Dynamic transitions in nonequilibrium work fluctuations of linear diffusion systems

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PRE(2011,2013)/ PRL(2013)/ …

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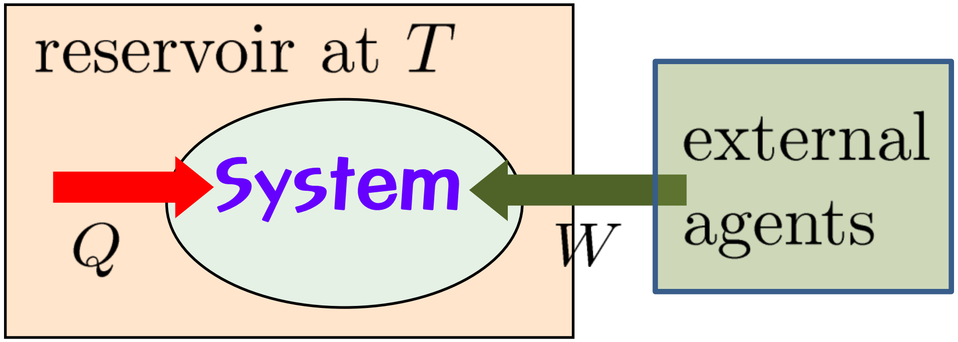
Dynamics processes & Fluctuation theorems



Q: heat, W: work ($\Delta E = Q + W$)

start from $p_0(\mathbf{x})$ for system and evolve over time t.

Integral fluctuation theorems $\langle e^{-R} \rangle = 1$ (i.c.)

$$\langle e^{-\Delta S_{tot}} \rangle = 1 \; (S_{tot} = S + S_r\text{: total entropy}) \quad \text{(any i.c.)}$$

$$\langle e^{-\beta W_d} \rangle = 1 \; (W_d = W - \Delta F\text{: dissipated work}) \text{(EQ i.c.)}$$

$$R = -\beta Q_{hk}, \; \Delta S - \beta Q_{ex}, \cdots$$

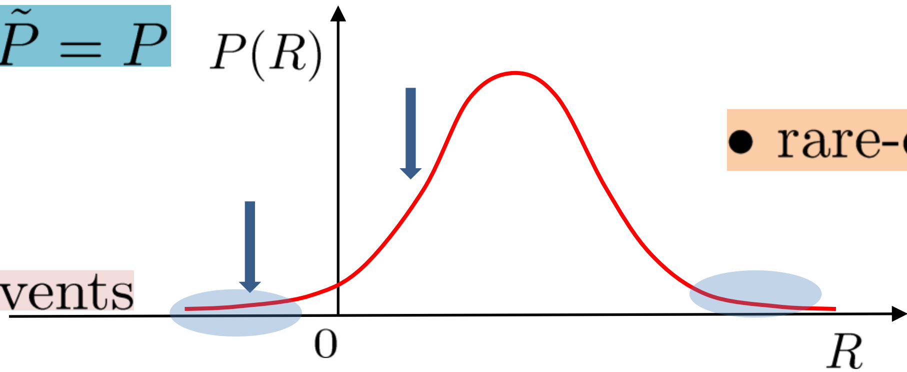
Thermodynamic 2nd laws $\langle R \rangle \geq 0.$ ⬅ Jensen's inequality

Dynamics processes & Fluctuation theorems

Detailed fluctuation theorems $(R = \Delta S_{tot}, \beta W_d = \beta W - \Delta F, \cdots)$

$$\frac{P(R)}{\tilde{P}(-R)} = e^{R}$$ ($\tilde{P}$ for 'reverse' process for ΔS_{tot}, βW_d)

when $\tilde{P} = P$



- rare-event prob. $\leftrightarrow$ frequent-event prob.

- Generating function $G(\lambda) = \langle e^{-\lambda R} \rangle = \int dR\, P(R)\, e^{-\lambda R}$

$\Rightarrow$ $G(\lambda) = G(1-\lambda)$

- Tail usually decays exponentially.

$P(R) \sim e^{-aR}$

Singularites of $G(\lambda)$ characterize tail shape at $\lambda = -a$

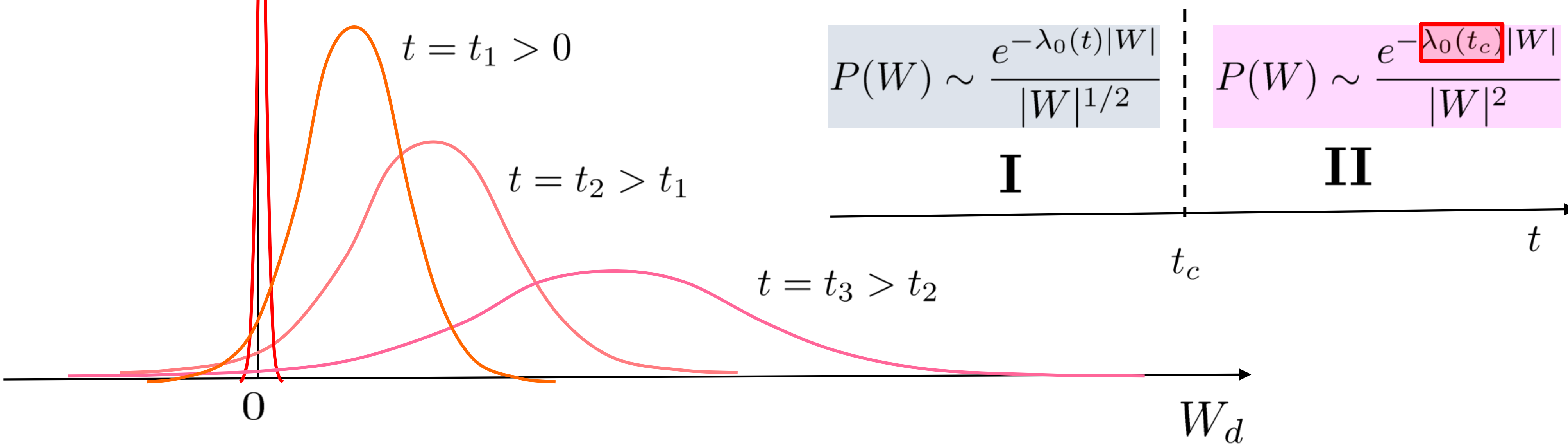
(also at $\lambda = 1 + a$) (DFT)

One-page summary of our analytic results

- We consider a simple linear dffusion system without time-dep. protocol and watch the $P(W_d)$ tail as function of time t.

$\tilde{P} = P$ & $W_d = W$

$P(W_d)$ tail shape changes as t increases not smoothly, but sharply through dynamic locking-unlocking transitions.



- More surprisingly, we find sequences of dynamic transitions, sometimes infinitely many transitions, **I**→**II**→**I**→ $\cdots$ at $t_{c1}, t_{c2}, t_{c3}, \cdots$ depending on specific details of linear diffusion processes.

Linear Diffusion Systems

Brownian dynamics

$$m\ddot{\mathbf{x}} = -\gamma\dot{\mathbf{x}} + \mathbf{f}(\mathbf{x}) + \boldsymbol{\xi} \qquad \langle \boldsymbol{\xi}(t)\boldsymbol{\xi}^T(t')\rangle = 2\mathsf{D}\delta(t-t')$$

Diffusion dynamics (overdamped limit)

$$\gamma\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \boldsymbol{\xi} \qquad \mathbf{f} = \mathbf{f}_c + \mathbf{f}_{nc} = -\boldsymbol{\nabla} E + \mathbf{f}_{nc}$$

(high dim. > 1)

$$\int_0^t d\tau\ \dot{\mathbf{x}}^T \cdot \mathbf{f}_c = -\Delta E \qquad \int_0^t d\tau\ \dot{\mathbf{x}}^T \cdot \mathbf{f}_{nc} \equiv W \qquad -\Delta E + W = -Q$$

Linear force

→ Analytically solvable

$$\mathbf{f} = -\mathsf{F}\cdot\mathbf{x}$$

$\mathsf{F} = \mathsf{F}_c + \mathsf{F}_{nc}$ (force matrix)

multivariate Ornstein-Uhlenbeck process

$$\mathsf{F}_c = \mathsf{F}_c^T \text{ and } E(\mathbf{x}) = \frac{1}{2}\mathbf{x}^T\cdot\mathsf{F}_c\cdot\mathbf{x}$$

Exact $P(\mathbf{x},t)$, $\mathbf{J}(\mathbf{x},t)$

$\mathsf{F}_{nc} \neq \mathsf{F}_{nc}^T$ → NEQ steady state with rotating current

Linear Diffusion Systems

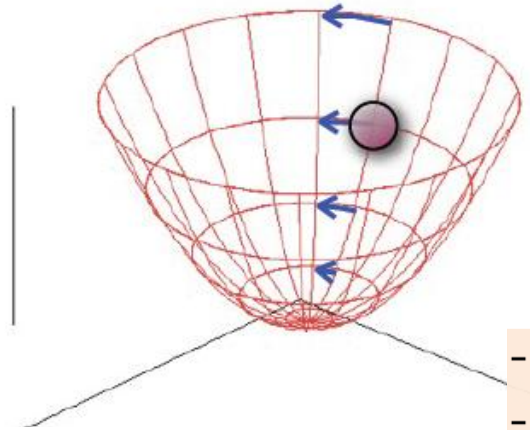
- simple examples

Particle dynamics trapped in a harmonic potential and driven by a swiring force in 2D

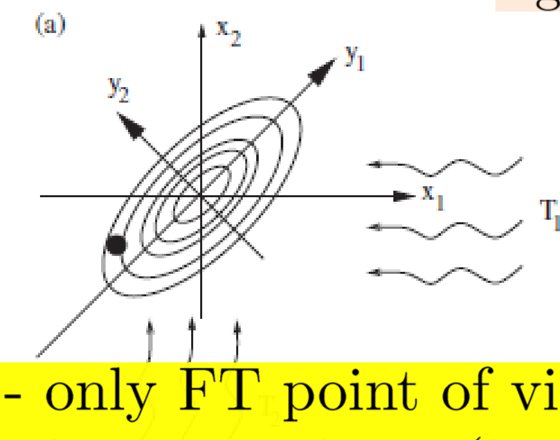
$$\gamma\dot{\mathbf{x}} = -\mathsf{F}_c \cdot \mathbf{x} - \mathsf{F}_{nc} \cdot \mathbf{x} + \boldsymbol{\xi}$$

$$\mathsf{F}_c = \begin{pmatrix} 1+a & b \\ b & 1-a \end{pmatrix}$$

$$\mathsf{F}_{nc} = \begin{pmatrix} 0 & q \\ -q & 0 \end{pmatrix}$$



- molecular motor
- global climate system



two diff. T reservoirs

underdamped

Brownian gyrator: nano heat engine
(Filliger and Reimann, PRL 2007)

Molecular refrigerator
(Kim and Qian , PRL 2004/PRE 2007)

Time-dependent harmonic potentials
(Zon/Cohen, Nickelsen/Engel, ..)

- only FT point of view
- long-time limit (large deviation)
- no interesting transient behavior

Linear Diffusion Systems

- Set $\gamma = \mathsf{D} = \mathsf{I}$ (scaling & rotation with $\beta = 1$)

$$\dot{\mathbf{x}} = -\mathsf{F} \cdot \mathbf{x} + \boldsymbol{\xi} \qquad (\mathsf{F} = \mathsf{F}_c + \mathsf{F}_{nc}) \qquad \langle \boldsymbol{\xi}(t) \boldsymbol{\xi}^T(t') \rangle = 2\mathsf{I}\, \delta(t - t')$$

- Path-integral formulation (Onsager-Machlup)

$$P_t(\mathbf{x}) = \int d\mathbf{x}_0 P_0(\mathbf{x}_0) \int D[\mathbf{x}] e^{-\int_0^t d\tau L(\mathbf{x}, \dot{\mathbf{x}})}$$

(all Gaussian integrals)

$$L(\mathbf{x}, \dot{\mathbf{x}}) = \frac{1}{4} (\dot{\mathbf{x}} + \mathsf{F} \cdot \mathbf{x})^T \cdot (\dot{\mathbf{x}} + \mathsf{F} \cdot \mathbf{x})$$

$$P_t(\mathbf{x}) \sim e^{-\frac{1}{2} \mathbf{x}^T \cdot \mathsf{A}(t) \cdot \mathbf{x}}$$

with $\mathsf{A}(0) = \mathsf{F}_c$ (EQ)

$$\dot{\mathsf{A}} = -2\mathsf{A}^2 + \mathsf{A}\mathsf{F} + \mathsf{F}^T \mathsf{A} \quad \Rightarrow \quad \frac{d\mathsf{A}^{-1}}{dt} = 2\mathsf{I} - \mathsf{F}\mathsf{A}^{-1} - \mathsf{A}^{-1}\mathsf{F}^T$$

- Generating function

$$G(\lambda) = \langle e^{-\lambda W} \rangle = \int d\mathbf{x}_t d\mathbf{x}_0 P_0(\mathbf{x}_0) \int D[\mathbf{x}] e^{-\int_0^t d\tau [L(\mathbf{x}, \dot{\mathbf{x}}) + \lambda W]}$$

$$\tilde{L}(\mathbf{x}, \dot{\mathbf{x}}) = L(\mathbf{x}, \dot{\mathbf{x}}) - \lambda \dot{\mathbf{x}}^T \cdot \mathsf{F}_{\mathrm{nc}} \cdot \mathbf{x}$$

$$\dot{\tilde{\mathsf{A}}} = -2\tilde{\mathsf{A}}^2 + \tilde{\mathsf{A}}\mathsf{F} + \mathsf{F}^T \tilde{\mathsf{A}} + \boldsymbol{\Lambda}$$

$$W = \int_0^t d\tau\, \dot{\mathbf{x}}^T \cdot \mathsf{F}_{nc} \cdot \mathbf{x}$$

Linear Diffusion Systems

Crucial: Nonlinear Inhomogeneous Matrix DE to solve

$$\dot{\tilde{\mathsf{A}}} = -2\tilde{\mathsf{A}}^2 + \tilde{\mathsf{A}}\tilde{\mathsf{F}} + \tilde{\mathsf{F}}^T\tilde{\mathsf{A}} + \boldsymbol{\Lambda}$$

$$\tilde{\mathsf{F}} = \mathsf{F} - \lambda(\mathsf{F} - \mathsf{F}^T)$$

$$\Lambda = (\mathsf{F}^T\mathsf{F} - \tilde{\mathsf{F}}^T\tilde{\mathsf{F}})/2$$

$$\tilde{\mathsf{A}}(0) = \mathsf{F}_c + \lambda(\mathsf{F}_{nc} + \mathsf{F}_{nc}^T)/2$$

Exactly solvable for general F by translation and inversion.

In 2D, explicit form is available, but looks horrible.

$$G(\lambda) = \langle e^{-\lambda W} \rangle$$

Gaussian integrals → Product of determinants

$$\ln G(\lambda;t) = \int_0^t d\tau \, \mathrm{Tr}(\tilde{\mathsf{A}}(\tau) - \tilde{\mathsf{F}}) - \frac{1}{2}\ln\frac{\det[\tilde{\mathsf{A}}(t) - \lambda(\mathsf{F}_{nc} + \mathsf{F}_{nc}^T)/2]}{\det \mathsf{F}_c}$$

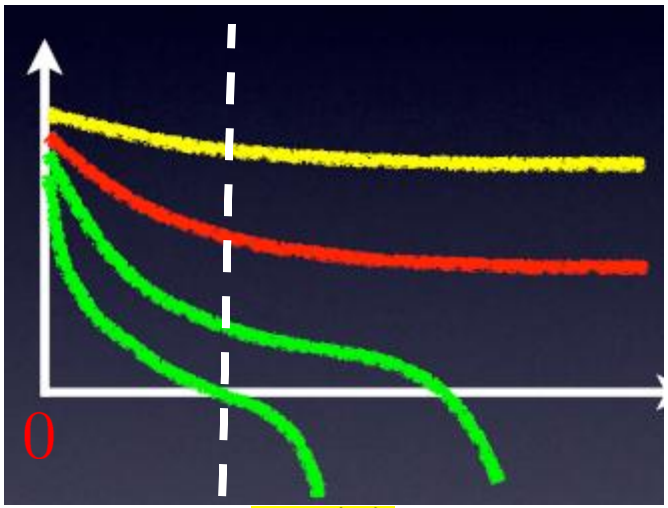
Generating function and PDF

$$\ln G(\lambda;t) = \int_0^t d\tau\ \mathrm{Tr}(\tilde{\mathsf{A}}(\tau) - \tilde{\mathsf{F}}) - \frac{1}{2}\ln\frac{\det\left[\tilde{\mathsf{A}}(t) - \lambda(\mathsf{F}_{nc} + \mathsf{F}_{nc}^T)/2\right]}{\det \mathsf{F}_c}$$

$z = \det\left[\tilde{\mathsf{A}}(t) - \lambda(\mathsf{F}_{nc} + \mathsf{F}_{nc}^T)/2\right]$

$G(\lambda, t)$

z

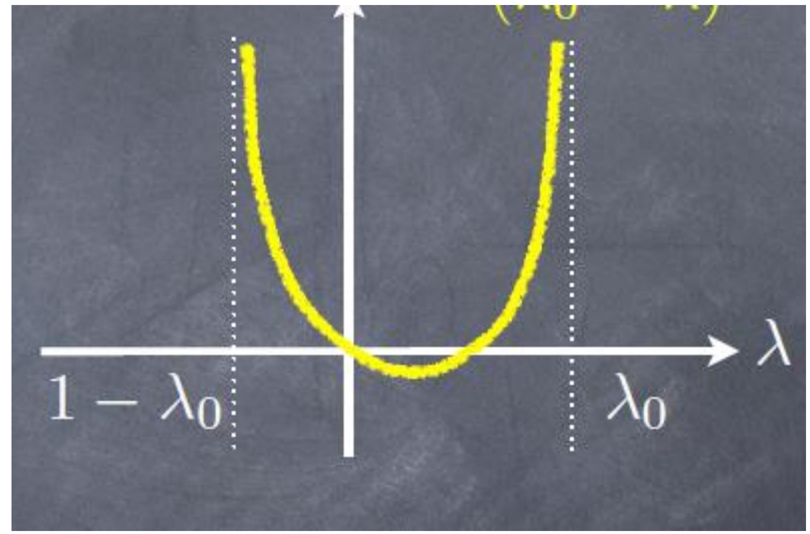


$\lambda < \lambda_c$

$\lambda = \lambda_c$

t

$\lambda_0(t)$ $\lambda > \lambda_c$



For fixed t, $z = 0$ at $\lambda = \lambda_0(t)$

Near $\lambda = \lambda_0(t)$, $z(\lambda;t) \sim (\lambda_0(t) - \lambda)$

- $\lambda_0(t)$ decreases continuously with t approaches λ_c.

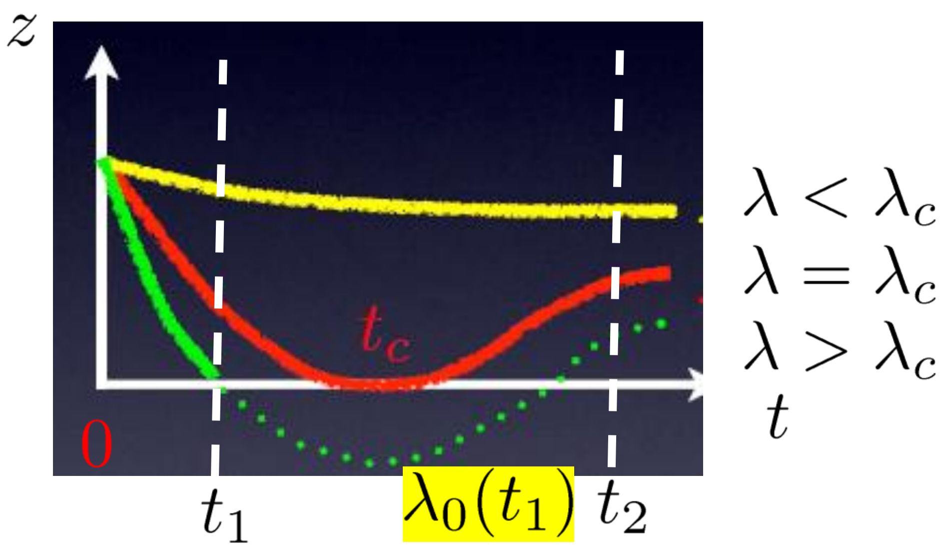
$G(\lambda, t) \sim (\lambda_0(t) - \lambda)^{-1/2}$

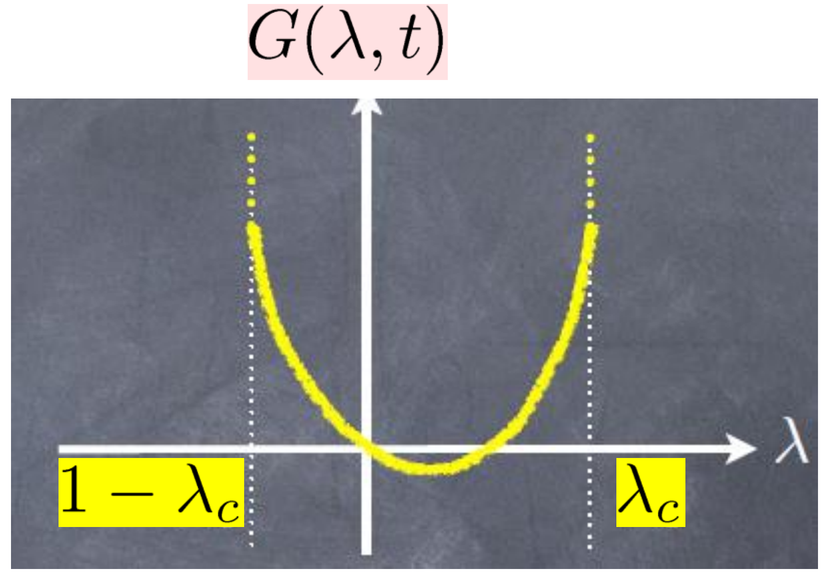
$P(W, t) \sim |W|^{-1/2} e^{-\lambda_0(t)|W|}$

Type I

Generating function and PDF

$$\ln G(\lambda;t) = \int_0^t d\tau \ \mathrm{Tr}(\tilde{\mathsf{A}}(\tau) - \tilde{\mathsf{F}}) - \frac{1}{2}\ln \frac{\det[\tilde{\mathsf{A}}(t) - \lambda(\mathsf{F}_{nc} + \mathsf{F}_{nc}^T)/2]}{\det \mathsf{F}_c}$$





For $t_1 < t_c$, $z = 0$ at $\lambda = \lambda_0(t_1)$

Near $\lambda = \lambda_0(t)$, $z(\lambda;t) \sim (\lambda_0(t) - \lambda)$

$G(\lambda, t) \sim (\lambda_0(t) - \lambda)^{-1/2}$

$P(W,t) \sim |W|^{-1/2} e^{-\lambda_0(t)|W|}$ **Type I**

For $t_2 > t_c$, $z > 0$ at $\lambda = \lambda_c$

G diverges discontinuously.

$P(W,t) \sim |W|^{-2} e^{-\lambda_c |W|}$

- $\lambda_c = \lambda_0(t_c)$ constant. **Type II**

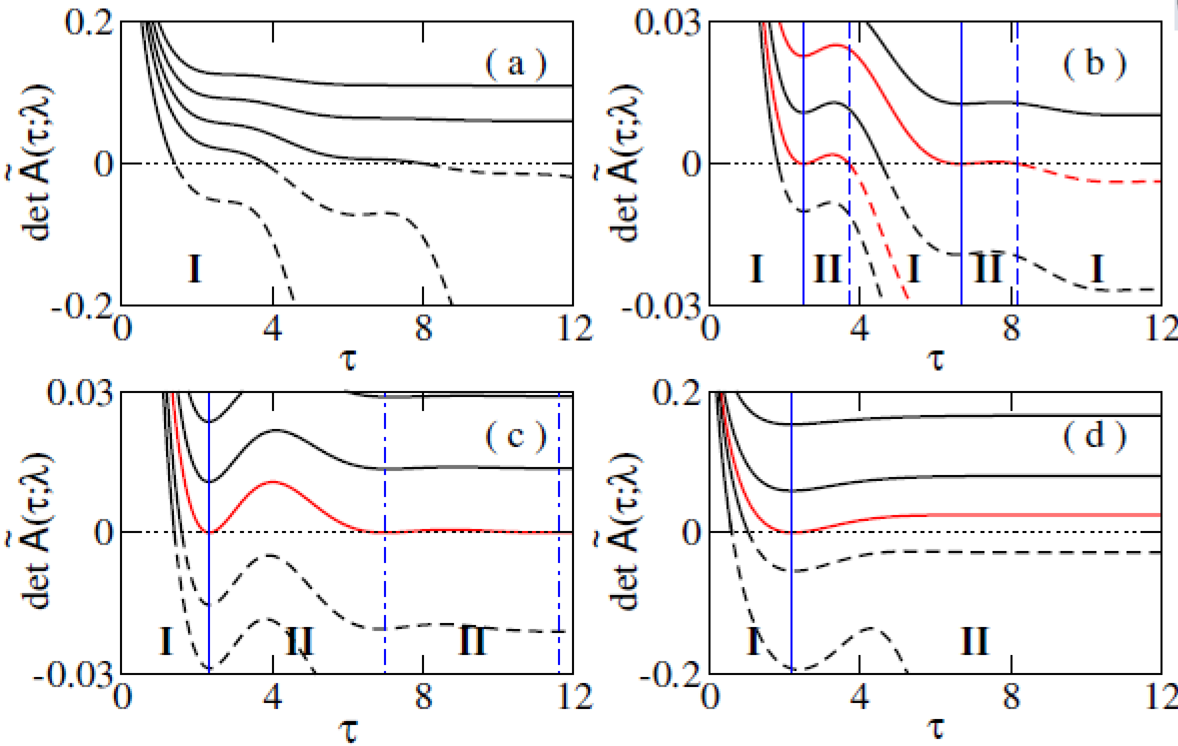
2D Linear Diffusion Systems

- simple case $\dot{\mathbf{x}} = -\mathsf{F}\cdot\mathbf{x} + \boldsymbol{\xi}$

$$\mathsf{F}_c = \begin{pmatrix} 1+y & 0 \\ 0 & 1-y \end{pmatrix} \quad \mathsf{F}_{nc} = \begin{pmatrix} 0 & q \\ -q & 0 \end{pmatrix}$$

$$z = \det[\tilde{\mathsf{A}}(t) - \lambda(\mathsf{F}_{nc} + \mathsf{F}_{nc}^T)/2]$$

$q = 0.3$



(a) $y = 0.65$

oscillation & mono. decreasing

irrelevant oscillation

(b) $y = 0.7$

oscillation relevant & complex tr.

(c) $y = \sqrt{109/200}$

Boundary & inf. tangential pts.

(d) $y = 0.8$

"strong" anisotropy

No (irrelevant) oscillation

1st overshooting dominant.

2D Linear Diffusion Systems

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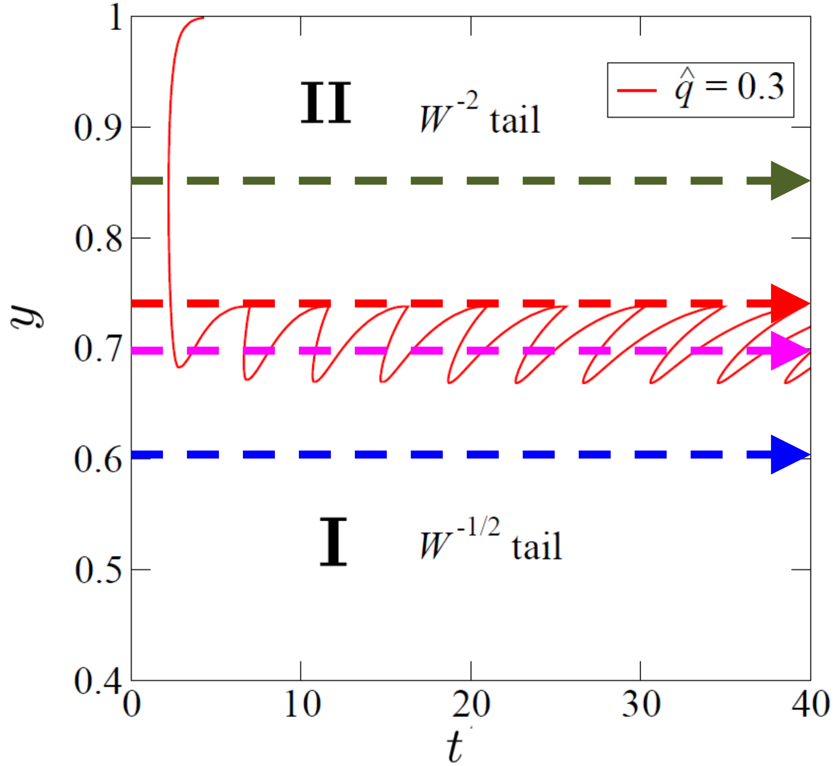


$$y^* = \sqrt{(1+q^2)/2},\ \lambda_c^* = (1+q)/(2q),$$

$$T^* = 2\pi/\sqrt{2(1-q^2)} = \pi/y^*,$$

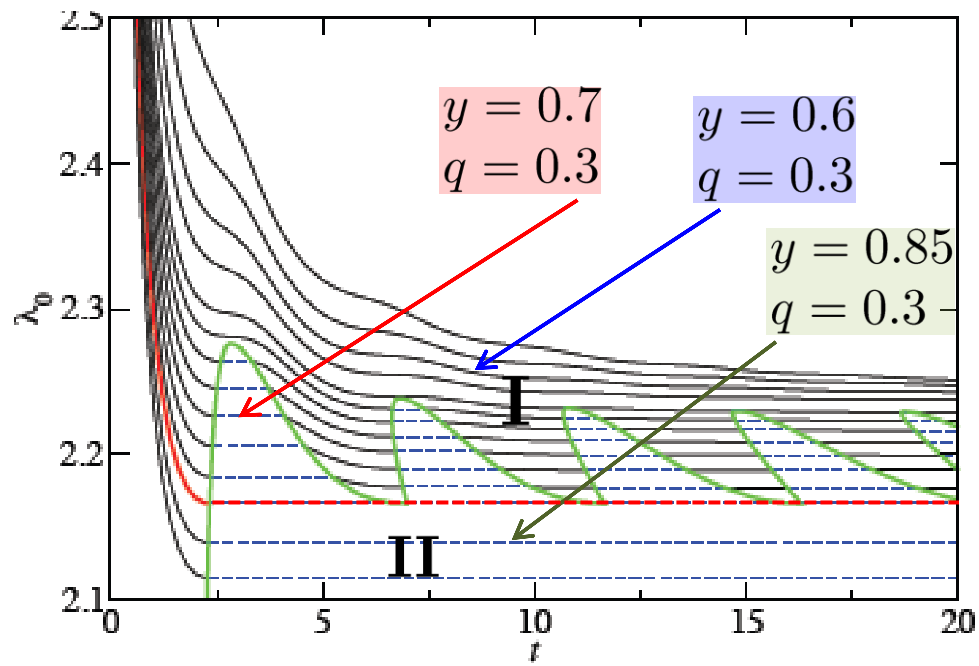
I $\quad G(\lambda) \sim (\lambda_0(t) - \lambda)^{-1/2}$

$$P(W) \sim \frac{e^{-\lambda_0(t)|W|}}{|W|^{1/2}}$$

II $\quad G(\lambda) \sim$ finite for $\lambda < \lambda_0(t_c)$

$\infty \quad$ for $\lambda > \lambda_0(t_c)$

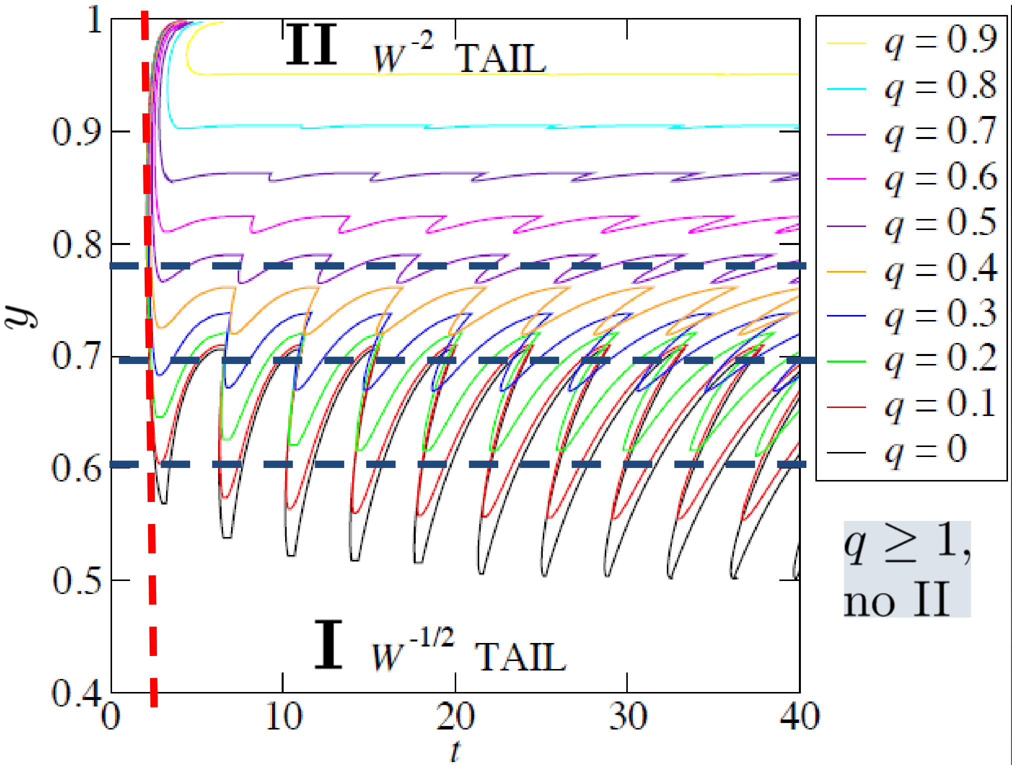
$$P(W) \sim \frac{e^{-\lambda_0(t_c)|W|}}{|W|^2}$$



2D Linear Diffusion Systems

- simple case $\dot{\mathbf{x}} = -\mathsf{F}\cdot\mathbf{x} + \boldsymbol{\xi}$

$$\mathsf{F}_c = \begin{pmatrix} 1+y & 0 \\ 0 & 1-y \end{pmatrix} \quad \mathsf{F}_{nc} = \begin{pmatrix} 0 & q \\ -q & 0 \end{pmatrix}$$



$q \geq 1$, no II

$y^* = \sqrt{(1+q^2)/2}$, $\lambda_c^* = (1+q)/(2q)$,

$T^* = 2\pi/\sqrt{2(1-q^2)} = \pi/y^*$,

I $P(W) \sim \dfrac{e^{-\lambda_0(t)|W|}}{|W|^{1/2}}$ $(q \geq 1)$

II $P(W) \sim \dfrac{e^{-\lambda_0(t_c)|W|}}{|W|^2}$

- Origin for locking transitions?
  - rotational mode by torque & decaying mode by anisotropy
  - **II**: torque is small enough to feel decaying mode
  - why locking like Shapiro steps?
- Ongoing and future works
  - tilted washboard potential ?
  - i.c. dependence - $P(Q)$
  - underdamped
  - time-dependent protocol