Poisson equation for nonreversible Markov jump processes and its applications

Christian Maes

Faezeh Khodabandehlou

Department of Physics and Astronomy,
KU Leuven, Belgium

Karel Netocny

Institute of Physics of the Czech Academy of Sciences,
Prague, Czech Republic

Poisson equation

For a given centered function f, what is V?

$$L\,V(x) + f(x) = 0 \qquad x \in K$$

$$\langle f \rangle = 0$$

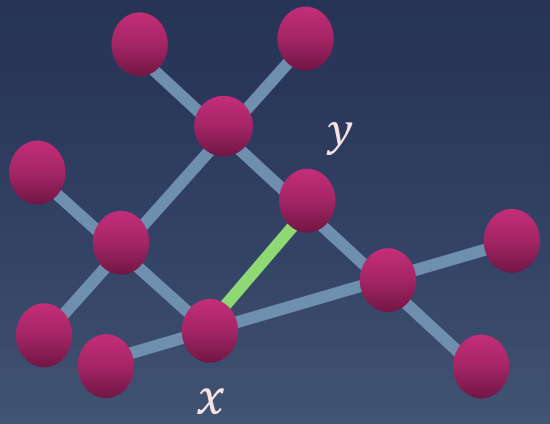
Markov jump process generator

vertices of irreducible graph

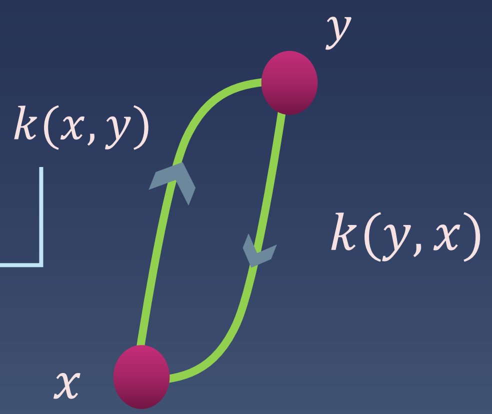
$$\langle f \rangle = \sum \rho(x) f(x)$$

Markov jump process

State space K



Transition rates



Probability per unit time
for x ➔ y

Markov jump process

Set of linear equations → $$\frac{d\rho_t(x)}{dt} = \sum_y [k(y,x)\rho_t(y) - k(x,y)\rho_t(x)] = \rho L\ (x)$$

Stationary distribution → $$L^*\rho^s = 0 \qquad \exists! \quad \rho^s > 0$$

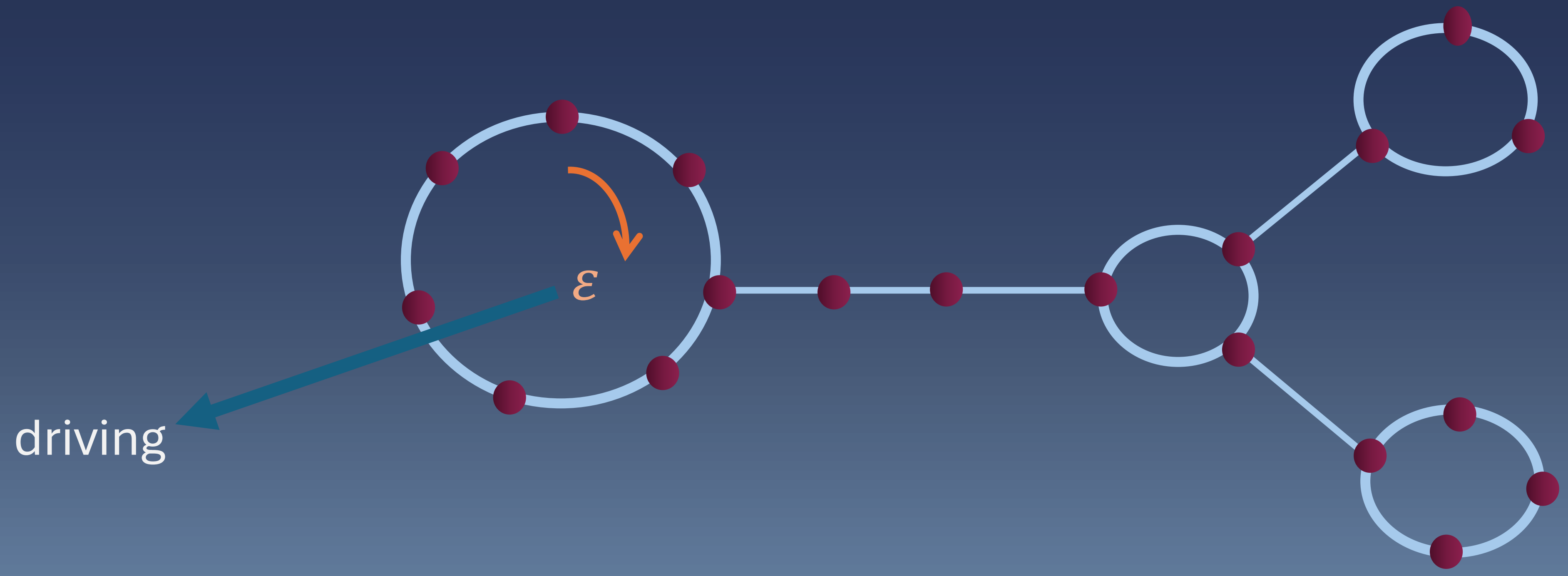
Backward generator → $$L = \begin{cases} L_{xy} = k(x,y) & x \neq y \\ L_{xx} = -\sum_y k(x,y) \end{cases}$$

Nonreversible Markov jump process

Breaking detailed balanced → $\rho^s(x)k(x,y) \neq \rho^s(y)k(y,x)$

Nonreversible Markov jump process

Breaking detailed Balanced → $\rho^s(x)k(x,y) \neq \rho^s(y)k(y,x)$



No simple expression for stationary distributions

applications

- Properties of V, such as behavior at large driving, e.g uniform boundedness in system parameters?
- Relation with mean first-passage times (helping to construct the solution V)
- Current –current relationship

Message of talk: potential theory for irreversible jump processes

1) There are interesting relations between nonequilibrium Currents

2) Graphical representations are available for solutions of Poisson equation and are most useful in asymptotic regimes of low-temperature (yet irreversible) Markov jump processes.

Poisson equations and solutions:

I. Quasipotential

II. First-passage time

Quasipotential!

Quasipotential

$$L\,V(x) + f(\mathrm{x}) = 0 \qquad \mathrm{x} \in \mathrm{K}$$

$$\langle f \rangle = 0$$

has unique centered solution
(the quasipotential corresponding to f)

$$V(x) = \int_0^\infty dt\, e^{t\,L}\, f(x)$$

Resolvent inverse

$V = -L^{-1} f$ formally...

$$|L| = 0$$

L is not invertible: how to represent solution??

Method 1: via graphical representation of resolvent inverse

(forest extension of tree theorem=Kirchhoff formula):

Matrix-forest theorem

Resolvent inverse of Laplacian

$$\frac{1}{I - \alpha L}$$

Matrix-forest theorems

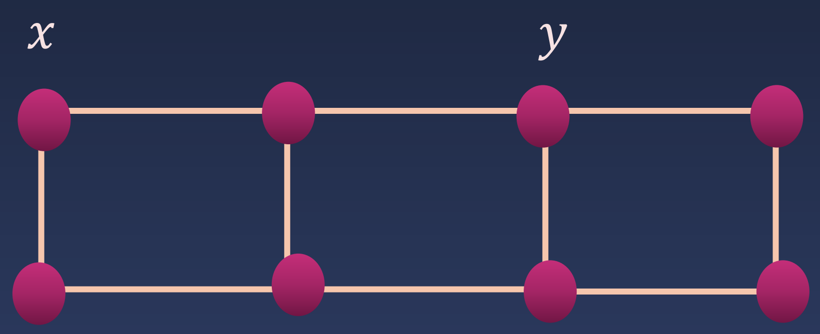
$$\left(\frac{1}{I - \alpha L}\right)_{xy} = \frac{\sum_{m=0}^{n-\gamma} \alpha^m w\left(F_m^{x \to y}\right)}{\sum_{m=0}^{n-\gamma} \alpha^m w(F_m)}$$

$$L^{-1} f = \left(\lim_{\alpha \to \infty} \frac{-\alpha}{I - \alpha L}\right) f$$

P. Chebotarev and E. Shamis. Matrix-forest theorems. arXiv, 0602575 [math.CO], (2006).

Illustration of matrix forest theorem for simple example

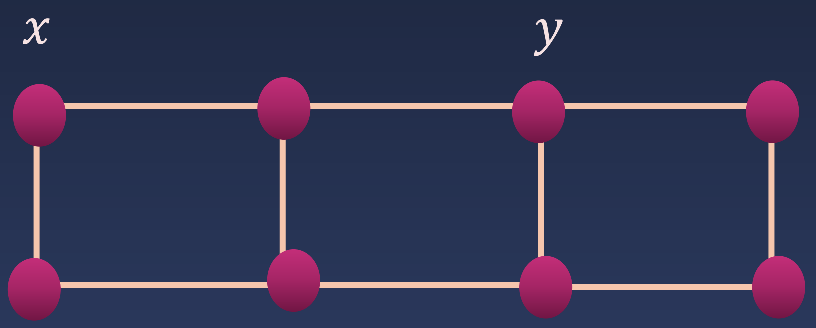
$$V(x) = \frac{\sum_y w(x \to y) f(y)}{W}$$



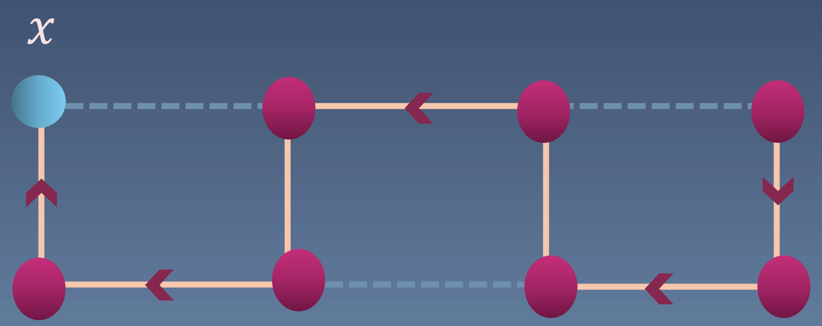
Quasipotential

$$V(x) = \frac{\sum_y w(x \to y) f(y)}{W}$$

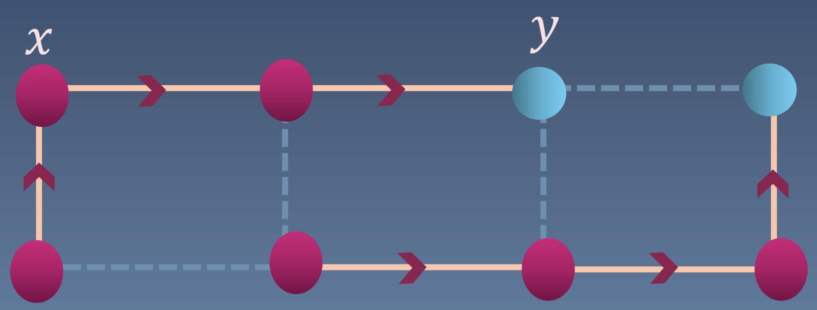
Products over edges of the rates



W : Weight of all rooted spanning trees

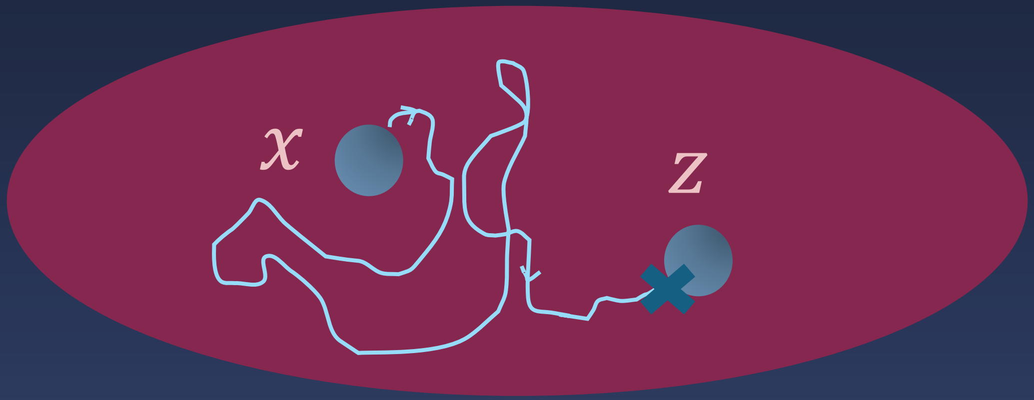


$w(x \to y)$: Weight of all spanning forests rooted at y such that x is in the same tree with y



Method 2 (of representing solution (quasoipotential) of Poisson eq: First passage time!

Mean-First passage time



The mean of the first time that process started from x hits state z = $\tau(x, z)$

$$L\tau\,(z) + 1 = 0$$

$$\sum_y k(x,y)[\tau(y,z) - \tau(x,z)] + 1 = 0, \quad x \neq z, \qquad \tau(z,z) = 0$$

Quasipotential and mean first-passage time

$$V(x) - V(y) = \sum_z \rho^s(z)\, f(z)\big(\tau(y,z) - \tau(x,z)\big)$$

Upper bound $|V(x) - V(y)| \leq ||f||\, \min\{\tau(x,y), \tau(y,x)\}$

Quasipotential bounds:

$$V(x) - V(y) = \sum_z \rho^s(z)\, f(z)\big(\tau(y,z) - \tau(x,z)\big)$$

Upper bound $|V(x) - V(y)| \leq ||f||\, \min\{\tau(x,y), \tau(y,x)\}$

If for any two neighboring states, the difference of quasipotentials is bounded, then also the quasipotential of every state is bounded. (lemma)

APPLICATION: Extended Third Law (Theorem)

The extended Third Law states that the nonequilibrium heat capacity, under two conditions, vanishes at absolute zero:

$$C(T) \underset{T\downarrow 0}{\longrightarrow} 0$$

I. Unique dominant state

II. Accessibility (boundedness of quasipotential)

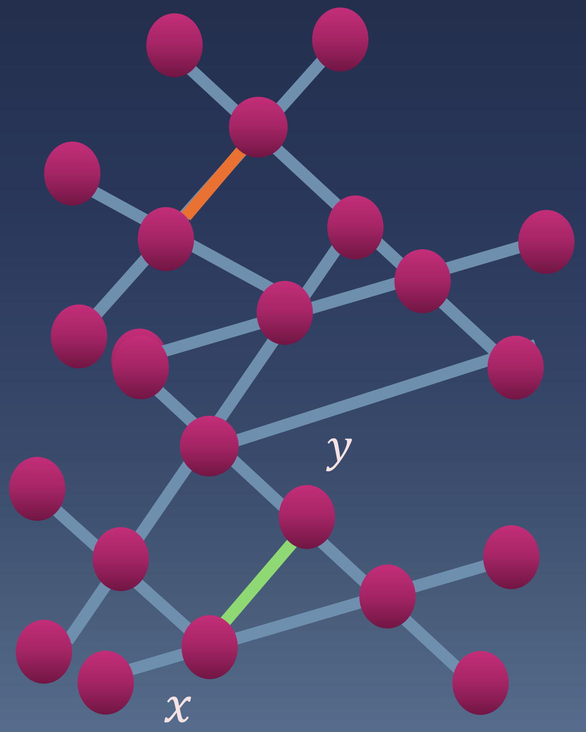
Application 2

Current-current relation

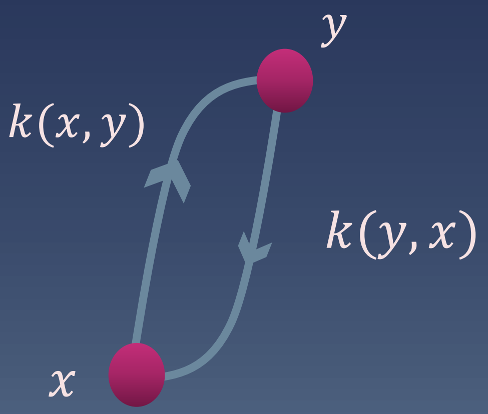
KU LEUVEN

Steady current

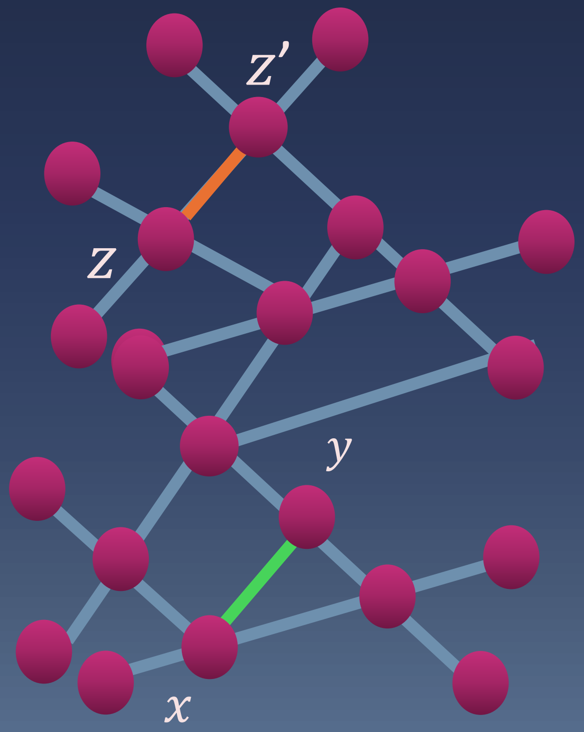
$$j(x,y) = \rho^s(x)k(x,y) - \rho^s(y)k(y,x)$$



Transition rate



Current-current relation

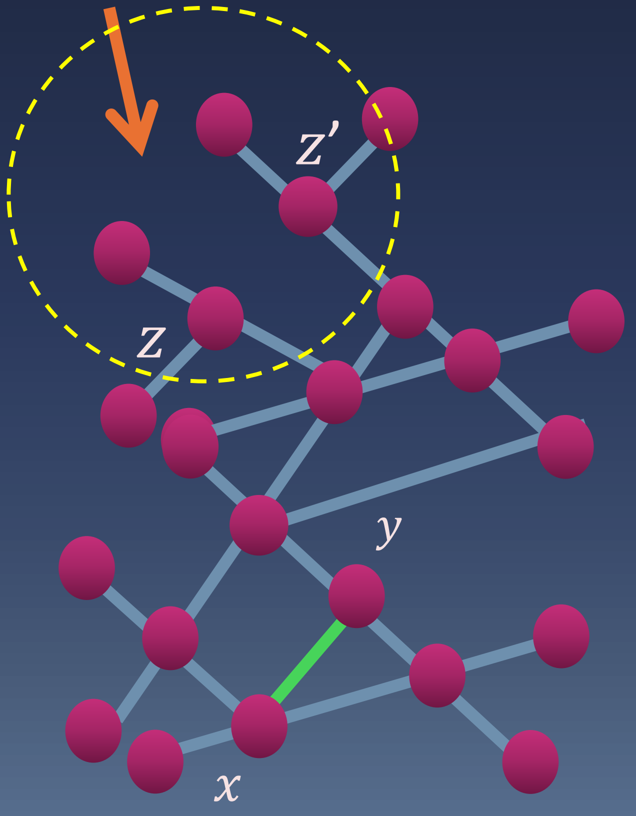


$$j(x,y) = \alpha + \lambda\, j(z,z')$$

Mutual Linearity of Nonequilibrium Network Currents. Pedro E. Harunari, Sara Dal Cengio, Vivien Lecomte, and Matteo Polettini. Phys. Rev. Lett. 2024.

KU LEUVEN

Current-current relation

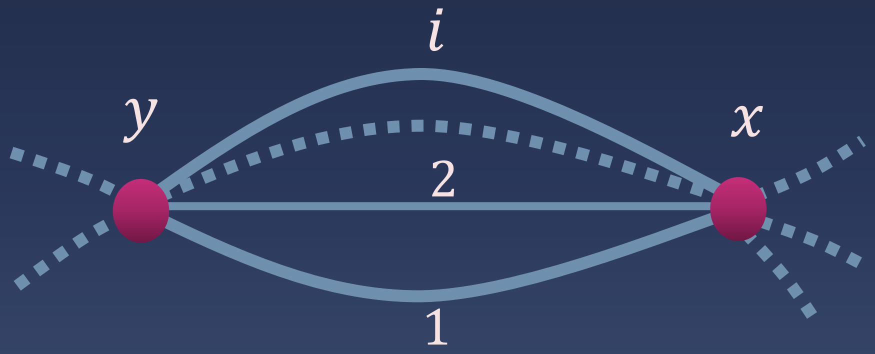


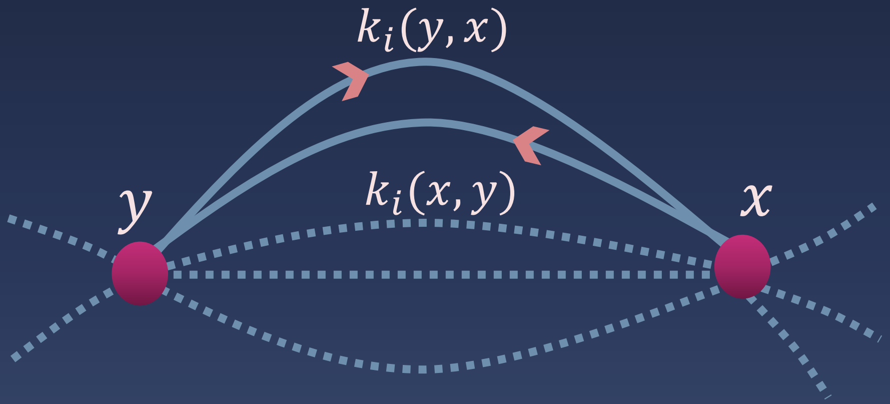
$$j(x,y) = \alpha + \lambda\, j(z,z')$$

Current over the edge (x,y) in the graph where {z,z'} is removed.

Susceptibility depends neither on k(z, z') nor k(z', z). Interestingly, λ can also be expressed in term of quasipotential (solution of Poisson eq)

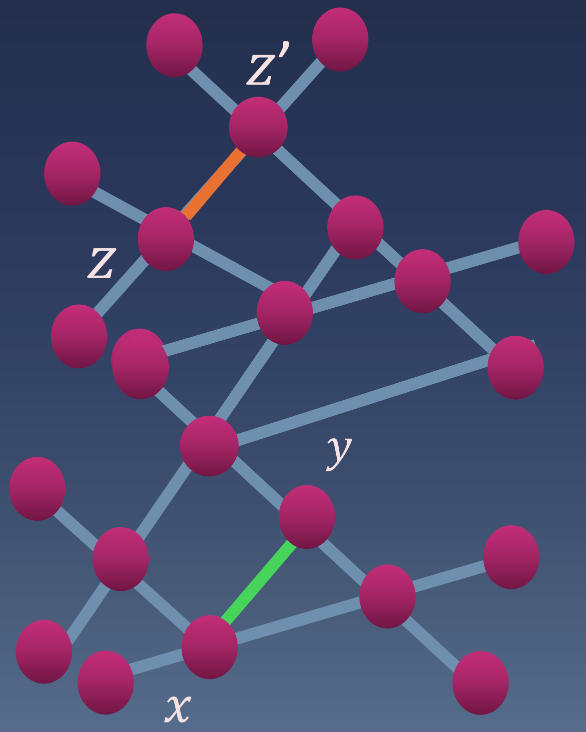
Perturbing the rates





$$k_i(x,y) = k_i^0(x,y) + \Delta_i(x,y)$$

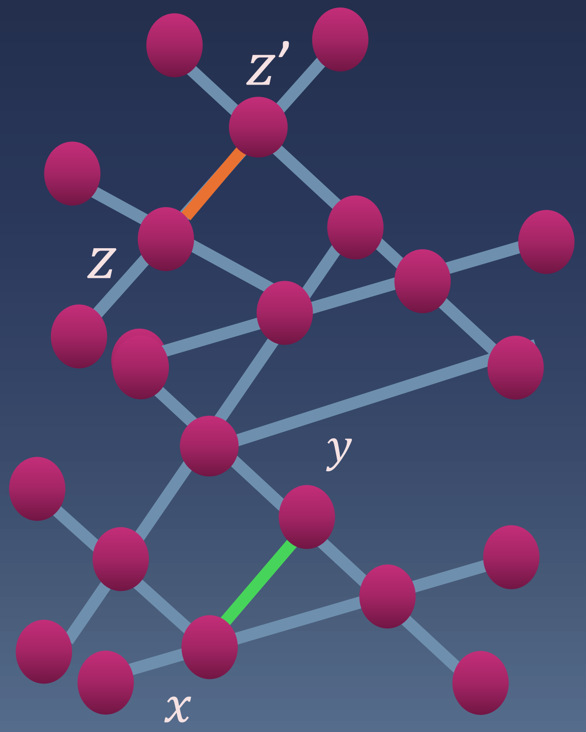
Current-current relation (First passage time)



$$j_i(x,y) = j_i^0(x,y) + \sum_{(z,z')} \lambda_i^0\big(zz',(x,y)\big)\, j_\Delta(z,z')$$

$$\lambda_i^0\big(zz',(x,y)\big) = \frac{1}{2}\begin{pmatrix} \rho^0(x)k_i^0(x,y)[\tau^0(z,x)-\tau^0(z',x)] \\ -\rho^0(y)k_i^0(y,x)[\tau^0(z,y)-\tau^0(z',y)] \end{pmatrix}$$

Current-current relation (Quasipotential)



$$j(x,y) = j^0(x,y) + \left(V^0_{xy}(z') - V^0_{xy}(z)\right) j(z,z')$$

$$L^0 V^0(z) = j^0(x,y) - n(z)$$

$$n(z) = \lim_{t \to 0^+} \frac{\langle N_{xy}(t) \rangle^0_z}{t} = \begin{cases} k^0(x,y) & if \quad z = x \\ -k^0(y,x) & if \quad z = y \\ 0 & otherwise \end{cases}$$

1. Nernst heat theorem for nonequilibrium jump processes. F. Khodabandehlou, C. Maes, K. Netočný. J. Chem. Phys. (2023).

2. The vanishing of excess heat for nonequilibrium processes reaching zero ambient temperature. F. Khodabandehlou, C. Maes, I. Maes and K. Netočný, Annales Henri Poincaré (2023).

3. Exact computation of heat capacities for active particles on a graph. F. Khodabandehlou, S. Krekels, I. Maes. J. Stat. Mech. (2022).

4 . On the Poisson equation for nonreversible Markov jump processes, F. Khodabandehlou, C. Maes, K. Netočný. J. Math. Phys. (2024).

5. Trees and forests for nonequilibrium purposes: an introduction to graphical representations. F.Khodabandehlou, C. Maes, I. Maes and K. Netočný, J. Stat. Phys. (2022).

6. Drazin-inverse and heat capacity for driven random walkers on the ring. F. Khodabandehlou, I. Maes. Stochastic Processes and their Applications, (2023).

7. Current relations. F. Khodabandehlou, C. Maes, K. Netočný. Preperation (2024)