Slow thermalization in a chain of classical oscillators

François Huveneers

DAUPHINE UNIVERSITÉ PARIS | CEREMADE UMR CNRS 7534

ICTS Bangalore, November 2019

Joint work with

Jani Lukkarinen
(University of Helsinki)

Main goals

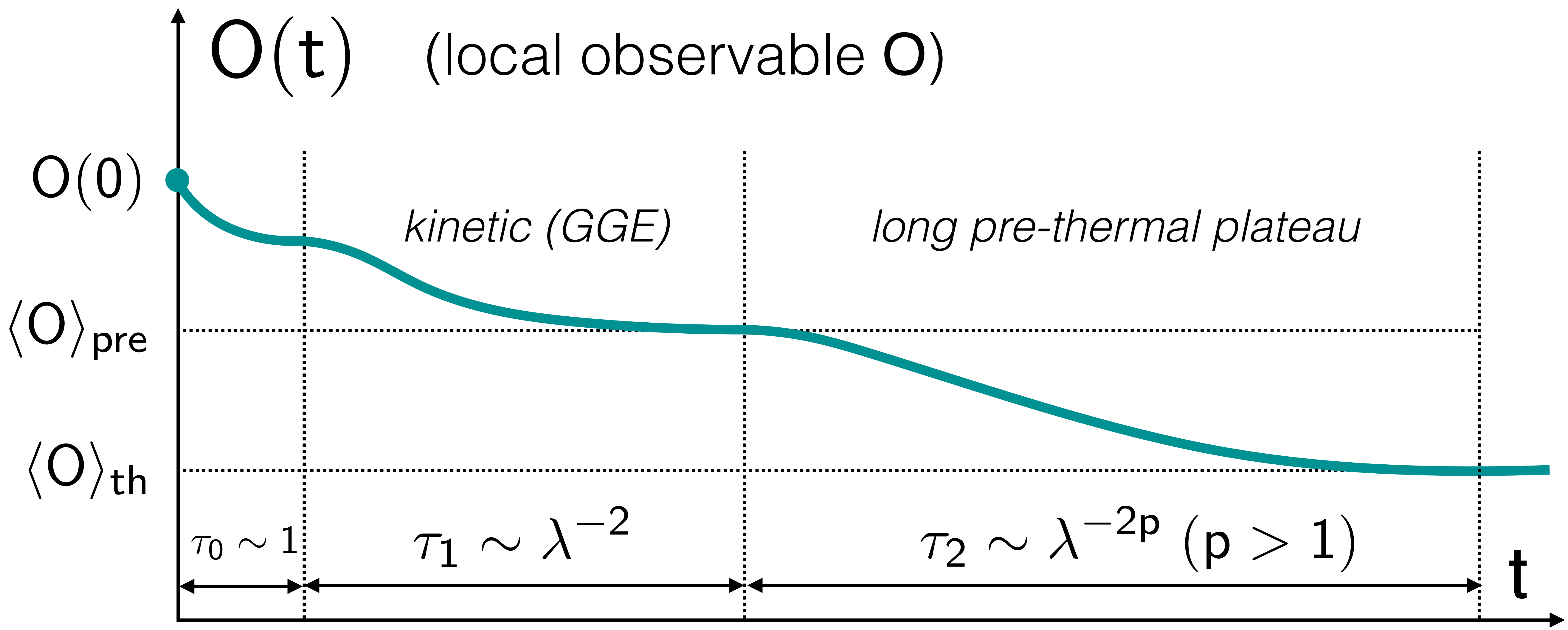
- New example of “astonishingly” *slow relaxation* in a Hamiltonian system (cfr. *W.W. Ho, A. Das…*)
- Apply recent ideas designed for *quantum* systems to a *classical* system
- Extend the description from *kinetic theory* to longer time scales (cfr. *M. Rigol*, K. Mallayya et al. PRX9)

general picture

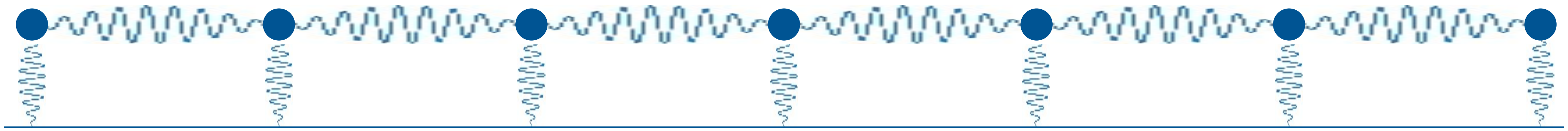
$$H = H_0 + \lambda V$$

integrable (H_0)

weak integrability breaking (λV)



Anharmonic chain of oscillators



$$H = \sum_{x=1}^{L} \left[\frac{p_x^2}{2} + \frac{\omega_0^2 q_x^2}{2} - \delta\omega_0^2 q_x q_{x+1} + \lambda \frac{q_x^r}{r} \right] \qquad r = 4, 6$$

kinetic energy — harmonic pinning — harmonic coupling — anharmonic interaction

units: $\omega_0 = 1$

weak coupling regime: $\lambda \to 0$

'Similar' to Fermi-Pasta-Ulam-Tsingou '53

classical dynamics

Newton's equations:

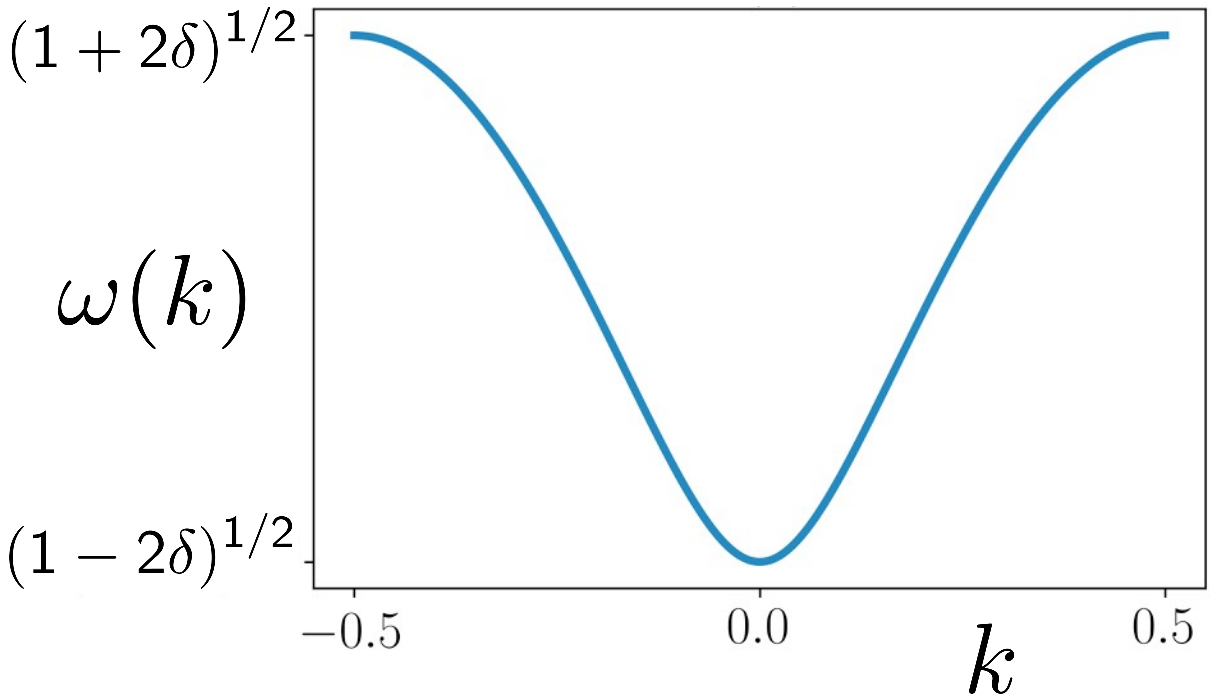
$$\frac{d^2 q_x}{dt^2} = -(1-2\delta)q_x + \delta(\Delta q)_x - \lambda q_x^{r-1}$$

$$0 \le \delta \le 0.5\,, \qquad \lambda \ge 0 \qquad (\text{stability})$$

λ=0: harmonic ~ classical phonon field:

$$H_0 = \int_{BZ} dk\, \omega(k) |a(k)|^2$$

$$\frac{da(k)}{dt} = -i\omega(k)a(k)$$



interacting phonons

$\lambda > 0$: interaction among phonons: $\quad H = H_0 + \lambda V$

$$V = \frac{1}{16} \int \frac{dk_1 \dots dk_4}{(\omega_1 \dots \omega_4)^{1/2}} \delta(k_1 + \cdots + k_4) \sum_{\sigma_i = \pm} a^{\sigma_1}(k_1) \dots a^{\sigma_4}(k_4) \qquad (r = 4)$$

$$\text{with} \quad a^-(k) = a(k), \quad a^+(k) = a^*(-k)$$

Only the energy **H** is conserved, so the number of phonons

$$N_0 = \int_{BZ} dk \, |a(k)|^2$$

is **not** preserved (terms with $\sigma_1 + \cdots + \sigma_4 \neq 0$)

Remark on locality

Observable $A = \int_{BZ} dk\, \varphi(k) |a(k)|^2$, $\varphi(k)$ analytic

In real space:

$$A = \sum_{x,y} \hat{\varphi}(x-y) a(x) a^*(y)\,, \qquad |\hat{\varphi}(x-y)| \sim e^{-|x-y|/\ell_0}$$

and **a(x)** quasi-local as well.

In particular, the number of phonons N_0 is local.

Generalized Gibbs ensemble (GGE)

Initial state: translation invariant and zero average

All the $|a(k)|^2$ are conserved at **λ=0**

State of the system after a time $\tau_0 \sim 1$:

$$\rho_0 \;\sim\; \exp\left(-\int_{BZ} dk \frac{|a(k)|^2}{W(k)}\right) \qquad \text{(GGE)}$$

where **W(k)** is called the *Wigner* function.

Boltzmann-Peierls description

Usually: proper thermalization on a time $\tau_1 \sim \lambda^{-2}$

(aka kinetic time scale, Fermi golden rule)

Reason:

(1) $\frac{d}{dt}|a(k)|^2 = \lambda\, J(k) \qquad \langle J(k)\rangle_{\rho_0} = 0 \qquad \text{for all GGE } \rho_0$

(2) Assume $\qquad \rho_t = \rho_0 \times \left[1 + \lambda f_1 + \mathcal{O}(\lambda^2)\right]$

(3) Thus $\qquad \frac{d}{dt}\langle |a(k)|^2\rangle_{\rho(t)} = \lambda^2 \langle J(k) f_1\rangle_{\rho_0} + \mathcal{O}(\lambda^3)$

(4) Thus λf_1 is stationary and is determined by expressing this.

The rate $\langle J(k) f_1\rangle_{\rho_0}$ becomes a *current-current* correlator

Boltzmann-Peierls description (cont'd)

Alternatively, one may express how the GGE, i.e. how the Wigner function, evolves with time (Boltzmann equation for phonons):

$$\partial_t W(k,t) = \lambda^2 \mathcal{C}(W(\cdot,t))(k) + \mathcal{O}(\lambda^3)$$

collision operator with **r=4,6** phonons

Cfr. Spohn, Lukkarinen, Lefevere…

The rate may accidentally vanish!

For q_x^4: $$\frac{d}{dt}\langle N_0 \rangle_{\rho_t} = 0 \times \lambda^2 + \mathcal{O}(\lambda^3)$$

Is it generic?

No: q_x^6 interaction , $0.3 < \delta < 0.5$

or q_x^4 and different dispersion relation $\omega(k)$

Yes: for δ small enough

Pre-thermal state if N_0 pseudo-conserved:

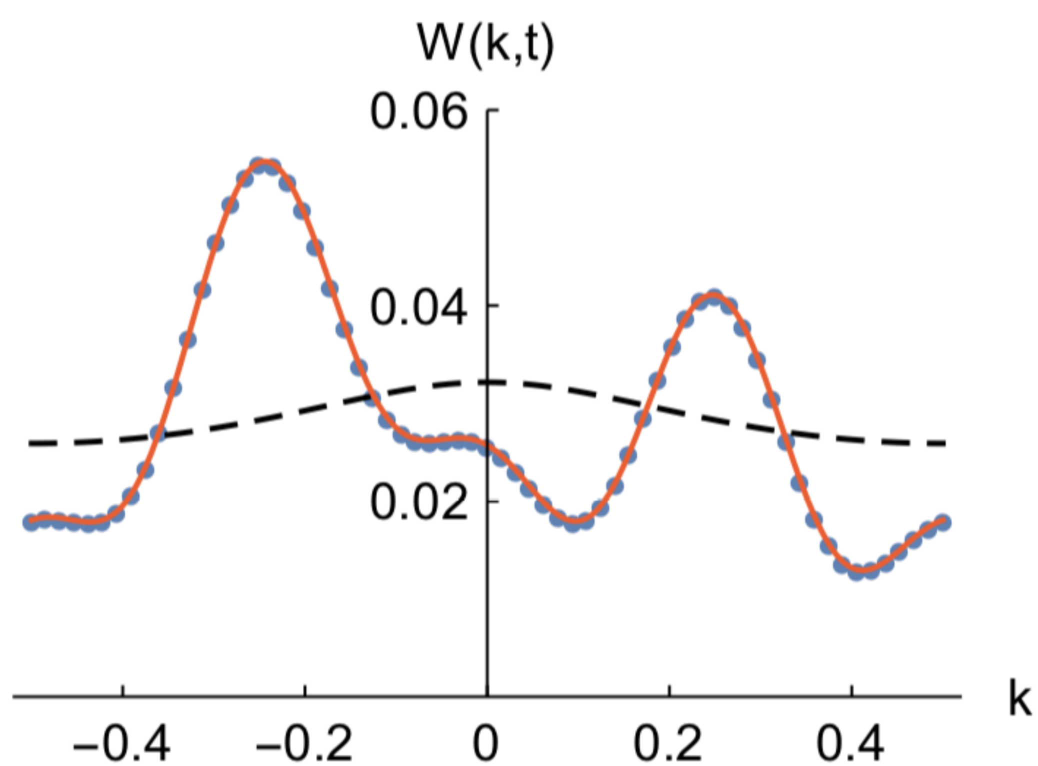
$$\rho_{pre} \sim e^{-\beta(H_0 - \mu N_0)}$$

When does it relax to proper equilibrium?

Kinetic time scales

Validity of the Boltzmann equation for spatially homogeneous initial conditions:

$$\mathsf{a}(\mathsf{k},0) \;=\; \sqrt{\mathsf{W}(\mathsf{k},0)}\,\mathsf{e}^{\mathsf{i}\varphi_\mathsf{k}} \qquad \varphi_\mathsf{k} \text{ random iid}$$

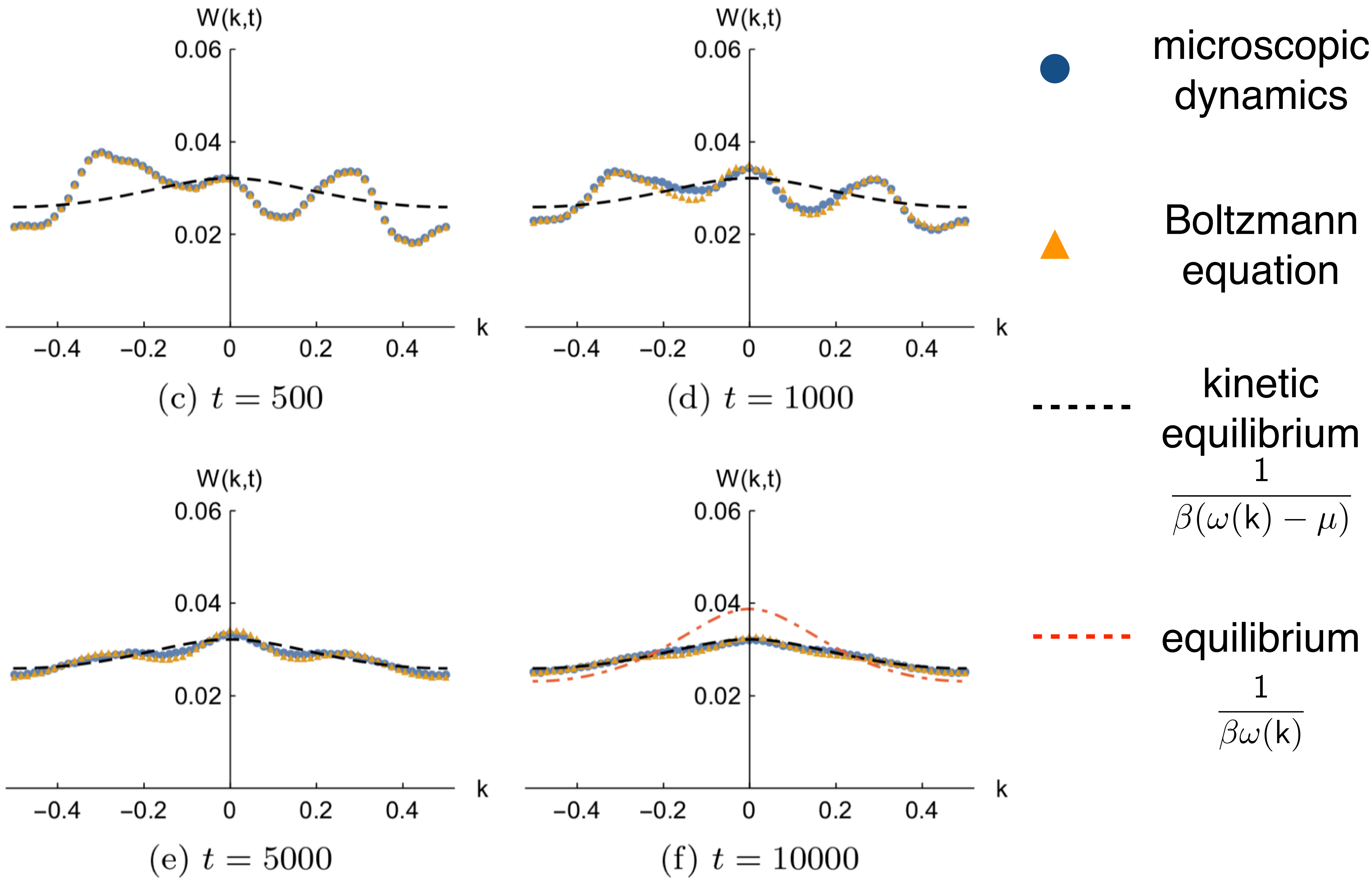


(a) $t = 0$

W(k,0)

$$\mathsf{W}_\infty(\mathsf{k}) \;=\; \frac{1}{\beta(\omega(\mathsf{k}) - \mu)}$$

Mendl, Lu and Lukkarinen, PRE '16



$t_{kin} \sim 1000$

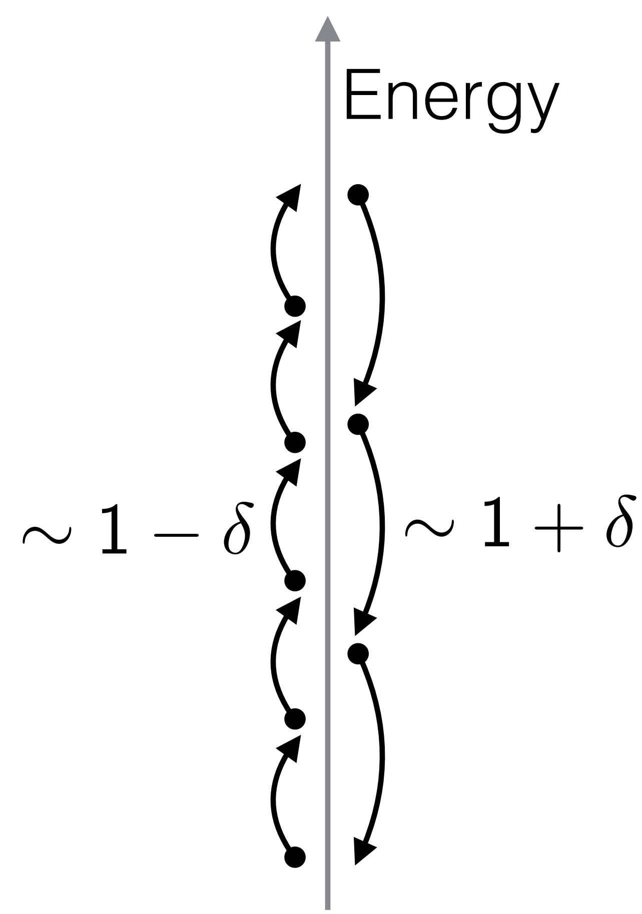
Mendl, Lu and Lukkarinen, PRE '16

Physical explanation, for *quantized* phonons!

- Only resonant processes (preserving $\mathbf{H_0}$) do change the number of phonons when $\lambda \to 0$
- The energy band becomes narrow for small δ: W $\sim 2\delta$

Creating **2** phonons through a **2n**-order process:

create **n+1** low energy phonons



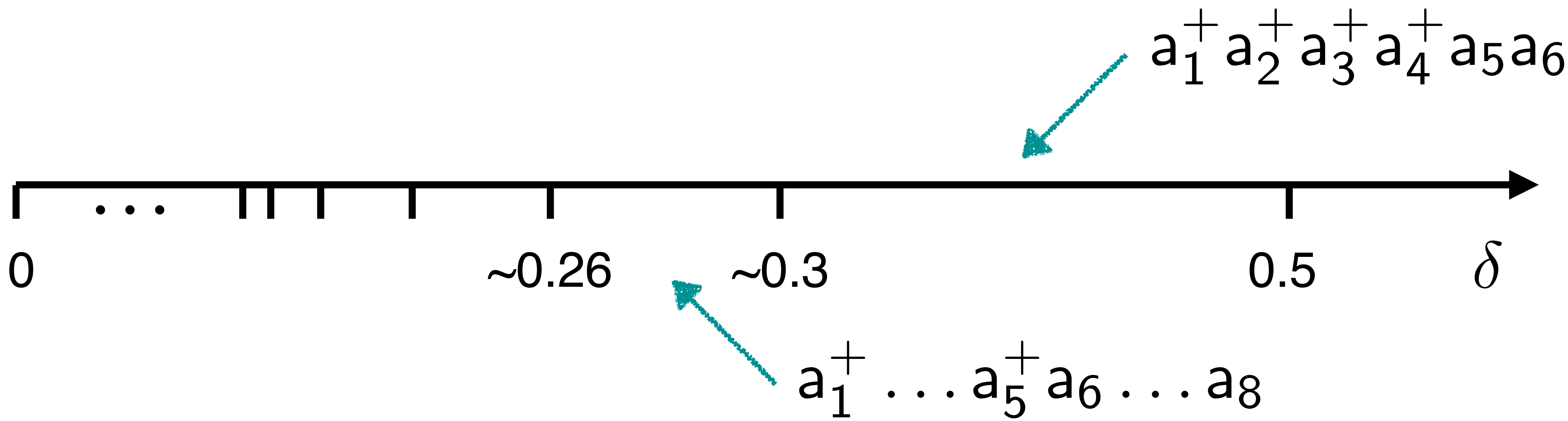
annihilate **n-1** high energy phonons

Need for high order processes

translation invariance: $k_1 + \cdots + k_{2n} = 0$

resonance: $(\omega_1 + \cdots + \omega_{n+1}) - (\omega_{n+2} + \cdots + \omega_{2n}) = 0$

$a_1^+ a_2^+ a_3^+ a_4$: impossible to satisfy both constraints



As $\delta \to 0$, need for a process of order $n \sim 1/\delta$

Scaling as a function of λ

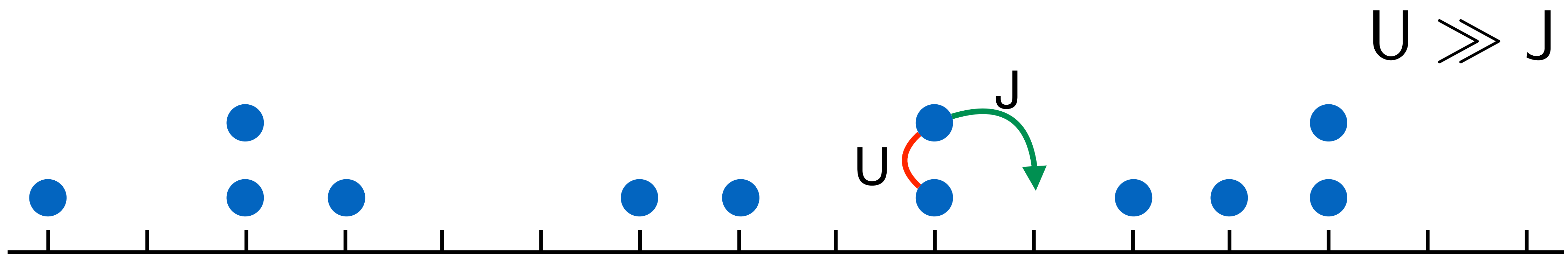
Strength of the processes dissipating the number of phonons:

anharmonic interaction / harmonic coupling	λq_x^4	λq_x^6
$0.3 < \delta \leq 0.5$	$\sim \lambda^2$	$\sim \lambda$
$0.26 < \delta < 0.3$	$\sim \lambda^3$	$\sim \lambda^2$
$\cdots < \delta < 0.26$	$\sim \lambda^4$	$\sim \lambda^2$

This is **not** yet the instantaneous **rate** of dissipation!

Inspiration for a rigorous formulation

Number of doublons N_d in the Fermi-Hubbard chain:



Unitary transformation to get rid of non-dissipative (non-resonant) processes:

$$[H, N_d] \sim J \qquad \text{to} \qquad [\tilde{H}, N_d] \sim J\, e^{-U/J}$$

D. Abanin, W. De Roeck, W.W. Ho and F.H, PRB '17, CMP '17

Pseudo-conserved quantity

Change frame = perform a canonical change of variables:

There exists $\mathsf{G} = \mathcal{O}(\lambda)$ such that

$$\tilde{\mathsf{H}} = e^{\{\mathsf{G},\cdot\}}\mathsf{H} \qquad \text{and} \qquad \{\tilde{\mathsf{H}}, \mathsf{N}_0\} \sim \lambda^{\mathsf{p}}$$

Back to the original coordinates:

There exists $\mathsf{N} = \mathsf{N}_0 + \mathcal{O}(\lambda)$ such that $\{\mathsf{H}, \mathsf{N}\} \sim \lambda^{\mathsf{p}}$

with $\mathsf{p} = \mathsf{p}(\delta)$ as on the table before $(\mathsf{p} \sim 1/\delta$ as $\delta \to 0)$

Questions

Q1: N_0 is not quantized, why does it work?

The spectrum of $\{N_0, \cdot\}$ is, when applied on polynomials in $a^\pm$

$$\{N_0, a^{\sigma_1}(k_1)\dots a^{\sigma_n}(k_n)\} = \big(\sigma_1 + \dots + \sigma_n\big)\, a^{\sigma_1}(k_1)\dots a^{\sigma_n}(k_n)$$

Q2: What means $\{H, N\} \sim \lambda^{p^\star+1}$?

translation invariance

$$\{H, N\} = \lambda^p \int dk_1 \dots dk_n\, \delta(k_1 + \dots + k_n) \sum_{\sigma_i=\pm1} \varphi(k_1, \dots, k_n, \sigma_1, \dots, \sigma_n)\, a^{\sigma_1}(k_1)\dots a^{\sigma_n}(k_n), \qquad n \sim p$$

analytic

Dissipation rate

We mimic the approach to kinetic regime: $\tau_2 \sim \lambda^{-2p}$

1) Assume that the system is in the state

$$\rho_t = \rho_0 \times \left[1 + \lambda^p f + \mathcal{O}(\lambda^{p+1})\right]$$

$$\rho_0 \sim e^{-\beta(\tilde{H} - \mu N_0)}$$

2) We notice that

$$\frac{dN_0}{dt} = \lambda^p J, \qquad \langle J \rangle_{\rho_0} = 0$$

Dissipation rate (cont'd)

3) We conclude that

$$\frac{d}{dt}\langle N_0\rangle_{\rho(t)} \;=\; \lambda^{2p}\langle Jf\rangle_{\rho_0} + \mathcal{O}(\lambda^{2p+1})$$

4) We deduce that **f** is stationary, and this allows to find it:

$$\frac{d}{dt}\langle N_0\rangle_{\rho(t)} \;=\; \lambda^{2p}(-\mu\beta)\int_0^\infty dt\, e^{-t/\tau}\langle J(t)J(0)\rangle_0 \;+\; \mathcal{O}(\lambda^{2p+1})$$

with $\langle\cdot\rangle_0 \sim e^{-\beta(H_0-\mu N_0)}$ and $J(t) = e^{\{H_0,\cdot\}t}J$

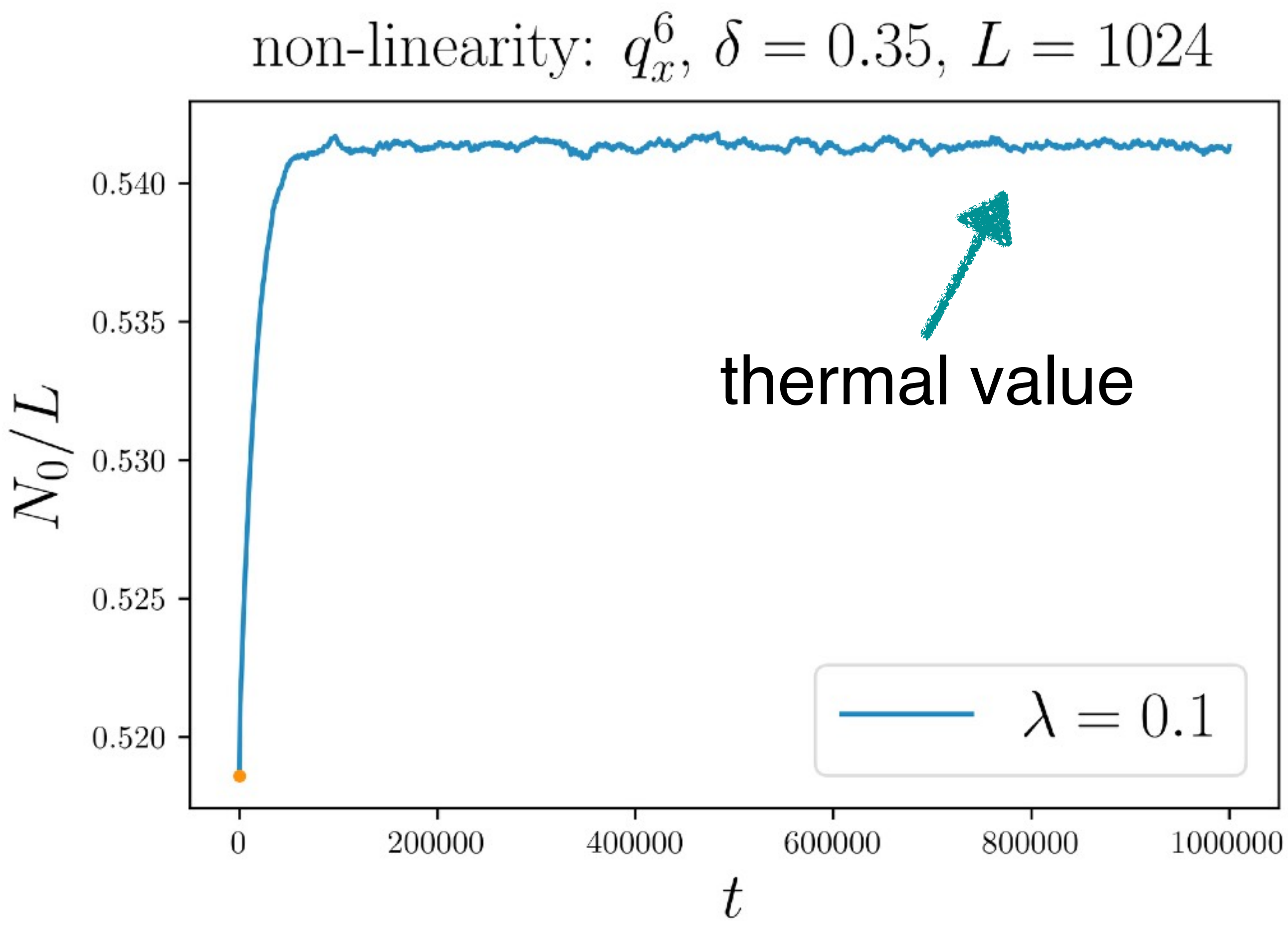
cfr. also K. Mallayya, M. Rigol, W. De Roeck, Phys. Rev. X 9, 2019

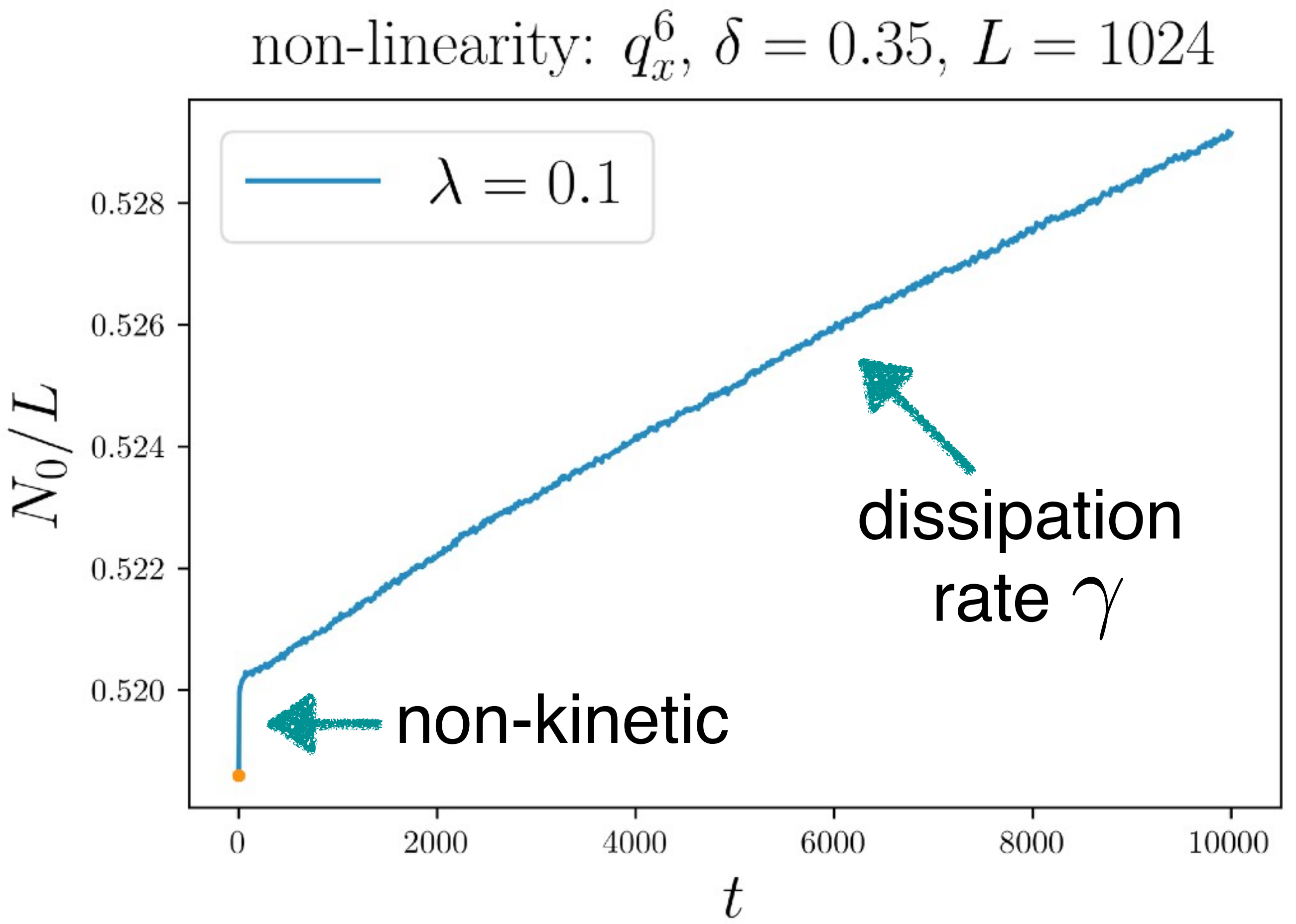
Numerical protocol

Initial state:

$$\mathsf{a}(\mathsf{k}) \;=\; \sqrt{\mathsf{W}(\mathsf{k})}\,\mathsf{e}^{\mathsf{i}\varphi_\mathsf{k}} \quad (\varphi_\mathsf{k} \text{ random iid}), \qquad \mathsf{W}(\mathsf{k}) \;=\; \frac{1}{\beta(\omega(\mathsf{k})-\mu)}$$

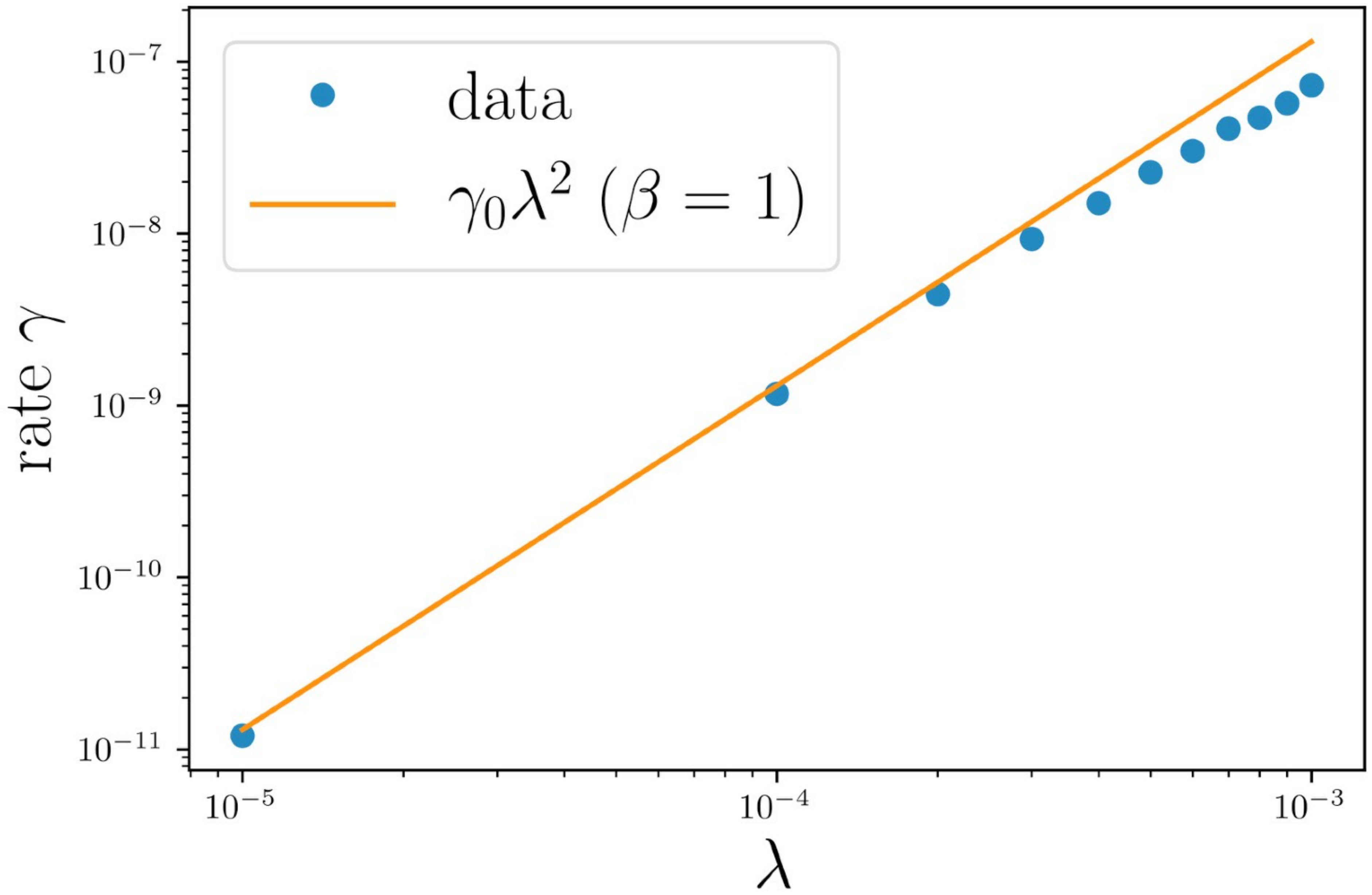
various β, $\mu = -1$ (out of equilibrium), $\mathsf{L} = 1024$





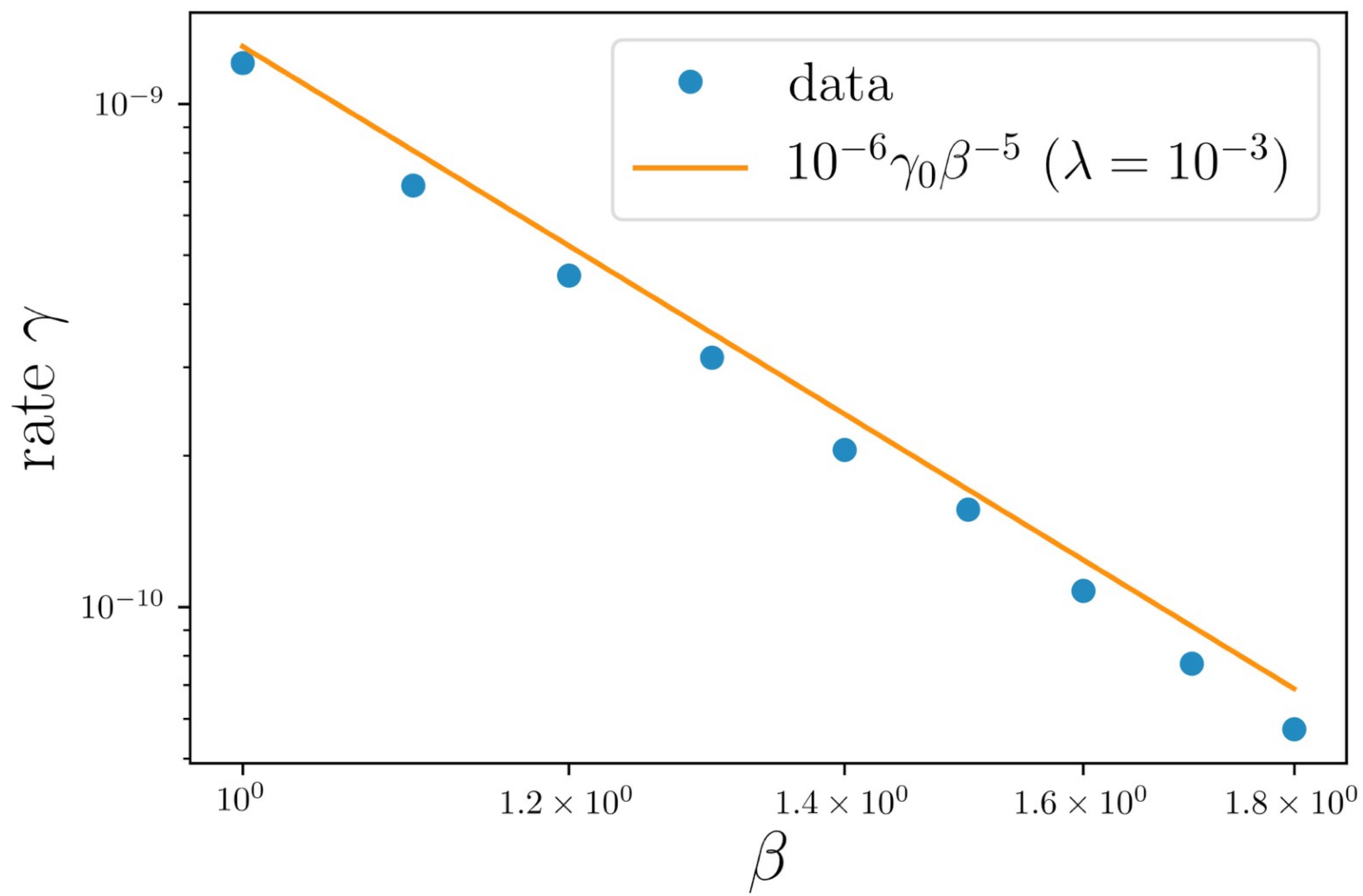
$\text{Case 1}: \quad \text{non}-\text{linearity}: \; q_x^6, \quad \delta = 0.35 \quad (L = 1024)$

$$\text{theory}: \quad \gamma = \gamma_0 \beta^{-5} \lambda^2 \;(\text{kinetic}), \quad \gamma_0 \simeq 0.13$$



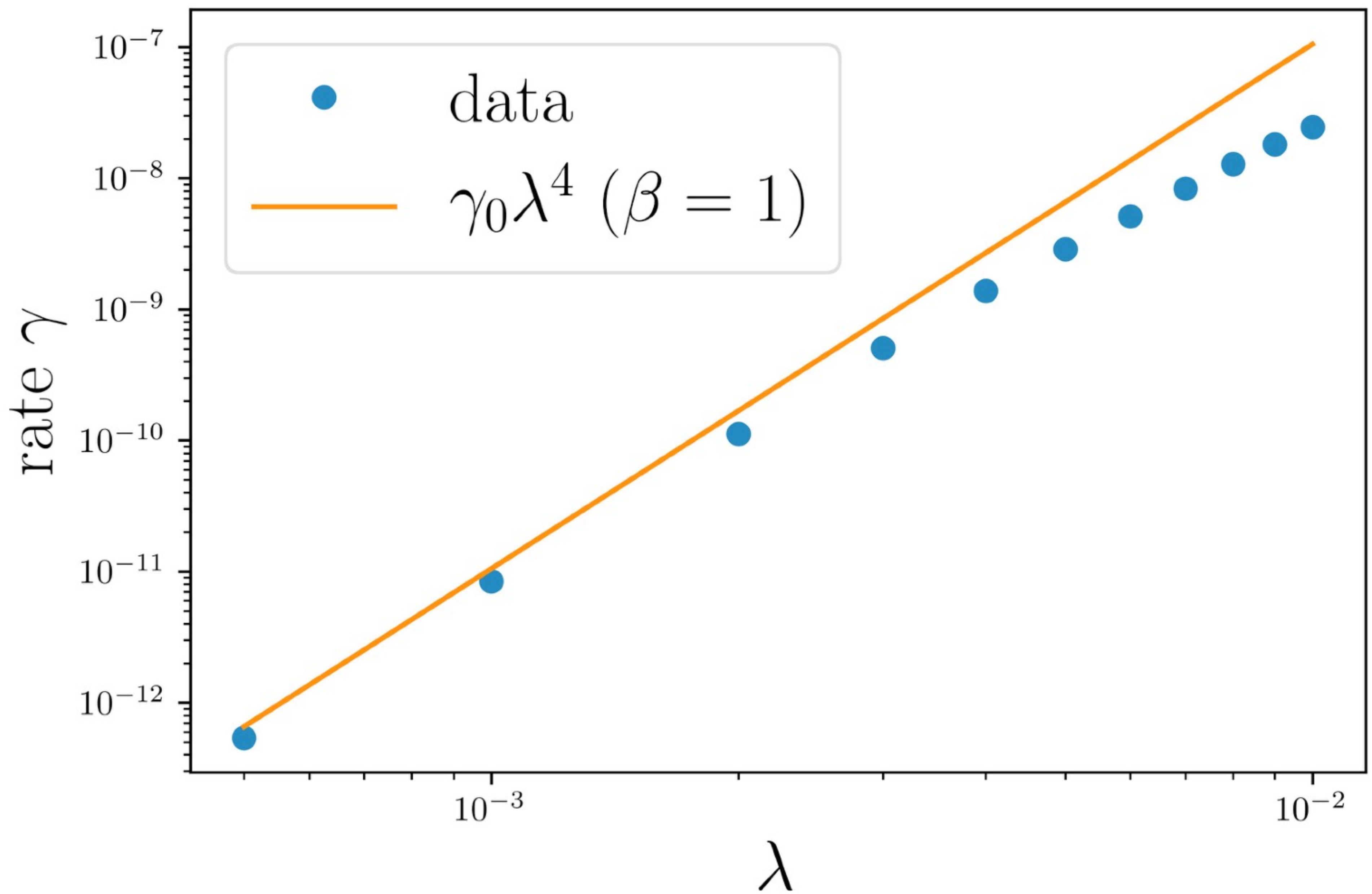
$$\text{Case 1 :} \quad \text{non} - \text{linearity :} \ q_x^6 , \quad \delta = 0.35 \quad (L = 1024)$$

$$\text{theory :} \quad \gamma \ = \ \gamma_0 \beta^{-5} \lambda^2 \ (\text{kinetic}), \quad \gamma_0 \simeq 0.13$$



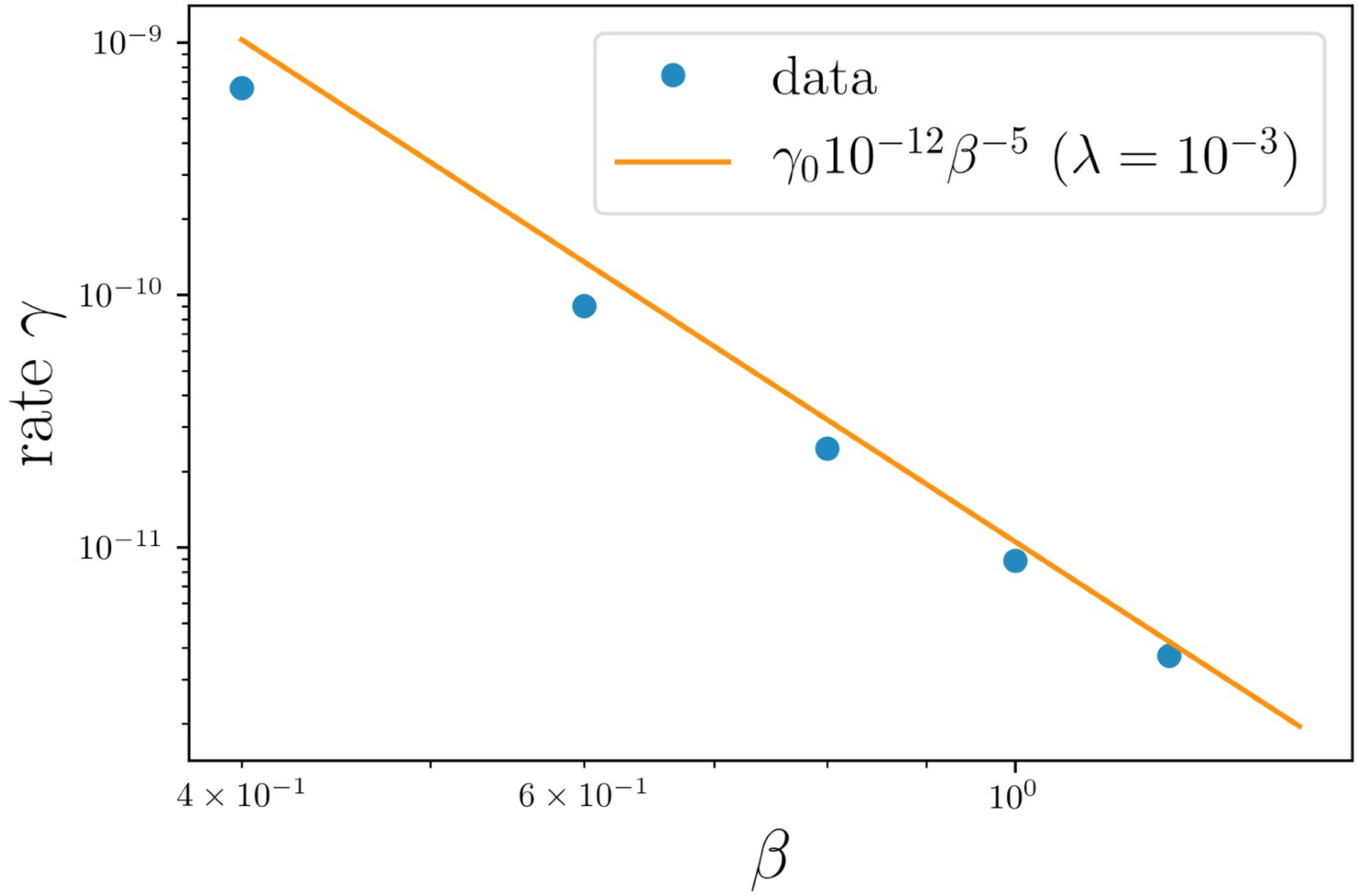
$\boxed{\text{Case 2 :} \quad \text{non} - \text{linearity :} \ q_x^4, \quad \delta = 0.45 \quad (L = 1024)}$

$$\text{theory :} \quad \gamma = \gamma_0 \beta^{-5} \lambda^4 \ \text{(non – kinetic)}, \quad \gamma_0 \simeq 10.5$$



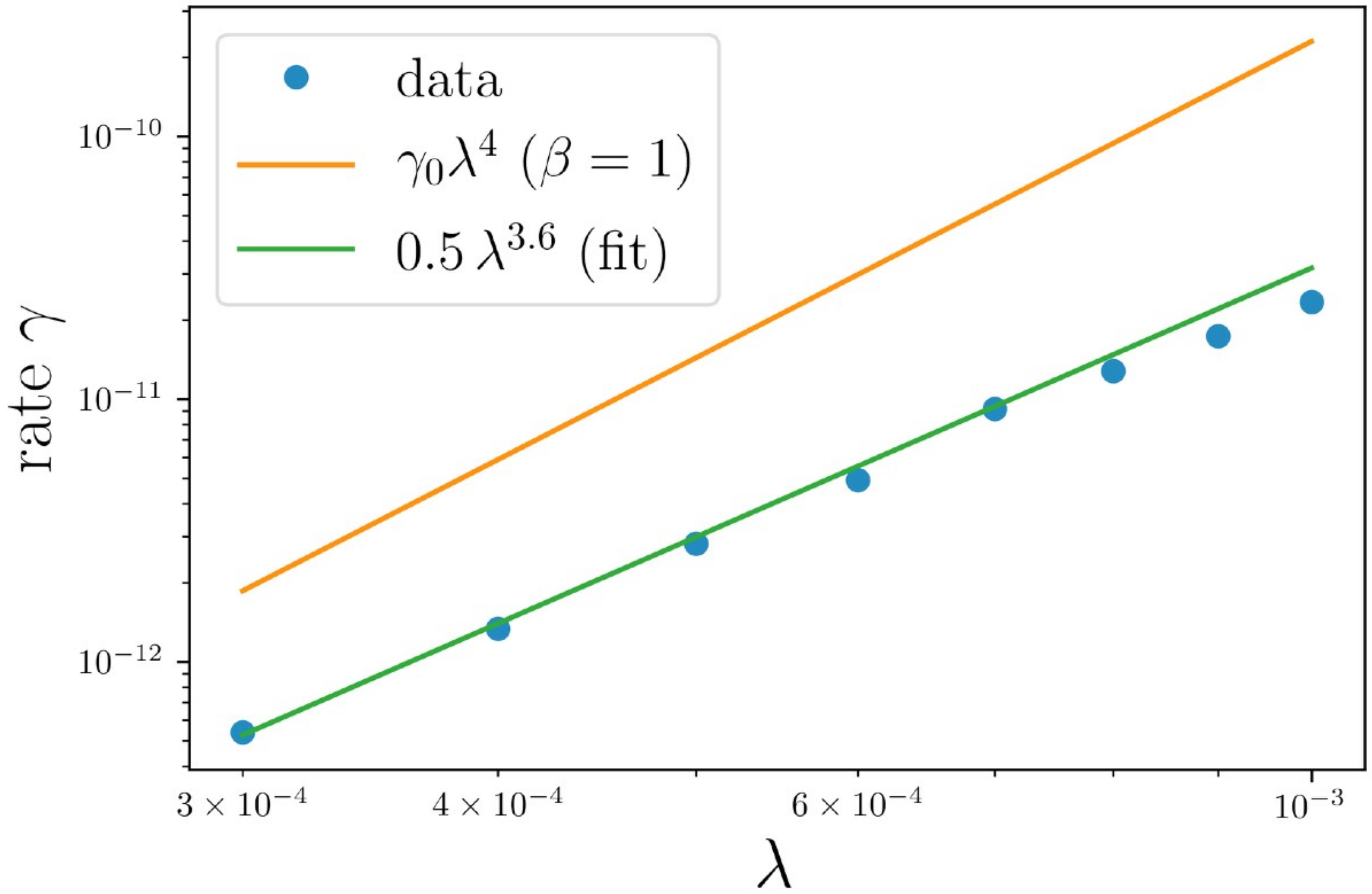
Case 2 : non − linearity : q_x^4, $\delta = 0.45$ $(L = 1024)$

theory : $\gamma = \gamma_0 \beta^{-5} \lambda^4$ (non − kinetic), $\gamma_0 \simeq 10.5$



Case 3 : non − linearity : q_x^6, $\delta = 0.28$ $(L = 1024)$

theory : $\gamma = \gamma_0 \beta^{-9} \lambda^4$ (non − kinetic), $\gamma_0 \simeq 230$

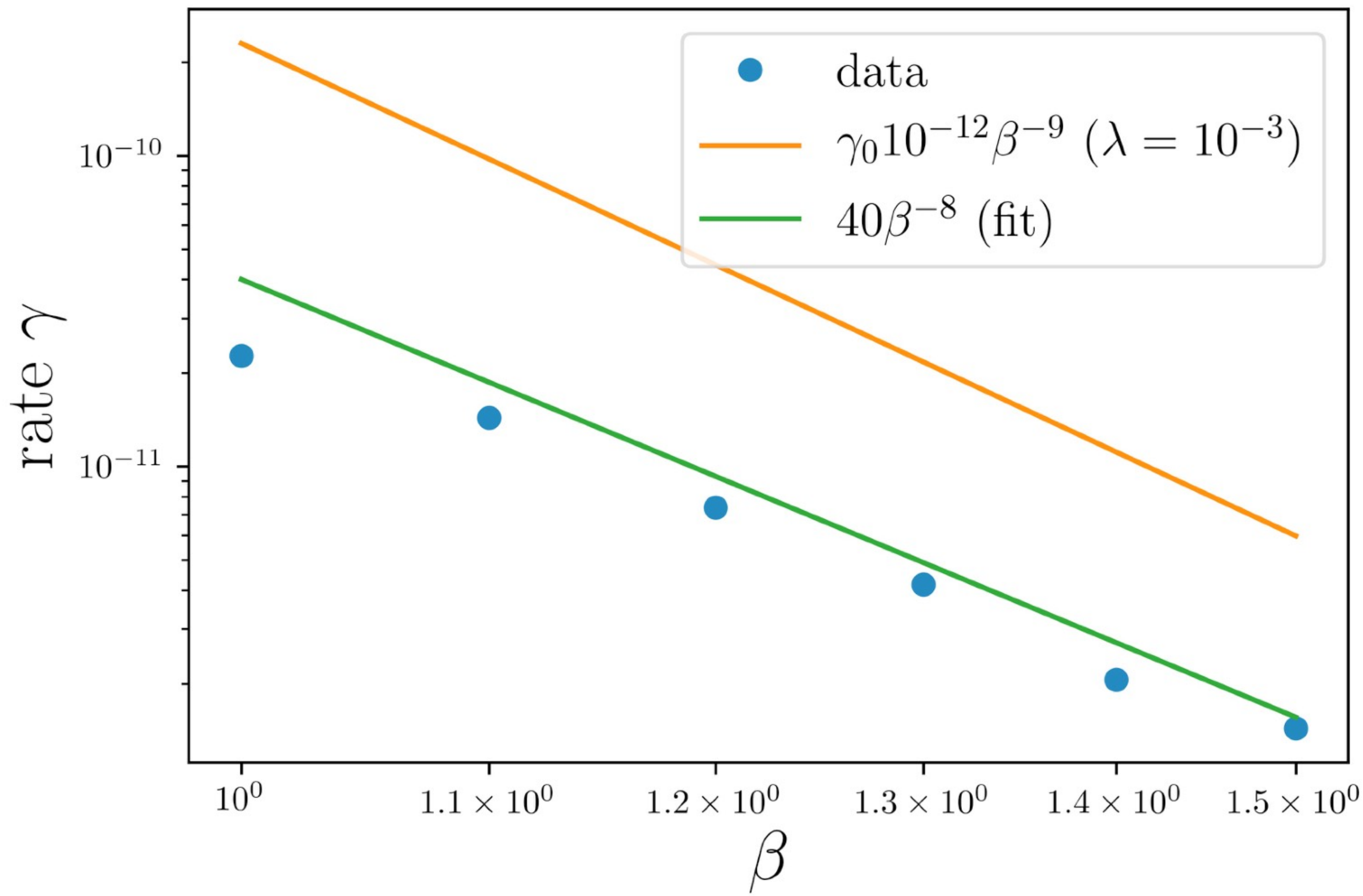


Two scenarios:

1) The theory is incorrect
2) The theory will eventually become correct for much smaller λ (not reachable)

$$\text{Case 3}: \quad \text{non-linearity}: \; q_x^6, \quad \delta = 0.28 \quad (L = 1024)$$

$$\text{theory}: \quad \gamma = \gamma_0 \beta^{-9} \lambda^4 \; \text{(non-kinetic)}, \quad \gamma_0 \simeq 230$$



Same possible two interpretations

Consistency of the main assumption?

Reminder: the theory is based on the assumption

$$\rho_t \sim e^{-\beta_t(\tilde{H}-\mu_t N_0)}(1+\mathcal{O}(\lambda^p)) = \rho_t^0 \times (1+\mathcal{O}(\lambda^p))$$

1) We predict:

$$v_1 = \frac{d}{dt}(\beta_t, \mu_t) \sim \lambda^{2p}$$

2) Fast (kinetic) relaxation towards the pseudo-equilibrium:

$$v_2 = \frac{d}{dt}(\rho_t - \rho_t^0) \sim \lambda^2 \, \lambda^p$$

kinetic rate

distance to ρ_t^0

OK if $v_2 > v_1$

$p = 1$ **not OK**

$$v_1 \sim \lambda^2 \gg \lambda^3 \sim v_2$$

Good sanity check: kinetic regime.

$\gamma \sim \lambda^2$ with different pre-factor

$p = 2$ **marginal**

$$v_1 \sim \lambda^4 \sim v_2$$

$p > 2$ **OK**

$$v_1 \sim \lambda^{2p} \ll \lambda^{p+2} \sim v_2$$

Conclusions

- Basic understanding of the slow thermalization in a classical chain of anharmonic oscillators
- Use of new methods from Quantum Mechanics in a classical set-up
- Proposal for the time scales for thermalization based on numerical and theoretical analysis
- Quantitative agreement between theory and numerics, at least in some cases