Temperature Gradient in Non-equilibrium Steady States in Open Quantum System

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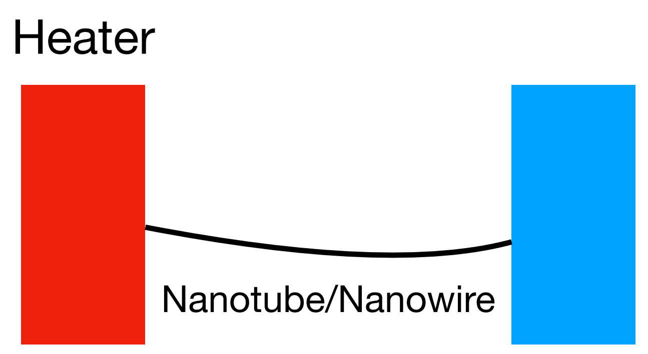
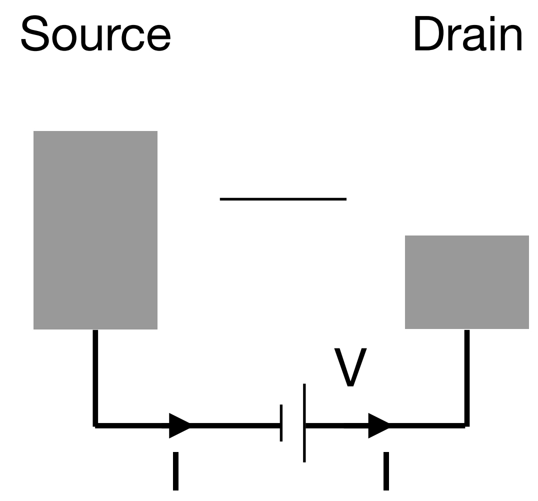
Non-equilibrium Statistical Mechanics

There are many non-equilibrium phenomena in nature:

- Heat transport
- Electronic transport
- Chemical Reaction
- … etc.

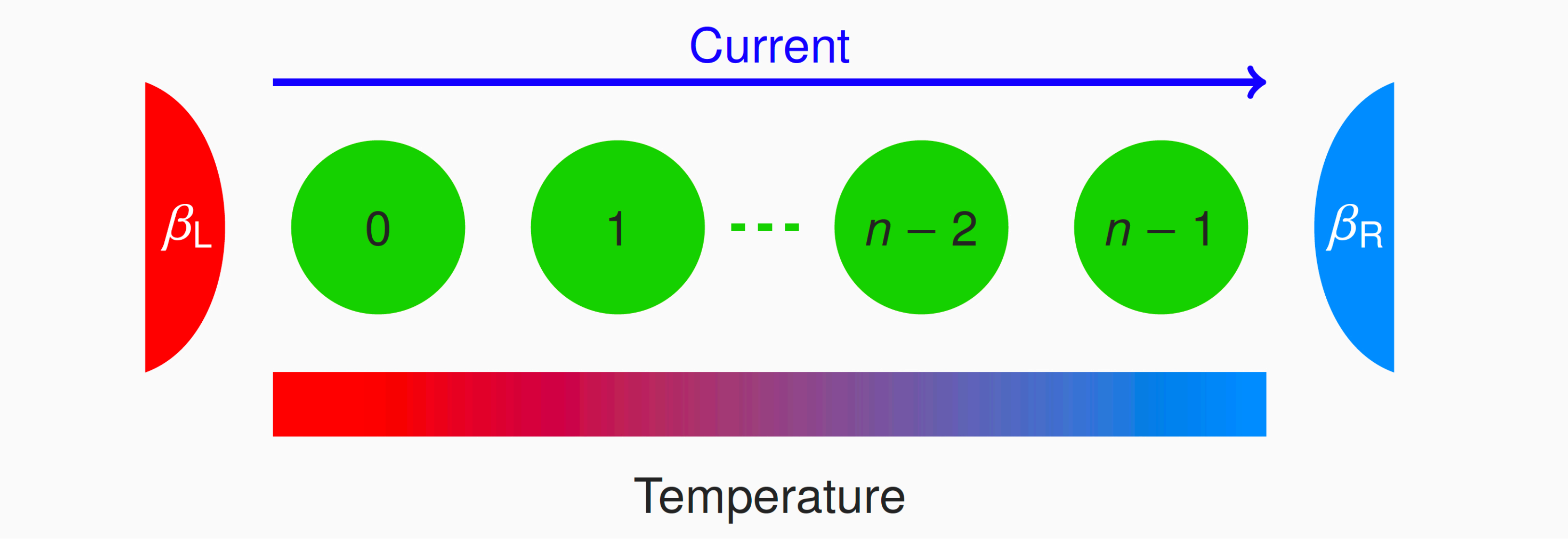




As a first step, we want to develop the theory for (quantum) non-equilibrium **steady** states.

(i.e. energy current of the system is constant.)

Setup



XXZ Hamiltonian (XX couplings are random variables)

$$H = \sum_p \omega Z_p + \sum_p \left\{ v_{p,p+1}\left(X_p X_{p+1} + Y_p Y_{p+1}\right) + \Delta Z_p Z_{p+1} \right\}$$

,where

$$A_p := \underbrace{I \otimes \cdots \otimes I}_{p-1} \otimes A \otimes \underbrace{I \otimes \cdots \otimes I}_{n-p-1}$$

X, Y, Z: Pauli matrices

- $v_{p,p+1}$ is randomly given by Gaussian distribution: $N(\mu, \alpha^2)$

$$f(y) = \frac{1}{\sqrt{2\pi}\alpha} \exp\left(-\frac{\left(y-\mu\right)^2}{2\alpha^2} \right)$$

- ZZ coupling is negligible: $\Delta \ll \mu$, $\Delta/\mu \sim 10^{-4}$

Setup

Non-equilibrium Steady States (NESS)

We have to calculate the NESS in order to get the temperature profile.
Eventually the NESS is the eigenvector corresponding to the zero eigenvalue:

$$L(\rho) = -i[H, \rho] + \sum_{p=0,n-1} \sum_{s=\pm} \left(V_{ps}\rho V_{ps}^{\dagger} - \frac{1}{2}\left\{ V_{ps}^{\dagger}V_{ps}, \rho \right\} \right)$$

(Environment effects)

Represent the L and ρ as the matrix and vector in the vector space of the linear operators.

$$L(\rho_{\textbf{NESS}}) = 0$$

$L : 2^{2n} \times 2^{2n}$ **matrix**

$\rho_{\textbf{NESS}} : 1 \times n$ **row vector**

However, this equation is hard to solve:
→ L contains $\mathcal{O}(2^{4n})$ elements
Thus, we have to use a perturbation theory and calculate numerically.

Calculation of the NESS

Perturbative approach: $L = L_0 + \epsilon L_1$, $\rho = \sum_{m=0}^{\infty} \epsilon^m \rho^{(m)}$

Calculate 0th order of the NESS $\rho^{(0)}$

$$\begin{cases} L_0(\rho^{(0)}) = 0, \\ L_0(\rho^{(1)}) + L_1(\rho^{(0)}) = 0. \end{cases}$$

$\Rightarrow \rho^{(0)} \in \ker(PL_1P)$,

where P is the projection onto $\ker(L_0)$.

PL_1P contains $\mathcal{O}(2^{2n})$ elements.

Calculate m th order of the NESS $\rho^{(m)}$

$$\begin{cases} L_0(\rho^{(m)}) + L_1(\rho^{(m-1)}) = 0, \\ L_0(\rho^{(m+1)}) + L_1(\rho^{(m)}) = 0. \end{cases}$$

$\Rightarrow \rho^{(m)} = [(PL_1P)^{-1}L_1 - 1](QL_0Q)^{-1}L_1\rho^{(m-1)} + c_m\rho^{(0)}$,

where $Q = 1 - P$. c_m is given by $\mathrm{Tr}(\rho^{(m)}) = 0$.

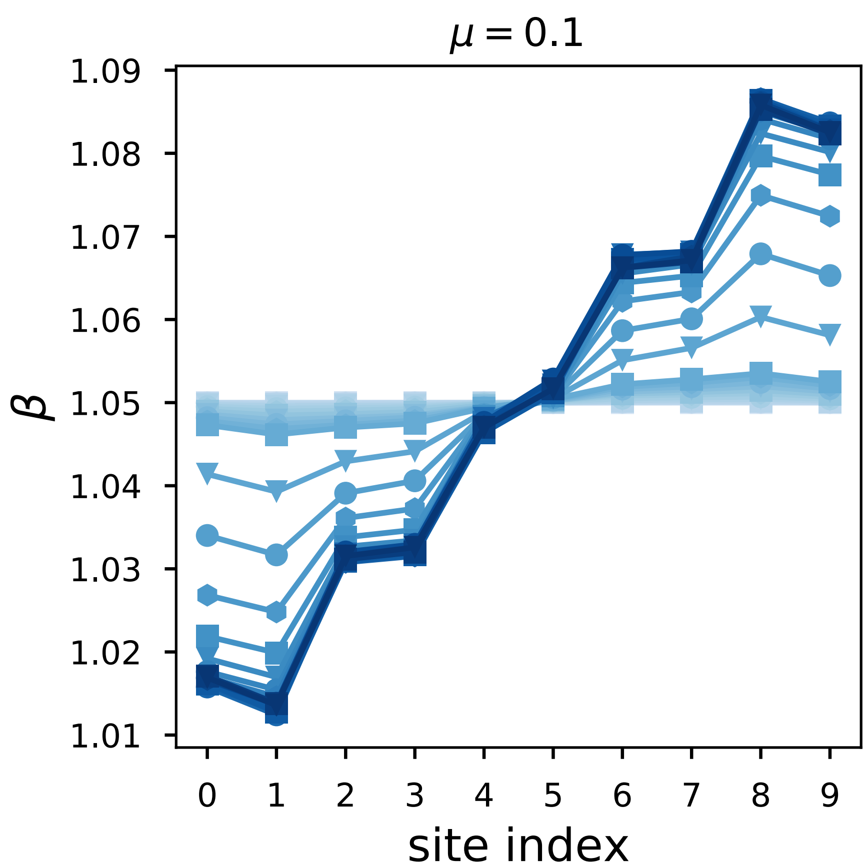
Error

$$\begin{aligned} \text{Error} &= ||L(\rho)|| \\ &= \epsilon^{m+1}||L_1(\rho^{(m)}|| \\ &\sim 10^{-7}, \end{aligned}$$

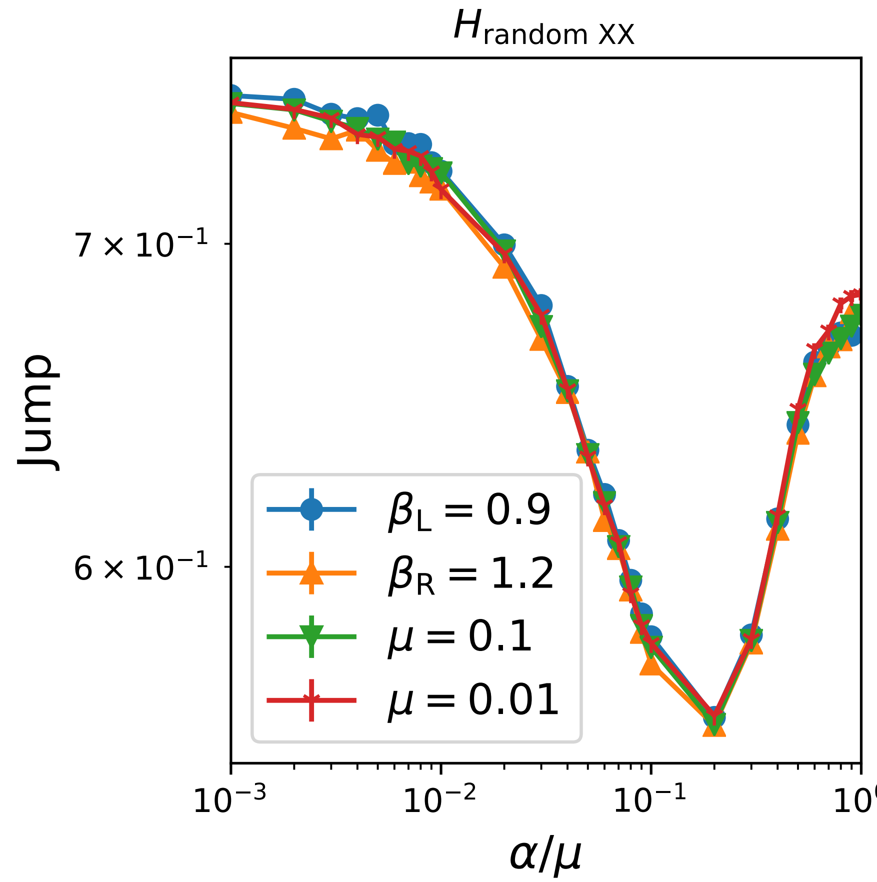
where ||A|| := $\sqrt{\mathrm{Tr}(A^\dagger A)}$

Relationship btw temperature profile and fluctuation

Averaged Temperature Profiles and Fluctuation



Averaged Jumps in Temperature Profiles and Fluctuation



Jump$:= \max_k |\beta_{k+1}^{\mathbf{norm}} - \beta_k^{\mathbf{norm}}|$

$$\beta_k^{\mathbf{norm}} := \frac{\beta_k - \min_i \beta_i}{\max_i \beta_i - \min_i \beta_i}$$

We calculated the temperature profiles 10000 times a parameter set.

- The more α, the more clearly the temperature gradient appears.
- There is a parameter range in which the temperature profiles is smooth.

Future Issues:

- Calculate other non-equilibrium properties. e.g. enegry current
- Calculate non-equilibrium observables using another approach