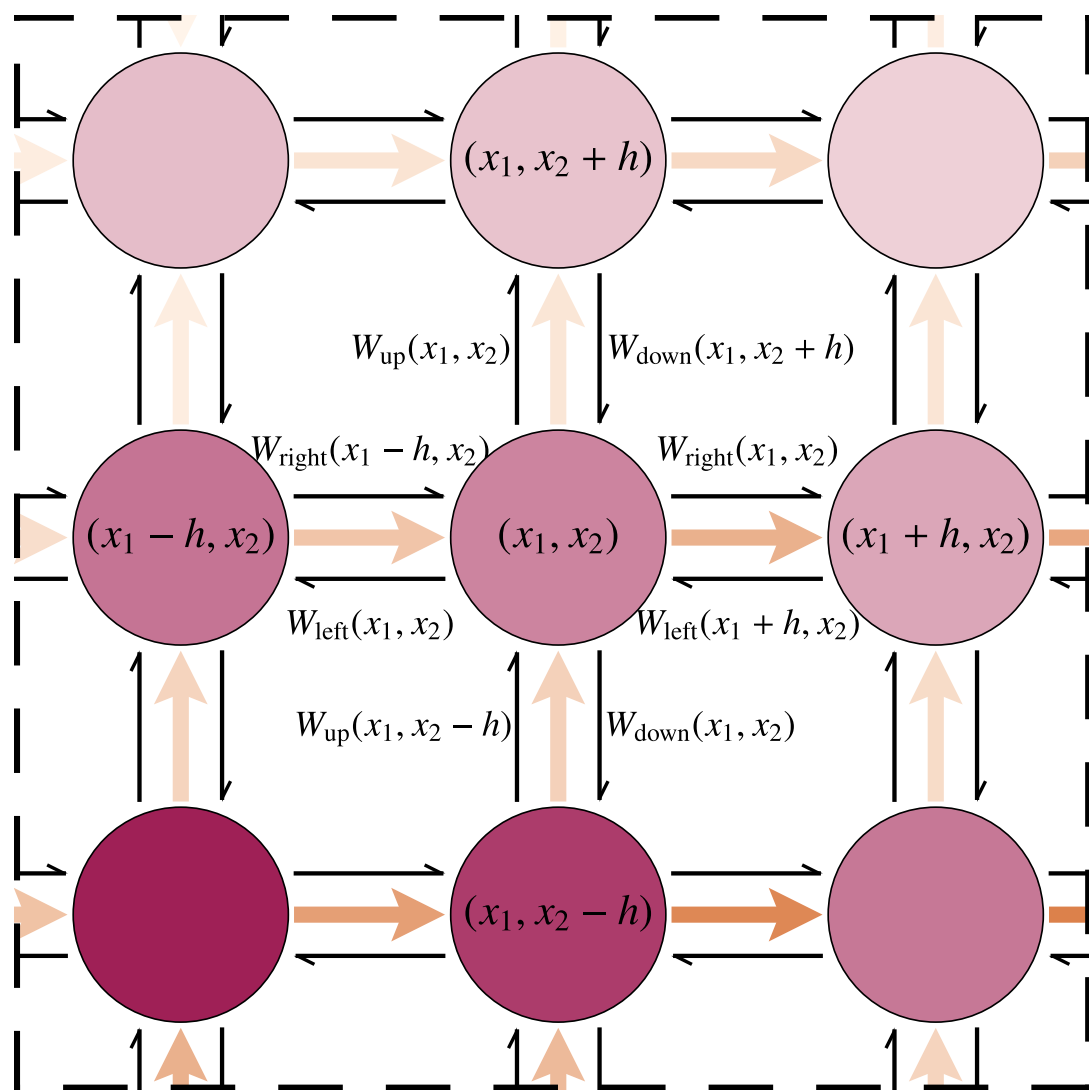
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Small deviations corollary (thermodynamic uncertainty):

$$\frac{\text{Var}(J_d)}{\langle J_d \rangle^2} = \frac{1}{j_d^\pi T I''(j_d^\pi)} \geq \frac{2}{T \Sigma^\pi}$$

What about diffusions?

Construct a jump process which limits to the desired diffusion.



$$W_{\text{right}}(\mathbf{x}) = \frac{\mu f_1(\mathbf{x})}{2h} + \frac{D}{h^2}$$

$$W_{\text{left}}(\mathbf{x}) = \frac{-\mu f_1(\mathbf{x})}{2h} + \frac{D}{h^2}$$

$$W_{\text{up}}(\mathbf{x}) = \frac{\mu f_2(\mathbf{x})}{2h} + \frac{D}{h^2}$$

$$W_{\text{down}}(\mathbf{x}) = \frac{-\mu f_2(\mathbf{x})}{2h} + \frac{D}{h^2}$$

Jump process quadratic bound

$$I(\mathbf{p}, \mathbf{j}) \leq \begin{cases} \sum_{y < z} \frac{(j(y, z) - j^p(y, z))^2 \sigma^p(y, z)}{4j^p(y, z)^2}, & \mathbf{j} \text{ conservative} \\ \infty, & \text{otherwise} \end{cases}$$

$$\Downarrow \begin{array}{l} \text{Lattice spacing} \\ \text{to zero limit} \end{array} \quad \mathcal{J}^\rho(\mathbf{x}) = D\rho(\mathbf{x})\mathcal{F}^\rho(\mathbf{x})$$

Diffusion process quadratic bound becomes an equality

$$\mathcal{I}[\rho, \mathcal{J}] = \int d\mathbf{x} \frac{\sigma^\rho(\mathbf{x})}{4\mathcal{J}^\rho(\mathbf{x})^2} (\mathcal{J}(\mathbf{x}) - \mathcal{J}^\rho(\mathbf{x}))^2.$$

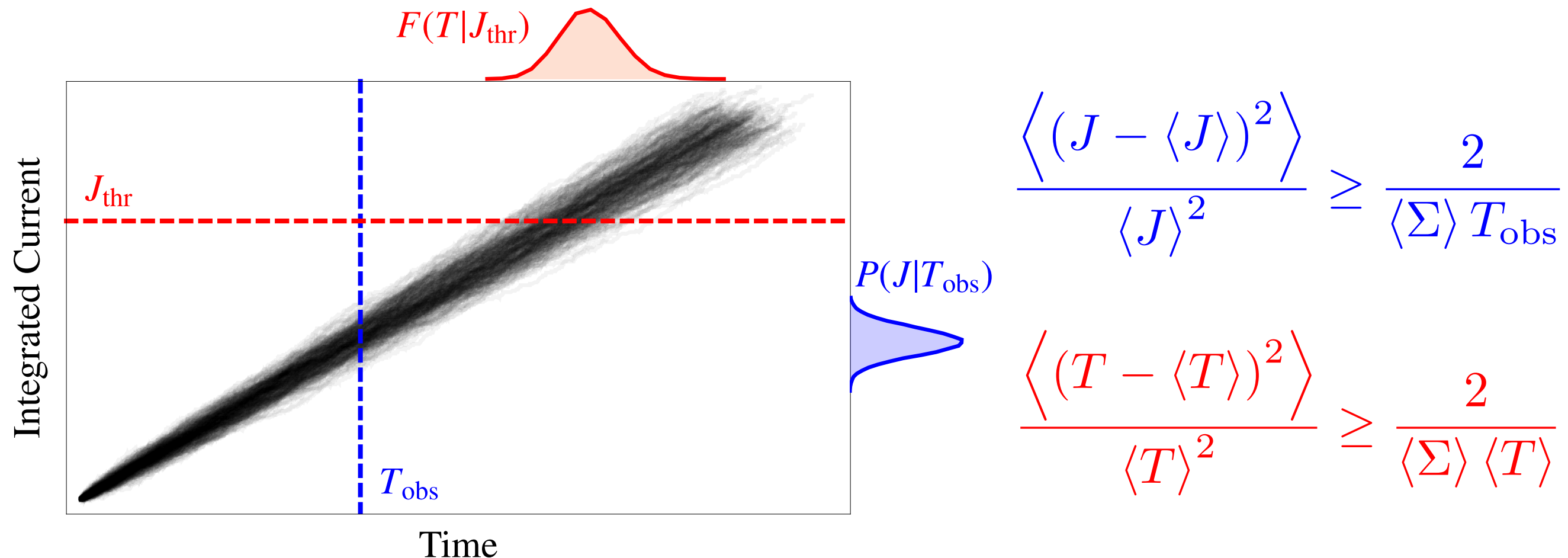
(again conservative currents)

$$= \int d\mathbf{x} \frac{1}{4D\rho(\mathbf{x})} (\mathcal{J}(\mathbf{x}) - \mathcal{J}^\rho(\mathbf{x}))^2.$$

And now, something different
(well not too different)

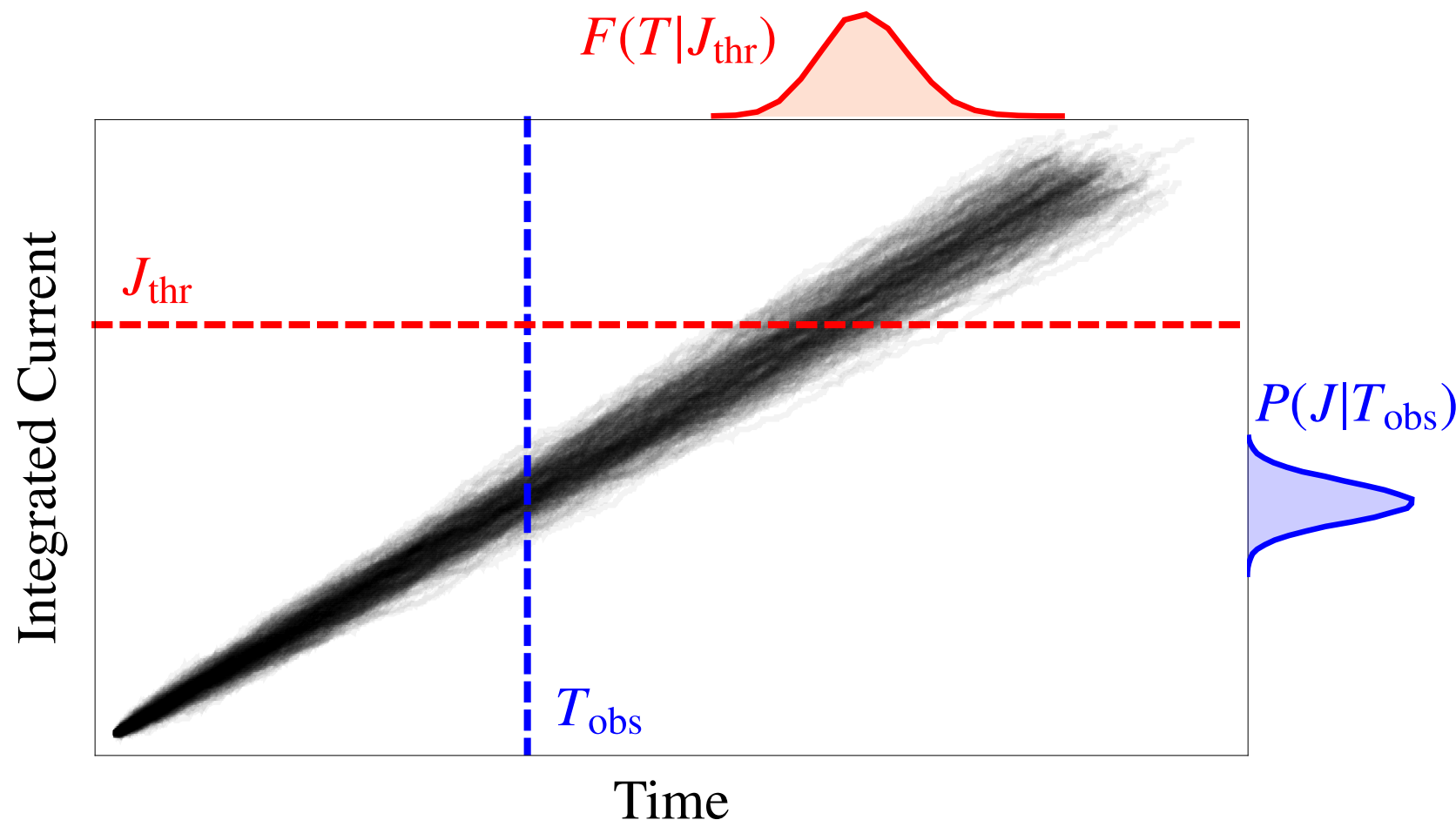
First passage time fluctuations

J.P. Garrahan, *PRE*, 95, 032134, 2017; K. Saito and A. Dhar, *EPL*, 115, 50004, 2016.



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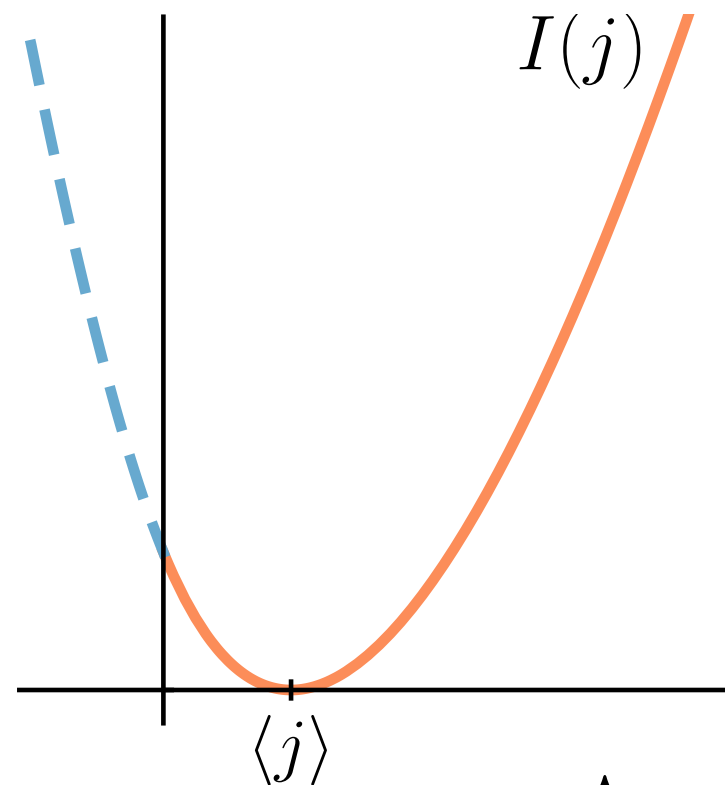


$$\frac{\langle (J - \langle J \rangle)^2 \rangle}{\langle J \rangle^2} \geq \frac{2}{\langle \Sigma \rangle T_{\text{obs}}}$$

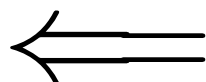
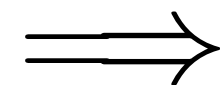
$$\frac{\langle (T - \langle T \rangle)^2 \rangle}{\langle T \rangle^2} \geq \frac{2}{\langle \Sigma \rangle \langle T \rangle}$$

$$F(T|J_{\text{thr}}) \asymp \begin{cases} e^{-J_{\text{thr}} \phi_+(T/J_{\text{thr}})}, & J_{\text{thr}} > 0 \\ e^{J_{\text{thr}} \phi_-(-T/J_{\text{thr}})}, & J_{\text{thr}} < 0 \end{cases}$$

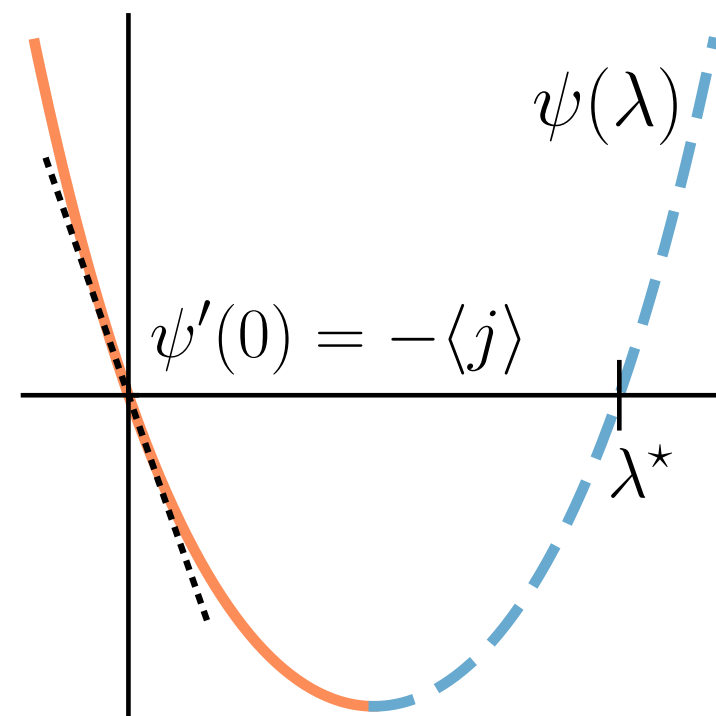
$$\phi_{\pm}(t) = tI(\pm 1/t)$$



$$\psi(\lambda) = -\min_j (I(j) + \lambda j)$$

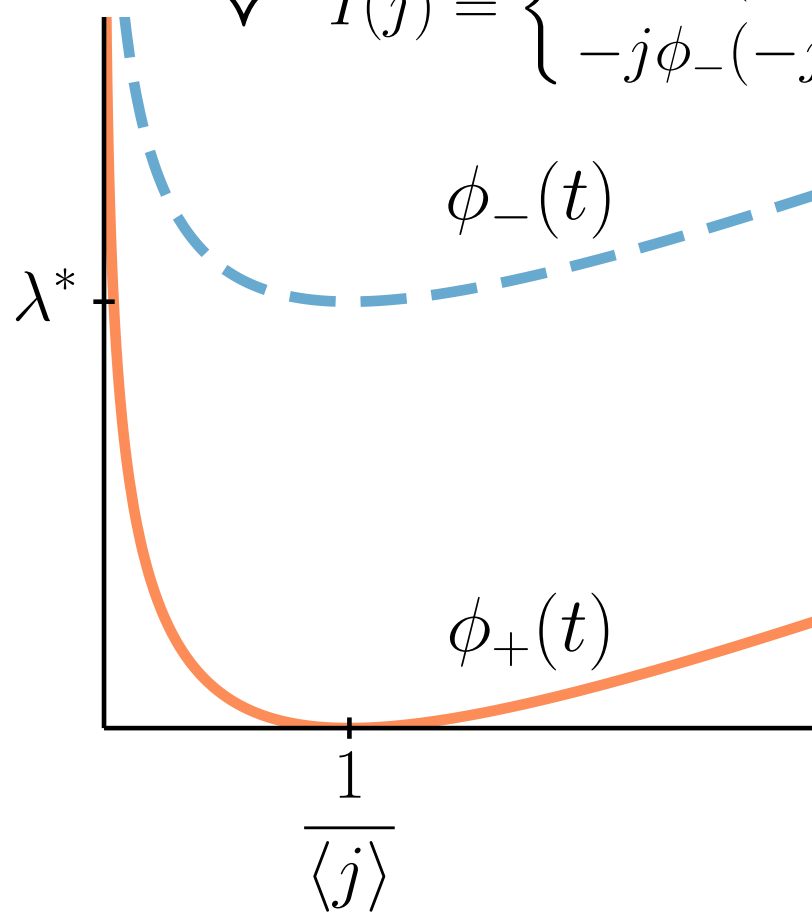


$$I(j) = -\min_\lambda (\psi(\lambda) + \lambda j)$$

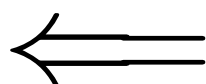
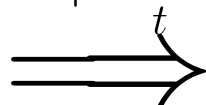


$$\phi_\pm(t) = tI(\pm t^{-1}) \quad \Uparrow$$

$$\Downarrow \quad I(j) = \begin{cases} j\phi_+(j^{-1}), & j \geq 0 \\ -j\phi_-(-j^{-1}), & j < 0 \end{cases}$$



$$g_\pm(\mu) = \mp \min_t (\phi_\pm(t) \pm \mu t)$$



$$\phi_\pm(t) = \mp \min_\mu (g_\pm(\mu) \pm \mu t)$$

$$\psi = g^{-1} \quad \Uparrow \Downarrow \quad g = \psi^{-1}$$

