Scaling and fragility of the rates of rare events

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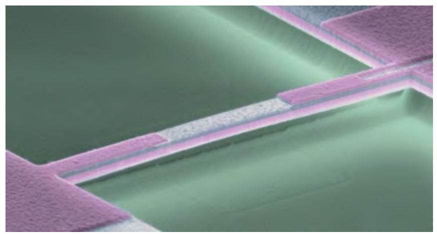
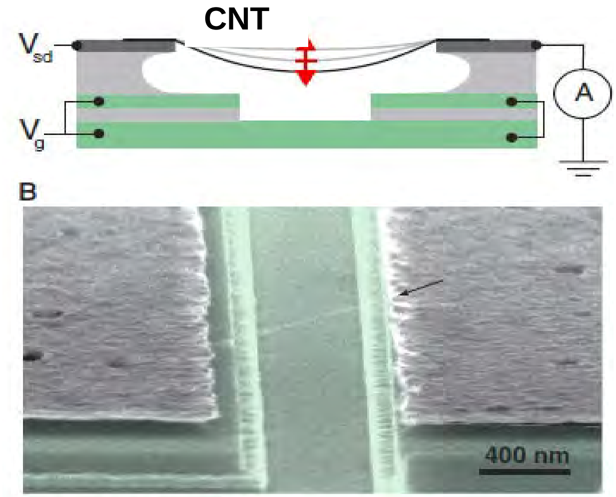
Mesoscopic oscillators

Vibrational systems that are

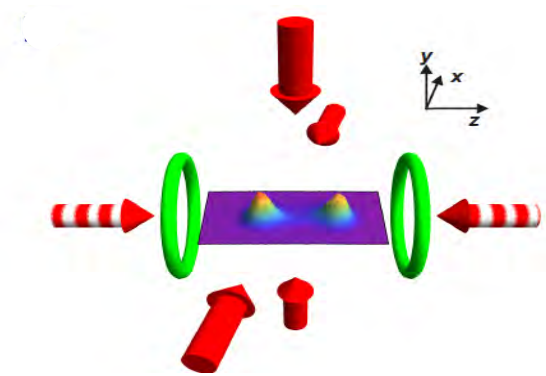
- **sufficiently large to be individually accessed**
- **small, so that classical and quantum fluctuations are substantial**



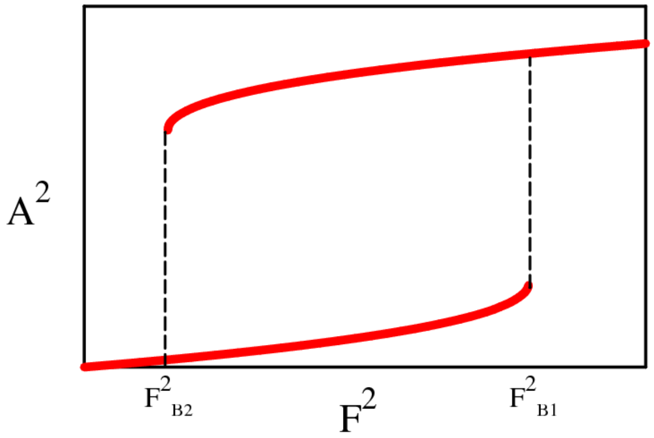


Frequencies 0.1 – 10 GHz

$$Q = \frac{\text{angular frequency}}{\text{decay rate}} \sim 10^3 - 10^7$$



- means to learn new classical and quantum physics far from equilibrium with well-characterized systems

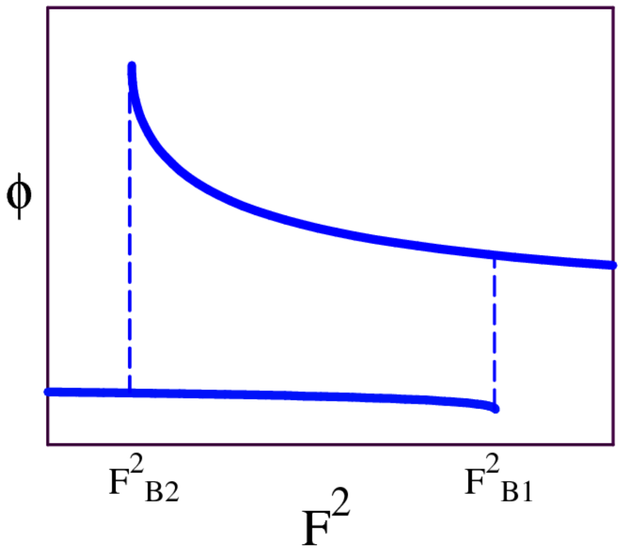


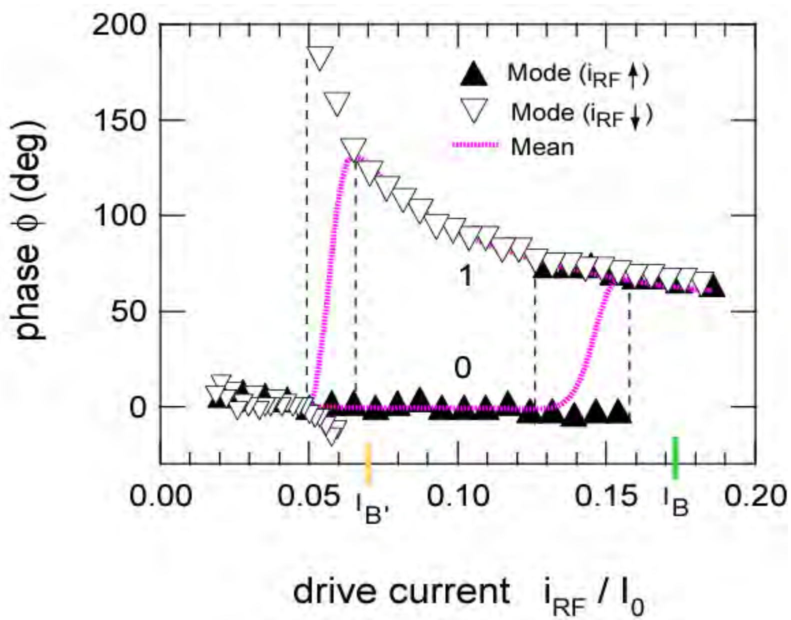
$$\ddot{q} + 2\Gamma\dot{q} + \omega_0^2 q + \gamma q^3 = F\cos\omega_F t$$

Periodic state: $q = A\cos(\omega_F t + \phi)$

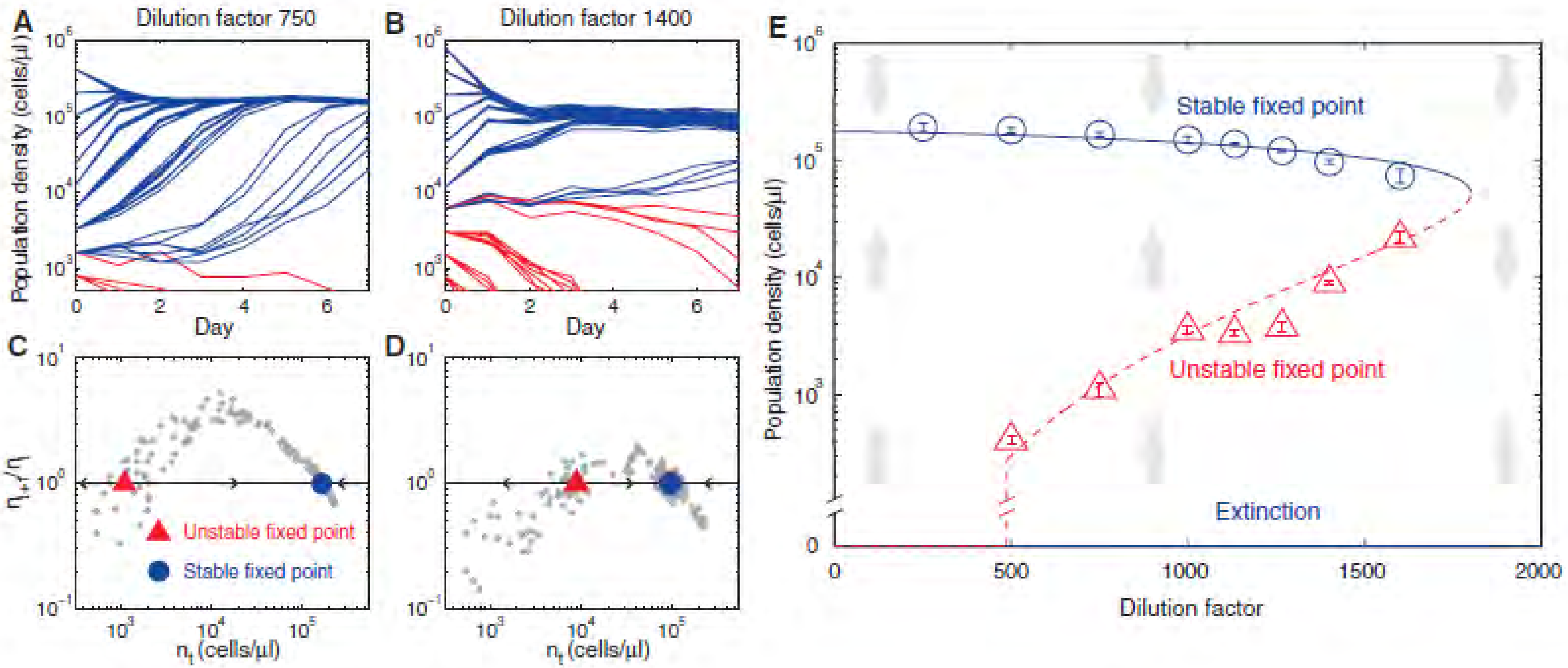
Both A and ϕ **display hysteresis**

A Josephson junction based nonlinear oscillator
(Siddiqi *et al*. PRL 2004, 2005)



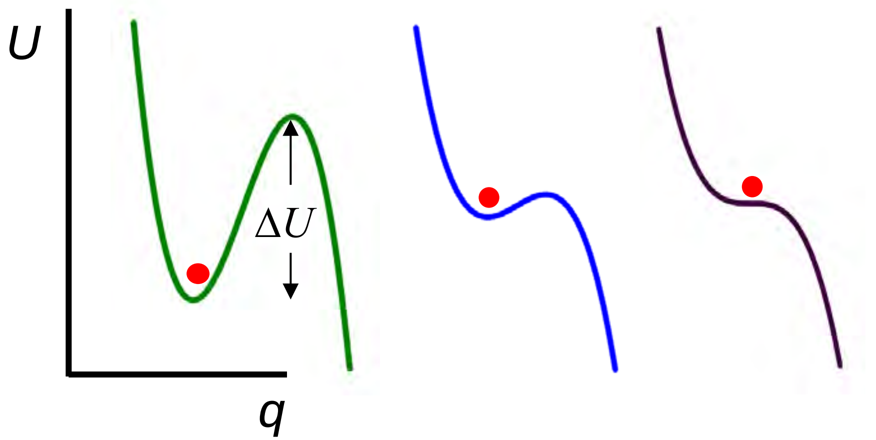


Bifurcation amplifier broadly used in quantum measurement



Lei Dai, Daan Vorselen, Kirill S. Korolev, Jeff Gore (2012)

Near bifurcation points one of the motions is **slow, a soft mode** ⇨ **universal behavior of the escape rate**

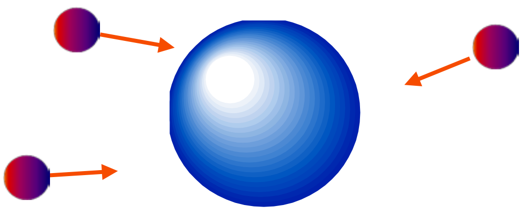


A **multivariable** system can be mapped onto a 1D overdamped (no inertia) Brownian particle

$$\dot{q} = -\partial_q U_b + f(\tau), \quad U_b(q) = -\tfrac{1}{3}q^3 + \eta q, \quad \langle f(\tau) f(\tau')\rangle = 2D\,\delta(\tau - \tau')$$

noise

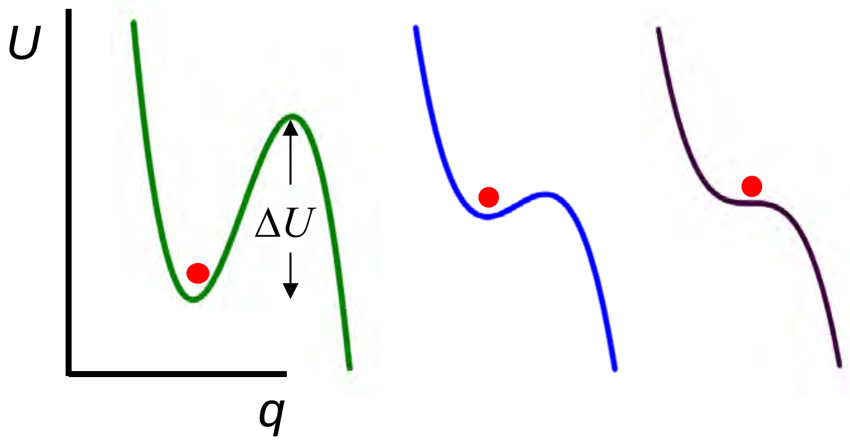
thermal noise: $D = k_B T$



a Brownian particle colliding with molecules

Switching rate near bifurcation points

Near bifurcation points one of the motions is **slow, a soft mode** ⇒ **universal behavior of the escape rate**



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$$\dot{q} = -\partial_q U_b + f(\tau), \quad U_b(q) = -\tfrac{1}{3}q^3 + \eta\, q, \quad \langle f(\tau) f(\tau') \rangle = 2D\,\delta(\tau - \tau')$$

noise

thermal noise: $D = k_B T$

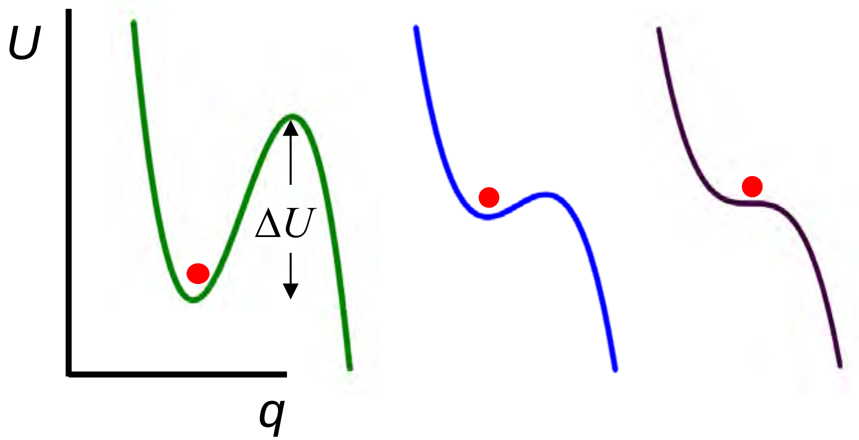
If the noise is Gaussian, the switching rate is

$$W = \Omega_e \exp\left(-\Delta U_b / k_B T\right), \quad \Delta U_b = \frac{4}{3}\eta^{\xi}, \quad \Omega_e \propto \eta^{\zeta}, \qquad \xi = 3/2, \quad \zeta = 1/2$$

Josephson junctions, static potential, no ac modulation: Kurkijarvi (1972).

General case of a nonequilibrium system/soft mode near a bifurcation point: MD & Krivoglaz (1980)

Near bifurcation points one of the motions is **slow, a soft mode** ➡ **universal behavior of the escape rate**



A multivariable **reaction** system can be mapped onto a 1D overdamped (no inertia) Brownian particle

slowly varying combination of populations:

$$\dot{q} = -\partial_q U_b + f(\tau), \quad U_b(q) = -\tfrac{1}{3}q^3 + \eta q, \quad \langle f(\tau) f(\tau')\rangle = 2D\,\delta(\tau - \tau')$$

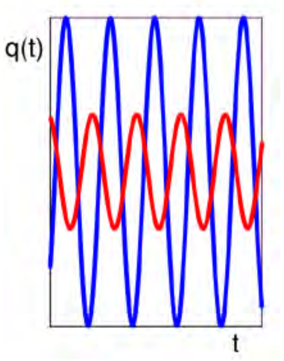
noise

noise: $D \propto 1/N$ – inverse total number of particles

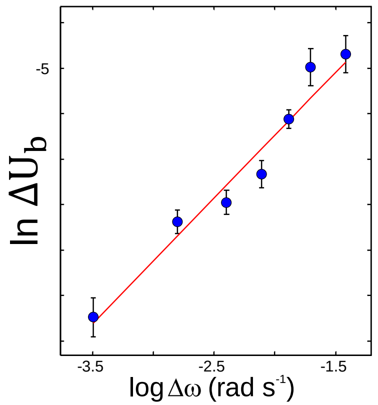
If the noise is Gaussian, the switching rate is

$$W = \Omega_e \exp(-\Delta U_b / D), \quad \Delta U_b = \frac{4}{3}\eta^{\xi}, \qquad \xi = 3/2$$

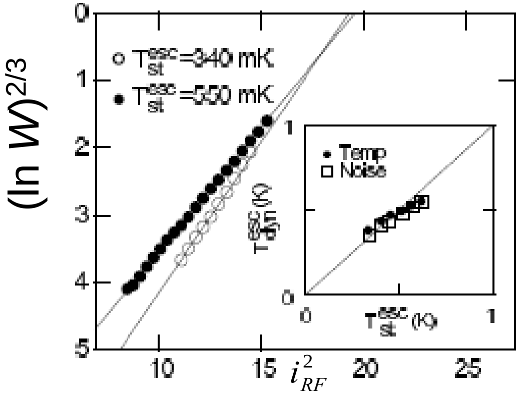
MD, Mori, Ross, & Hunt (1994)



For resonant modulation, $\Delta U_b \propto \eta^{3/2}$ close to bifurcation points.

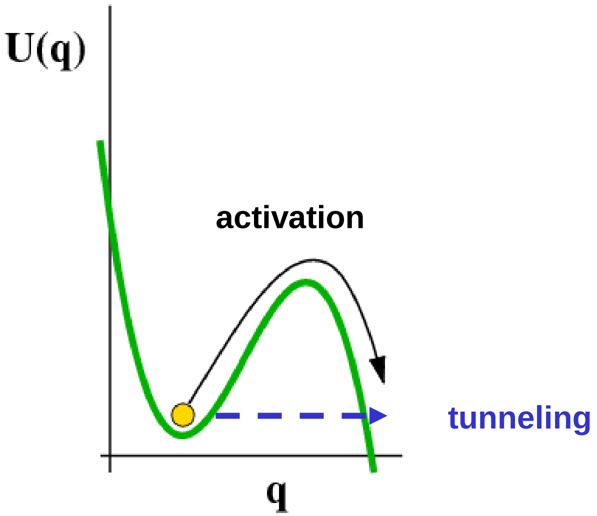


MEMS (Chan & Stambaugh, 2005/2006)



Josephson junctions (Siddiqi et al., 2005)

Low temperatures: conventionally, escape occurs via tunneling

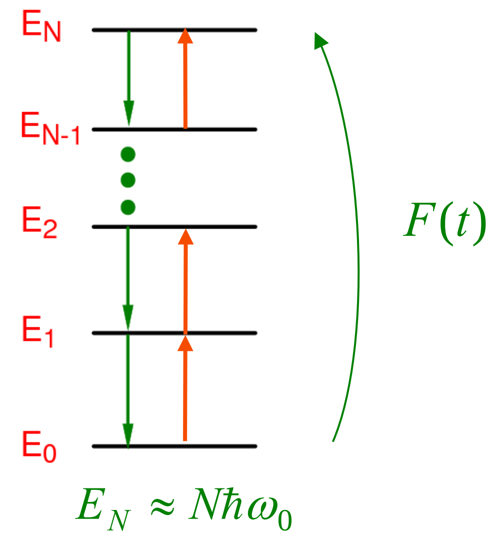


$$W \propto \exp(-\Delta U / k_B T) \Rightarrow \exp(-2S_{\text{tun}} / \hbar)$$

$W << \Gamma$, **the relaxation rate**

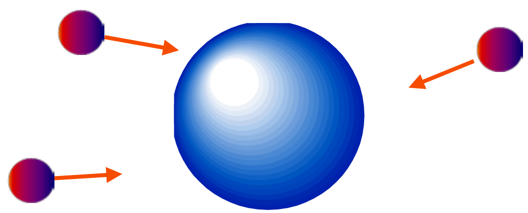
Oscillator Hamiltonian: $H_0 = \frac{1}{2}p^2 + \frac{1}{2}\omega_0^2 q^2 + \frac{1}{4}\gamma q^4 - qF\cos\omega_F t$

+ coupling to a thermal bath



Relaxation: transitions between the energy levels due to the coupling

Transitions happen **at random.** Classically, a "kick" to the oscillator coordinate and momentum



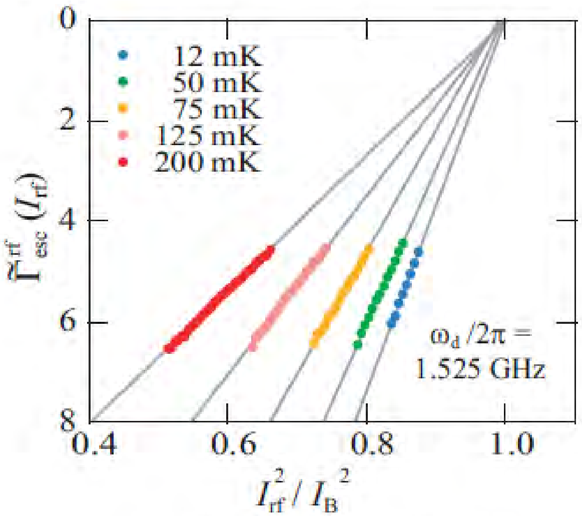
à la Brownian particle colliding with molecules

"Noise intensity" is the total transition rate (emission / absorption of bath excitations)

$$k_B T \Rightarrow k_B T_{\rm eff} = \hbar\omega_0(2\bar{n}+1)/2, \quad \bar{n} = \left[\exp(\hbar\omega_0/k_B T) - 1\right]^{-1}$$

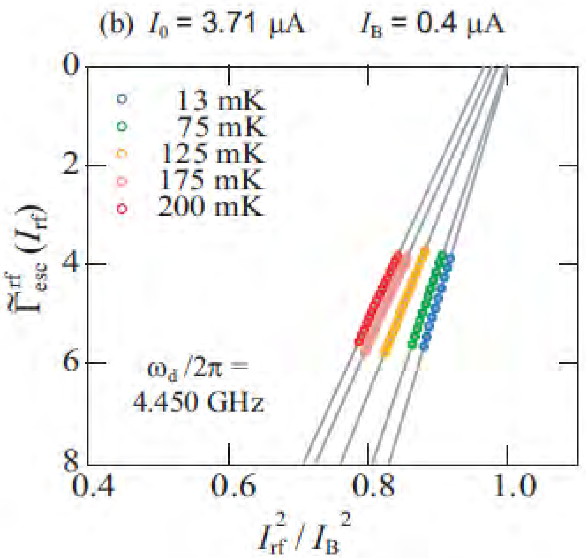
The picture applies only near bifurcation points; one dynamical variable + many short collisions; *ultra-strong squeezing* classical dynamics with Gaussian quantum noise

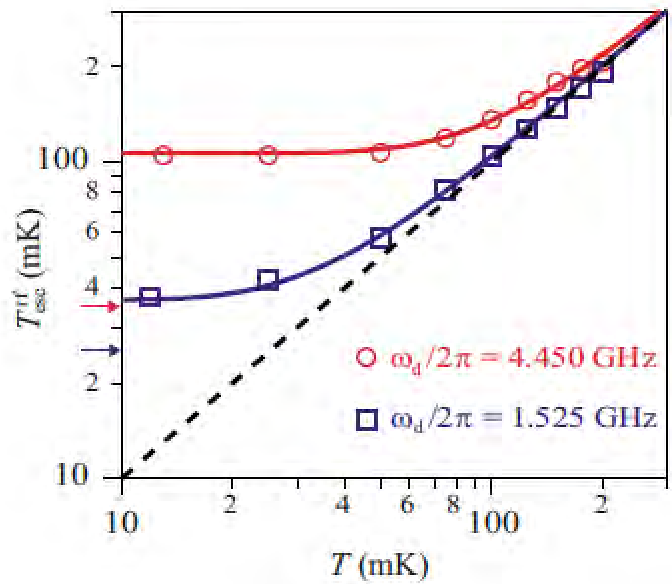
MD, 2007, 2012



$$W_A \propto \exp(-\Delta U_A / k_B T_{\rm eff}), \qquad \Delta U_A \propto |F - F_B|^{3/2}$$

$$k_B T_{eff} = \hbar\omega_0(\bar{n} + \tfrac{1}{2}), \; \bar{n} = \left[\exp(\hbar\omega_0 / k_B T) - 1\right]^{-1}$$





$$\tilde{\Gamma}^{rf}_{\rm esc} = [\log(\omega_{\rm attempt} / W_A)]^{2/3}$$

Vijay et al. (2009)

(Bio)chemistry,

population dynamics

$$\mathbf{X} \xrightarrow{W(\mathbf{X};\mathbf{r})} \mathbf{X} + \mathbf{r} \qquad \mathbf{X} = (X_1, X_2, \ldots X_m)$$

numbers of individuals/molecules

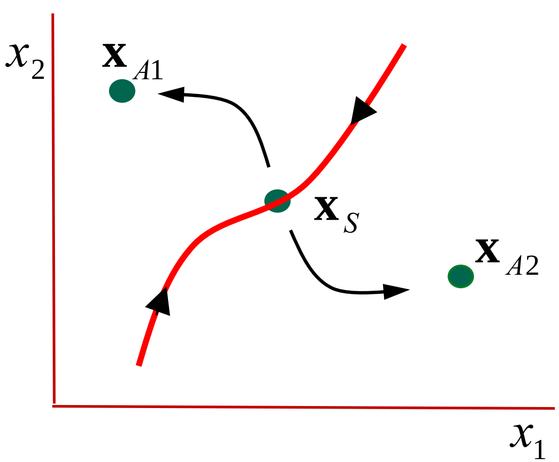
Mean-field equation of motion

$$\dot{\mathbf{X}} = \sum_{\mathbf{r}} \mathbf{r}\, W(\mathbf{X};\mathbf{r})$$

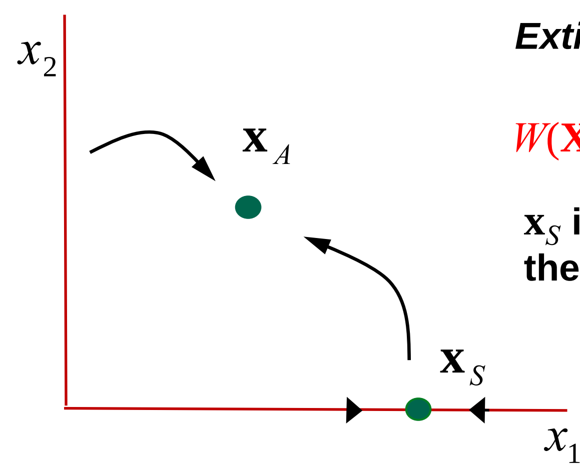
Scaled population: $\mathbf{x} = \mathbf{X}/N$

$$\dot{\mathbf{x}} = \sum_{\mathbf{r}} \mathbf{r}\, w(\mathbf{x};\mathbf{r}) \qquad w(\mathbf{x};\mathbf{r}) = W(\mathbf{X};\mathbf{r})/N$$

Bistability



Extinction



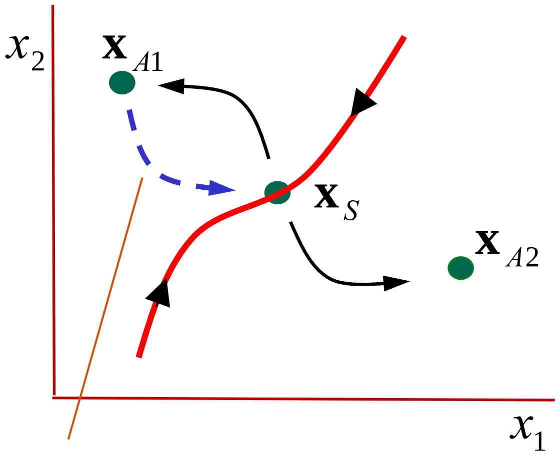
Extinction plane $X_E = 0$:

$W(\mathbf{X};\mathbf{r}) = 0$ for $r_E \neq 0$

$\mathbf{x}_S$ is a stable state in the extinction plane

$$\mathbf{X} \xrightarrow{W(\mathbf{X};\mathbf{r})} \mathbf{X} + \mathbf{r} \quad \Rightarrow \quad \frac{\partial \rho(\mathbf{X})}{\partial t} = \sum_{\mathbf{r}} [W(\mathbf{X}-\mathbf{r};\mathbf{r})\rho(\mathbf{X}-\mathbf{r}) - W(\mathbf{X};\mathbf{r})\rho(\mathbf{X})]$$

$$= \sum_{\mathbf{r}} [\exp(-\mathbf{r}\partial_{\mathbf{X}}) - 1] W(\mathbf{X};\mathbf{r})\rho(\mathbf{X})]$$



Switching: **rare event, requires a large fluctuation,**

switching rate: $W_{sw} << t_r^{-1}$

Hamilton-Jacobi equation for action s

Eikonal approximation: $\rho(\mathbf{X}) = \exp[-Ns(\mathbf{x})], \quad \dot{s} = -H(\mathbf{x}, \partial_{\mathbf{x}} s), \quad \mathbf{x} = \mathbf{X}/N$

$$H(\mathbf{x},\mathbf{p}) = \sum_{\mathbf{r}} w(\mathbf{x};\mathbf{r})[\exp(\mathbf{pr}) - 1], \quad \mathbf{p} = \partial_{\mathbf{x}} s$$

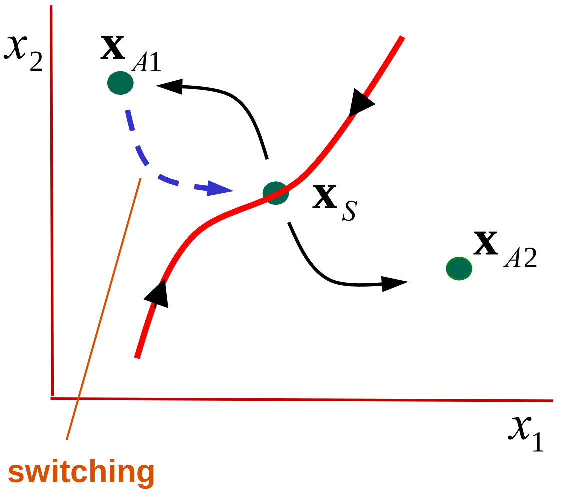
Hamiltonian dynamics of an auxiliary system with action $s(\mathbf{x})$ $[\, w(\mathbf{x};\mathbf{r}) = W(\mathbf{X};\mathbf{r})/N \,]$

- describes the *least improbable* sequence of reactions leading to switching

$$\mathbf{X} \xrightarrow{W(\mathbf{X};\mathbf{r})} \mathbf{X} + \mathbf{r}$$

$$\frac{\partial \rho(\mathbf{X})}{\partial t} = \sum_{\mathbf{r}} [W(\mathbf{X}-\mathbf{r};\mathbf{r})\rho(\mathbf{X}-\mathbf{r}) - W(\mathbf{X};\mathbf{r})\rho(\mathbf{X})]$$

$$= \sum_{\mathbf{r}} [\exp(-\mathbf{r}\partial_{\mathbf{X}}) - 1] W(\mathbf{X};\mathbf{r})\rho(\mathbf{X})]$$



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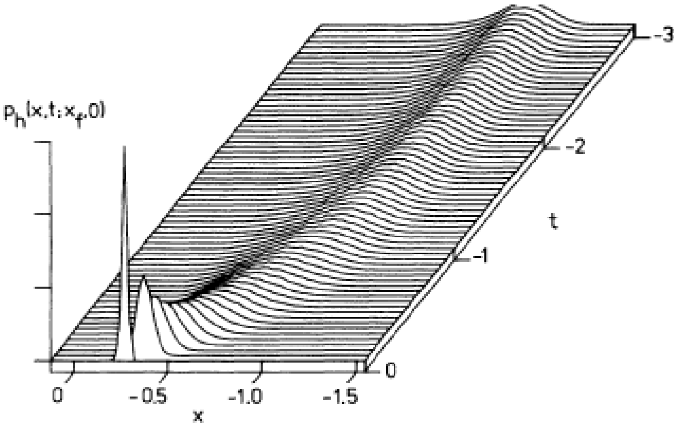
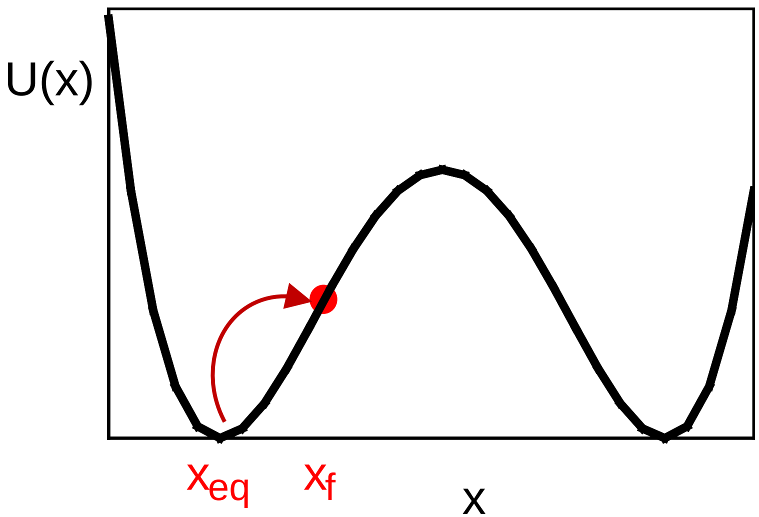
$$H(\mathbf{x},\mathbf{p}) = \sum_{\mathbf{r}} w(\mathbf{x};\mathbf{r})[\exp(\mathbf{pr}) - 1], \quad \mathbf{p} = \partial_{\mathbf{x}} s$$

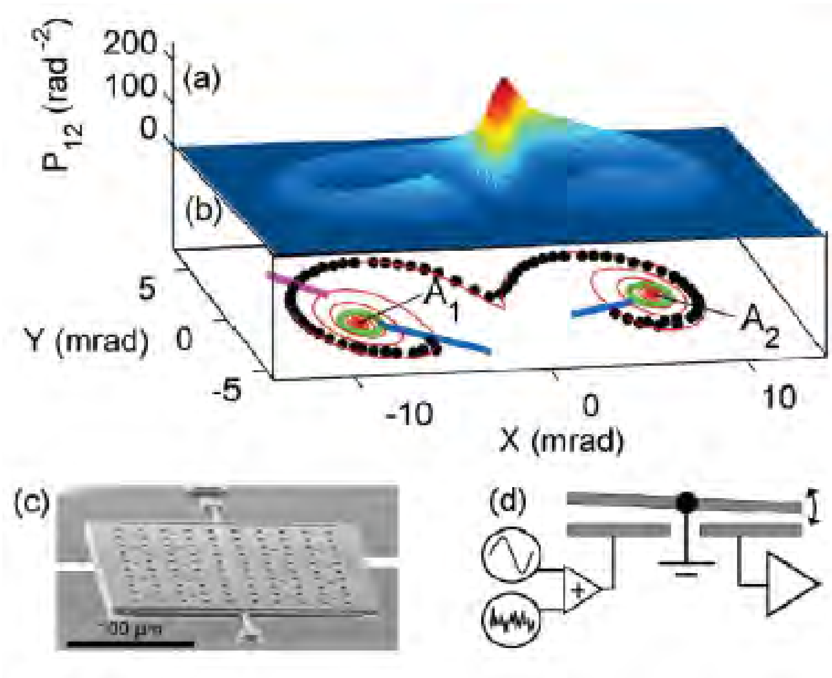
p **is the fluctuational force that drives the system against the “mean-field” force**



$$\dot{x} = -U'(x) + f(t), \qquad \langle f(t)f(t')\rangle = 2D\delta(t-t'),$$
$$U(x) = -\frac{1}{2}x^2 + \frac{1}{4}x^4$$

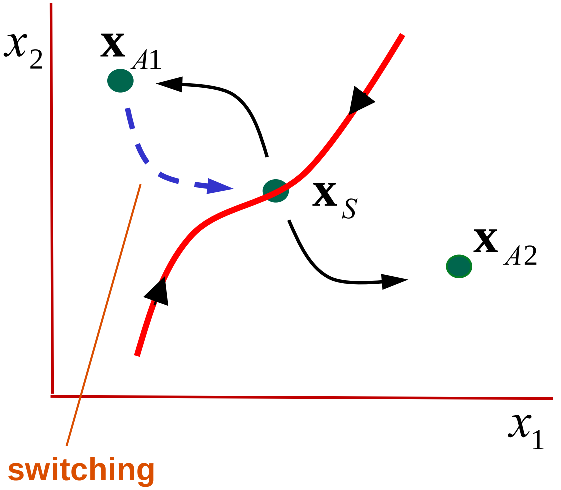


MD, McClntock, Smelyanskiy, Stein, & Stocks (1991)



Chan, MD,& Stambaugh (2008)

Switching rate: $W_{sw} = C\exp(-NR_{sw}), \quad R_{sw} = s(\mathbf{x}_S) - s(\mathbf{x}_A)$



Optimal switching path: from $\mathbf{x}_A$ to $\mathbf{x}_S$

$$\mathbf{x} \to \mathbf{x}_A, \mathbf{p} = \partial_{\mathbf{x}} s \to \mathbf{0} \text{ for } t \to -\infty;$$

$$\mathbf{x} \to \mathbf{x}_S, \mathbf{p} \to \mathbf{0} \text{ for } t \to \infty$$

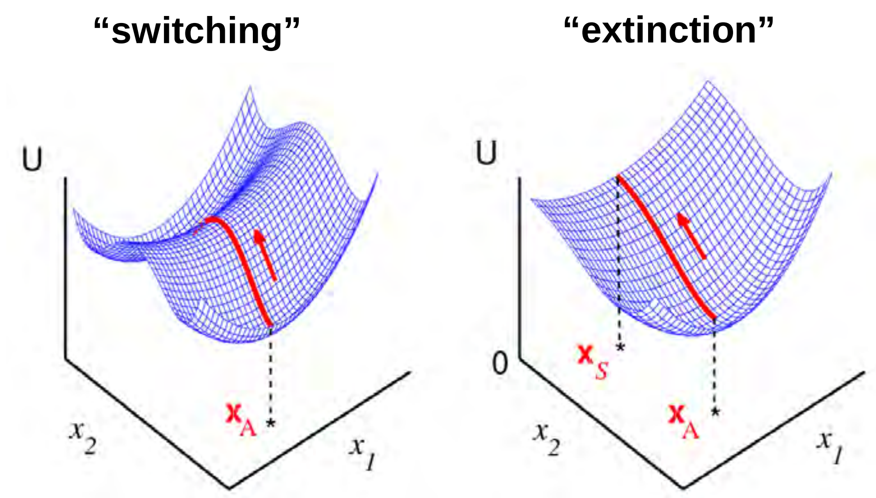
the probability current is continuous across the saddle, no accumulation near the saddle point, as for switching in white-noise driven continuous dissipative systems

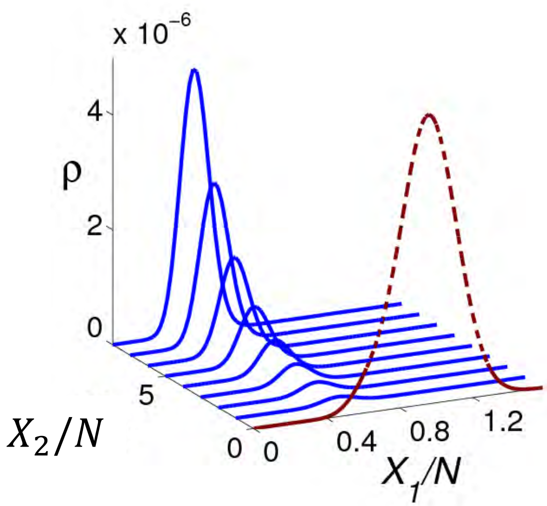
MD, Mori, Ross, & Hunt (1994)

Extinction also requires a large fluctuation

$$\frac{\partial \rho(\mathbf{X})}{\partial t} = \sum_{\mathbf{r}} [W(\mathbf{X}-\mathbf{r};\mathbf{r})\rho(\mathbf{X}-\mathbf{r}) - W(\mathbf{X};\mathbf{r})\rho(\mathbf{X})]$$

Individuals/molecules that have reached the extinction plane $X_E = 0$ **accumulate there,** $\dot{\rho} = -\nabla \mathbf{J} \neq 0$





Snapshot of the distribution tail for the SIS model, t/t_r = 9, N = 50 (Khasin & MD, 2009)

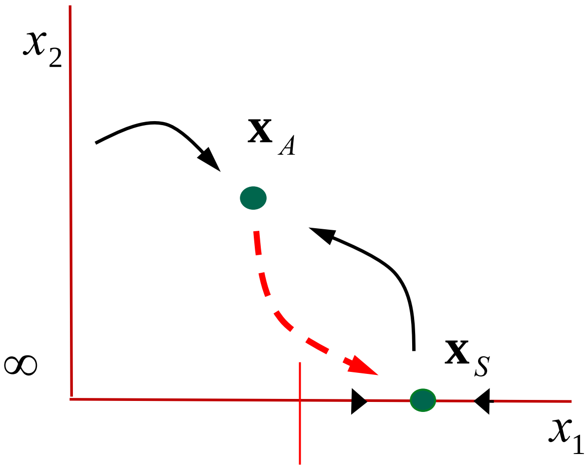
Extinction rate $W_e << t_r^{-1}$. **For** $t_r << t << W_e^{-1}$ **the distribution is quasistationary away from the extinction plane. The in-plane population is** $W_e t$.

Boundary conditions for the optimal extinction path

Eikonal approximation: $\rho(\mathbf{X}) = \exp[-Ns(\mathbf{x})],\ \dot{s} = -H(\mathbf{x}, \partial_{\mathbf{x}} s) \equiv -H(\mathbf{x}, \mathbf{p})$

Quasistationary distribution away from the extinction plane: $H(\mathbf{x},\mathbf{p}) = \sum_{\mathbf{r}} w(\mathbf{x};\mathbf{r})[\exp(\mathbf{pr})-1] = 0$

Extinction rate: $W_e = C\exp(-NR_e),\ R_e = s(\mathbf{x}_S) - s(\mathbf{x}_A)$



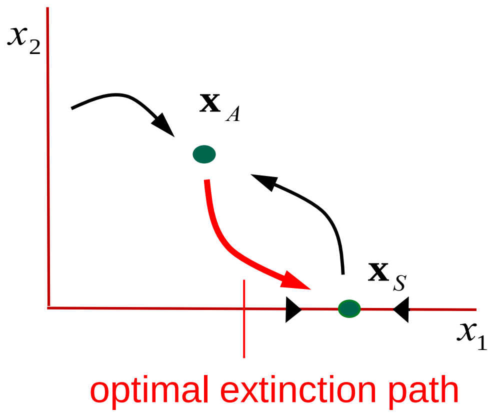
Optimal extinction path $\mathbf{x}_e(t), \mathbf{p}_e(t)$:

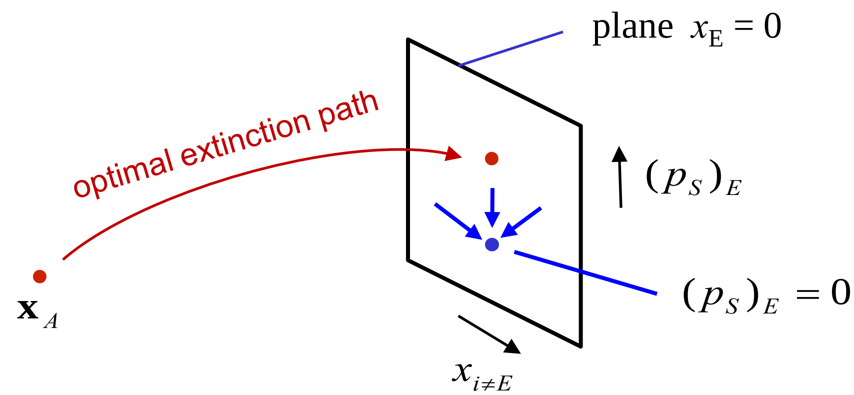
$\mathbf{x}_e \to \mathbf{x}_A, \mathbf{p}_e \to \mathbf{0}$ for $t \to -\infty$; $\mathbf{x}_e \to \mathbf{x}_S, \mathbf{p}_e \to \mathbf{p}_S$ for $t \to \infty$

$s(\mathbf{x})$ is minimal in the extinction plane **for** $\mathbf{x} = \mathbf{x}_S$.

$(p_S)_{i\neq E} = 0,\ (p_S)_E \neq 0$ from equation: $\sum_{\mathbf{r}} w(\mathbf{x};\mathbf{r})\{\exp[(p_S)_E r_E]-1\} = 0$ for $\mathbf{x}\to\mathbf{x}_S$

The normal momentum component is not equal to zero!





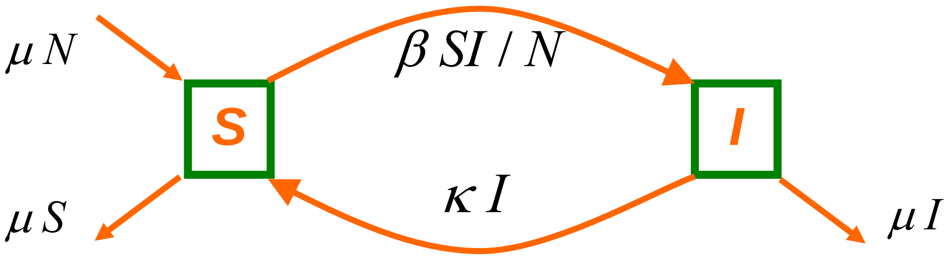
The system **first** approaches $(\mathbf{x}_S, \mathbf{p}_S)$, and **then** moves to $(\mathbf{x}_S, \mathbf{p}=\mathbf{0})$, with no change in Q_e.

Specific systems: van Herwaarden & Grassman (1995); Elgar & Kamenev (2004)

General: MD, Schawrtz, & Landsman (2008); periodically modulated systems: Khasin, MD, & Meerson (2010)

"Anomalous" scaling of the extinction exponent R_e with the distance η to the bifurcation point where $\mathbf{x}_A$ and $\mathbf{x}_S$ merge: $R_e \propto \eta^2$ instead of the scaling $R_{sw} \propto \eta^{3/2}$

MD, Schawrtz, & Landsman (2008)



S: susceptible

I: infected

μ: birth and death rate

β: contact rate between S and I

κ: recovery rate

Birth-death transition rates: $W(\mathbf{X};(1,0)) = N\mu,\quad W(\mathbf{X};(-1,0)) = \mu X_1,\quad W(\mathbf{X};(0,-1)) = \mu X_2$

Infection-recovery transition rates: $W(\mathbf{X};(-1,1)) = \beta X_1 X_2 / N,\quad W(\mathbf{X};(1,-1)) = \kappa X_2$

Disease extinction: $I = X_2 \equiv X_E \to 0$

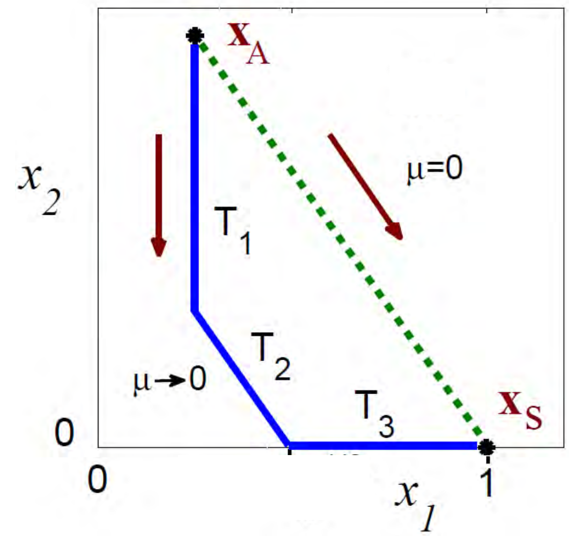
$\mu = 0$ - conserved total population, $X_1 + X_2 = N$

[Weiss & Dishon (1971), Leigh (1981), Doering, Sargsyan, & Sander (2005), …]

Explicit solution for the optimal extinction path gives: $(p_S)_E \equiv (p_S)_2 = 0,\ (p_S)_1 = \ln(\beta/\kappa)$

inconsistent with $(p_S)_{i \neq E} = 0,\ (p_S)_E \neq 0$

Optimal extinction paths without and with birth-death processes, $\mu = 0$ **and** $\mu > 0$



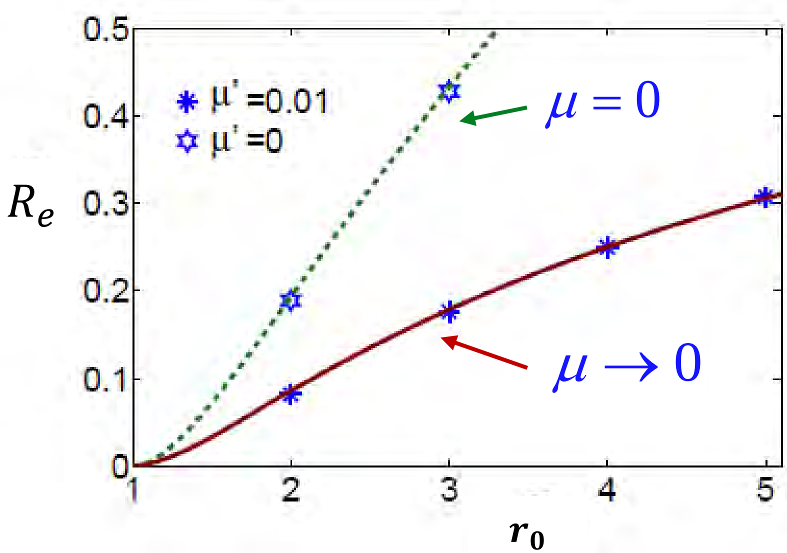
$r_0 = \beta/(\mu+\kappa)$, infection reproductive rate

Extinction exponents [$W_e = C_e \exp(-NR_e)$]:

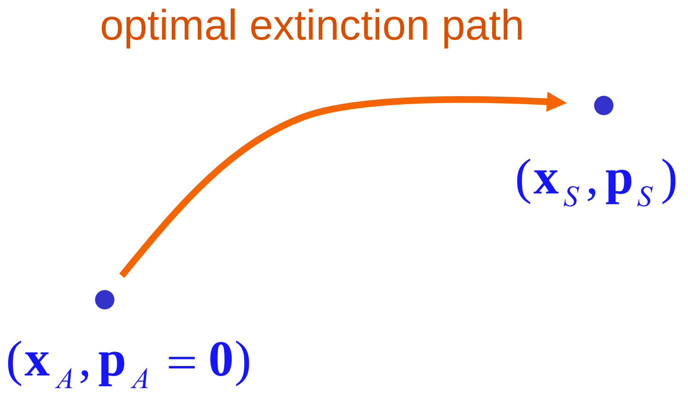
$$R_e\Big|_{\mu=0} = \ln r_0 - 1 + r_0^{-1}$$

$$R_e\Big|_{\mu\to 0} = \left(r_0^{1/2} - 1\right)^2 / r_0$$

$$\mu >> W_e$$



Solutions with $(p_S)_{i \neq E} \neq 0$ are *fragile*



Perturbation: $W(\mathbf{X};\mathbf{r}) \to W(\mathbf{X};\mathbf{r}) + \mu W^{(1)}(\mathbf{X};\mathbf{r})$

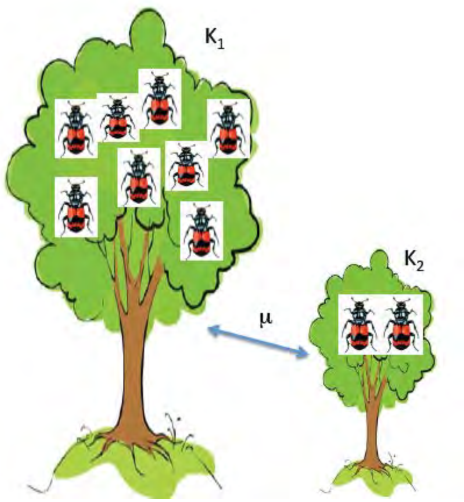
$$|\mu| << 1$$

Perturbed Hamiltonian: $H \to H + \mu H^{(1)}$

$$H^{(1)}(\mathbf{x},\mathbf{p}) = \sum_{\mathbf{r}} w^{(1)}(\mathbf{x};\mathbf{r})[\exp(\mathbf{p}\,\mathbf{r}) - 1]$$

Perturbed extinction exponent: $R^{(1)} = -\mu \int_{-\infty}^{\infty} dt\, H^{(1)}(\mathbf{x}_e^{(0)}(t), \mathbf{p}_e^{(0)}(t))$

If $(p_S)_{i \neq E} \neq 0$ and $w^{(1)}(\mathbf{x}_S;\mathbf{r}) \neq 0$ the integral **diverges** for $t \to \infty$

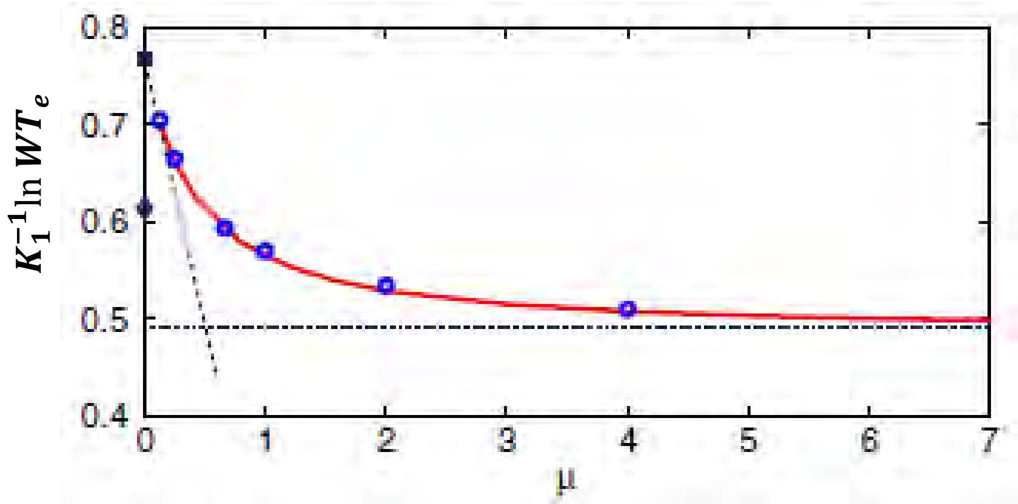


$$\overset{W}{A \to 2A,} \qquad \overset{W/K_i}{2A \to 0}$$

$\boldsymbol{\mu}$ − **migration rate**

mean-field equations for populations x, y **scaled by** K_1

$$W\dot{x} = x - x^2 - \mu(x - y), \qquad W\dot{y} = y - \frac{K_1}{K_2} y^2 + \mu(x - y)$$



Khasin, Meerson,Khain,& Sander, 2012

Oscillator isolated from the thermal reservoir: Floquet (quasienergy) states

$$H(t) = \tfrac{1}{2}(p^2 + \omega_0^2 q^2) + \tfrac{1}{4}\gamma q^4 - qF\cos(\omega_F t), \qquad i\hbar\dot{\psi} = H(t)\psi,$$

$$\psi_\varepsilon(t) = e^{-i\varepsilon t/\hbar}\, u_\varepsilon(t), \qquad u_\varepsilon\left(t + \frac{2\pi}{\omega_F}\right) = u_\varepsilon(t)$$

↑ quasienergy

Values of ε are quantized, $\varepsilon \to \varepsilon_n$; discrete states of the modulated oscillator are ψ_{ε_n}

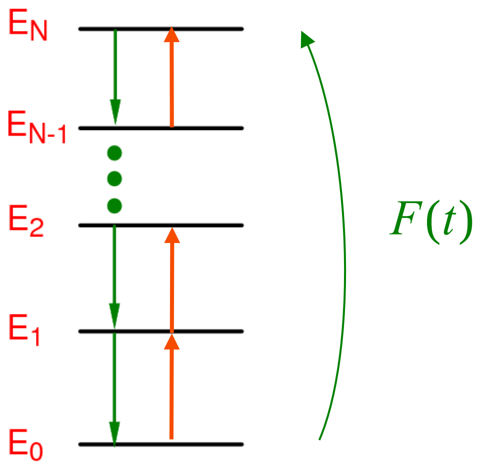
Underdamped oscillator in the rotating frame:

$$H(t) = \tfrac{1}{2}\left(p^2 + \omega_0^{\,2} q^2\right) + \tfrac{1}{4}\gamma q^4 - qF\cos(\omega_F t) \xrightarrow{\text{RWA}} C_g\, g(Q,P),$$

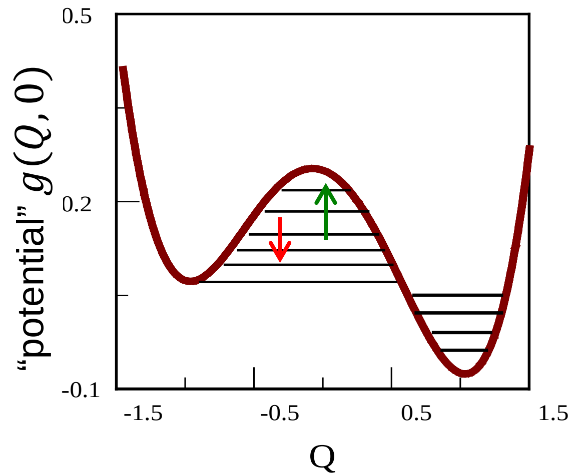
energy states

$$\varepsilon_n \propto (\omega_F - \omega_0)^2 g_n$$

quasi-energy states

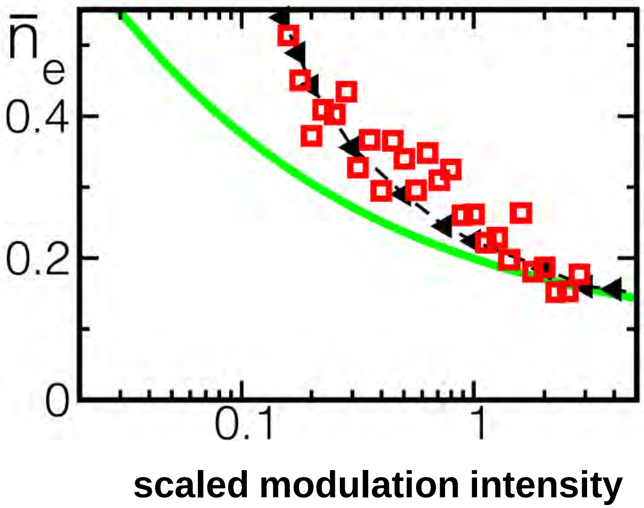


$$E_N \approx N\hbar\omega_0$$

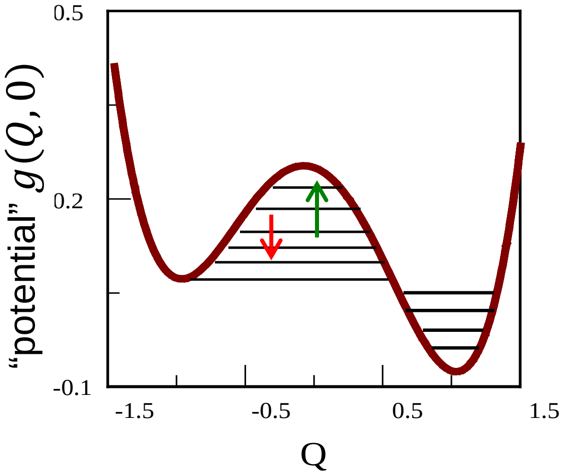


Quasienergy states are linear combinations of Fock states. Inter-level transitions $|N_{\mathrm{Fock}}\rangle \to |N_{\mathrm{Fock}} - 1\rangle$ **correspond to inter-quasi-energy level transitions** $|n\rangle \to |n \pm m\rangle$ ➡

drift and quantum diffusion over quasienergy even for T = 0

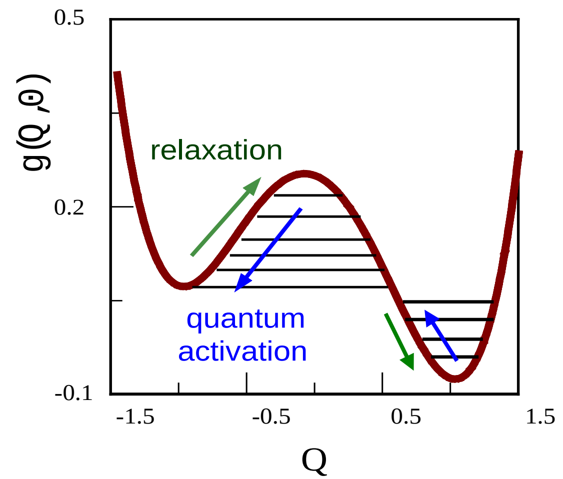


T=0



$\bar{n}_e$ – "Planck number" of the distribution over quasienergy states (experiment: Ong et al, 2013; theory: MD, Marthaler, & Peano, 2011; MD 2012; Peano & MD 2014)

near extremum: $\rho_n \propto \exp(-g_n/k_B T_e)$



Balance equation **for populations ρ_n of quasienergy states**

$$\partial_t \rho_n = \sum [W(n-k;k)\rho_{n-k} - W(n;k)\rho_n]$$
$$= \sum \left(e^{-k\partial_n} - 1\right) W(n;k)\rho_n$$

Many "intrawell" states $N \propto \tilde{\hbar}^{-1} \propto \hbar^{-1}$

dimensionless Planck constant

Far tail: steep distribution, $\rho_n = \exp\left(-R_n/\tilde{\hbar}\right) \quad (\tilde{\hbar} \ll 1)$

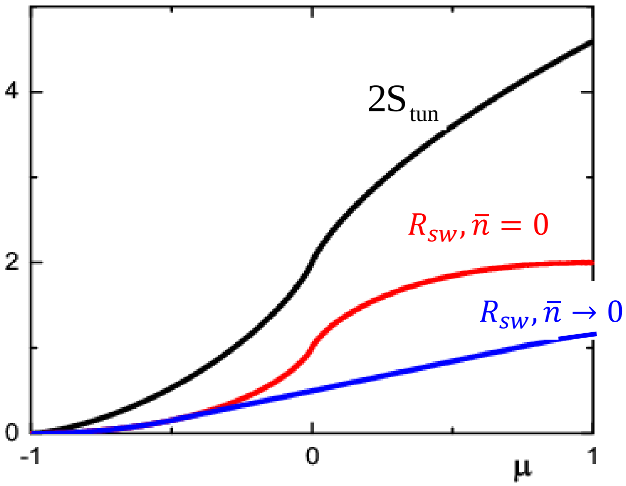
Eikonal approximation: smooth $R_n, \quad R_n \equiv R(g_n), \; |R_{n\pm1} - R_n| \sim \tilde{\hbar} \ll 1$

Switching rate $W_{sw} \propto \Gamma \exp(-R_{sw}/\tilde{\hbar}), \; R_{sw} = R(g_S) - R(g_A)$

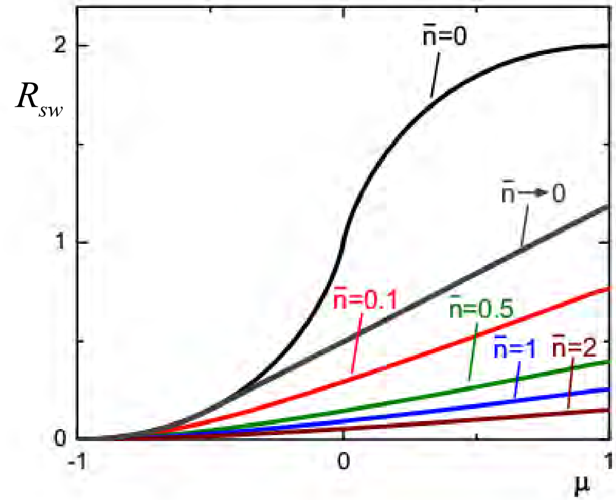
(MD & Smelyanskiy, 1988)

Modulated oscillator: quantum activation vs tunneling*

$$W_{\rm tun} \propto \exp(-2S_{\rm tun}/\tilde{\hbar})$$



$$W_{sw} \propto \exp(-R_{sw}/\tilde{\hbar})$$



$$\bar{n} = [\exp(\hbar\omega_0/kT) - 1]^{-1}$$

Surprise #1: Activation energy < tunneling exponent!

Surprise # 2: Fragility - in the WKB limit

$$R_{sw}(T=0) \neq R_{sw}(T\to 0)$$

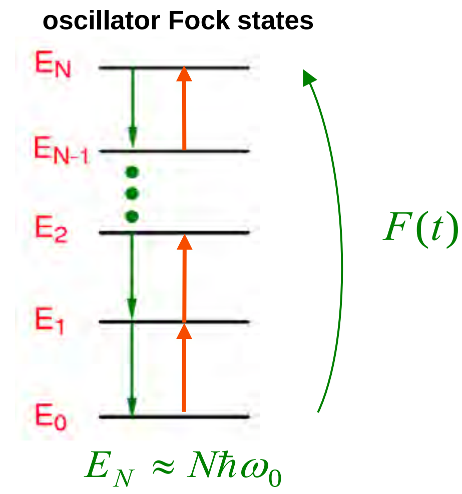
***The plots refer to a parametric oscillator; Marthaler & MD (2006)**

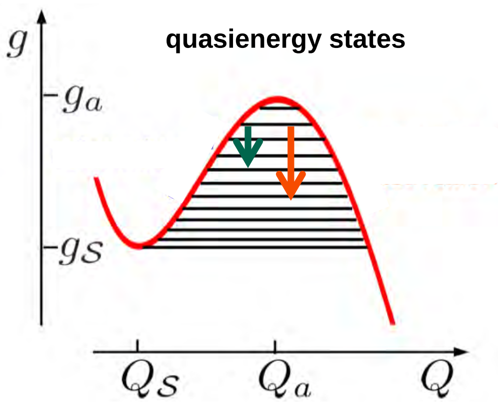
Balance equation: $\dot{\rho}_n = \sum[W(n-k;k)\rho_{n-k} - W(n;k)\rho_n]$

Contribution to transition rates from "photon" emission and absorption:

$W(n;k) = W^{(e)}(n;k) + W^{(abs)}(n;k),$ $W^{(abs)} \propto \bar{n} \propto \exp(-\hbar\omega_0/k_B T)$

$\bar{n} \ll 1$





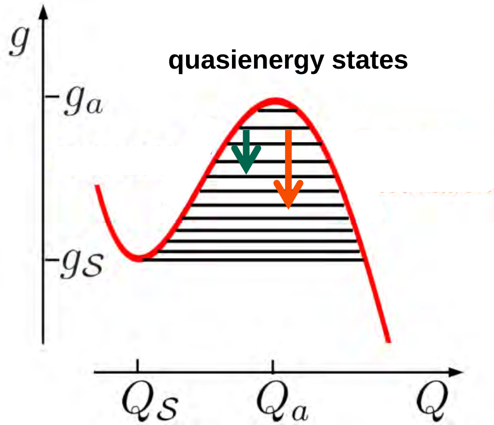
The absorption-induced transitions have longer "decay length"

$W^{(e)}(n;k) \propto \exp[-k/\xi^{(e)}(n)],$

$W^{(abs)}(n;k) \propto \exp[-k/\xi^{(abs)}(n)],$ $\boldsymbol{\xi^{(e)} < \xi^{(abs)}}$

The perturbation theory in $\bar{\boldsymbol{n}}$ breaks down for $\boldsymbol{T > T_{c1} \propto \hbar^2}$,
$\ln \bar{\boldsymbol{n}} \propto -\hbar^{-1}$

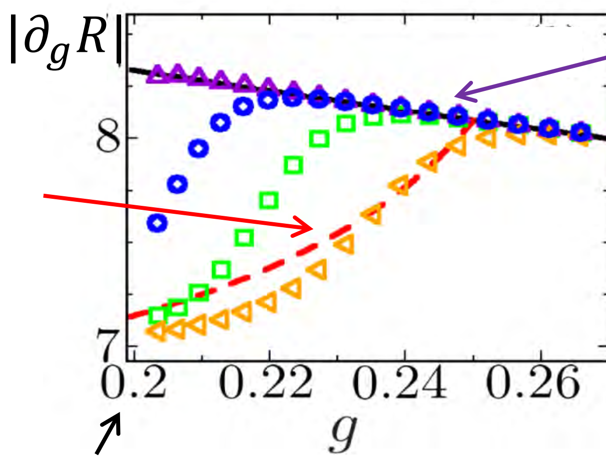
T>$T_{cr} \propto \hbar^2$: onset of a kink



Breakdown of the eikonal approach for $\mathrm{T} > \mathrm{T}_{c1}$:

starting with some $n^* \equiv n^*(T)$, state populations are determined by the absorption-induced influx from states close to the extremum of g

➡ **inter-instanton kink at $\mathbf{n}^*(\boldsymbol{T})[\boldsymbol{g}_{\boldsymbol{n}^*} = \boldsymbol{g}(\boldsymbol{n}^*(\boldsymbol{T}))]$, which moves with T**



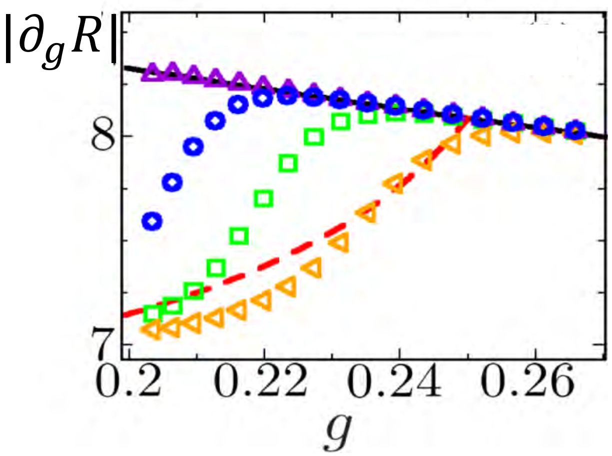
$T = 0$ solution

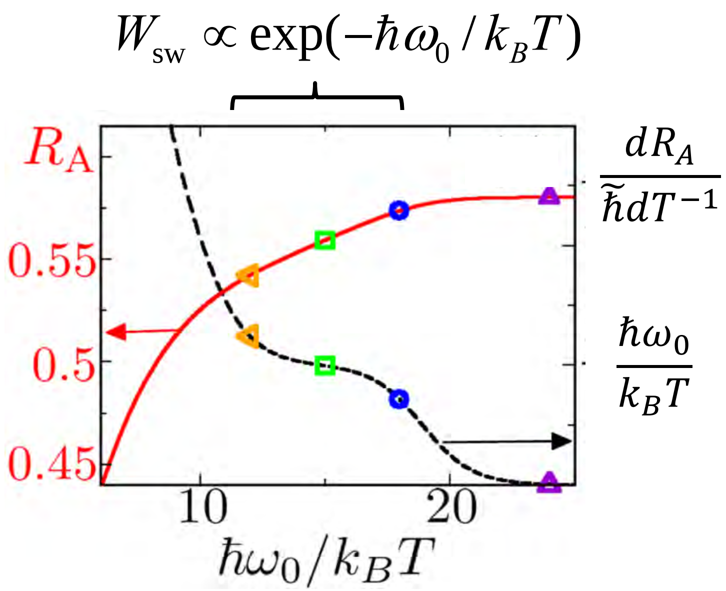
$T > T_{c2} \propto \hbar/|\log \tilde{\hbar}|, \bar{n} \ll 1$

g_s, saddle state

g_{max}, stable vibrational state

L. Guo, V. Peano, M. Marthaler, and MD (2013) inter-instanton kink, which moves with temperature





General fragility condition for the instanton Hamiltonian $\mathcal{H}(x,p) = \mathcal{H}^{(0)}(x,p) + \epsilon \mathcal{H}^{(1)}(x,p)$.

The instanton is "fragile" for $\int dt\, \mathcal{H}^{(1)}\left(x^{(0)}(t), p^{(0)}(t)\right) \to \infty$

as in the problem of population extinction, although the mechanism is different

Conclusions

- **The exponents and prefactors of switching rates scale as a power of the distance to the bifurcation point. Different scaling for extinction**

- **Switching and extinction rates in systems lacking detailed balance display fragility: a *parametrically large* change of the rate exponent occurs in an *extremely narrow* parameter range – the beauty of real-time instantons. Watch out for fragility**

- ***Quantum relaxation comes with noise*. Escape of modulated quantum oscillators occurs via quantum activation – a restriction on JBA-based quantum measurements**