Activity driven energy transport

Urna Basu
S. N. Bose National Centre for Basic Sciences, Kolkata

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Joint works with ***Ritwick Sarkar*** *&* ***Ion Santra***

1. R. Sarkar, I. Santra, and UB, arXiv 2404.00615
2. R. Sarkar, I. Santra, and UB, Phys. Rev. E 107, 014123 (2023)
3. I. Santra and UB, SciPost Phys. 13, 041 (2022)

Outline

- Energy transport in thermally driven harmonic chain
- Active reservoir model: harmonic chain of RTP oscillators
- Effective probe dynamics: violation of FDT
- Activity driven harmonic chain
  - Characterisation of the NESS
  - Spatio-temporal correlations
  - Energy current
- Conclusions

Energy transport in one dimension

- Macroscopic system subjected to temperature difference: energy transport
- Theoretical model: Oscillator chain connected to equilibrium thermal reservoirs, satisfy Fluctuation-Dissipation Theorem
- Relevant questions:
    - Energy current — thermal conductivity? Fourier Law?
    - Local temperature?
    - Velocity / position fluctuations?
- Paradigmatic example (in 1D): Harmonic chain connected to Langevin baths with different temperatures

Rieder, Lebowitz, Lieb, J Math Phys 1967

Harmonic chain under temperature gradient

- Chain of N harmonically coupled identical oscillators with displacement $\{x_l\}$
- Boundary oscillators $l = 1, N$ coupled to reservoirs with temperatures T_1, T_N
- Reservoirs exerting forces: '*thermal noise*' and '*dissipation*'
- Equilibrium reservoirs: Fluctuation-dissipation theorem (FDT) relates noise and dissipation

Langevin Bath

- Simple model —

constant dissipation and Gaussian white noise at boundary

$$
\begin{aligned}
m\ddot{x}_1 &= -k(2x_1 - x_2) - \gamma_1 \dot{x}_1 + \sqrt{2\gamma_1 T_1}\,\xi_1(t), \\
m\ddot{x}_l &= -k(2x_l - x_{l-1} + x_{l+1}), \quad \forall l \in [2, N-1], \\
m\ddot{x}_N &= -k(2x_N - x_{N-1}) - \gamma_N \dot{x}_N + \sqrt{2\gamma_N T_N}\,\xi_N(t)
\end{aligned}
$$

Mass m

Coupling constant k

Rieder, Lebowitz, Lieb,
J Math Phys 1967
Dhar, Phys Rev Lett 2001

- Linearity and Gaussianity allow exact solution
- Current carrying Gaussian nonequilibrium stationary state
- In the thermodynamic limit $N \to \infty$ constant energy current $J_{\text{th}} \propto (T_1 - T_N)$ flows through the system

$$J_{\text{th}} = \frac{k(T_1 - T_N)}{2\gamma}\left[1 + \frac{mk}{2\gamma^2} - \frac{mk}{2\gamma^2}\sqrt{1 + \frac{4\gamma^2}{mk}}\right].$$

Rieder, Lebowitz, Lieb
J Math Phys 1967,
Dhar, Phys Rev Lett. 2001

- Uniform temperature at the bulk $T = \frac{1}{2}(T_1 + T_N)$

Correlated bath

Rubin, J Math Phys 1961
Rubin & Greer
J Math Phys 1971

- Rubin-Greer model: Semi-infinite chain of harmonic oscillators at temperature T
- Generalised Langevin equations

$$
\begin{aligned}
m\ddot{x}_1 &= k(x_2 - x_1) - \int_{-\infty}^{t} ds\, \dot{x}_1(s)\, \gamma(t-s) + \eta_1(t), \\
m\ddot{x}_l &= k(x_{l-1} + x_{l+1} - 2x_l), \quad \forall\, l \in [2, N-1], \\
m\ddot{x}_N &= k(x_{N-1} - x_N) - \int_{-\infty}^{t} ds\, \dot{x}_N(s)\, \gamma(t-s) + \eta_N(t).
\end{aligned}
$$

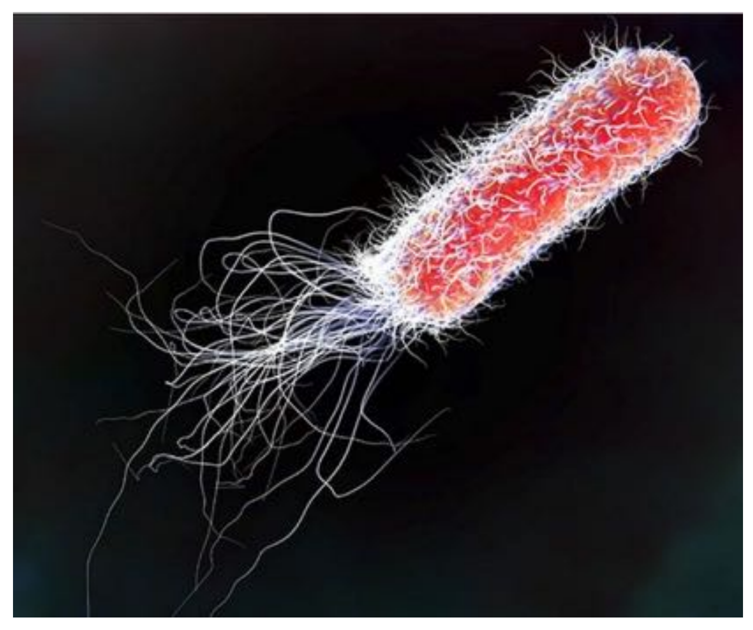
Dissipation kernel $\gamma(t)$

- FDT demands $\langle \tilde{\eta}_i(\omega)\tilde{\eta}_i(\omega')\rangle = 4\pi k_B T_i \,\mathrm{Re}[\gamma(\omega)]\delta(\omega + \omega')$
- Stationary current $\propto (T_1 - T_N)$

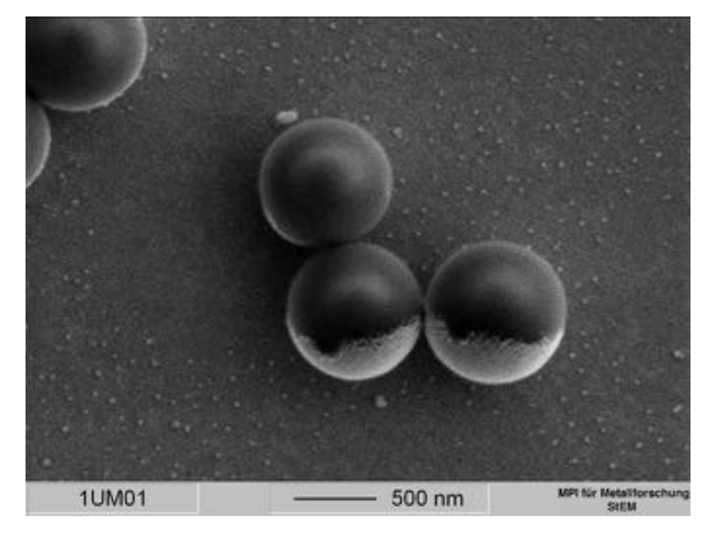
☆ What happens when reservoirs are away from equilibrium?

☆ Active reservoirs?

Active Reservoir



- Medium consisting of self-propelled active particles
- Active Particles: Generate directed motion consuming energy from environment at individual level



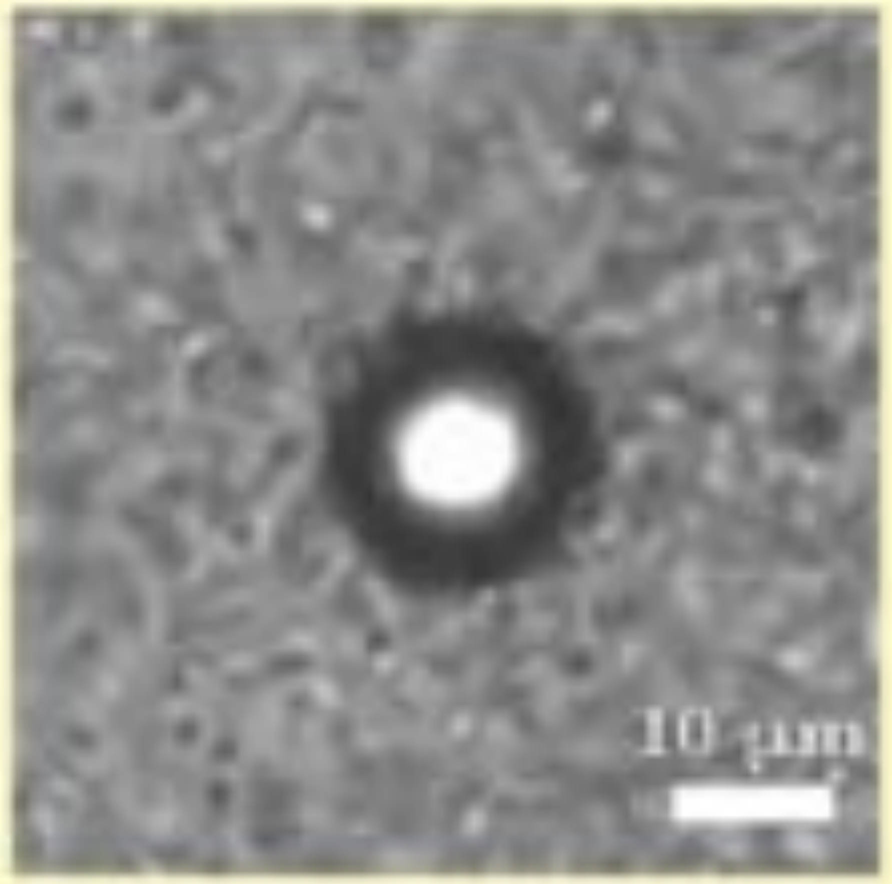
- Inherently nonequilibrium in nature
- Examples: at all scales
  - In nature: Bacteria, Bird flocks, Fish schools…
  - Artificial: Micro/nano swimmers, Janus particles…

Bechinger et al, RMP 2016
Ramaswamy 2017, …

- Motion of single probe particle in active reservoirs: theoretical and experimental studies

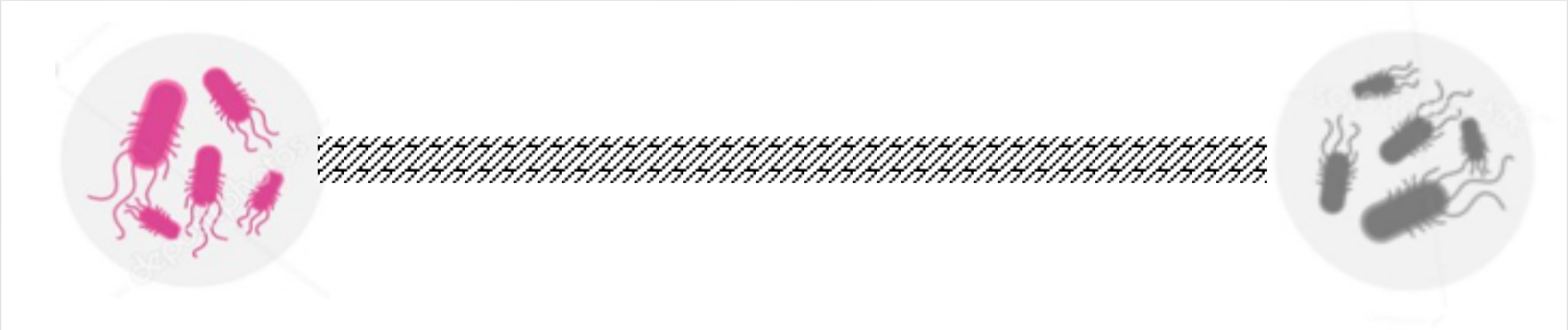
Maggi et al., PRL 2014,
Maes, PRL 2020,
Seyforth et al., PRR 2022,
Granek et al., PRL 2022,...

- Intriguing features:
  - Emergence of memory,
  - Modification of equipartition theorem,
  - Negative friction



Seyforth et al., PRR 2022

- How are transport properties of extended systems affected when connected to active reservoirs?

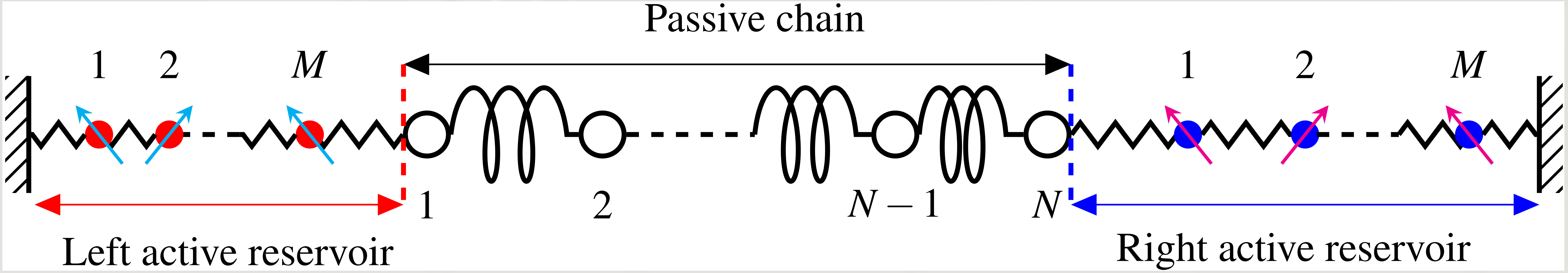


Courtesy: Ion Santra

- Simple, linear model: Activity driven harmonic chain

Set-up : Model

- Simple model of active reservoir: chain of identical Run-and-Tumble Particles (RTP)



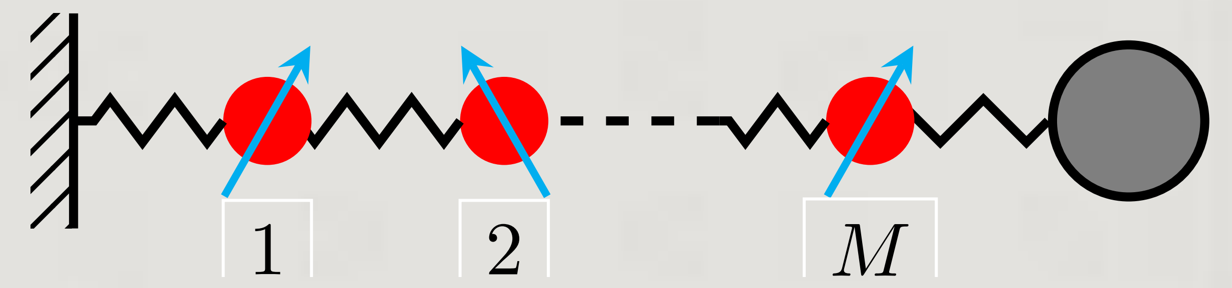
- Rubin-Greer like set-up
- 'Activity' of the reservoir : persistence time of constituents
- Conducting system — chain of passive oscillators — connected to two active reservoirs

Objective

- Characterise the active reservoir
  - Breaking of FDT?
  - Effective temperature?
- Characterise the nonequilibrium stationary state (NESS) of the passive chain
  - Velocity/position fluctuations?
  - Spatio-temporal correlations?
- Energy current flowing through the system

Characterisation of the active reservoir

- Active reservoir: Chain of harmonically coupled active particles



- Probe particle coupled to one end
- Reservoir particle dynamics: overdamped Langevin equation for $\{y_l\}$

$$\nu \dot{y}_l = \begin{cases} \lambda(y_{l+1} + y_{l-1} - 2y_l) + f_l(t), & \forall l \in [1, M-1], \\ \lambda(x_1 + y_{M-1} - 2y_M) + f_M(t), & \text{when } l = M, \end{cases}$$

  - Fixed boundary at one end ($y_0 = 0$)
  - Probe particle (x_1) attached at the other end

friction ν and
Coupling strength λ

- Stochastic dynamics with active noise $f_l(t)$: memory
- Stationary auto-correlation— persistence time-scale τ

measure of activity

$$\langle f(t) f(t') \rangle = h\left(\frac{|t-t'|}{\tau}\right)$$

No detailed balance

- Unrelated to dissipation — no fluctuation-dissipation relation
- Probe particle dynamics $m\ddot{x}_1 = \lambda(y_M - x_1),$

Effective description?

Effective probe dynamics

- Integrate out the bath degrees of freedom
  - Linear: exact solution of bath particles Langevin equations for given $x_1(t)$

$$y_M(t) = \frac{\lambda}{\nu}\int_{-\infty}^{t} ds\, x_1(s)\Lambda_{MM}(t-s) + \frac{1}{\nu}\int_{-\infty}^{t} ds \sum_{j=1}^{M} \Lambda_{Mj}(t-s)\, f_j(t),$$

- $M \times M$ matrix $\Lambda(z)$ with elements

$$\Lambda_{j\ell}(z) = \frac{2}{M+1}\sum_{k=1}^{M} \sin\frac{jk\pi}{M+1}\sin\frac{\ell k\pi}{M+1} e^{-\mu_k z/\nu}$$

with

$$\mu_k = 4\lambda\sin^2\left(\frac{k\pi}{2(M+1)}\right).$$

- Generalised Langevin equation for probe dynamics (in a correlated bath)

$$m\ddot{x}_1 = -\int_{-\infty}^{t} ds\,\dot{x}_1(s)\gamma(t-s) + \Sigma(t)$$

Dissipation kernel

Effective noise (active)

No time-scale separation assumed

- Use this effective description to study the extended system

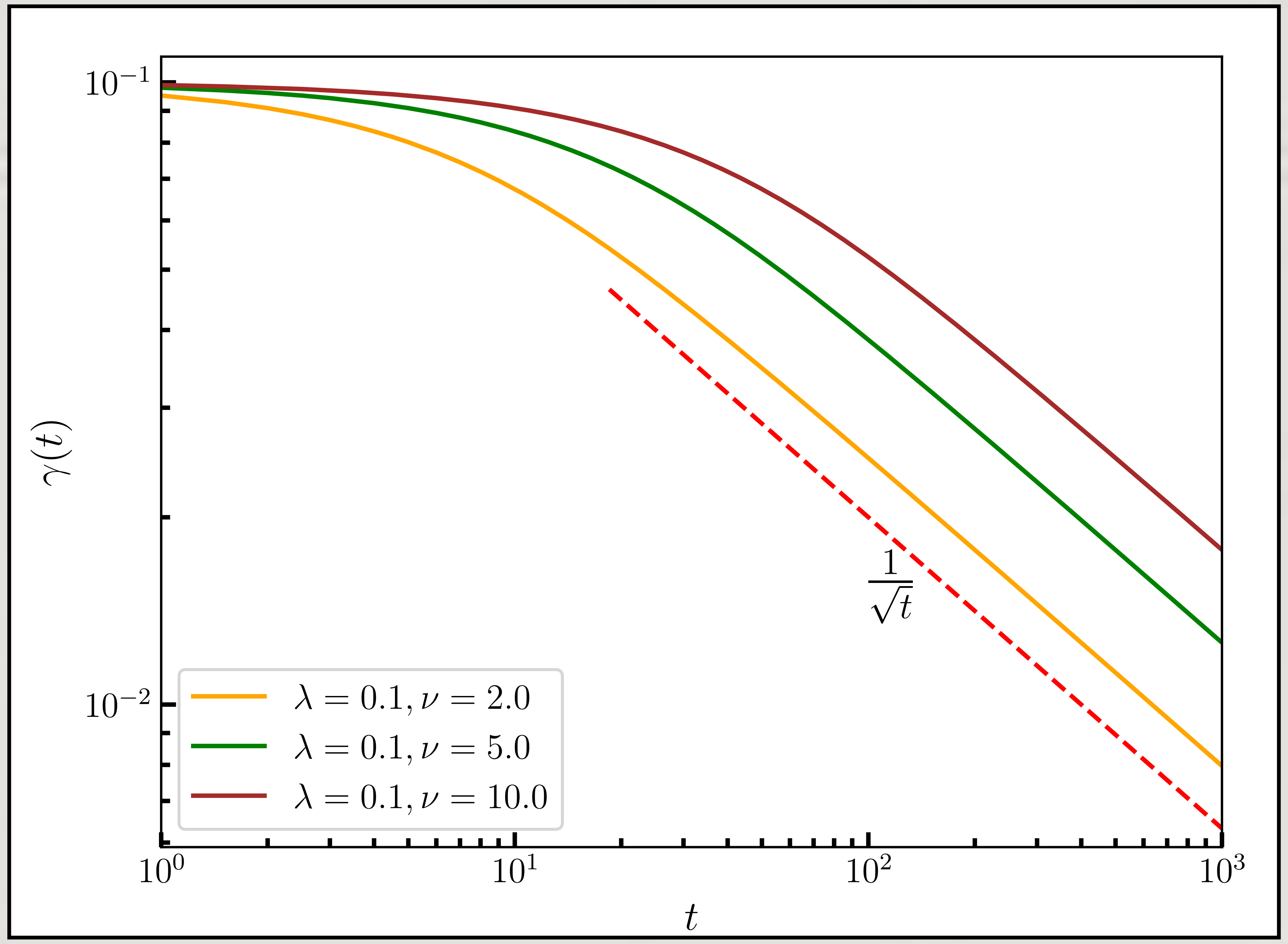
Properties in thermodynamic limit $M \to \infty$

Dissipation kernel

- Dissipation kernel

$$\gamma(t) = \lambda e^{-\frac{2\lambda t}{\nu}}\left[I_0\left(\frac{2\lambda t}{\nu}\right) + I_1\left(\frac{2\lambda t}{\nu}\right)\right]\Theta(t),$$

- At long-times $t \gg \nu/\lambda$: algebraic decay $t^{-1/2}$
- Irrespective of active nature, property of the chain structure
- Appears in various contexts including active baths



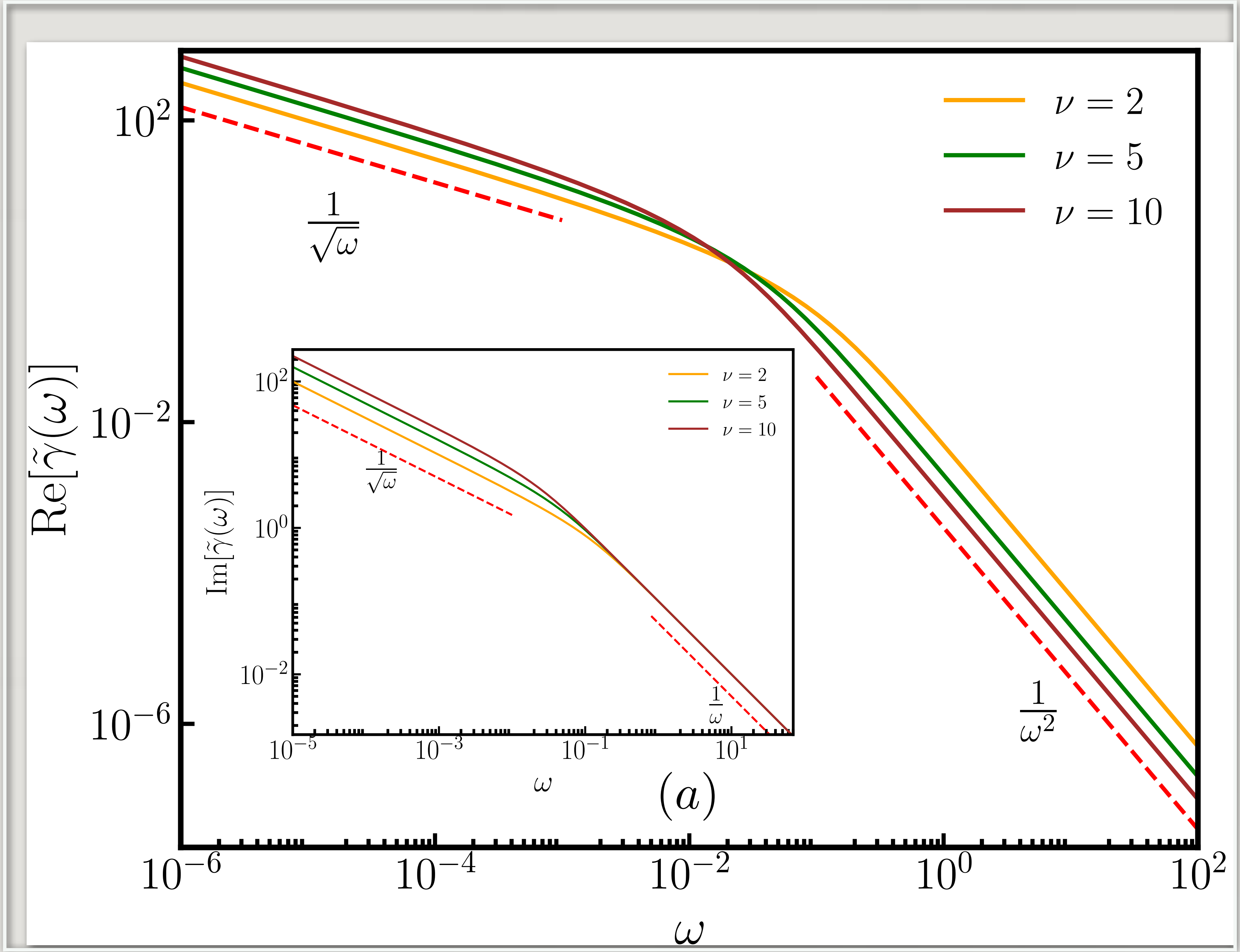
Overdamped Rubin-Greer Bath

Granek et al., PRL 2022,
Saito and Sakaue, PRE 2015
Lizana et al., PRE 2010...

- Spectral function $\tilde{\gamma}(\omega) = \int_0^\infty dt\, e^{-i\omega t}\gamma(t)$
- Symmetry properties $\mathrm{Re}[\tilde{\gamma}(-\omega)] = \mathrm{Re}[\tilde{\gamma}(\omega)]$ and $\mathrm{Im}[\tilde{\gamma}(-\omega)] = -\mathrm{Im}[\tilde{\gamma}(\omega)]$.
- For $\omega > 0$

$$\tilde{\gamma}(\omega) = -\frac{\nu}{2}\left[1 - \left(\sqrt{\frac{1}{4} + \frac{4\lambda^2}{\nu^2\omega^2}} + \frac{1}{2}\right)^{1/2}\right] + i\frac{\nu}{2}\left(\sqrt{\frac{1}{4} + \frac{4\lambda^2}{\nu^2\omega^2}} - \frac{1}{2}\right)^{1/2}.$$

- Asymptotic behaviour for small and large ω ...



Effective noise

$$\langle f(t)f(t')\rangle = h\left(\frac{|t-t'|}{\tau}\right)$$

- Effective noise acting on the probe

$$\Sigma(t) = \frac{\lambda}{\nu}\int_{-\infty}^{t} ds \sum_{j=1}^{M} \Lambda_{Mj}(t-s) f_j(s),$$

- Auto-correlation in the frequency space

$$\langle \tilde{\Sigma}(\omega)\tilde{\Sigma}(\omega')\rangle = 2\pi\delta(\omega+\omega')\,\tilde{g}(\omega)$$

with

$$\tilde{g}(\omega) = \frac{1}{\nu}\tilde{h}(\omega)\mathrm{Re}[\tilde{\gamma}(\omega)]$$

- Combination of active force $\tilde{h}(\omega)$ and chain structure through $\tilde{\gamma}(\omega)$
- Breaking of fluctuation-dissipation relation in a specific way

Reminder: for equilibrium baths $\langle \tilde{\eta}_i(\omega)\tilde{\eta}_i(\omega')\rangle = 4\pi k_B T_i \,\mathrm{Re}[\gamma(\omega)]\delta(\omega+\omega')$

Active noise: example

- Active noise $f_l(t)$: independent, run-and-tumble like process
- Dichotomous noise in 1D $f_l(t) = v_0 \sigma_l(t)$
- Intermittent 'tumbles' $\sigma \to -\sigma$ with constant rate
- Waiting time between consecutive tumbling events drawn from exponential distribution
- Auto-correlation $h_1(z) = v_0^2 e^{-z}$ and frequency spectra $\tilde{h}_1(\omega, \tau) = \frac{2v_0^2\tau}{1+\omega^2\tau^2}$
- Other dynamics: ABP, AOUP etc equivalent

Characteristic time τ

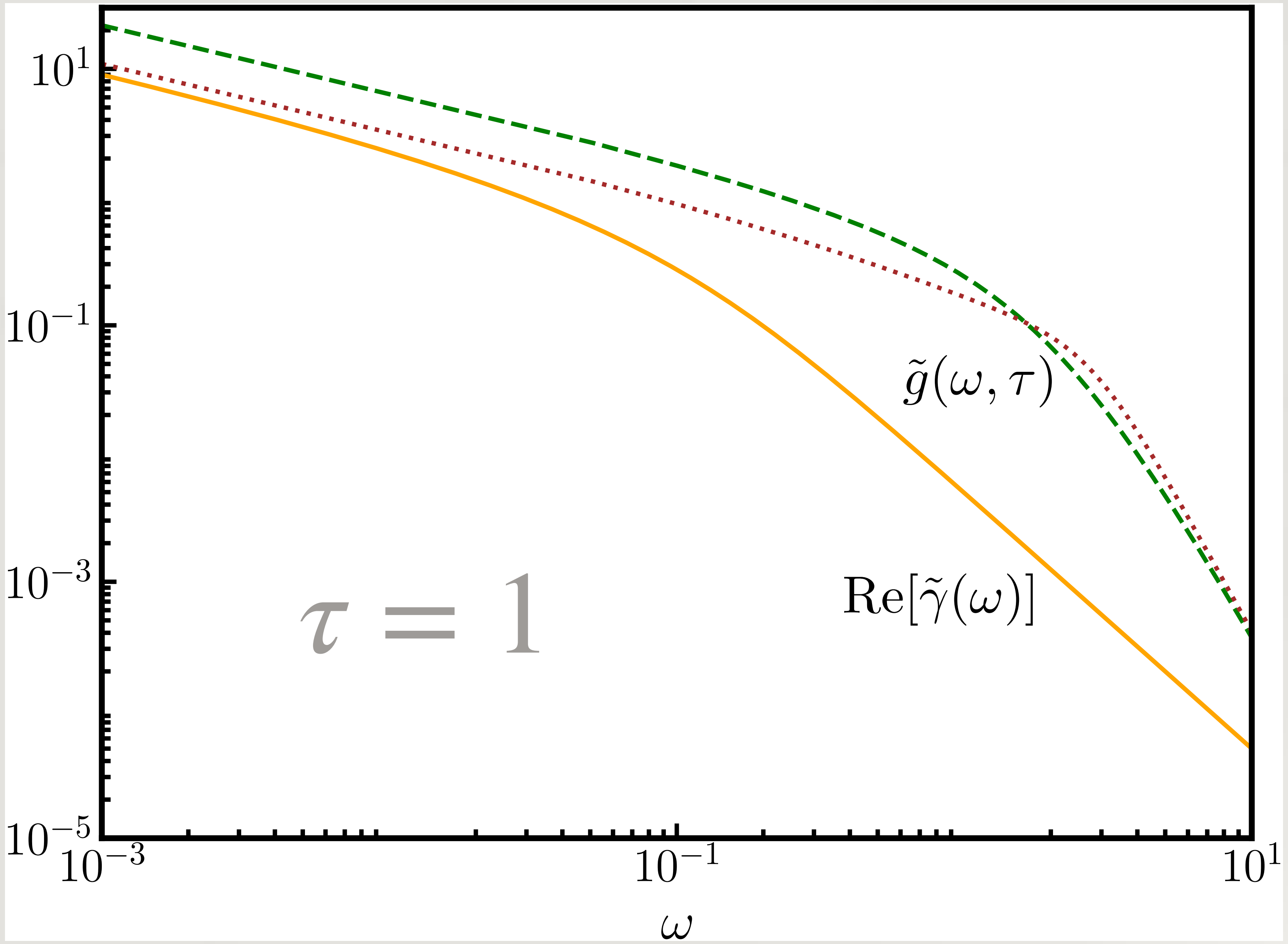
Modification of FDT

- Equilibrium thermal baths: FDT $\tilde{g}(\omega) \propto k_B T\, \mathrm{Re}[\tilde{\gamma}(\omega)]$

❖ Presence of active force modifies FDT

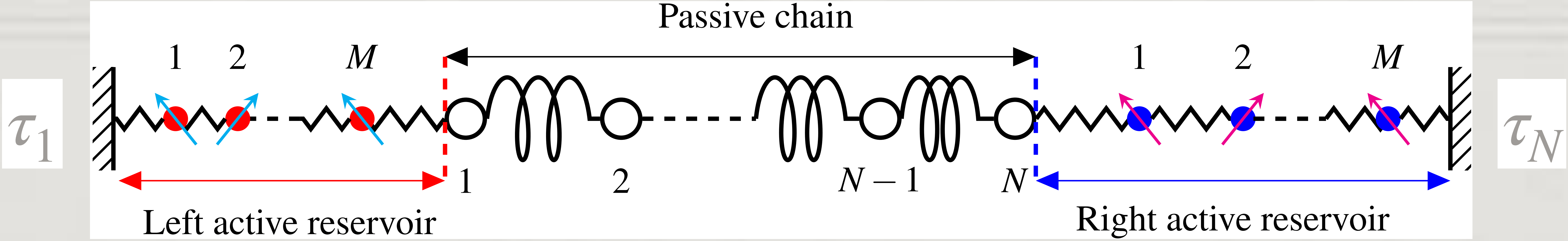
$$\tilde{g}(\omega) = \frac{1}{\nu}\tilde{h}(\omega)\mathrm{Re}[\tilde{\gamma}(\omega)]$$

- Effective temperature in passive limit $\tau \to 0$, $h(\omega) \propto v_0^2 \tau$



Effect of active bath on extended system?

Activity driven harmonic chain



- Passive conducting harmonic chain connected to two active reservoirs
- Reservoirs differ only in persistence times
- Langevin equations for displacements $\{x_l\}$

$$
\begin{aligned}
m\ddot{x}_1 &= k(x_2 - x_1) - \int_{-\infty}^{t} ds\, \dot{x}_1(s)\, \gamma(t-s) + \Sigma_1(t), \\
m\ddot{x}_l &= k(x_{l-1} + x_{l+1} - 2x_l), \quad \forall\, l \in [2, N-1], \\
m\ddot{x}_N &= k(x_{N-1} - x_N) - \int_{-\infty}^{t} ds\, \dot{x}_N(s)\, \gamma(t-s) + \Sigma_N(t).
\end{aligned}
$$

Objectives

- How is the nonequilibrium stationary state (NESS) different from the thermally driven scenario?
    - Local velocity fluctuations
    - Temperature profile
    - Spatio-temporal correlations
    - Average energy current

NESS

- Linearity allows exact computation of certain observables
- Use Fourier transform and matrix method introduced in Dhar, PRL 2001
- In the stationary state

$$x_l(t) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{i\omega t}[G_{l1}(\omega)\tilde{\Sigma}_1(\omega) + G_{lN}(\omega)\tilde{\Sigma}_N(\omega)]$$

Effective noise

with,

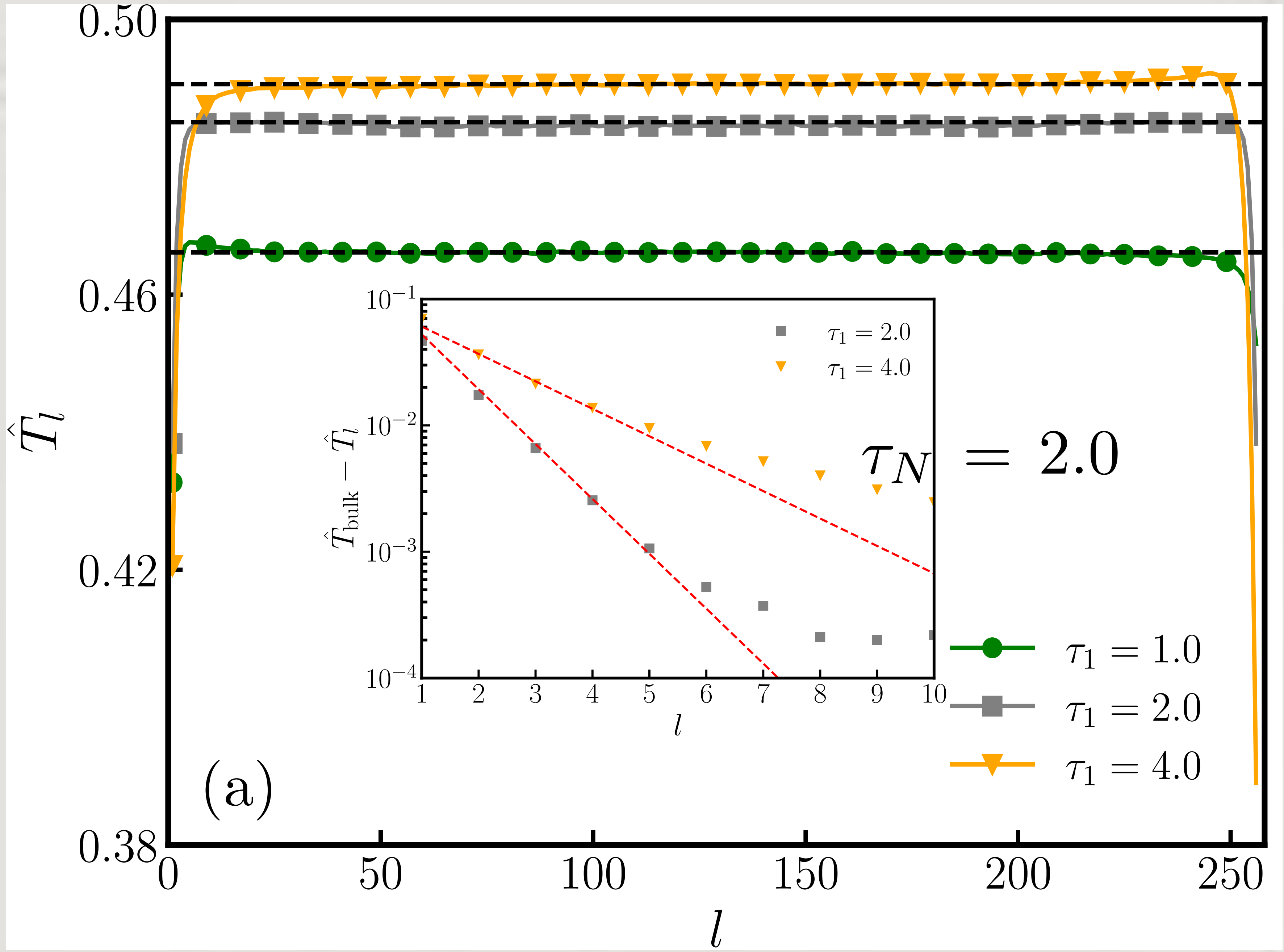
$$G(\omega) = \begin{bmatrix} -m\omega^2 + k - i\omega\tilde{\gamma} & -k & \cdots \\ -k & -m\omega^2 + 2k & \cdots \\ \vdots & \ddots & \cdots \\ 0 & \cdots & -m\omega^2 + k - i\omega\tilde{\gamma} \end{bmatrix}^{-1}$$

Kinetic temperature

- Average kinetic energy of oscillators $\hat{T}_l = \langle v_l^2 \rangle$
- Uniform at the bulk in thermodynamic limit, contribution from both reservoirs

$$\hat{T}_l = \sum_{i=1,N} \frac{v_0^2 \tau_i}{2\nu\sqrt{1 + \frac{4k}{m}\tau_i^2}}.$$

- Exponentially decaying boundary layer

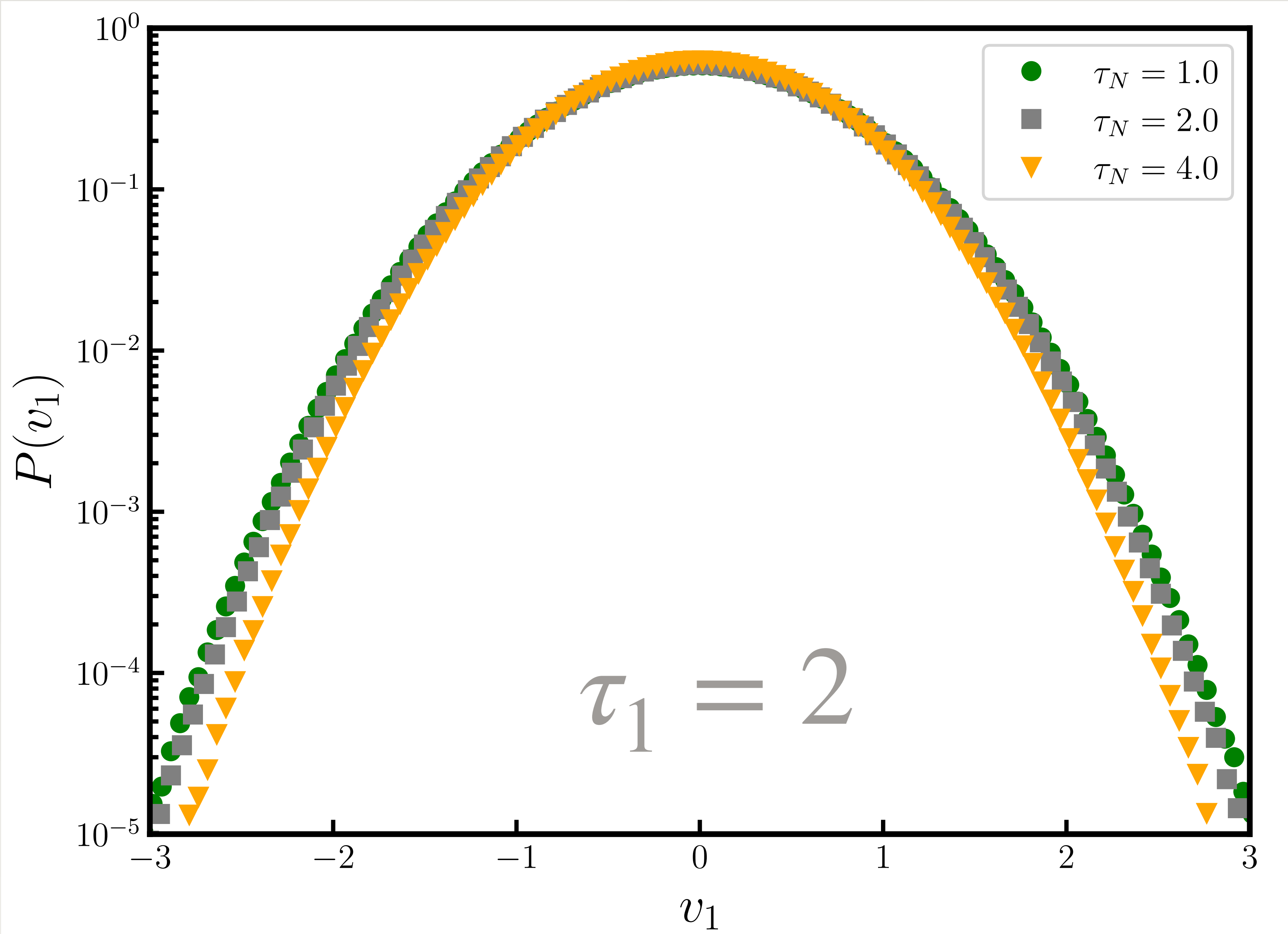


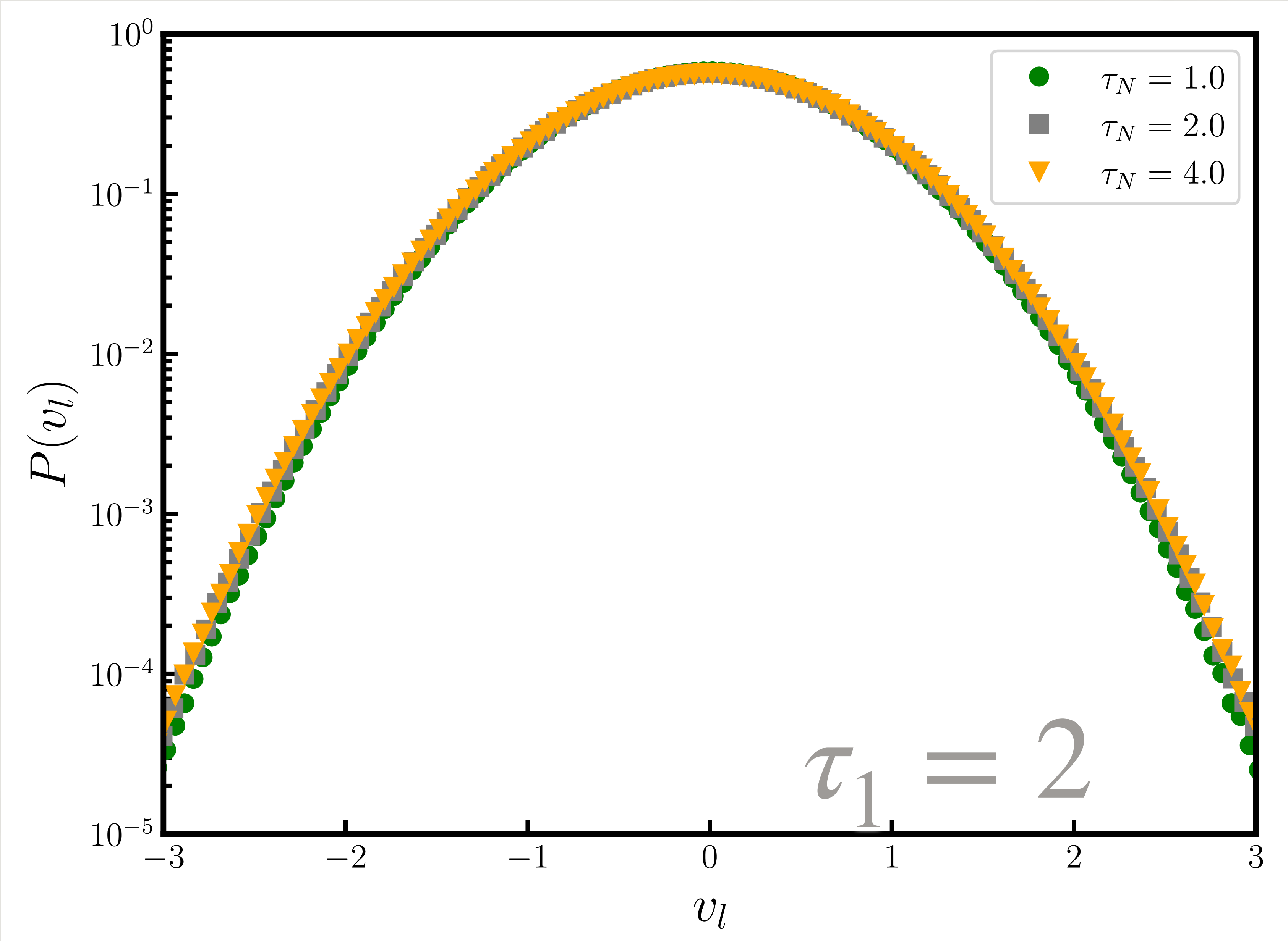
$M = N = 256$

Similar to thermally driven scenario

Velocity fluctuations

- Typical velocity fluctuations: Gaussian both in bulk and at boundary





$$M = N = 256$$

$$m = k = 1,\ \nu_1 = \nu_N = 1,\ \lambda_1 = \lambda_N = 1$$

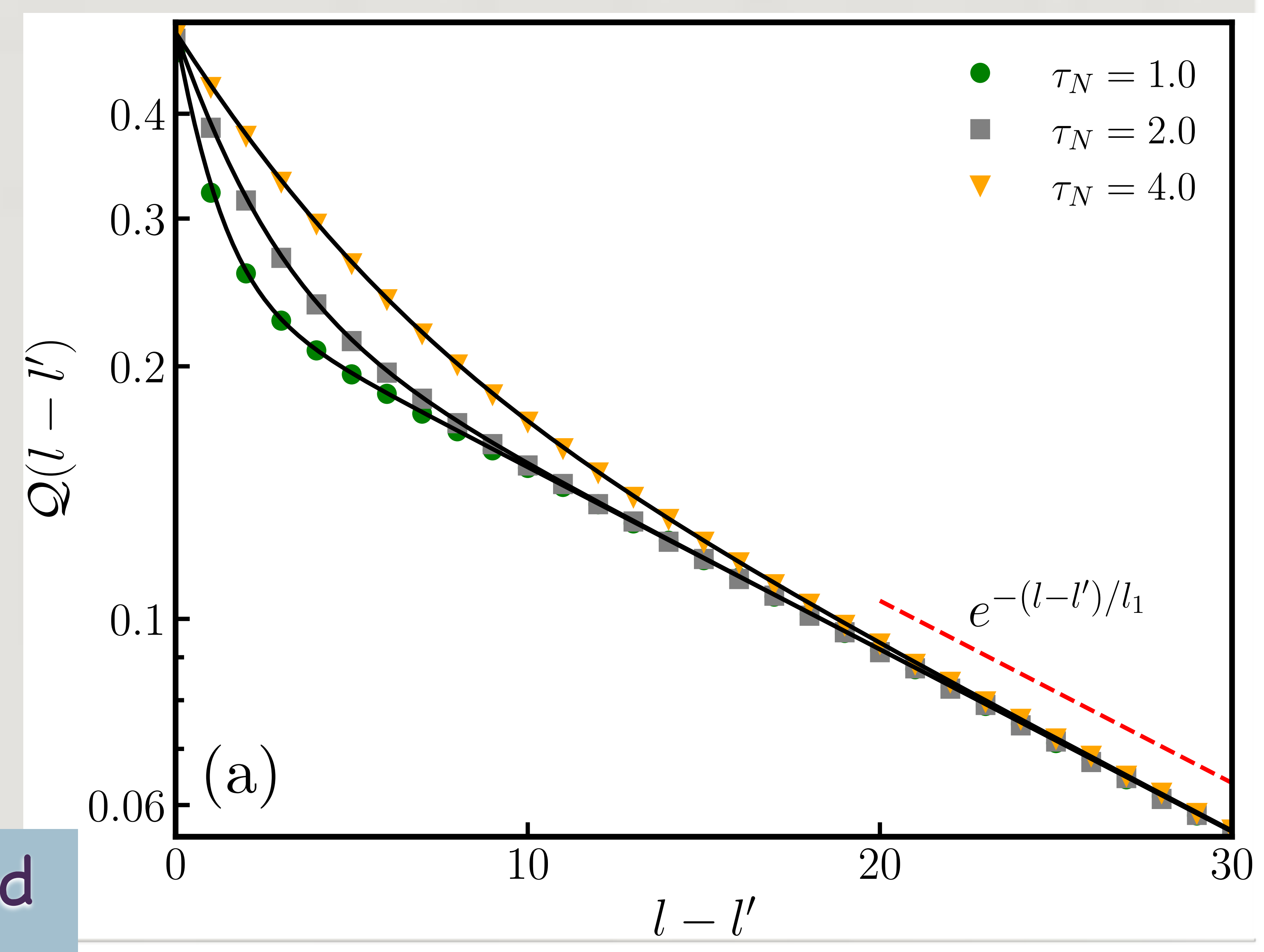
Similar to thermally driven scenario

Spatial correlation

- Stationary correlation $Q(l, l') \equiv \langle v_l v_{l'} \rangle$ in the bulk (in thermodynamic limit)
- For thermally driven chain— no spatial correlation $Q(l, l') = \delta_{l,l'} \frac{(T_1 + T_N)}{2}$
- Active reservoirs: new emergent length-scales

$$\mathcal{Q}(l - l') = \frac{v_0^2}{\nu\sqrt{8km}} \sum_{i=1,N} \exp\left(-\frac{|l - l'|}{\ell_i}\right)$$

$$\ell_i = \tau_i \sqrt{\frac{k}{2m}}.$$



Origin: Driving activity τ_1, τ_N

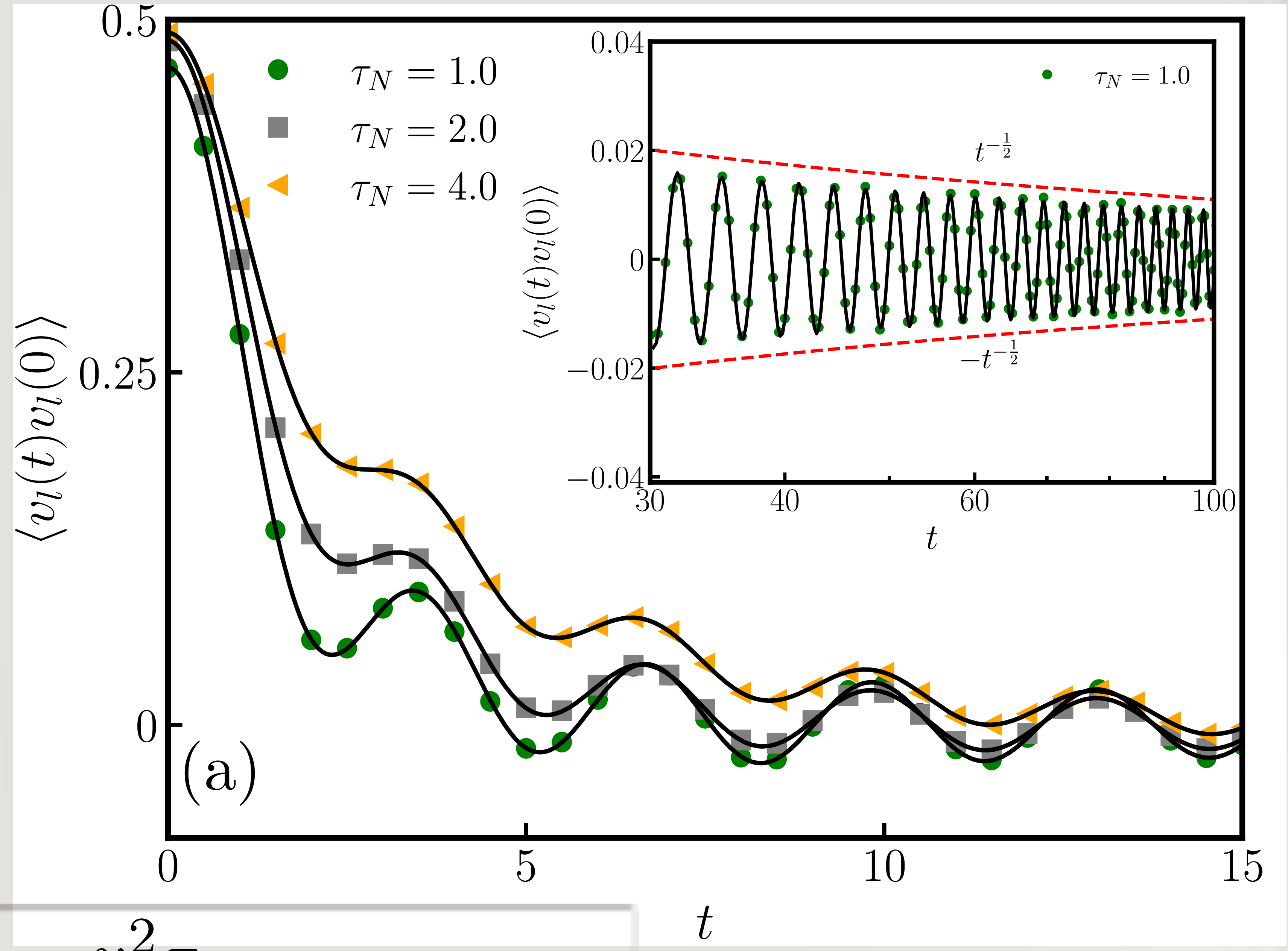
Characteristic frequency $\omega_c = \sqrt{\frac{2k}{m}}$

Correlated over a distance controlled by higher activity reservoir

Temporal correlation

- Two-time correlation $\langle v_l(0) v_l(t) \rangle$ of bulk oscillator velocity in NESS
- For thermally driven chain, in the thermodynamic limit $\langle v_l(0) v_l(t) \rangle = \dfrac{(T_1 + T_N)}{2m} J_0(\omega_c t)$
- For activity driven chain

$$\langle v_l(t) v_l(0) \rangle = \sum_{i=1,N} \int_0^{\omega_c} \frac{d\omega}{2\pi} \frac{\cos \omega t}{\sqrt{m(4k - m\omega^2)}} \tilde{h}(\omega, \tau_i)$$



Asymptotic behaviour:

- Signature of activity at short-times
- Thermal-like decay at late times— oscillations with $t^{-1/2}$ envelop

$$\langle v_l(t) v_l(0) \rangle \simeq \sum_{i=1,N} \frac{v_0^2 \tau_i}{2\nu(m + 4k\tau_i^2)} J_0(\omega_c t)$$

Energy current

- Energy current: average energy flowing (from the reservoirs) per unit time through the system

$$\mathcal{J}_l = \frac{k}{2}\langle (v_l + v_{l-1})(x_l - x_{l-1}) \rangle$$

$$\mathcal{J}_1 = \lambda(y_M^L - x_1)\dot{x}_1 \qquad \mathcal{J}_{N+1} = \lambda(y_1^R - x_N)\dot{x}_N$$

- Same for all oscillators (no source/dissipation in bulk)

$$J_{\text{act}} = \langle J_1 \rangle = \cdots = \langle \mathcal{J}_l \rangle = \cdots = -\langle \mathcal{J}_{N+1} \rangle.$$

- Finite current in thermodynamic limit $N \to \infty$, analytically computable

- Landauer-like formula for stationary current

$$J_{\rm act} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\omega^2 \Big|G_{1N}\Big|^2 \mathrm{Re}[\tilde{\gamma}(\omega)] \Big(\tilde{g}(\omega,\tau_1) - \tilde{g}(\omega,\tau_N)\Big)$$

Transmission coefficient

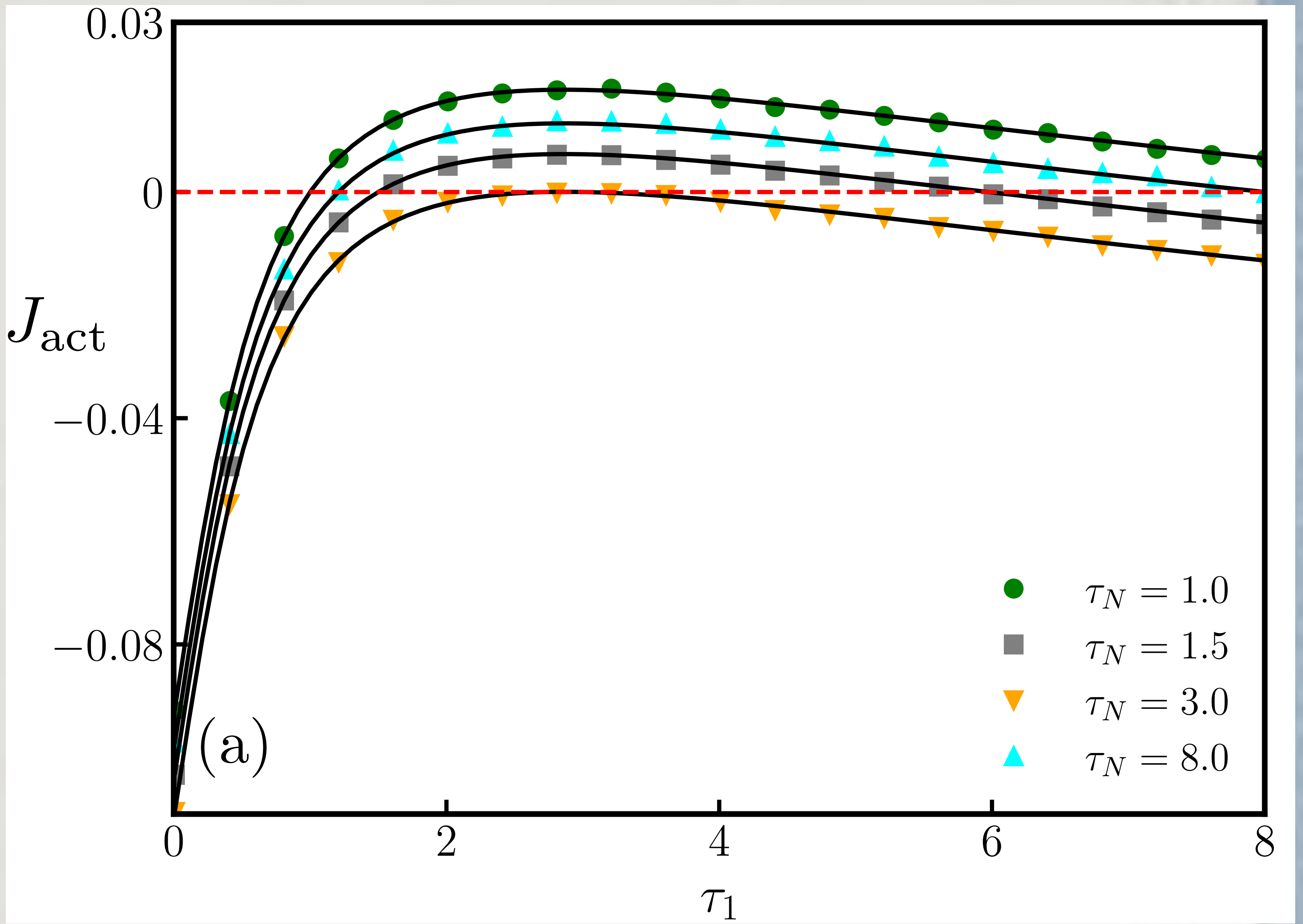
Reservoir spectra

- Depends on τ through reservoir spectra $\tilde{g}(\omega,\tau)$

- Additive contribution from both reservoirs

- In the thermodynamic limit $J_{\rm act} = \mathcal{J}_1 - \mathcal{J}_N,$

$$\mathcal{J}_i = \int_0^{\omega_c} \frac{d\omega}{4\pi} \frac{\sqrt{m(4k - m\omega^2)}}{mk + |\tilde{\gamma}|^2 - \mathrm{Im}[\tilde{\gamma}]m\omega} \tilde{g}(\omega, \tau_i).$$



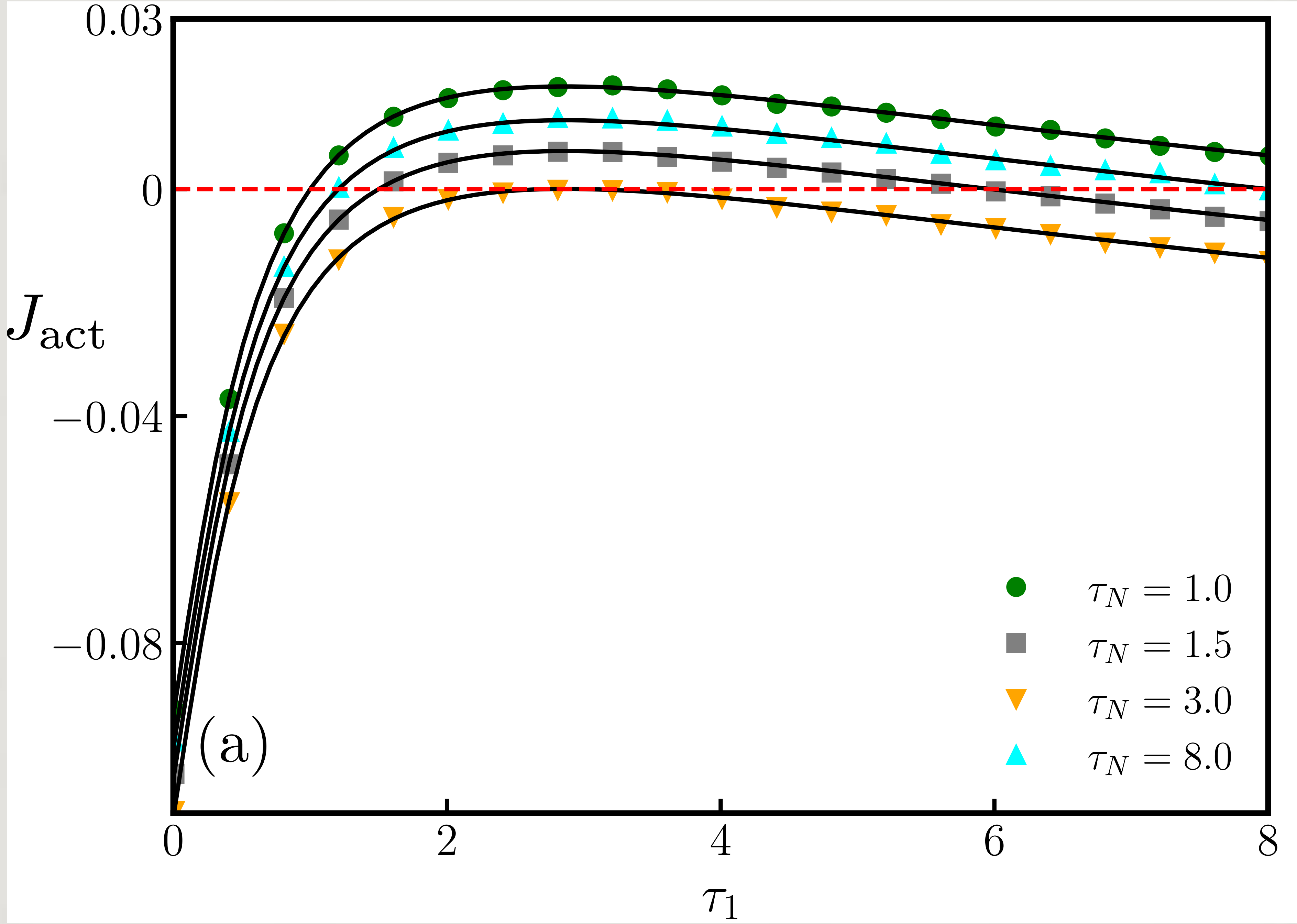
- No closed form, can be numerically evaluated
- No generic effective temperature description

$m = k = 1,\ \nu_1 = \nu_N = 1,\ \lambda_1 = \lambda_N = 1$

$M = N = 256$

- Effective temperature picture emerges in the passive limit

- Intriguing features :
  - Negative differential conductivity-
    - J_{act} changes non-monotonically with activity drive
    - Maximum at intermediate τ_m
  - Current reversal -
    - J_{act} changes direction at $\tau_1^* \neq \tau_N$ (additionally)



Plot of J_{act} vs τ_1 ($k = 2, m = \gamma = 1$)
Symbols: numerical simulation for RTP, M=N=256

Negative differential conductivity

- Differential conductivity $\frac{dJ_{\text{act}}}{d\tau_j} < 0$ in certain parameter regime
- NDC is a counterintuitive phenomenon, possible only away from equilibrium
- Known examples are in non-linear systems: rotor chain, presence of obstacles, kinetic constraints
- Activity drive leads to NDC in this linear system!
- Physical origin?

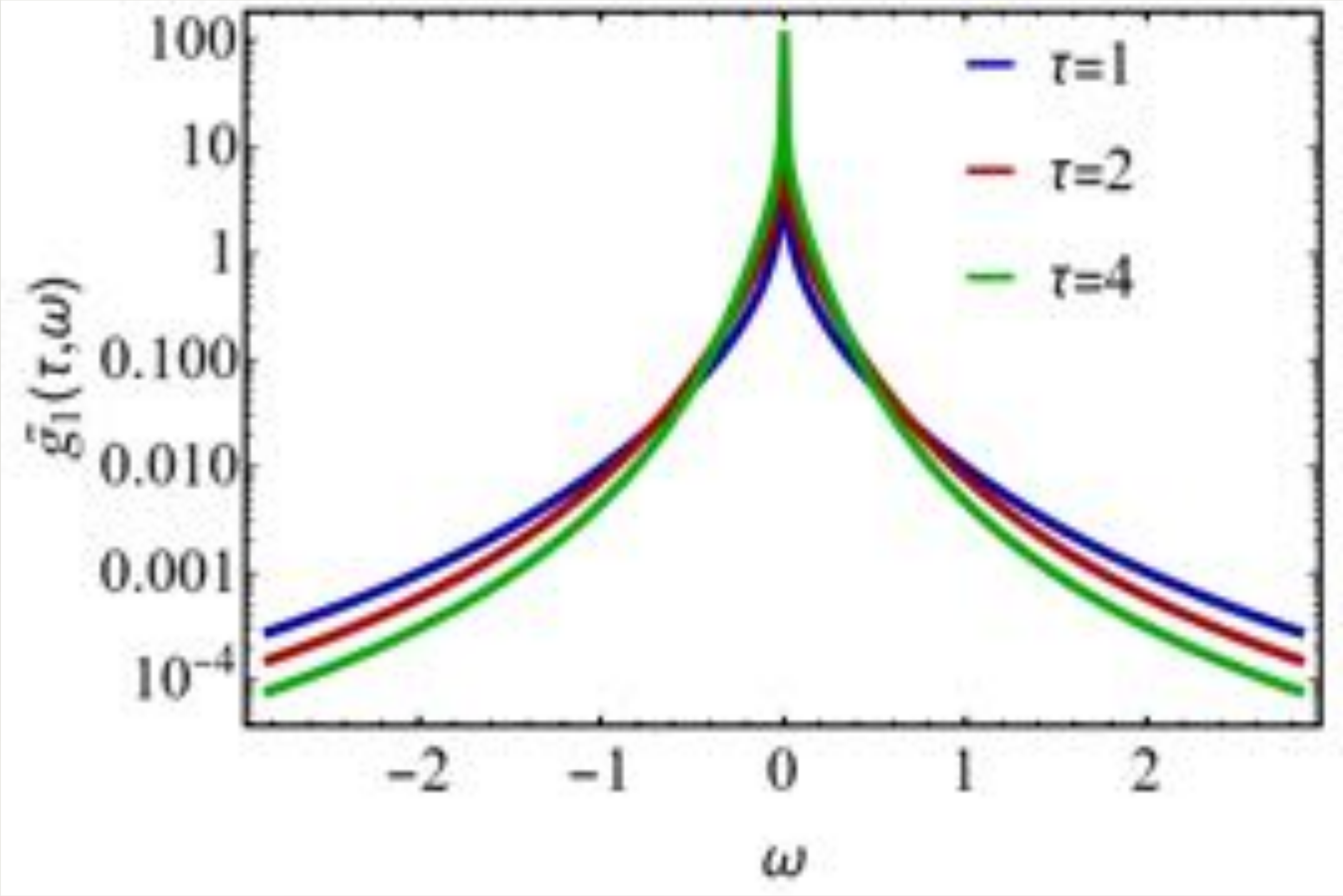
Barma & Dhar JPhysA 1984
Iacobucci et. al., PRE 2011
Leitmann & Franosch, PRL 2013
Baerts et. al., PRE 2013
Chatterjee et al, PRE 2018 ...

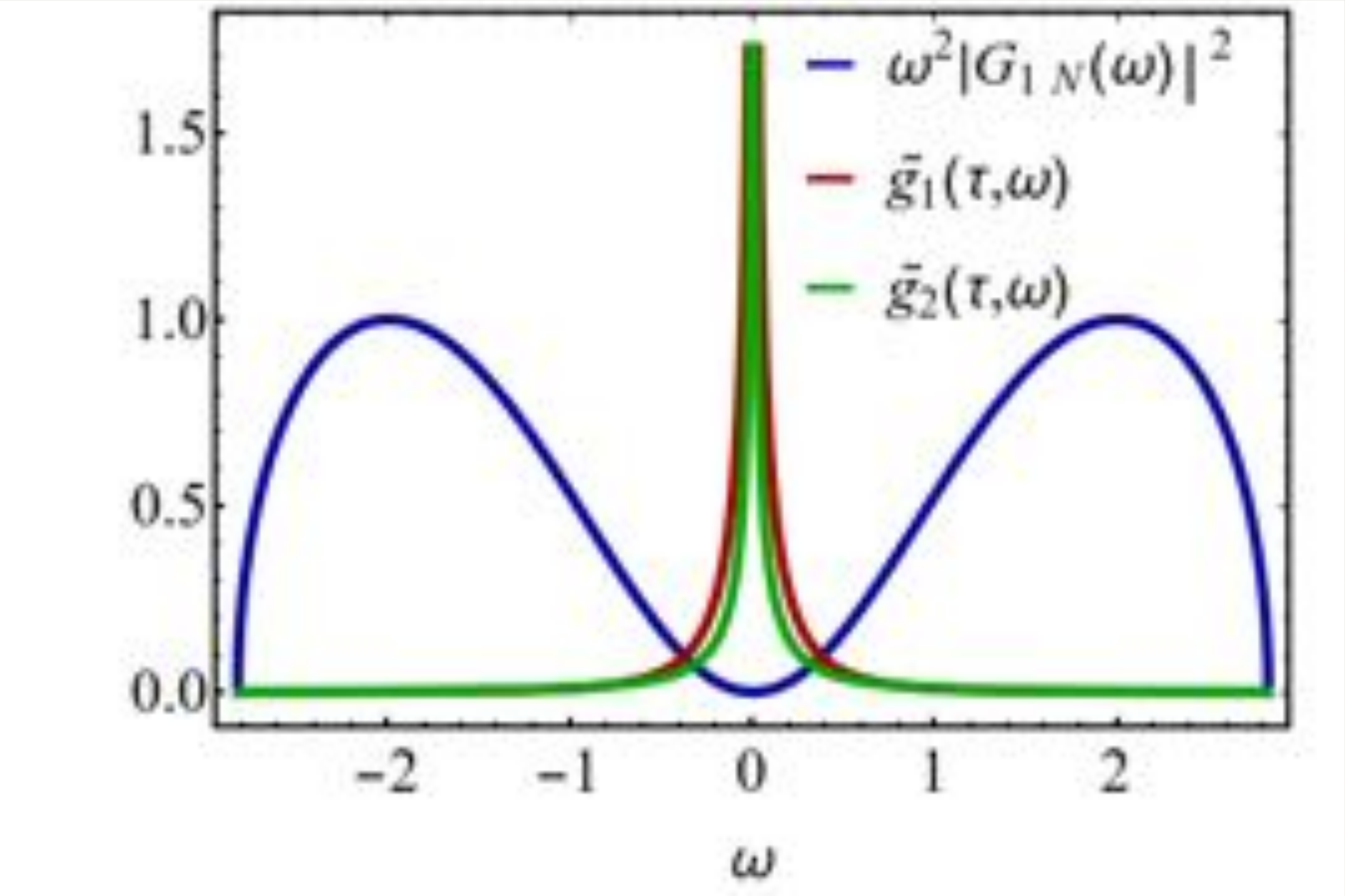
- System frequency spectrum is peaked near the characteristic frequency $\omega_c = 2\sqrt{k/m}$

$$J_{\text{act}} = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega^2 \left|G_{1N}\right|^2 \text{Re}[\tilde{\gamma}(\omega)] \left(\tilde{g}(\omega,\tau_1) - \tilde{g}(\omega,\tau_N)\right)$$

- Each reservoir spectrum is peaked at $\omega = 0$

- Overlap changes non-monotonically as activity is changed leading to NDC





Winning reservoir decides direction of current …

Conclusions

- Characterisation of active bath modelled by harmonic chain of RTPs
- Dissipation and noise kernels — modification of FDT
- NESS of harmonic chain driven by active reservoirs
- Emergent finite correlation length due to activity driving
- Transport properties: energy current reversal, NDC

Open questions

- What decides the direction? Thermodynamic understanding?
- Do the NDC and current reversal survive in higher dimensions?
- Effect of disorder?
- Effect of anharmonicity — what happens for FPUT chain?
- Coupling with thermal current?

Acknowledgements

Ritwick Sarkar
SNBose National Centre
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Kolkata, India

Ion Santra
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Göttingen, Germany

Joint works with ***Ritwick Sarkar*** *&* ***Ion Santra***

1. R. Sarkar, I. Santra, and UB, arXiv 2404.00615
Harmonic chain driven by active Rubin bath: transport properties and steady-state correlations
2. R. Sarkar, I. Santra, and UB, Phys. Rev. E 107, 014123 (2023)
Stationary states of activity driven harmonic chains
3. I. Santra and UB, SciPost Phys. 13, 041 (2022)
Activity driven transport in harmonic chains

Thank you!