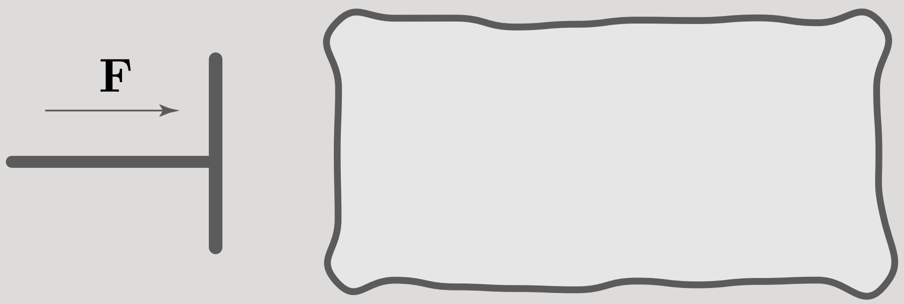
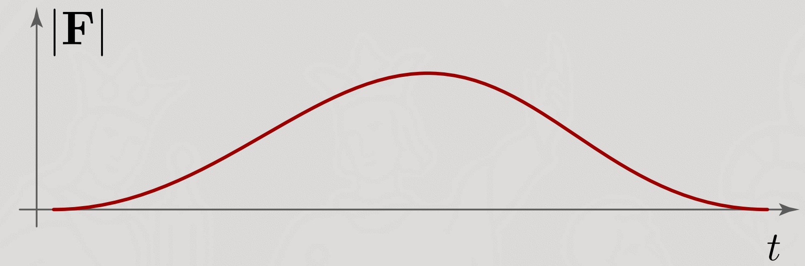
example: Jarzynski relation

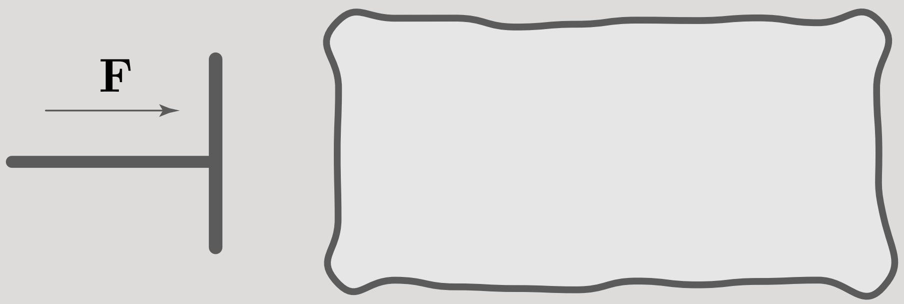


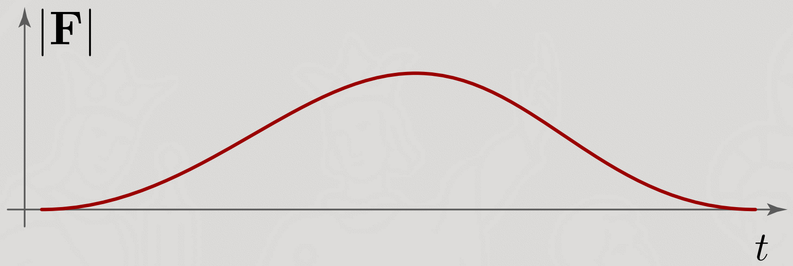


Work done: W

Free energy gain: ΔF

thermodynamics: $\langle W \rangle \geq \Delta F$





Work done: W

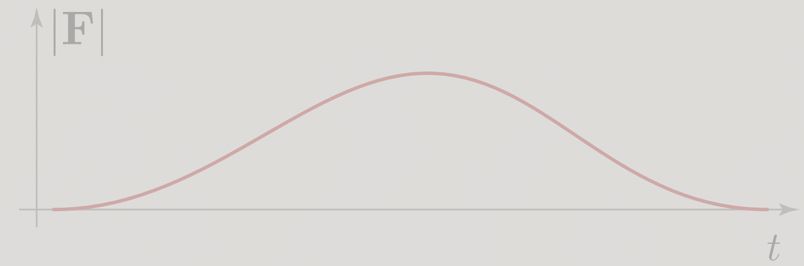
Free energy gain: ΔF

thermodynamics: $\langle W \rangle \geq \Delta F$

Jarzynski relation (1997):

$$\boxed{\left\langle e^{-\frac{1}{T}(W-\Delta F)} \right\rangle = 1}$$

implies existence of processes in which work is gained out of fluctuations!



FR: describe the interplay of fluctuations and dissipation out of equilibrium

Work done: W

Free energy gain: ΔF

thermodynamics: $\langle W \rangle \geq \Delta F$

Jarzynski relation (1997):

$$\boxed{\left\langle e^{-\frac{1}{T}(W-\Delta F)} \right\rangle = 1}$$

implies existence of processes in which work is gained out of fluctuations!

▷ literature: focus on fluctuation relations as rigorous bounds in nonequilibrium statistical mechanics

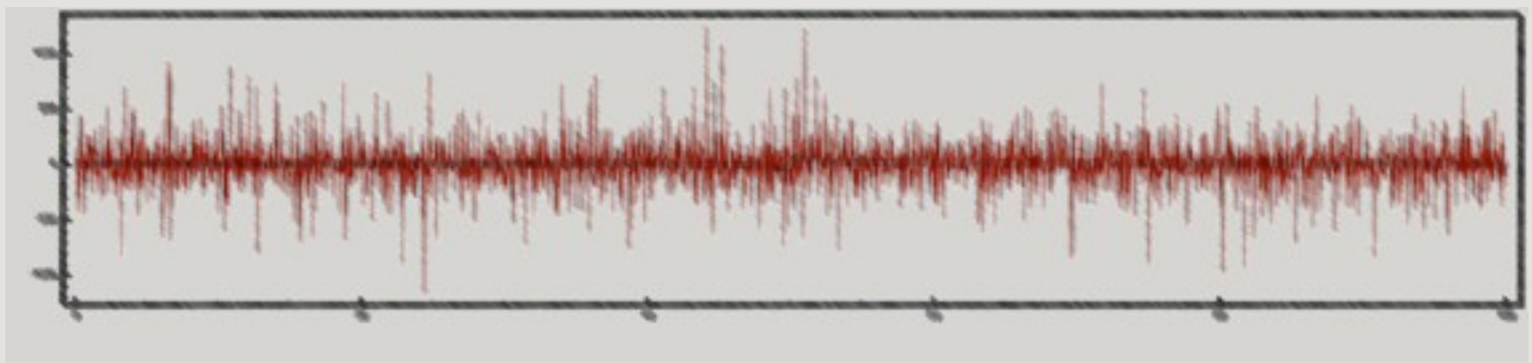
▷ here: FR as diagnostic tool in transport

transient fluctuation relations in transport

Chernogolovka, Sep. 20. 10

Boris Narozhny, Alessandro de Martino, Alexander Altland, Cologne University

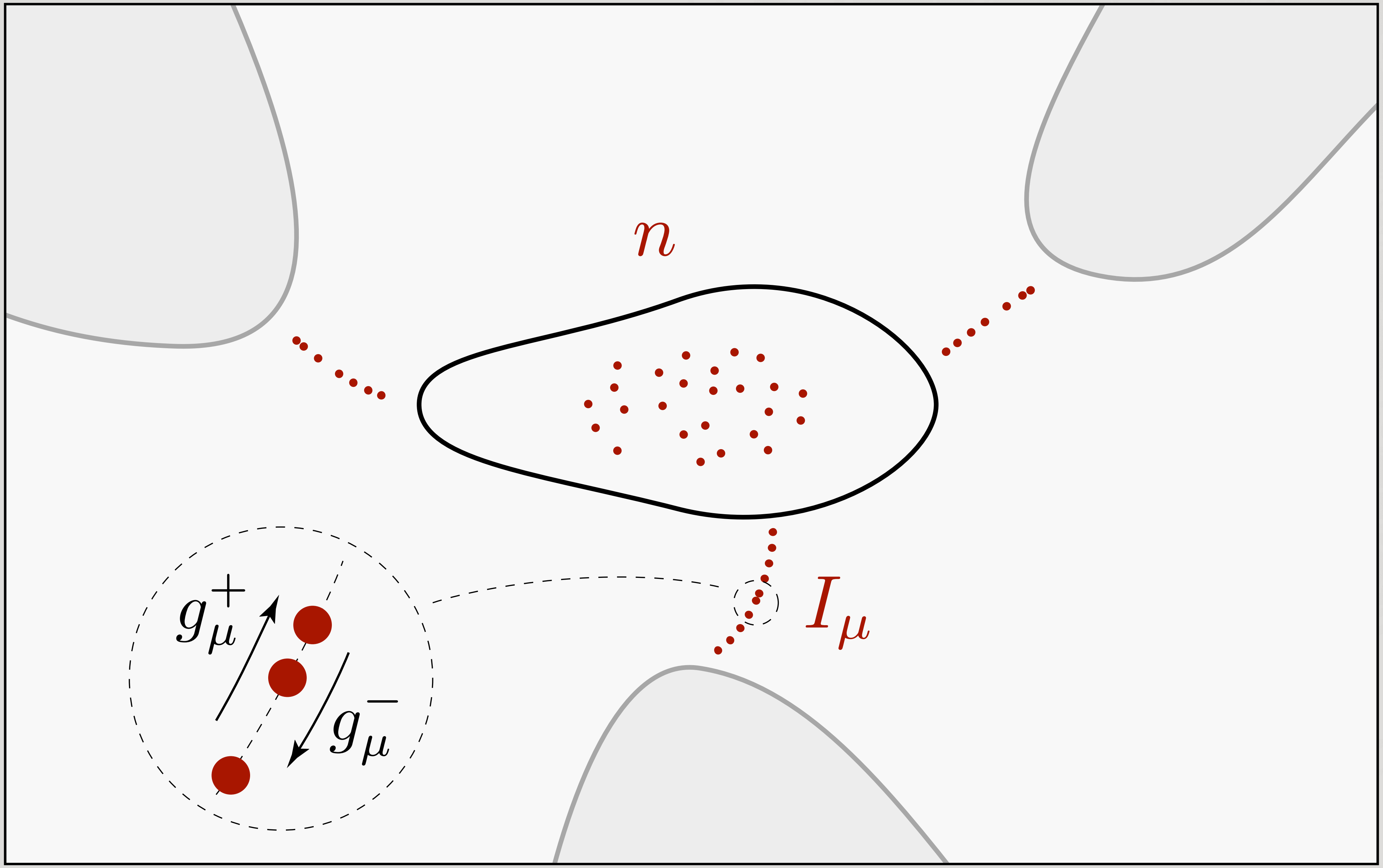
Reinhold Egger, Düsseldorf University



- ▷ master equation
- ▷ stochastic path integral
- ▷ fluctuation relations
- ▷ example: RC circuit

arXiv:1007.1826, 1005.4662

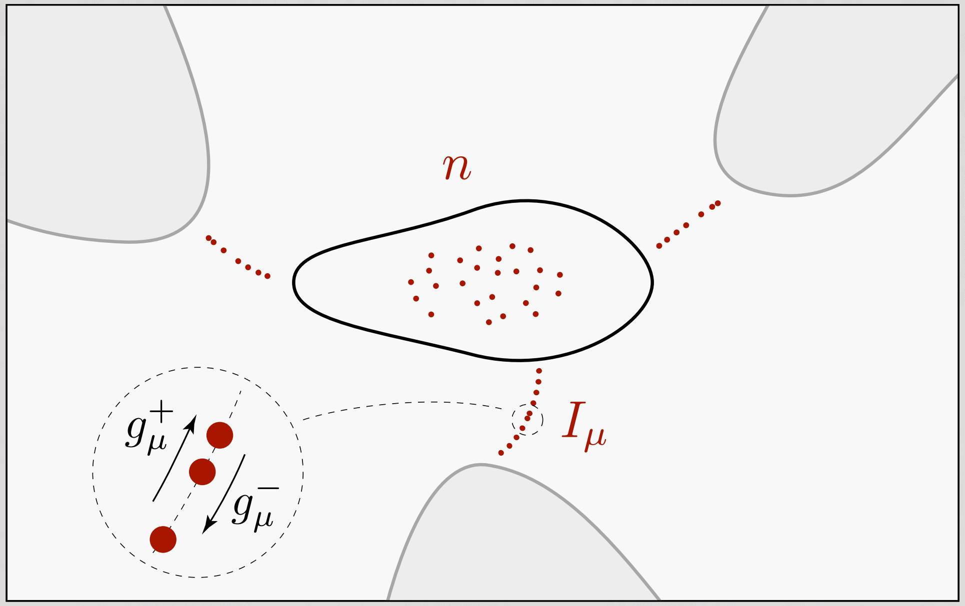
master equation
and
stochastic path integral


n
I_μ
g_μ^+
g_μ^-

setup

▷ describe setup in terms of system particle number and currents

$$d_t n + \sum_{\nu=1}^{M} I_\nu = 0$$



quantity of interest:

$$\{I_1, \ldots, I_\mu\}[g_1^\pm, \ldots, g_\mu^\pm]$$

setup

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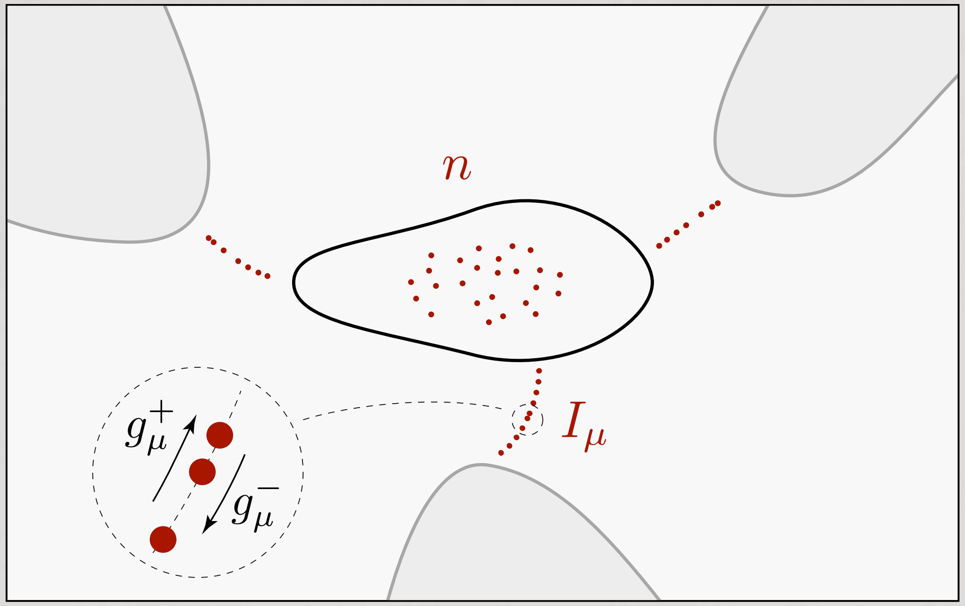

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- describe dynamics of particle currents in terms of rates

$$\frac{g_\nu^+}{g_\nu^-} = \exp\left(-\beta(\partial_n U - f_\nu)\right)$$

setup

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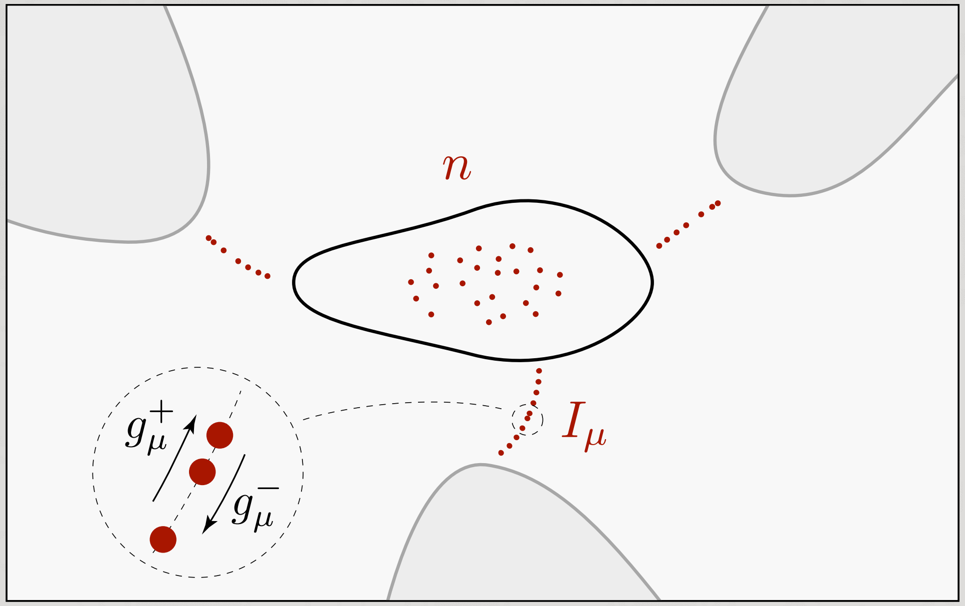

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▷ describe dynamics of particle currents in terms of rates

$$\frac{g_\nu^+}{g_\nu^-} = \exp\left(-\beta(\partial_n U - f_\nu)\right)$$

▷ local energy change due to entering particle:

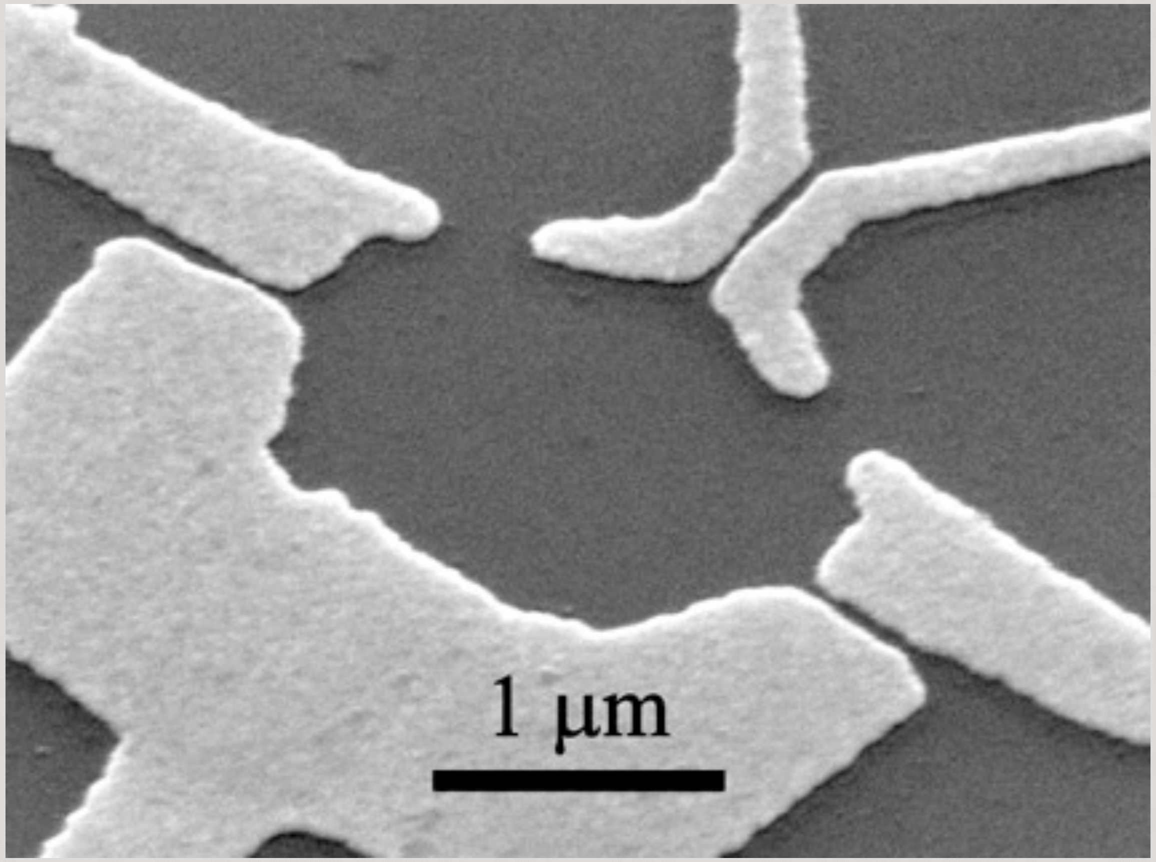
$$\Delta E_\nu(n) = U(n+1) - U(n) - f_\mu \simeq \partial_n U(n) - f_\nu$$

internal energy

driving force

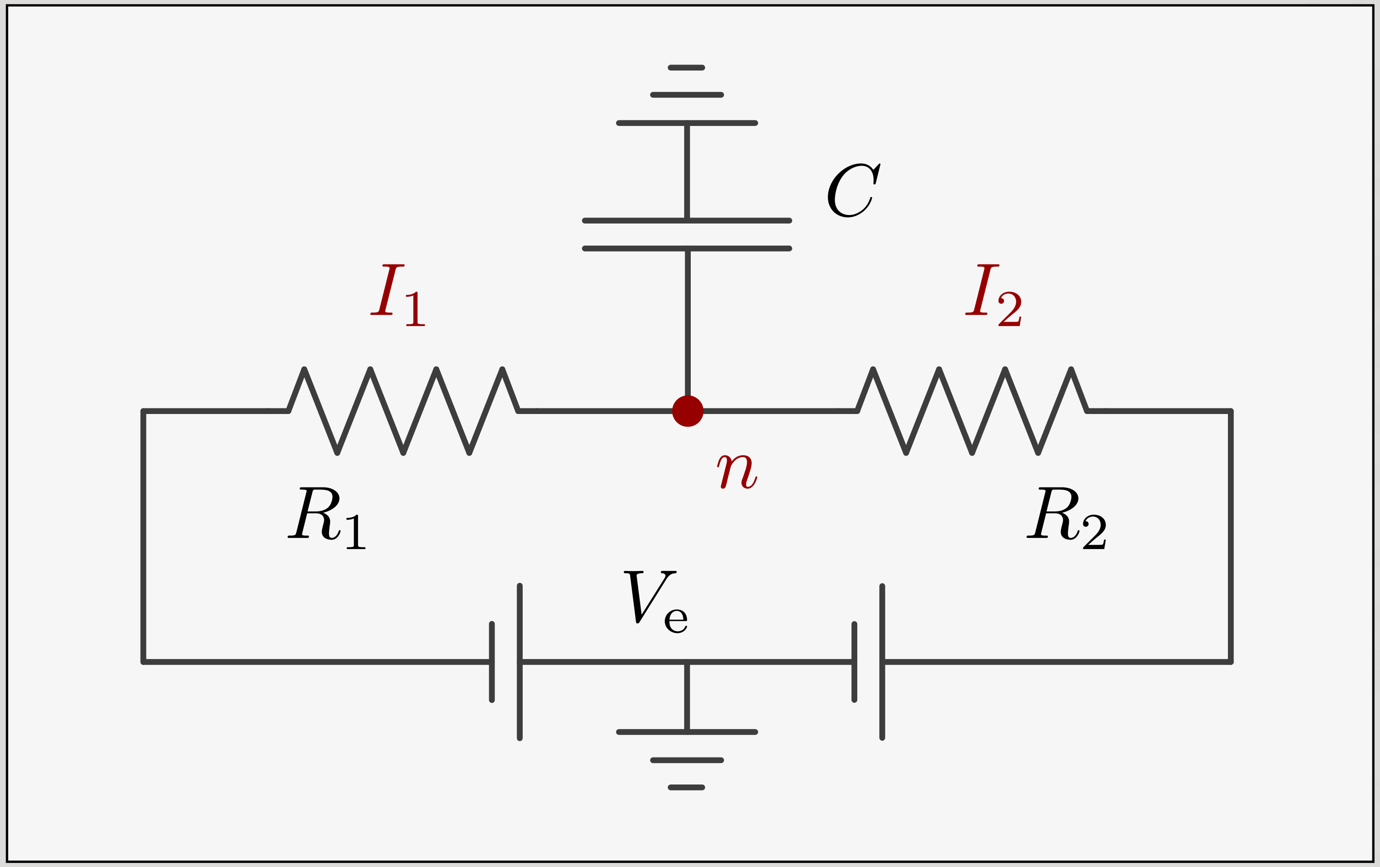
example

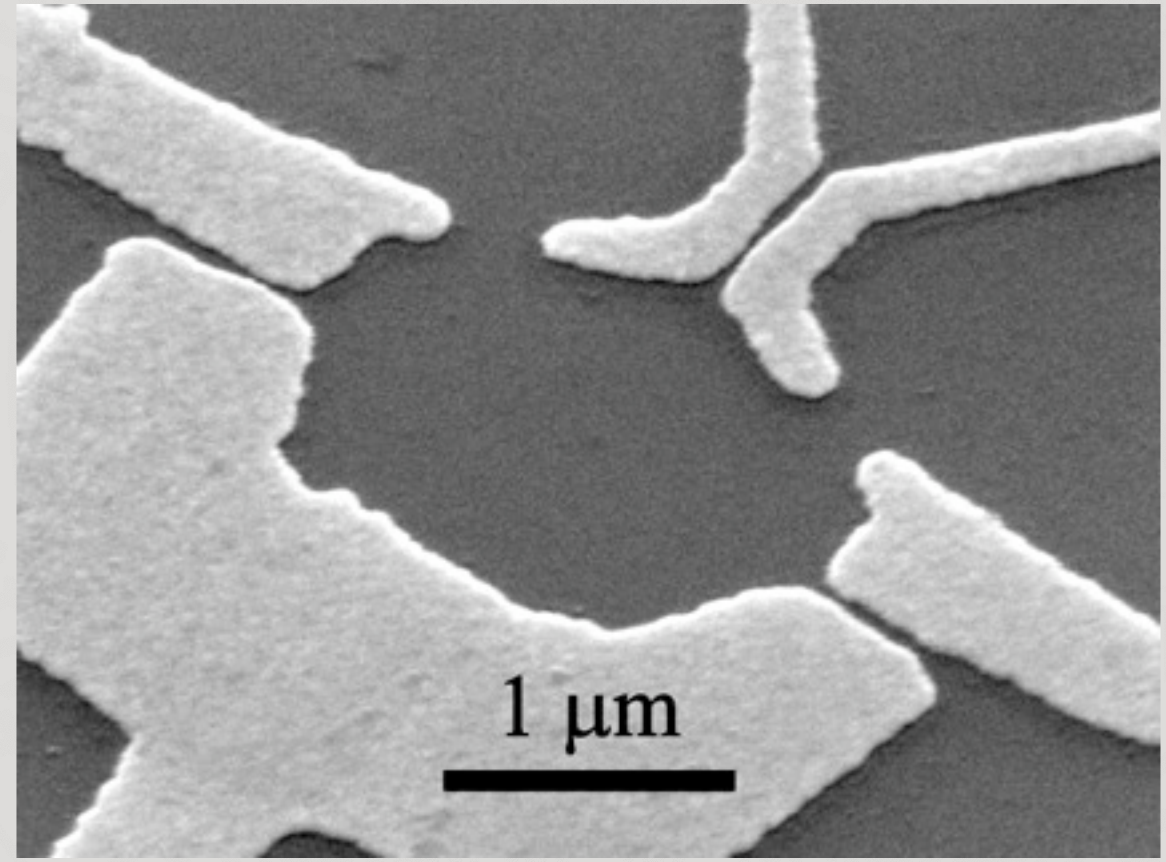
mesoscopic RC circuit



example

mesoscopic RC circuit





- island charge
- internal energy: $U(n) = \dfrac{n^2}{2C}$
- driving: $f_\nu = (-)^\nu \dfrac{V_\mathrm{e}}{2}$

System	Variable n	$U(n)$	f_ν
electronic circuits (see Sec. IV)	charge	charging energy	bias voltages
molecular motors[35]	mechanochemical state of motor protein	load potential	ATP concentration
chemical reaction networks[36]	number of reaction partners	internal energy	chemostat concentrations
adaptive evolution[37]	allele frequencies	log equilibrium dist.	fitness gradients

master equation

▷ consider probability $P_t(n)$

$$\partial_t P_t(n) = -\hat{H}_g P_t(n),$$

$$\hat{H}_g(n,\hat{p}) = \sum_{\pm,\nu=1}^{M} \left(1 - e^{\mp\hat{p}}\right) g^{\pm}_{\nu,t}(n),$$

(one step) master equation

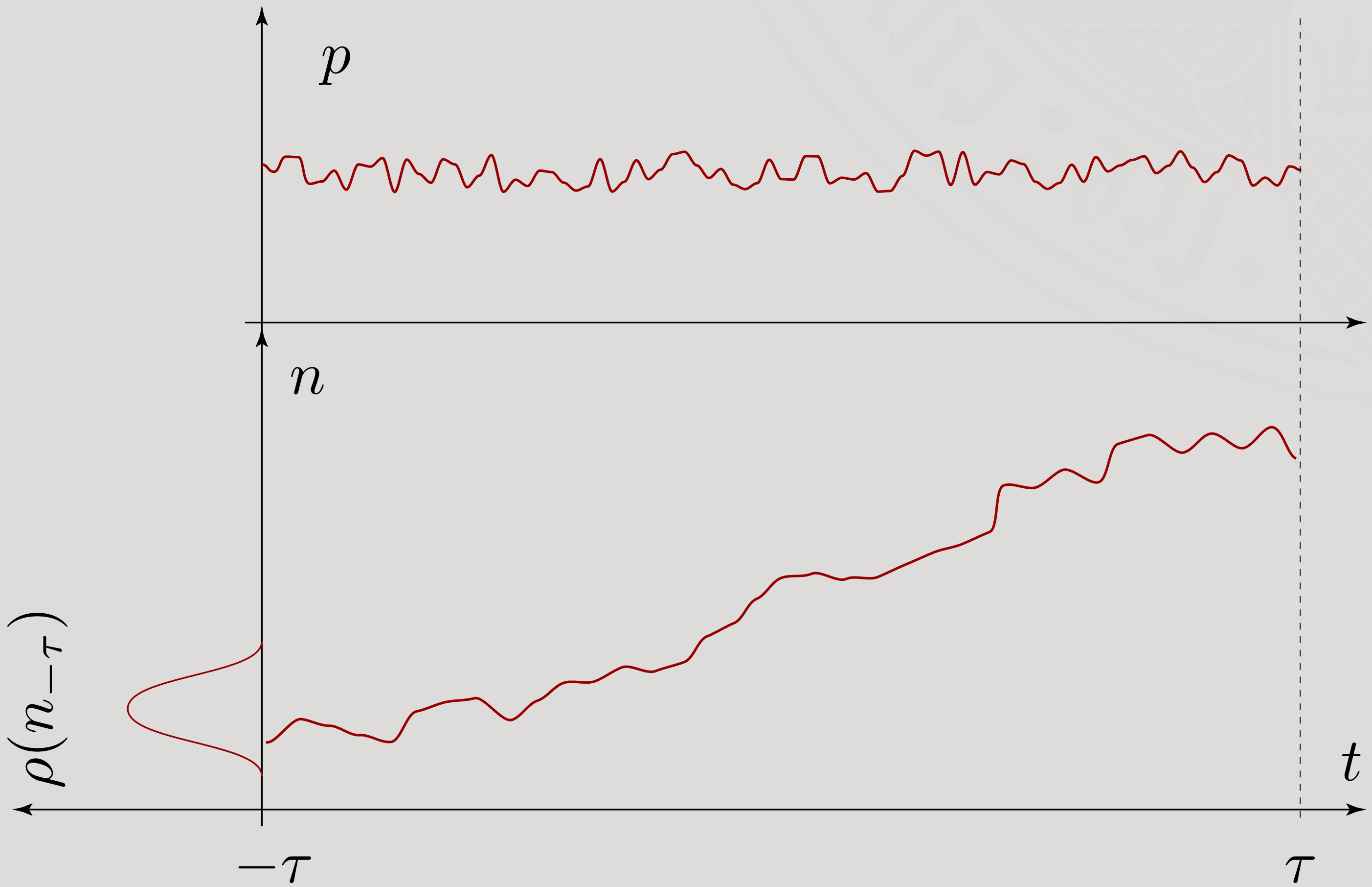
where $e^{\pm\hat{p}} f(n) = f((n \pm 1),$ $\qquad [\hat{p},\hat{n}] = 1$

stochastic path integral

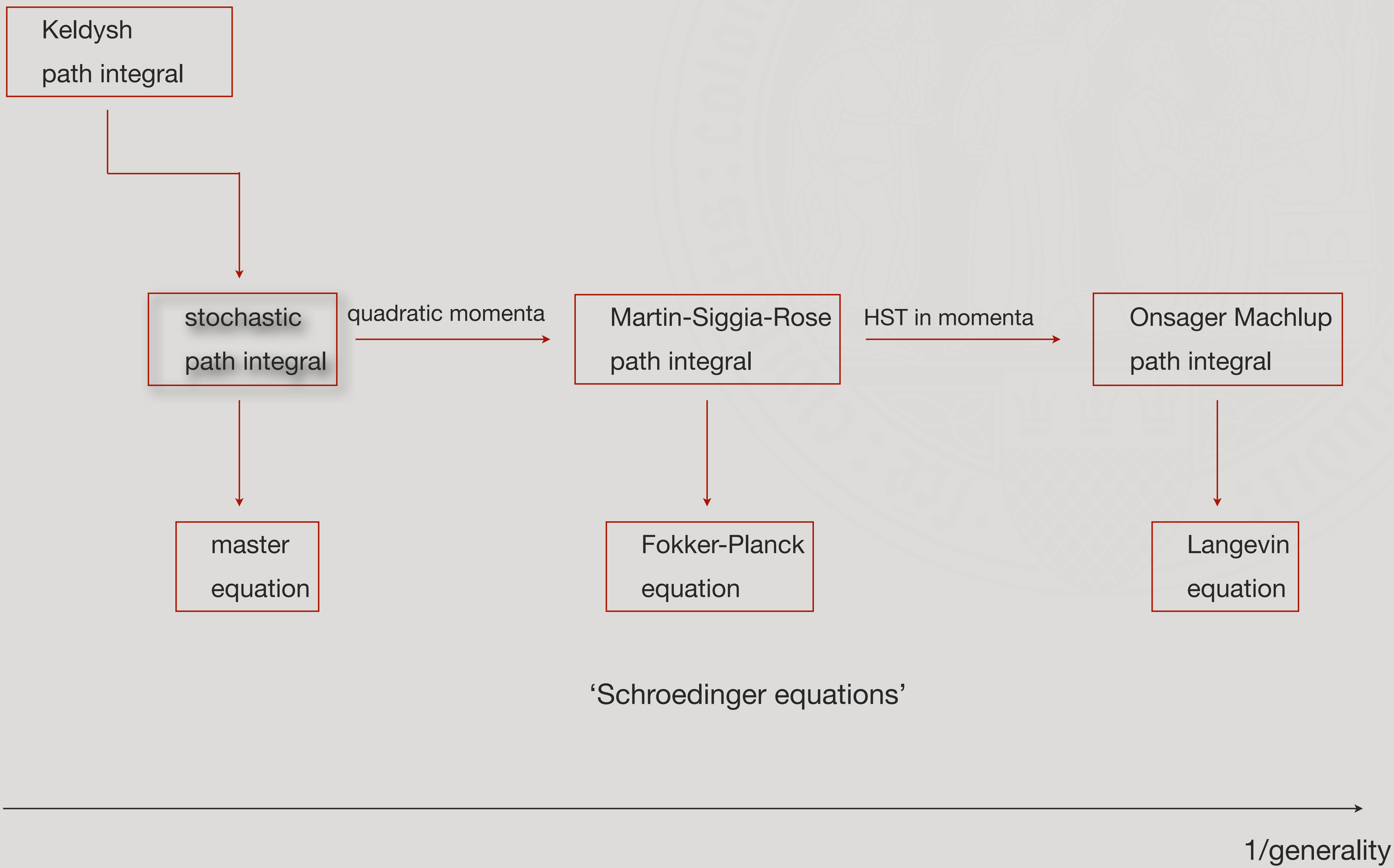
- represent probability in terms of (imaginary time) stochastic path integral

$$
\boxed{
\begin{aligned}
Z_f \equiv 1 = \sum_n P_t(n) &= \int D(n,p)\, e^{-S_g[n,p]} \rho(n_{-\tau}), \\
S_g[n,p] &= -\int_{-\tau}^{\tau} dt\, (p\dot{n} - H_g(n,p))
\end{aligned}
}
$$

Kubo et al., 73



ramifications



information from the path integral

- functional partition function normalized to unity. Want to obtain currents.

$$H_g(n,p) \to H_g(n,p,\chi) \equiv \sum_{\nu,\pm} \left(1 - e^{\mp(p - i\chi_\nu)}\right) g_\nu^\pm(n)$$

cf. vector potential

- generating functional (Pilgram et al. 03)

$$Z_f[\chi] = \int D(n,p)\, e^{-S_g[n,p,\chi]} \rho(n_{-\tau}),$$

$$S_g[n,p,\chi] \equiv - \int_{-\tau}^{\tau} dt\, (p\dot{n} - H_g(n,p,\chi))\,.$$

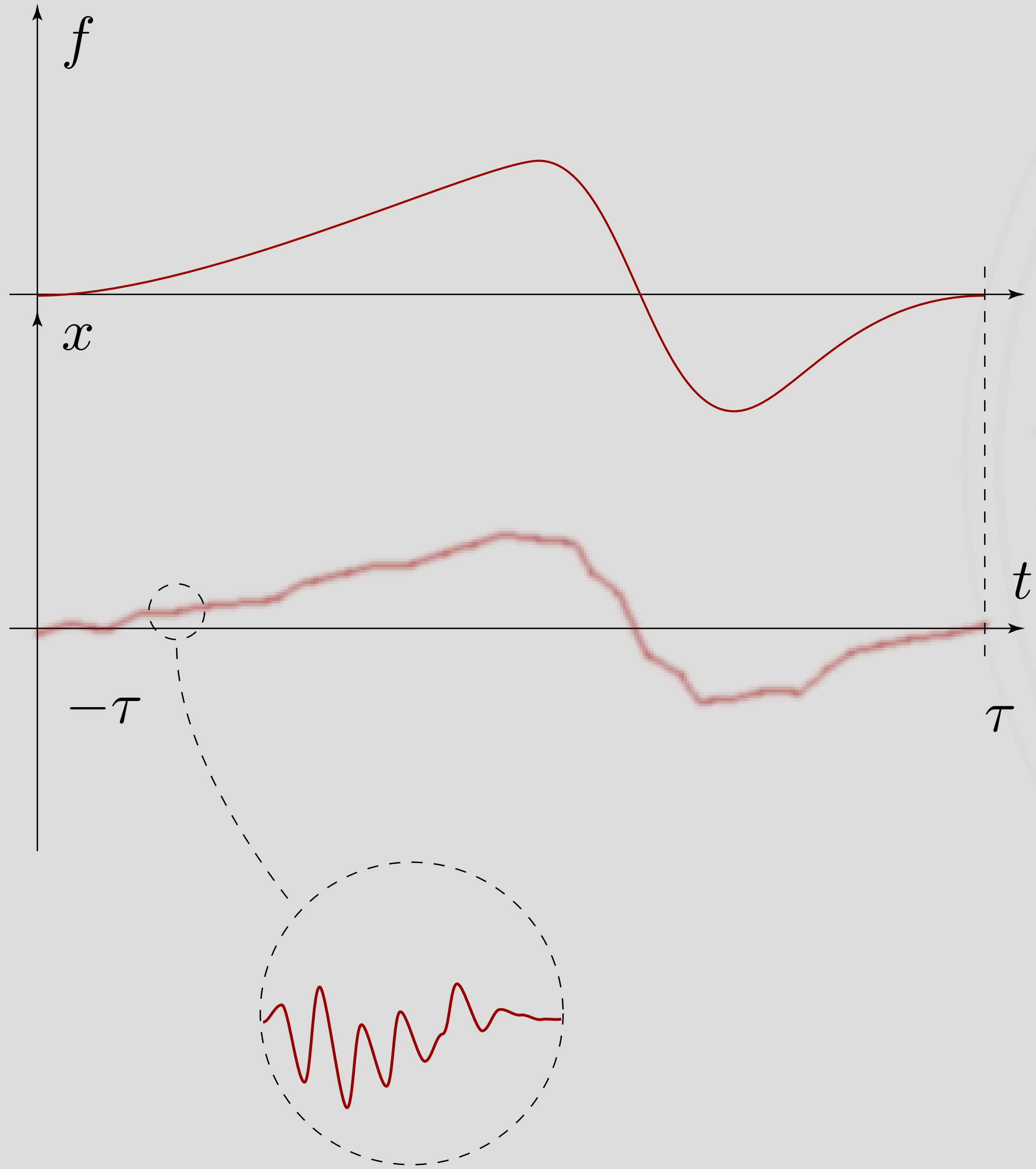
- current statistics

$$Z_f[\chi] = \left\langle e^{-i \sum_\nu \int_{-\tau}^{\tau} dt\, \chi_\nu I_\nu} \right\rangle_f ,$$

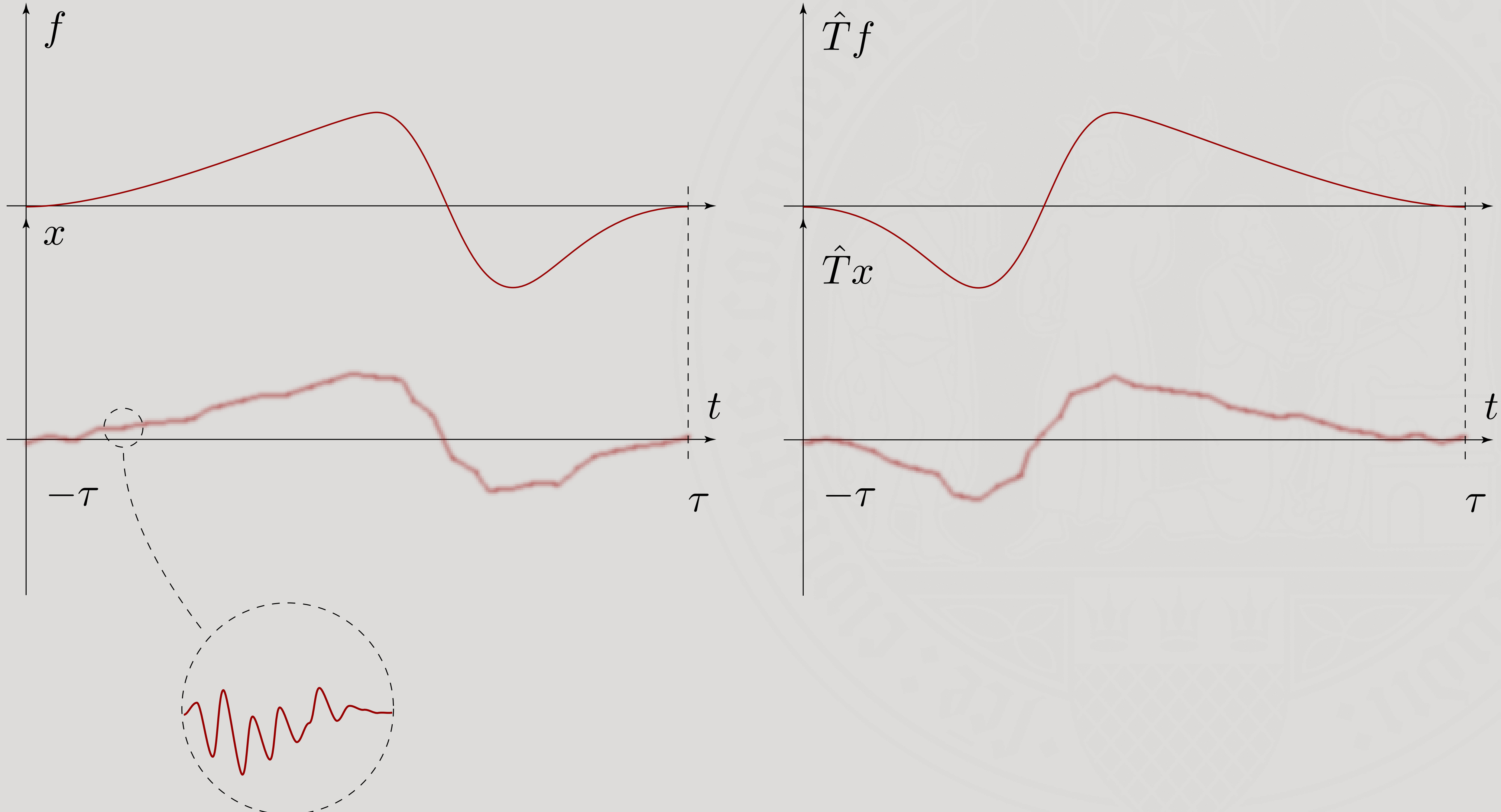
$$\langle I_{\nu_1,t_1} I_{\nu_2,t_2} \ldots \rangle = \frac{i\delta}{\delta\chi_{\nu_1,t_1}} \frac{i\delta}{\delta\chi_{\nu_2,t_2}} \ldots \Big|_{\chi=0} Z_f[\chi] \Leftrightarrow$$

fluctuation relations

fluctuation relations

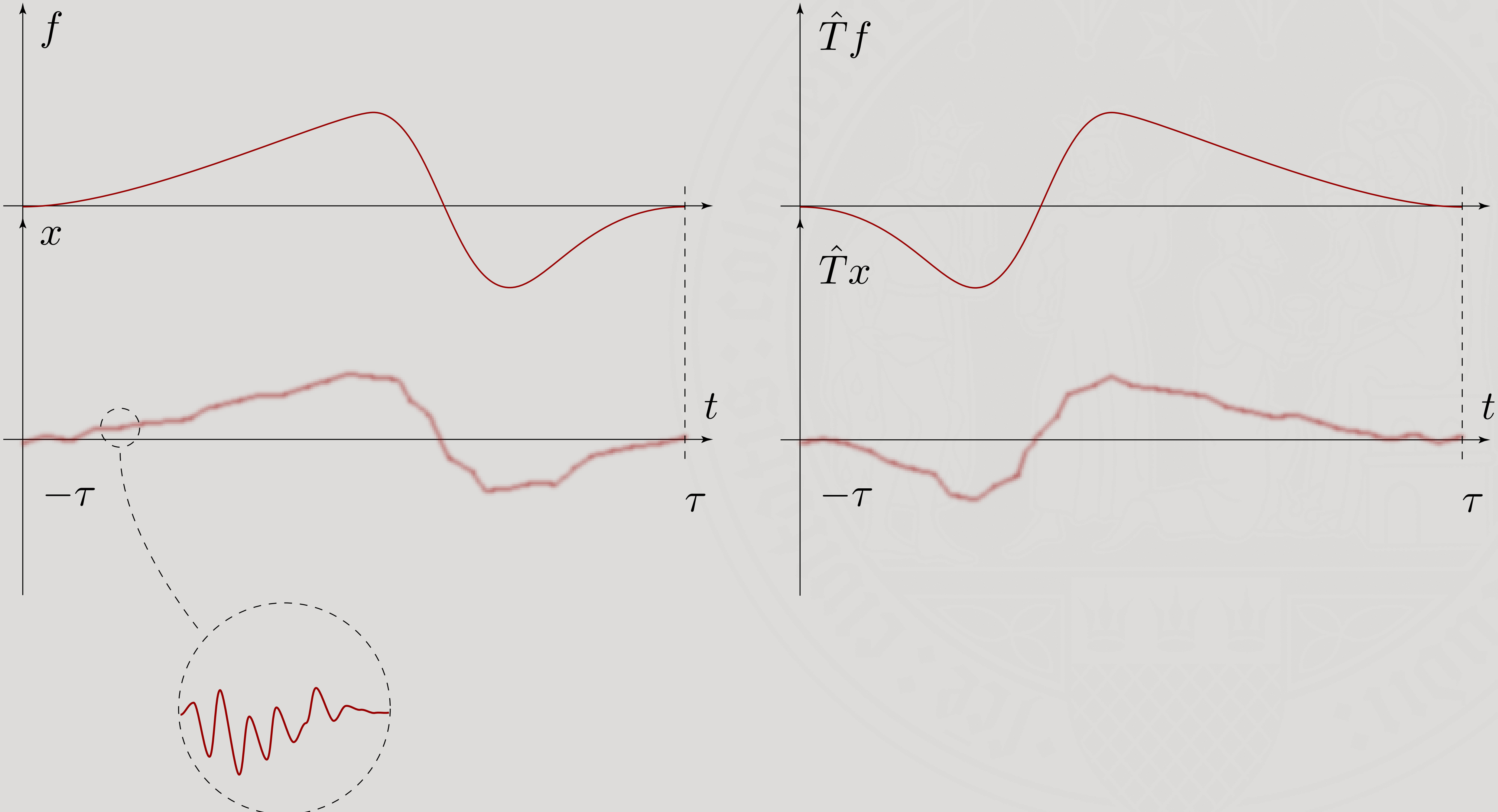


fluctuation relations

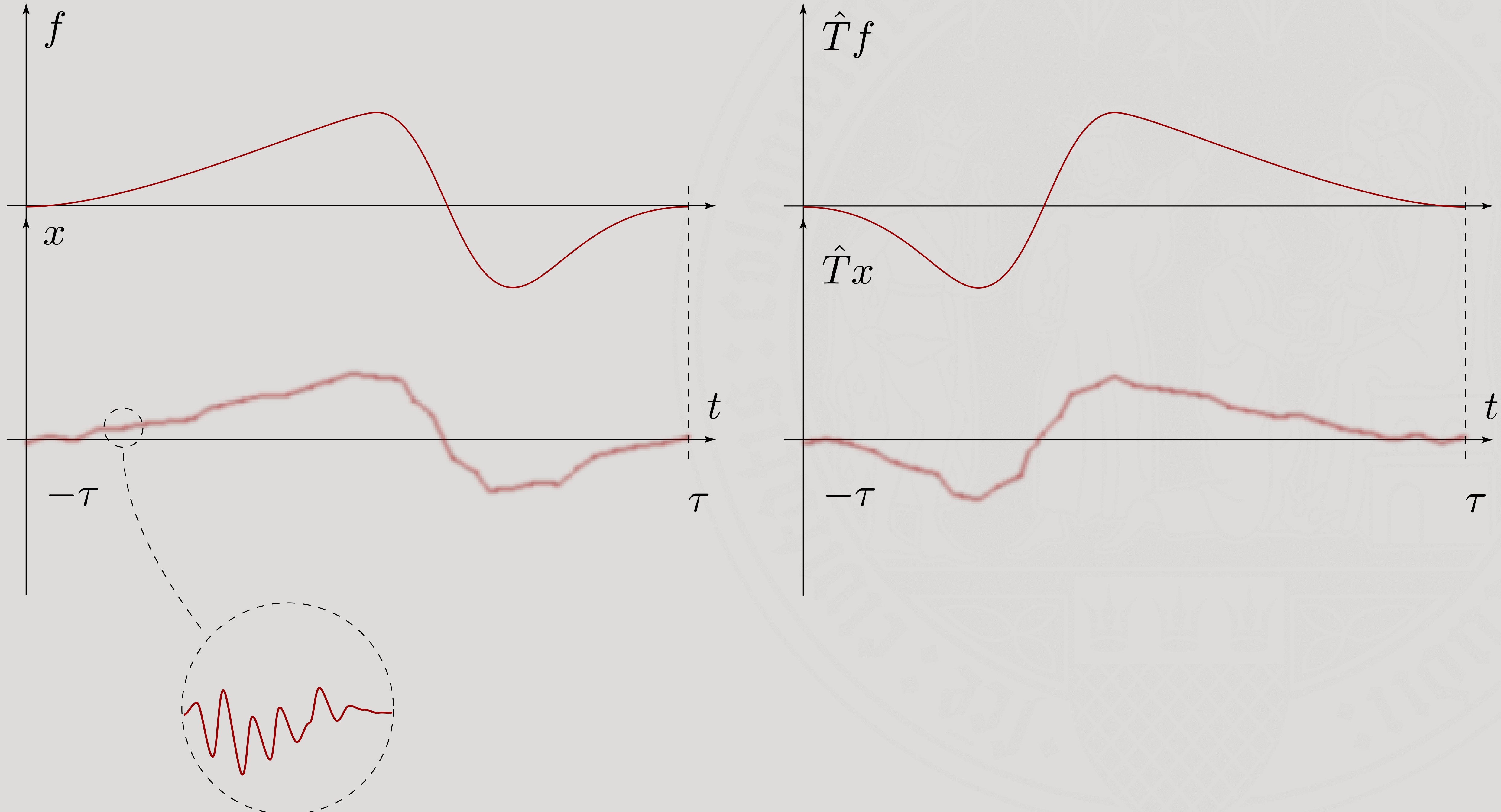


$$P_f[x] = P_b[\hat{T}x]$$

fluctuation relations



$$P_f[x] = P_b[\hat{T}x] \times e^{\beta Q[x]}$$



$$P_f[x] = P_b[\hat{T}x] \times e^{\beta Q[x]} \times e^{\beta(U[x]-\Delta F)} = P_b[\hat{T}x] \times e^{\beta(W[x]-\Delta F)}$$

time reversal

$$\boxed{S_g[n,p,\chi] \quad = \quad S_{\hat{T}g}[\hat{T}n, \hat{T}(p-\beta\partial_n U), \hat{T}(\chi+i\beta f)] + \beta[U(n_\tau)-U(n_{-\tau})].}$$

$$X = n, g, U \qquad X_t \to (\hat{T}X)_t = X_{-t}$$

$$X = p, \chi_\nu, I_\nu \qquad X_t \to (\hat{T}X)_t = -X_{-t}$$

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$$Z_f[\chi] \quad = \quad \int D(n,p) e^{-S_{\mathcal{T}g}[n,p,\mathcal{T}(\chi+i\beta f)]} \rho(n_{-\tau}) = Z_b[\mathcal{T}(\chi+i\beta f)].$$

$$\boxed{S_g[n,p,\chi] \quad = \quad S_{\hat{T}g}[\hat{T}n, \hat{T}(p-\beta\partial_n U), \hat{T}(\chi+i\beta f)] + \beta[U(n_\tau) - U(n_{-\tau})].}$$

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fluctuation relations

functional fluctuation relations

functional fluctuation relations

$$\boxed{P_f[I] = P_b[\hat{T}I]e^{-\beta\int_{-\tau}^{\tau}dt\,\sum_\nu f_\nu I_\nu}}$$

functional Crooks relation (cf. Bochkov & Kusovlev, 81)

$$\boxed{\left\langle e^{\beta\int_{-\tau}^{\tau}dt\,\sum_\nu f_\nu I_\nu}\right\rangle_f = 1}$$

functional Jarzynski relation

applications

- information on rare event statistics
- generalized Onsager relations for AC transport
- information on effective distributions prevalent in the system
- information on joint statistics of particle transport and energy

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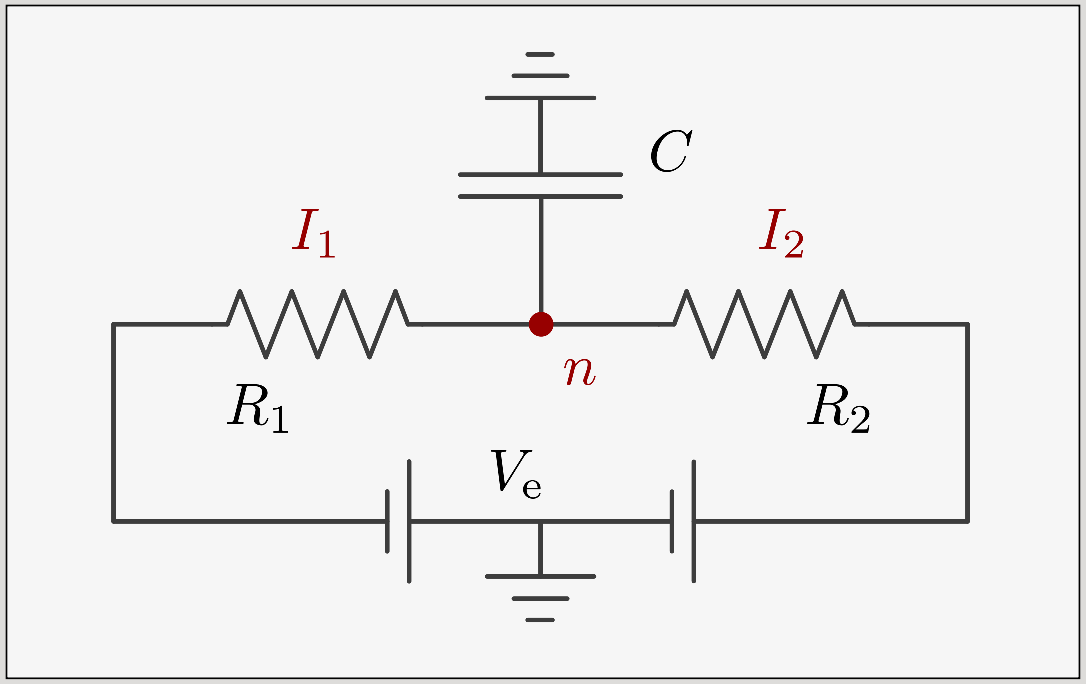
application: mesoscopic RC circuit



- two terminal setup
- system parameters: $G_\nu = 20\dfrac{e^2}{h}$

  V fluctuates at scales larger than RC-time

  V/T large (shot noise regime) or small (thermal regime)

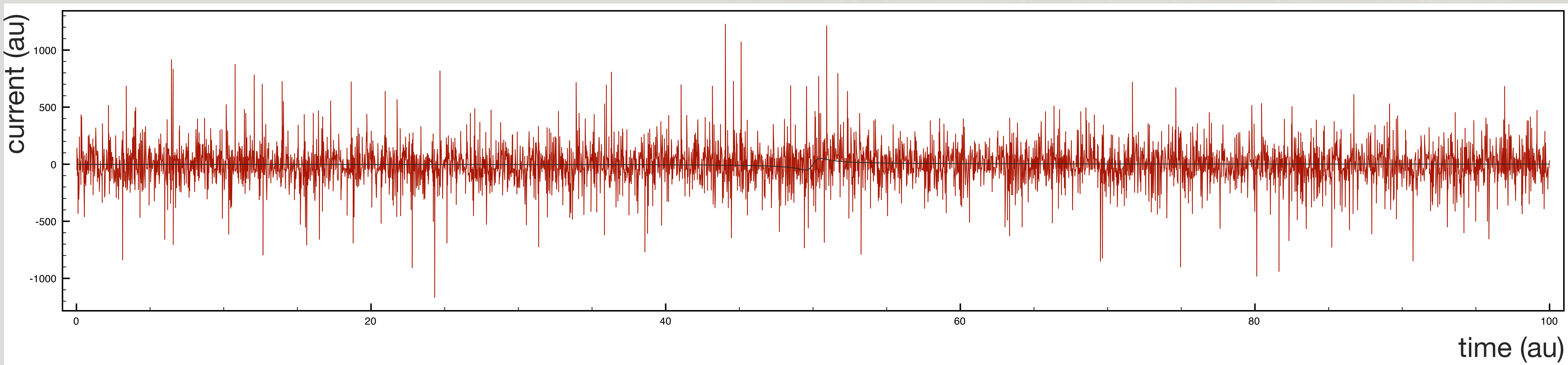
- microscopic description through master equation with rates

$$g^{\pm}_{\nu,t}(n) = G_\nu \frac{\pm\kappa_{\nu,t}(n)}{e^{\pm\beta\kappa_{\nu,t}(n)} - 1}, \quad \kappa_{\nu,t}(n) = \partial_n U(n) + (-)^\nu \frac{V_t}{2}.$$

applications I: rare event statistics

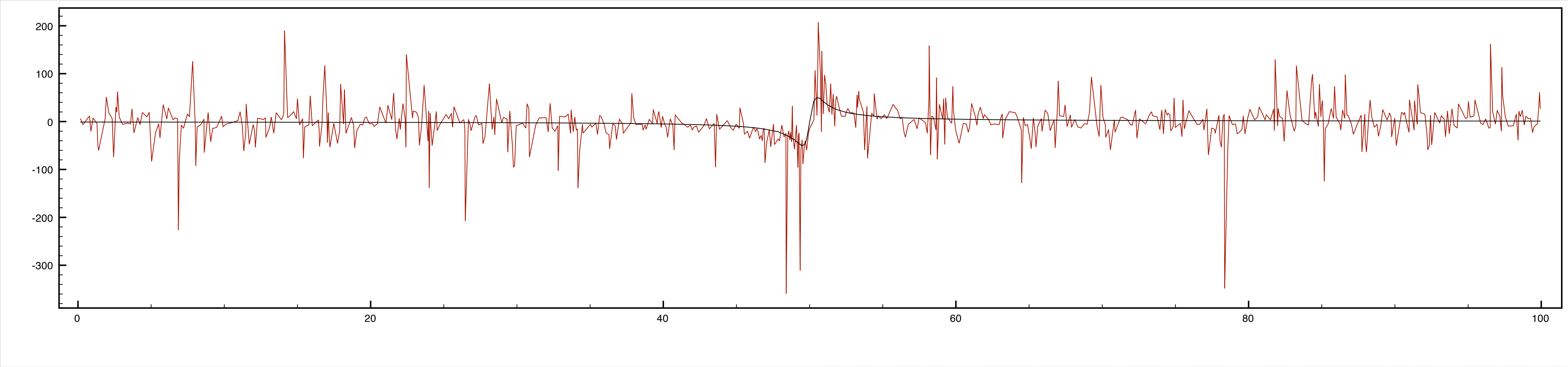
current fluctuations

- near equilibrium $T/V \gg 1$: thermal (Johnson-Nyquist) fluctuations



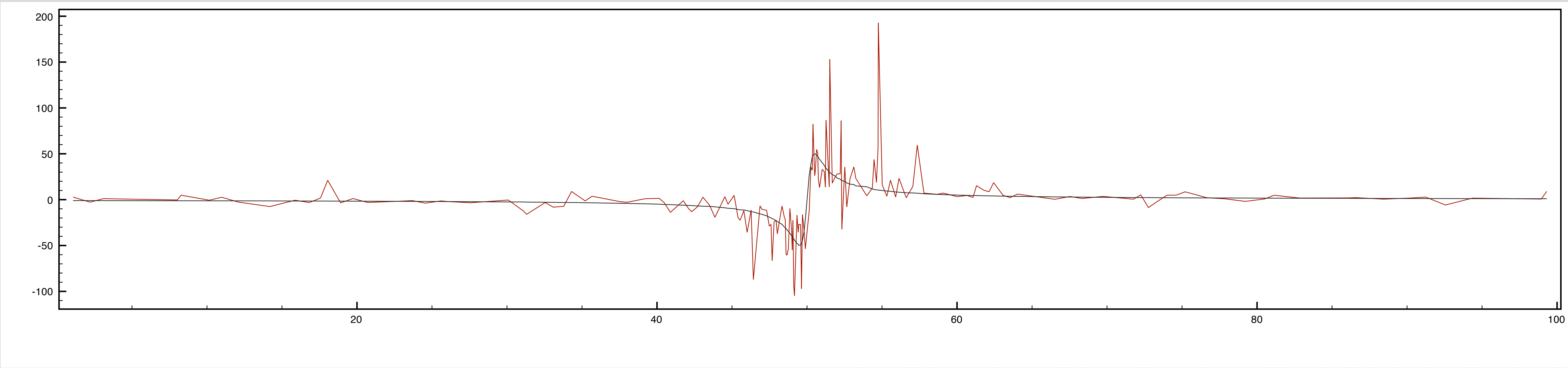
current fluctuations

- crossover regime $T/V \simeq 1$



current fluctuations

- out of equilibrium $T/V \ll 1$



current fluctuations vs. Jarzynski relation

$$\boxed{\left\langle e^{\beta \int_{-\tau}^{\tau} dt\, V(I_2 - I_1)} \right\rangle_f = 1}$$

functional Jarzynski relation

off equilibrium: probes rare events through variable $X \equiv e^{\beta \int_{-\tau}^{\tau} dt\, V(I_2 - I_1)}$

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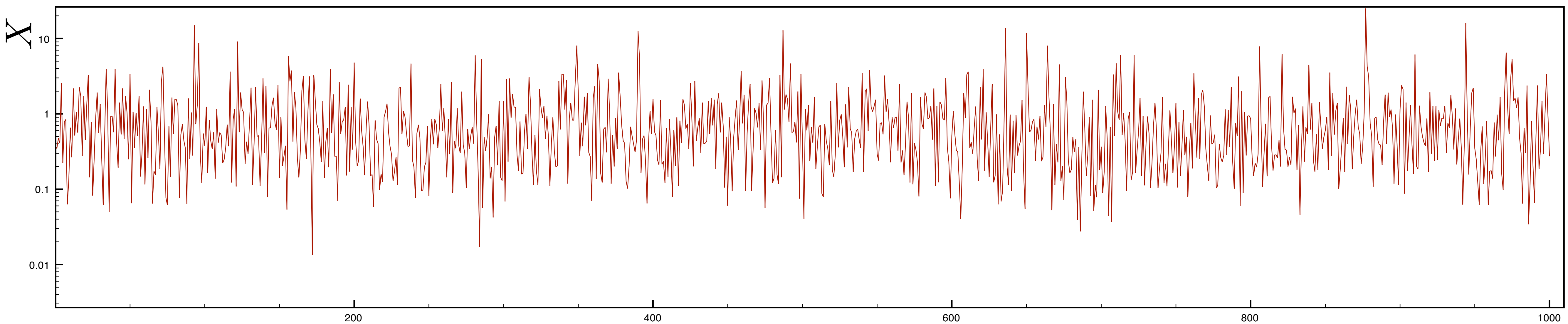


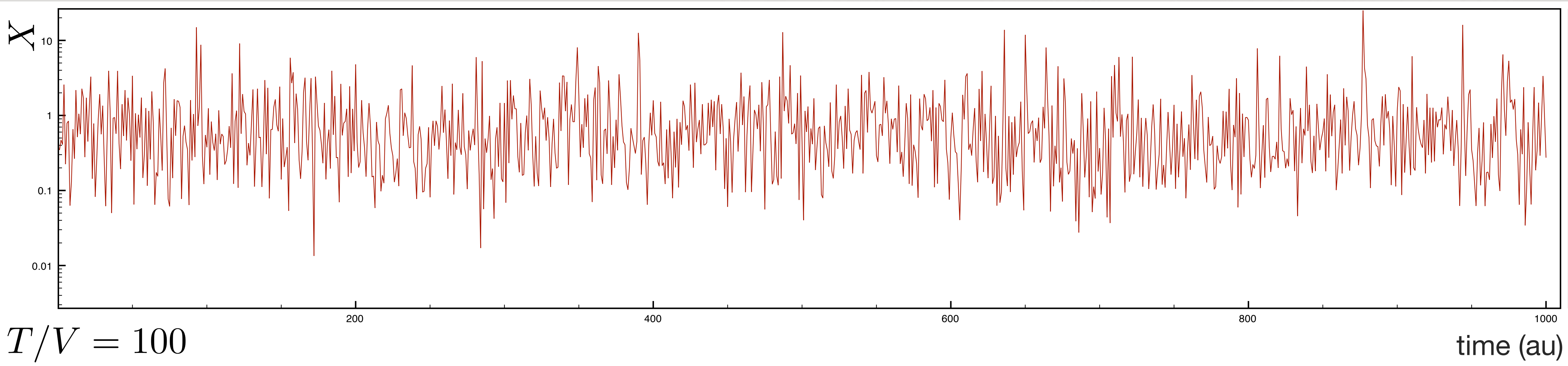
$T/V = 100$

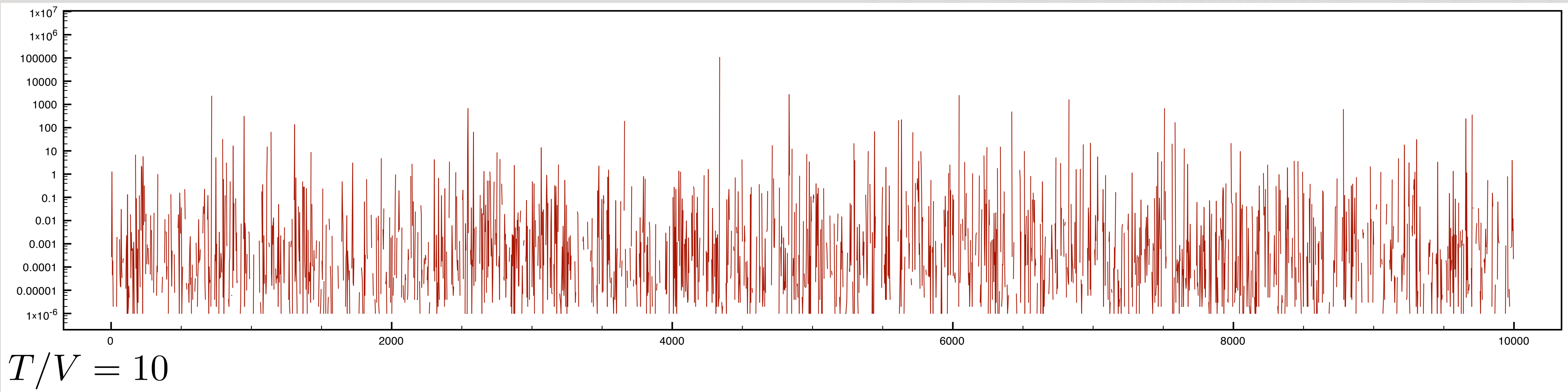
current fluctuations vs. Jarzynski relation

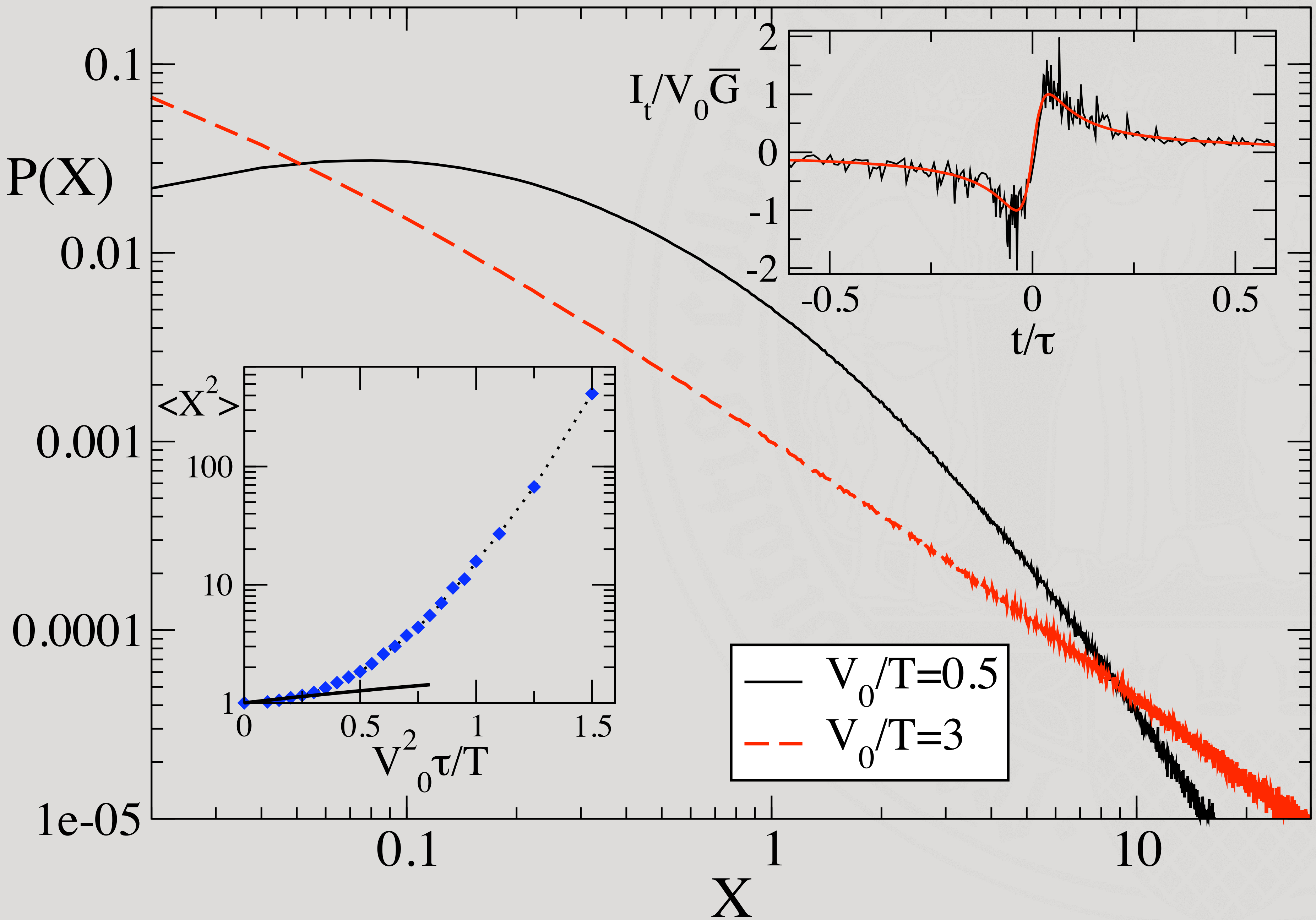
$$\boxed{\left\langle e^{\beta \int_{-\tau}^{\tau} dt\, V(I_2 - I_1)} \right\rangle_f = 1}$$

functional Jarzynski relation

off equilibrium: probes rare events through variable $X \equiv e^{\beta \int_{-\tau}^{\tau} dt\, V(I_2 - I_1)}$





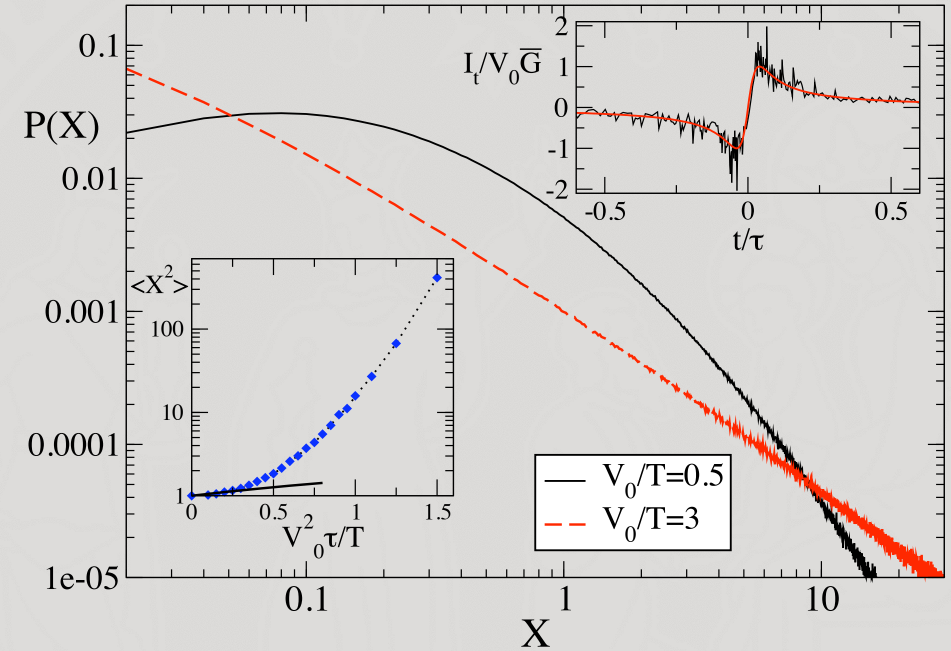


path integral can be applied to estimate fluctuations of X

thermal regime: $\langle X^2\rangle_f \sim e^{\tau\beta(f_1-f_2)^2\frac{g_1g_2}{g_1+g_2}}$

shot noise regime: $\langle X^2\rangle_f \sim e^{4\tau|\langle I_1\rangle\langle I_2\rangle|^{1/2}e^{\beta|f_1-f_2|/2}}$

fluctuation statistics



optimal fluctuation approach to path integral

thermal: Gaussian fluctuations around mean

$$\langle X^2 \rangle_f \sim e^{\tau \frac{V^2}{T} \frac{g_1 g_2}{g_1+g_2}} = e^{\tau \langle I \rangle \frac{V}{T}}$$

shot noise: rare event statistics

$$\langle X^2 \rangle_f \sim e^{4\tau |\langle I_1 \rangle \langle I_2 \rangle|^{\frac{1}{2}}} e^{\frac{V}{2T}}$$

fluctuation statistics of X sensitive probe of nonequilibrium transport processes

applications II: distribution diagnostics

use fluctuation relations to explore state of the system

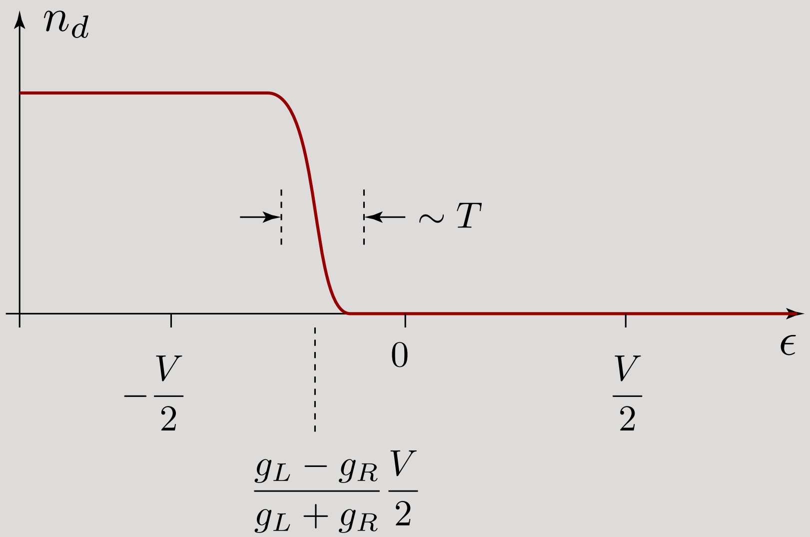
derivation of FRs based on balance relation $$\frac{g_\nu^+}{g_\nu^-} = \exp\left(-\beta(\partial_n U - f_\nu)\right)$$

model dot distribution functions

use fluctuation relations to explore state of the system

derivation of FRs based on balance relation $\dfrac{g_\nu^+}{g_\nu^-} = \exp\left(-\beta(\partial_n U - f_\nu)\right)$

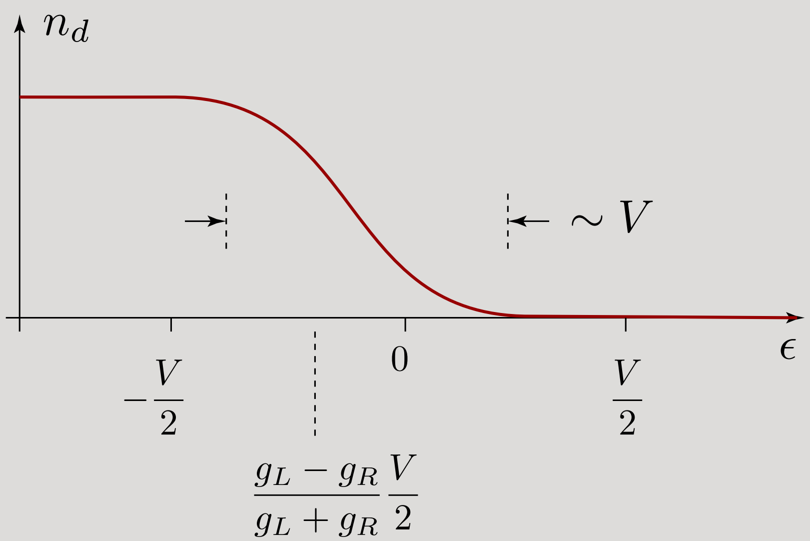
model dot distribution functions



$\tau_{ee} < \tau_d$, cooled

+

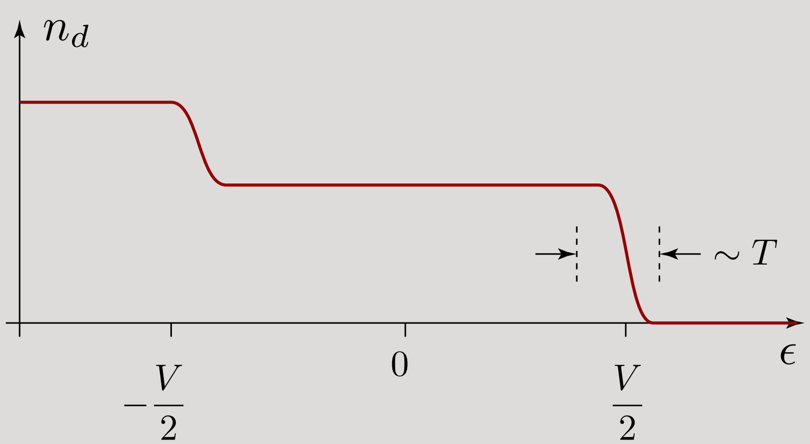
'standard' FR



$\tau_{ee} < \tau_d$, isolated

-

effective or extended FR



$\tau_{ee} > \tau_d$

(+)

standard FR

Effective fluctuation relations

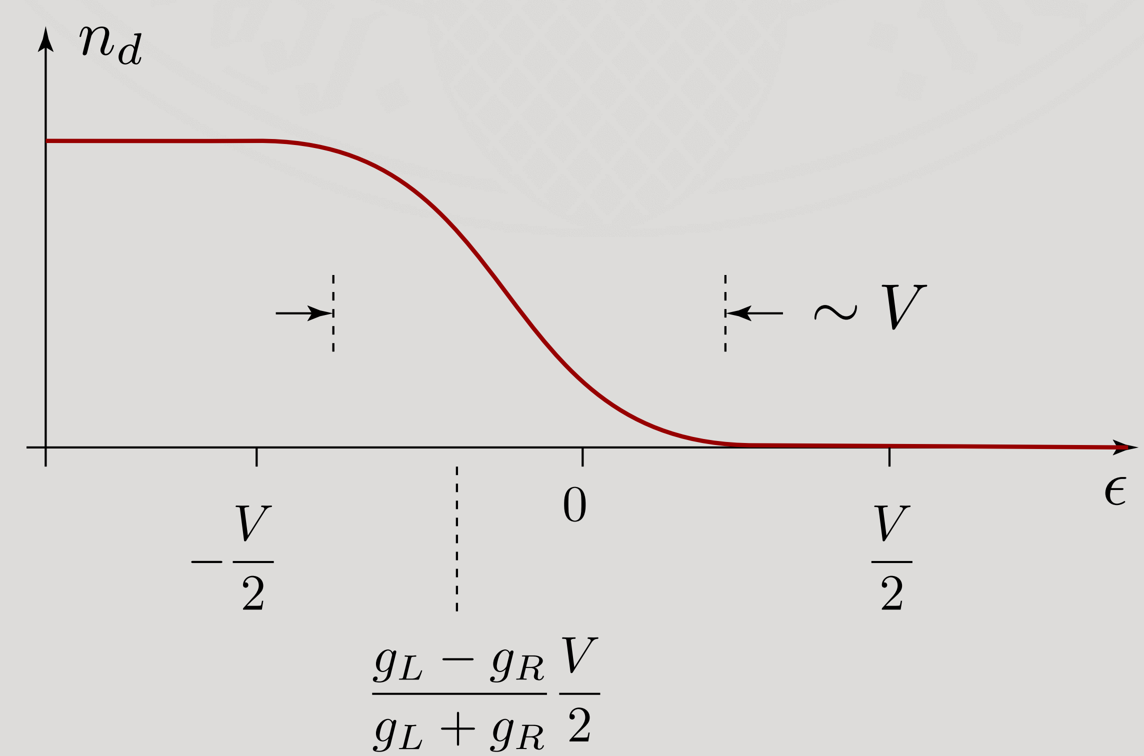
- breakdown of $\dfrac{g_\nu^+}{g_\nu^-} = \exp\left(\dfrac{1}{T}(\partial_n U - f_\nu)\right)$

- need to describe transport at higher resolution (e.g. particle & energy transport)
- *define* effective temperature through

$$\frac{g_\nu^+}{g_\nu^-} = \exp\left(\frac{1}{T_{\mathrm{eff},\nu}}(\partial_n U - f_\nu)\right)$$

phenomenology

comparison to (measured) fluctuation statistics contains information on mechanisms of nonequilibrium driving.



fluctuation relations in stochastic dynamics

- are useful when included in out of equilibrium theory of transport
- enable one to describe statistics of rare events