Quantum Stochastic Transport Along Chains

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Scope

- Consider a particle hopping on a tight-binding *chain* or *ring* in an Ohmic environment.
- The particle can hop due to both *stochastic* and *coherent* transitions.
- We find a non-monotonic dependence of the current (I) on the bias ($\mathcal{E}$).
- We highlight counter-intuitive enhancement of disorder due to coherent hopping.

The Model

The **dynamics** is generated by a master equation for the probability matrix (Ohmic master equation):

$$\frac{d\rho}{dt} = \mathcal{L}\rho = -i[\boldsymbol{H},\rho] + \mathcal{L}^{(B)}\rho$$

Coherent transitions – tight-binding Hamiltonian:

$$\boldsymbol{H} = U(\boldsymbol{x}) - c\cos(\boldsymbol{p}) = -\mathcal{E}\hat{\boldsymbol{x}} - c\cos(\boldsymbol{p})$$

Stochastic transitions – each bond x is coupled to a bath of intensity ν and temperature T, resulting in a dissipator:

$$\mathcal{L}^{(B)}\rho = -\frac{1}{2}\sum_x\left(\nu[\boldsymbol{W}_x,[\boldsymbol{W}_x,\rho]] + \eta\, i[\boldsymbol{W}_x,\{\boldsymbol{V}_x,\rho\}]\right) + O(\eta^2)$$

$$\boldsymbol{W}_x = \boldsymbol{D}_x + \boldsymbol{D}_x^\dagger \qquad \boldsymbol{V}_x = i[\boldsymbol{H},\boldsymbol{W}_x]$$

$$\boldsymbol{D}_x \equiv |x{+}1\rangle\langle x| \qquad \eta = \nu/(2T)$$

Adding **bias** generates non-symmetric stochastic transitions:

$$\omega_x^{\pm} = \nu\left(1 + \frac{\mathcal{E}_x}{2T}\right)$$

$$\frac{\omega^-}{\omega^+} \approx e^{-\mathcal{E}_x/T} \text{ (Boltzmann)} \qquad \mathcal{E}_x \equiv -(U(x+1) - U(x))$$

Mixed type transitions – There are many other transitions. For example "$c\eta$" terms and "ν" terms that couple off-diagonal elements to diagonal and off-diagonal elements of ρ.

$$\boldsymbol{V}_x = i\mathcal{E}_x\left(\boldsymbol{D}_x^\dagger - \boldsymbol{D}_x\right) - i\frac{c}{2}[(\boldsymbol{D}_{x+1}\boldsymbol{D}_x - \boldsymbol{D}_x\boldsymbol{D}_{x-1}) - h.c.]$$

Dynamics of the Pauli-type Master Equation

As a "first-order" approximation one can drop the coupling between the diagonal and off diagonal terms of ρ in the dissipator $\mathcal{L}^{(B)}$ – obtaining a Pauli-like master equation.

$$\mathcal{L}^{(\text{B,Pauli})}\rho = -(\omega^+ + \omega^-)\rho + \sum_x\left(\omega^+\boldsymbol{D}_x^\dagger\rho\boldsymbol{D}_x + \omega^-\boldsymbol{D}_x\rho\boldsymbol{D}_x^\dagger\right)$$

$\boldsymbol{c = 0}$: Take $\rho(t{=}0)$ Gaussian with momentum k_0, then $\rho(t)$ at the Wigner picture is

$$\rho_w(R,P,t) = e^{-\gamma_0 t}\left[G^c(R,P) - G^0(R,P)\right] + G^t(R,P)$$

$$G^c(R,P) = \frac{2}{L}\exp\left(-\frac{1}{2}\frac{R^2}{\sigma_0^2} - (P-k_0)^2\sigma_0^2\right)$$

$$G^t(R,P) = \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{\sigma_0^2 + 2Dt}}\exp\left(-\frac{1}{2}\frac{(R-vt)^2}{\sigma_0^2 + 2Dt}\right)$$

With drift and diffusion:

$$v = (\omega^+ - \omega^-) = 2\eta\mathcal{E}$$
$$D = (\omega^+ + \omega^-)/2 = \nu$$

$\boldsymbol{c \neq 0}$: Solving $\mathcal{L}\rho = -\lambda\rho$. The relaxation eigenvalues are [2]

$$\lambda_{q,0} = \gamma_0 - \sqrt{\gamma_q^2 - 4c^2\sin^2(q/2)}$$
$$\gamma_q = \gamma + \omega^+ e^{-iq} + \omega^- e^{iq}$$

Drift is the same. Diffusion gains another term:

$$D = \frac{1}{2}(\omega^+ + \omega^-) + \frac{c^2}{2\gamma_0} = \nu + \frac{(c/2)^2}{\nu + (\gamma/2)}$$

In this approximation D is independent of $\mathcal{E}$.

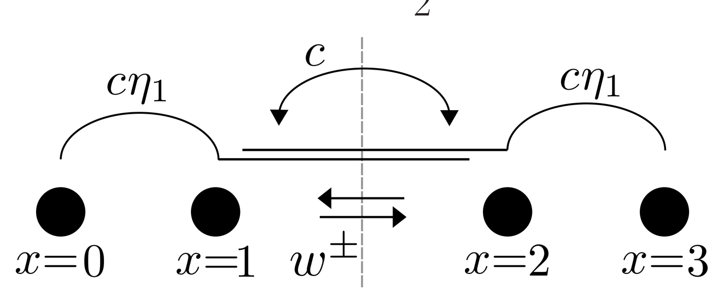
Expression for the Current

To express the current, the system is partitioned at the n-th bond. Define:

$$\boldsymbol{Q} = \sum_{x>n}|x\rangle\langle x|$$

The current flowing from left to right is $I = \langle\dot{\boldsymbol{Q}}\rangle = \mathrm{Tr}[\boldsymbol{Q}\mathcal{L}\rho]$:

$$I = \vec{I} - \overleftarrow{I} + c\,\mathrm{Im}[\rho_n(1)] + O(\eta^2)$$
$$\vec{I} = \omega_n^+ p_n - \frac{c\eta_n}{2}\mathrm{Re}[\rho_{n-1}(1)]$$
$$\overleftarrow{I} = \omega_n^- p_{n+1} - \frac{c\eta_n}{2}\mathrm{Re}[\rho_{n+1}(1)]$$



$$\rho_x(r) \equiv \langle x|\rho|x+r\rangle$$

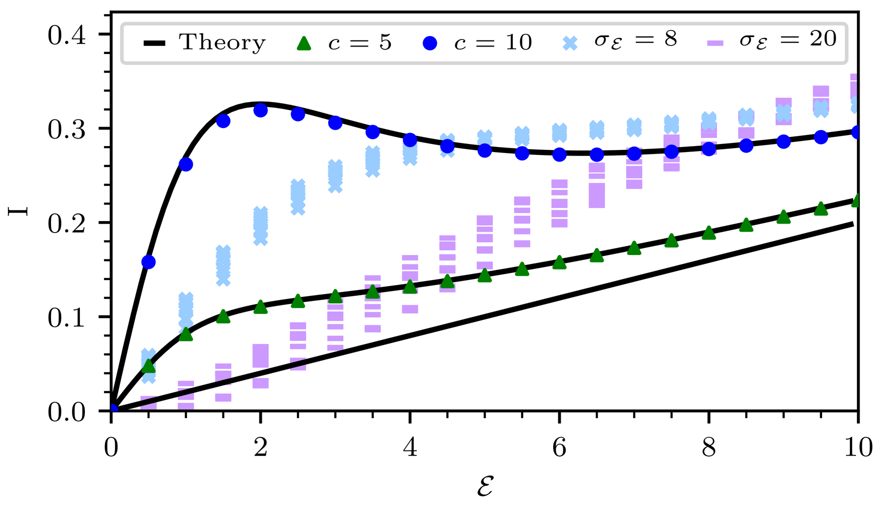
Non-Equilibrium Steady State and Current

The current is obtained by solving the steady state in first order in η, and applying $I[\rho]$.

$$\rho^{(\text{NESS})} = \frac{1}{L}\left(1 + \alpha_0 e^{+i\boldsymbol{p}} + \alpha_0^* e^{-i\boldsymbol{p}}\right)$$
$$\alpha_0 = \frac{3\nu - i\mathcal{E}}{3\nu^2 + \mathcal{E}^2}\eta c$$

NESS current is **non-monotonic**:

$$I_x = \frac{1}{L}\left((\omega_x^+ - \omega_x^-) + c\,\mathrm{Im}(\alpha_0)\right) = \frac{1}{L}\left[1 + \frac{c^2}{6\nu^2 + 2\mathcal{E}^2}\right]2\eta\mathcal{E}$$

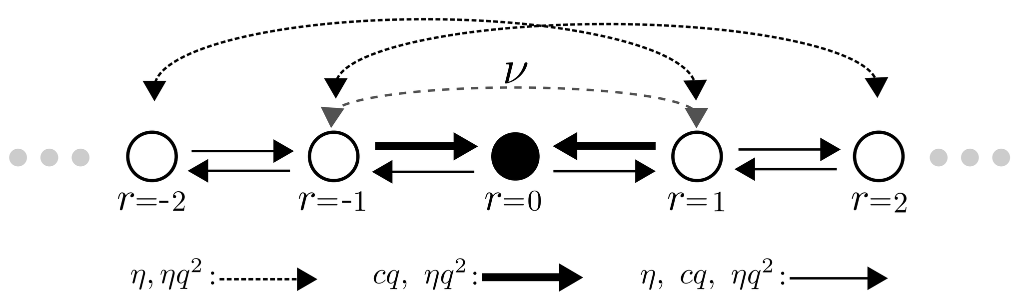


Relaxation Spectrum for the Clean Ring

The Lindblad operator for a uniform field $\mathcal{E}_x = \mathcal{E}$ is translation invariant.

Block-diagonal in Fourier: $\rho_q(r) = FT[\rho_x(r)]$
($\rho_x(r) \equiv \langle x|\rho|x+r\rangle$)

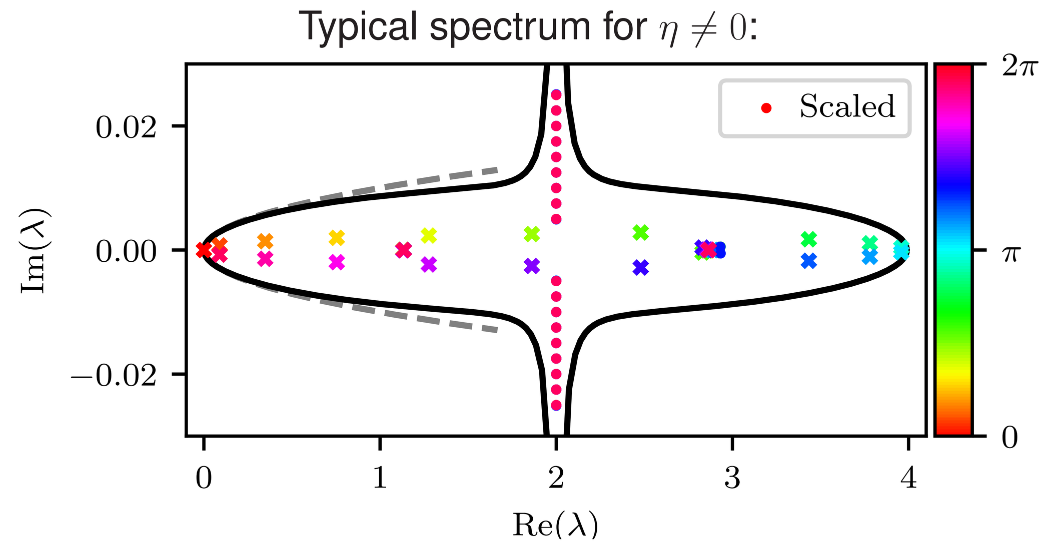
Schematic transitions for a given q ($q \ll 1$):



Eigenvalues for $q = 0$ and $\eta = 0$ ($\mathcal{L}\rho = -\lambda\rho$):

$$\lambda_{q=0,0} = 0 \quad \text{(NESS)}$$
$$\lambda_{q=0,\pm} = 2\nu \pm \sqrt{\nu^2 - \mathcal{E}^2}$$
$$\lambda_{q=0,s} = 2\nu + i\mathcal{E}s, \quad (s = \pm2, \pm3, \ldots)$$

Typical spectrum for $\eta \neq 0$:

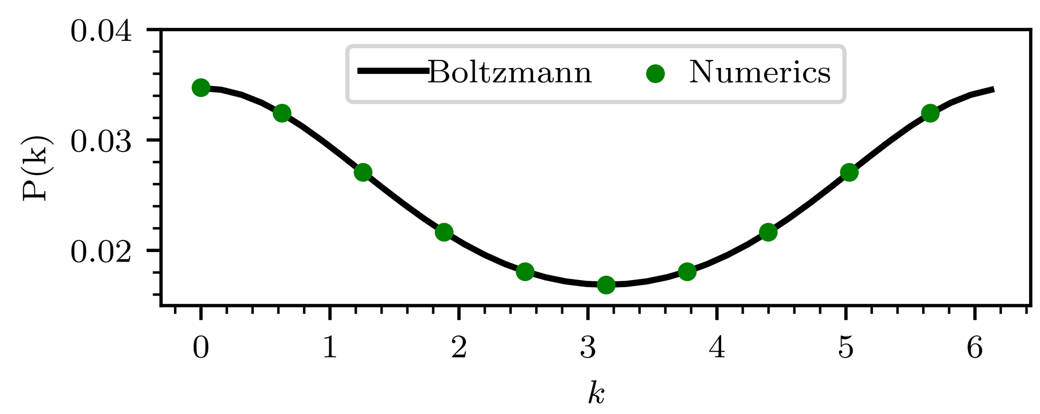


η-Correction for the Diffusion

The diffusion in zero order in η satisfies FDT: $v = D(\mathcal{E}/T)$. What is the $\boldsymbol{\eta}$**-correction** for the diffusion?

Naive treatment – The Drude type term in the expression for the diffusion is $\langle v_k^2\rangle\tau$. For finite T and $\mathcal{E} = 0$:

$$\left\langle v_k^2\right\rangle = \int_{-\pi}^{\pi}[c\sin(k)]^2 p(k)\,dk \approx \left[1 - \frac{1}{8}(\beta c)^2\right]\frac{c^2}{2}$$

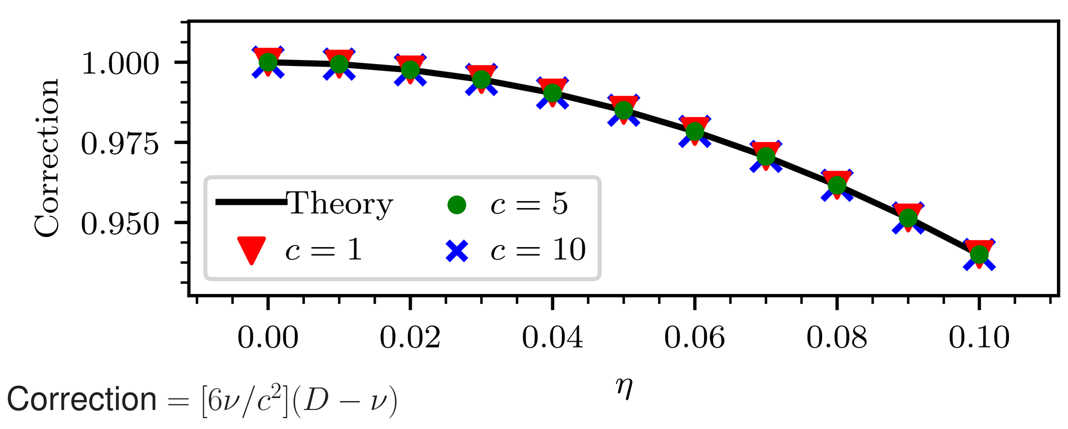


Exact treatment – Diffusion is obtained from the eigenvalues:

$$\lambda_{q,0} = ivq + Dq^2$$
$$v = \left[1 + \frac{c^2}{6\nu^2 + 2\mathcal{E}^2}\right]2\eta\mathcal{E}$$
$$D = \left[1 + \frac{c^2}{6\nu^2 + 2\mathcal{E}^2}\right]\nu + (\eta c)^2 D^{(\tilde{c})}$$

For $\mathcal{E} = 0$:

$$D = \nu + \left[1 - 6\eta^2\right]\frac{c^2}{6\nu}$$



Correction $= [6\nu/c^2](D - \nu)$

Disordered Enhanced-Current

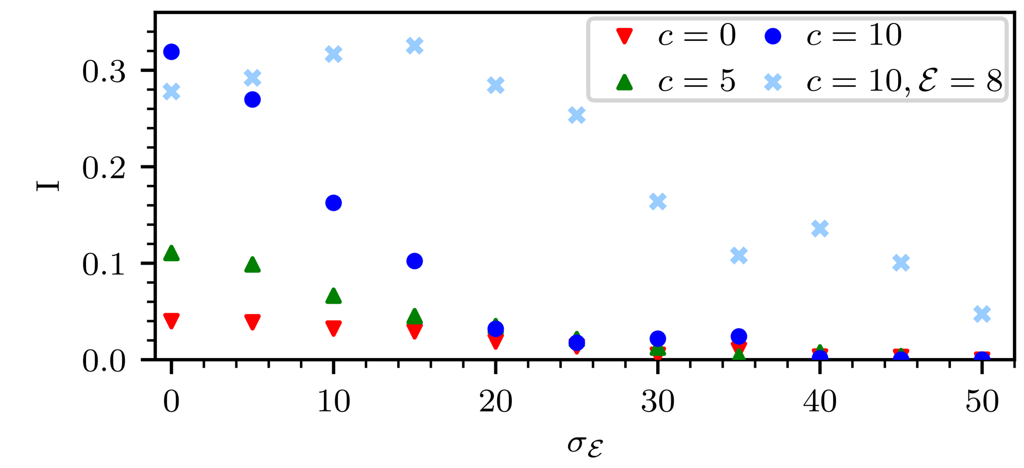
Disorder may **increase** the current for the same total bias.

Adding disorder:

$$\mathcal{E}_x = [-\sigma_\mathcal{E}, \sigma_\mathcal{E}] + \mathcal{E}$$

The non-monotonicity of $I(\mathcal{E})$ explains the enhanced current. A rough estimate:

$$I = \left[\sum_x \frac{1}{v(\mathcal{E}_x)}\right]^{-1}$$

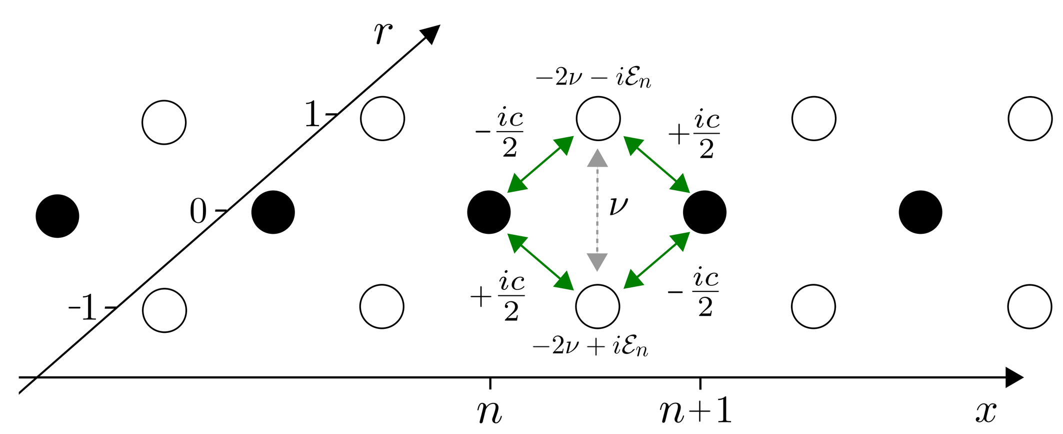


$\mathcal{E} = 6$ for the triangles and circle.

Effective Disorder

Increasing the hopping (c), for a given disorder, **increases** the effect of disorder on the relaxation spectrum.

Using a three-band model:



Reducing to an effective one-band:

$$H_{\text{eff}}(\lambda) = H_0 + W'G(\lambda)W$$

Resulting in a tight-binding probability-conserving model, with an added **Hermitian** disorder:

$$w_n^{\pm} = \nu + \nu_n \pm \eta\mathcal{E}_n$$
$$\nu_n = \frac{c^2}{2}\frac{\nu - \lambda}{(2\nu - \lambda)^2 + \mathcal{E}_n^2 - \nu^2}$$

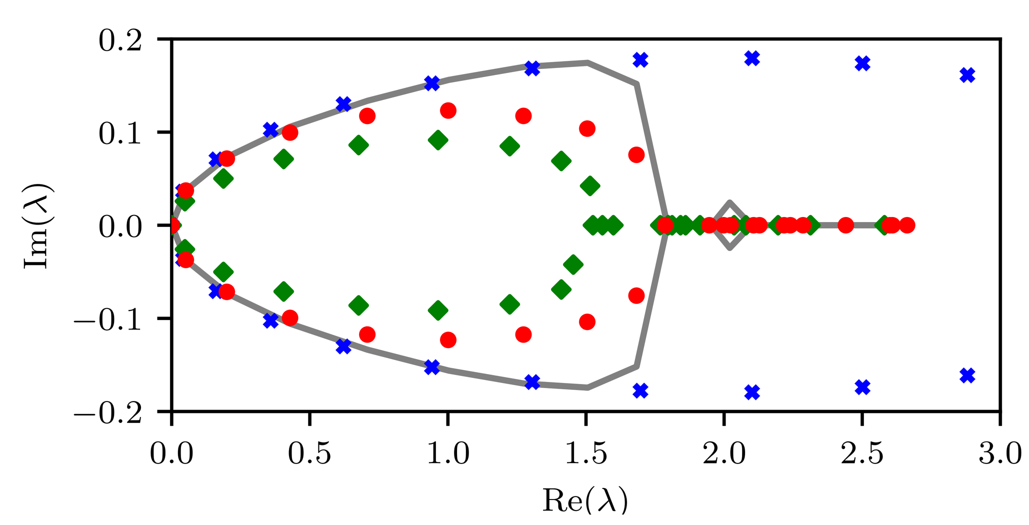
The spectrum becomes complex when the inverse localization length (κ) of the corresponding Hermitian matrix is smaller than $\eta\mathcal{E}$:

$$\kappa(\lambda) \approx \frac{1}{4}\left(\frac{\sigma_\perp}{\nu}\right)^2\frac{\lambda}{\nu}$$

Choosing a representative point in the spectrum ($\lambda = 2$):

$$w_n \approx \nu\frac{c^2}{2(\nu^2 - \mathcal{E}^2)}\left(1 + B\delta_n + C\delta_n^2\right)$$
$$\sigma_\perp^2 = \mathrm{Var}(w_n) \approx \left(\frac{c^2\nu}{2(\nu^2 - \mathcal{E}^2)}\right)^2\left(C_2\sigma_\mathcal{E}^2 + C_4\sigma_\mathcal{E}^4\right)$$

The spectrum becomes real because of the Hermitian disorder $\sim c^2$ which is independent of temperature.



The classical-relaxation spectrum with disorder. The green-diamond and blue-x correspond to $c{=}0$ and $c{=}2$. The red-dot and grey-line are the three-band and one-band approximations. ($L{=}31, \mathcal{E}{=}2, \sigma_\mathcal{E}{=}1.5, \nu{=}1, \eta{=}0.01$).

Conclusions

1. The NESS current is the sum of stochastic and quasi-coherent terms.
2. It displays non-monotonic dependence on the bias, due to crossover from Drude-type to hopping-type transport.
3. Disorder may increase the current due to convex property.
4. The interplay of stochastic and coherent transitions is reflected in the relaxation spectrum.
5. In the presence of disorder the quasi-coherent transitions enhance the localization of the relaxation modes.

References

[1] D. Shapira and D. Cohen (arXiv:1907.01993)
[2] M. Esposito and P. Gaspard (J. Stat. Phys. 121, 463 (2005))

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