Auto-correlations of spins in 1D East Model

Gang Huang

March 16, 2022

East Model is an example of kinetically constrained Ising model.

East model is a 1-D system of spins on lattice. For site i, $n_i = 0$ or 1. No static interactions between spins. (**Palmer 1984; Jaeckle, Eisinger 1991; Eisinger, Jaeckle 1993; Faggionato, Martinelli, Roberto, and Toninelli 2012**)
Boundary condition: PBC (**Sollich,2003**).
A given spin may only flip if the neighboring spin to the right is up, with an acceptance ratio A,

$$A = \begin{cases} e^{-\beta}, & \text{for } 01 \to 11 \\ 1, & \text{for } 11 \to 01. \end{cases} \tag{1}$$

East model shows glassy dynamics. (**Pitts and Andersen, 2001**)
Auto-correlation function

$$C(t) = \frac{\langle \delta n_i(t) \delta n_i(0) \rangle}{\langle \delta n_i(0)^2 \rangle} = \frac{\langle n_i(t) n_i(0) \rangle - c^2}{c - c^2} = \frac{\langle \delta n_i(t) \delta n_i(0) \rangle}{c(1-c)}. \tag{2}$$

$\langle \cdots \rangle$: Average for the equilibrium state; n_i: occupation number of site i; $c = \langle n_i \rangle$; $\langle n_i(t)^2 \rangle = \langle n_i(t) \rangle$.

Relation between β and c

Denote $c = \langle n_i \rangle_{\text{eq}}$ (**Eisinger and Jaeckle, 1991**),

$$c = \frac{e^{-\beta}}{1+e^{-\beta}} \Rightarrow \beta = \ln \frac{c}{1-c} \text{ for } c < 1/2. \tag{3}$$

(**Wu Jianlan, 2004, JPC**)

Theoretical and MC simulation (total steps: 3000) values of and c for given β's.

β	c (Theo.)	$c(N=32)$	$c(N=64)$	$c(N=128)$	$c(N=256)$
0.08	0.4800		0.4797	0.4800	0.4803
0.40	0.4013		0.4027	0.4006	0.4012
0.85	0.2994		0.2998	0.2992	0.3005
1.39	0.1994		0.2046	0.2034	0.2033
2.00	0.1192		0.1492	0.1576	0.1539
2.20	0.0997		0.1450	0.1487	0.1520

Q: Why is the values of c obtained by the Monte Carlo simulation too large at high β?
A: Because the system does not reach equilibrium!

To make sure we have calculated the $c(t)$ of equilibrated chain

Q2: How to make sure the system is in equilibrium?
A2: We set

$$\text{total steps} = \text{INT}[N_{\text{step}}(1+\beta)^2], \tag{4}$$

where $N_{\text{step}} = 3000$.
Then, for higher β, the total number of MC steps will be larger! The data for analyzing: the last $N_{\text{step}} \cdot \alpha = 3000 \times 0.8 = 2400$ steps.

Theoretical and MC simulation (total steps: 3000) values of and c for given β's.

β	c (Theo.)	$c(N=32)$	$c(N=64)$	$c(N=128)$	$c(N=256)$
0.08	0.4800		0.4797		
0.40	0.4013		0.4027		
0.85	0.2994		0.2998		
1.39	0.1994		0.2046		
2.00	0.1192		0.0959		
2.20	0.0997		0.0803		

For high β, the fluctuation of c is large! As β increase, we need longer trajectory to make sure the c from simulated data reaches the theoretical value. 3000 is too small for $\beta = 2.2$.

To make sure we have calculated the $c(t)$ of equilibrated chain(2)

Q3: Besides using long trajectory, how to know that the system is in equilibrium?
A3: We need longer trajectory for analyzing data. 3000 $\rightarrow$ 10000.

Theoretical and MC simulation (total steps: 10000) values of and c for given β's.

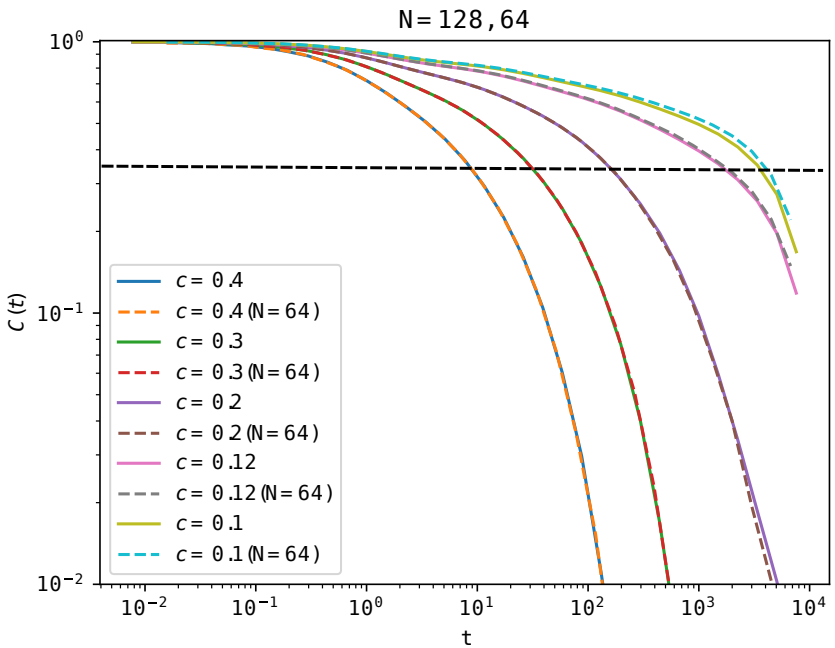
β	c (Theo.)	$c(N=32)$	$c(N=64)$	$c(N=128)$
0.08	0.4800	0.4798	0.4801	0.4799
0.40	0.4013	0.4014	0.4009	0.4012
0.85	0.2994	0.2999	0.2999	0.2998
1.39	0.1994	0.1983	0.2006	0.1993
2.00	0.1192	0.1117	0.1194	0.1214
2.20	0.0997	0.1074	0.0981	0.1030

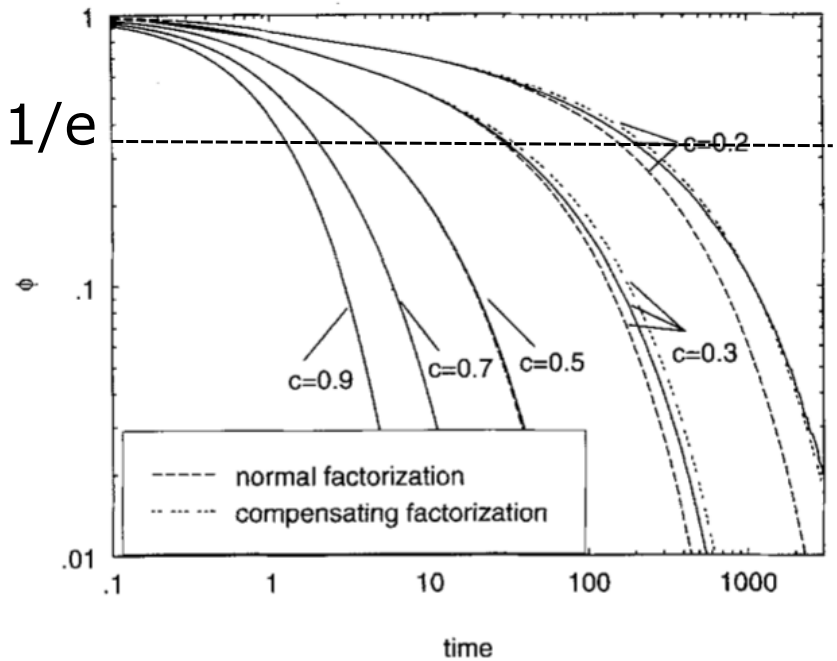
Conclusion: The total steps (10000) is large enough for high β (eg.,$\beta = 2.2$)!

MC Move Scheme for 1-dimensional East model

- N randomly chosen sites update one by one. Each update is labeled by index (time) i, $i = 1, 2, \cdots$. At each step i, we record the configuration.
- We only calculated the correlation function at the time (i) in the set $\{1, 2, 3, 5, 7, 11, 17, 25, 38, \cdots\}$, $\mathrm{INT}((3/2)^n)$, for $n = 0, 1, 2, 3, \cdots$. Therefore, the data of $C(t)$: $C(0), C(1), C(2), C(3), C(5), C(7), \cdots$.

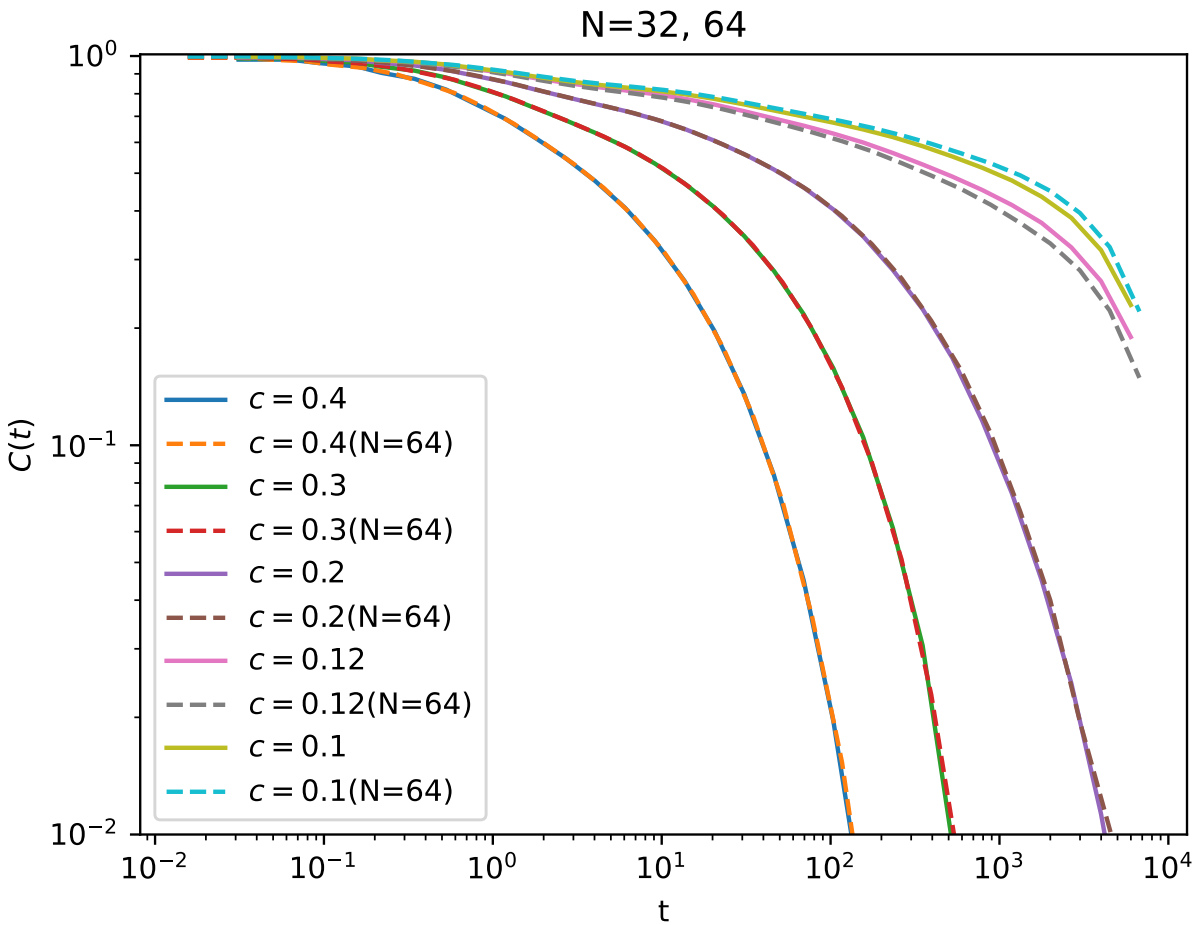
$C(t)$ for 1-dimensional East model





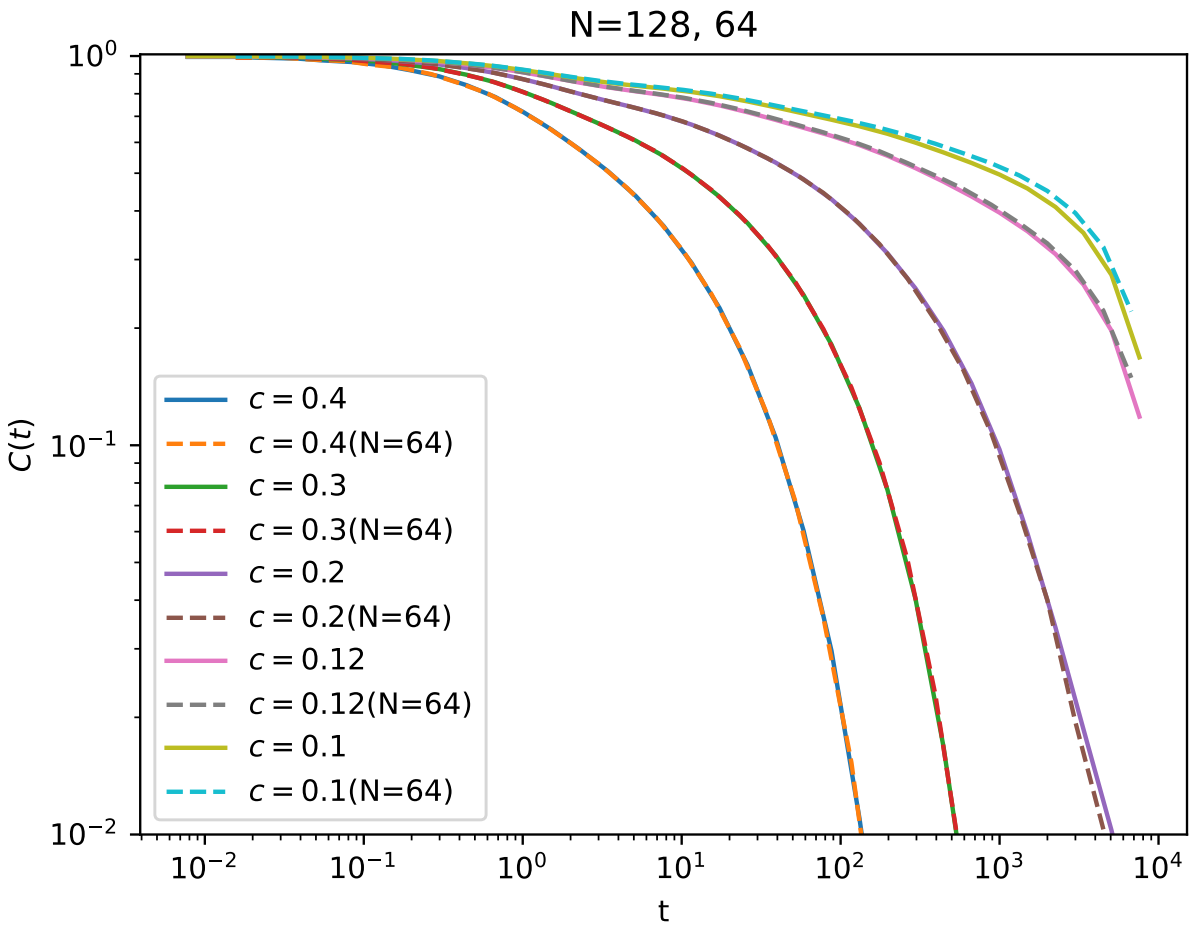
$C(t)$ from MC simulations of finite 1D East model (PBC) and from **Eisinger and Jaeckle (1993)** (semi-infinite chain).

$C(t)$ for 1-dimensional East model



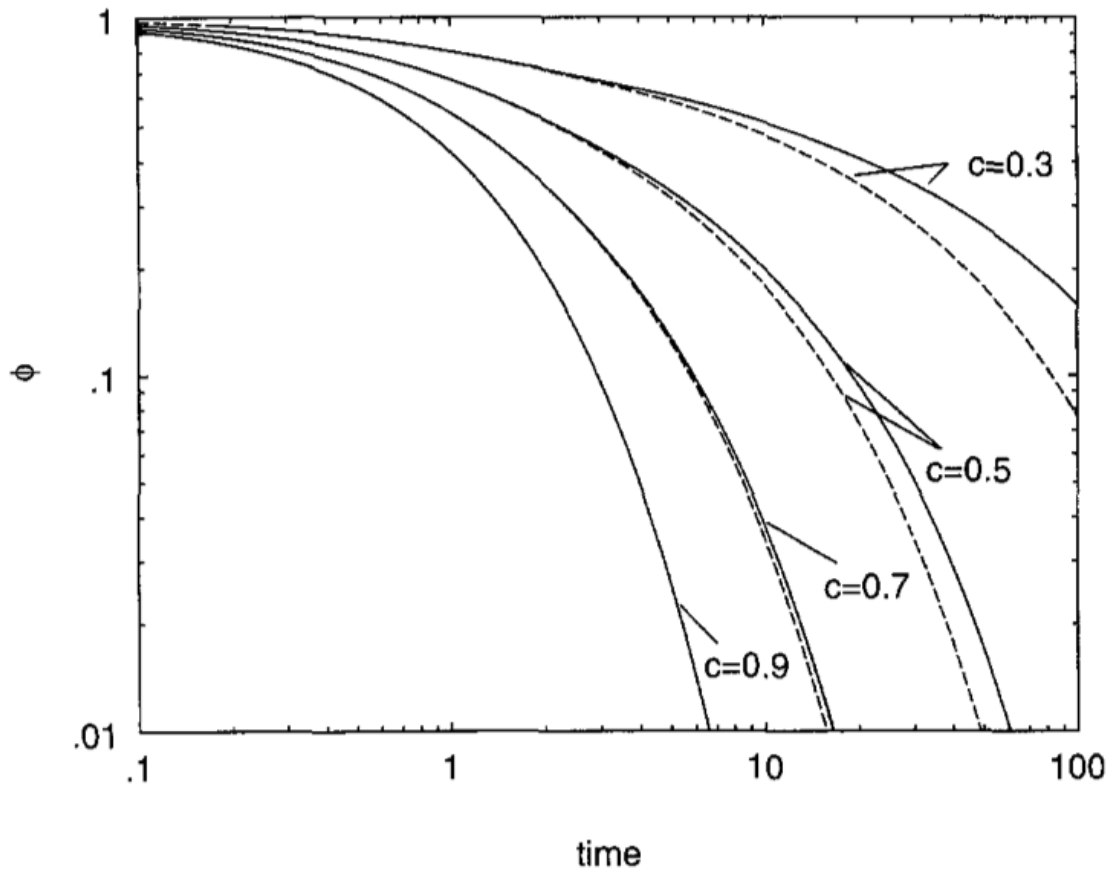
Compare $C(t)$ of $N = 32$ and 64 for different concentrations c. From MC simulations of finite 1D East model (PBC).

$C(t)$ for 1-dimensional East model



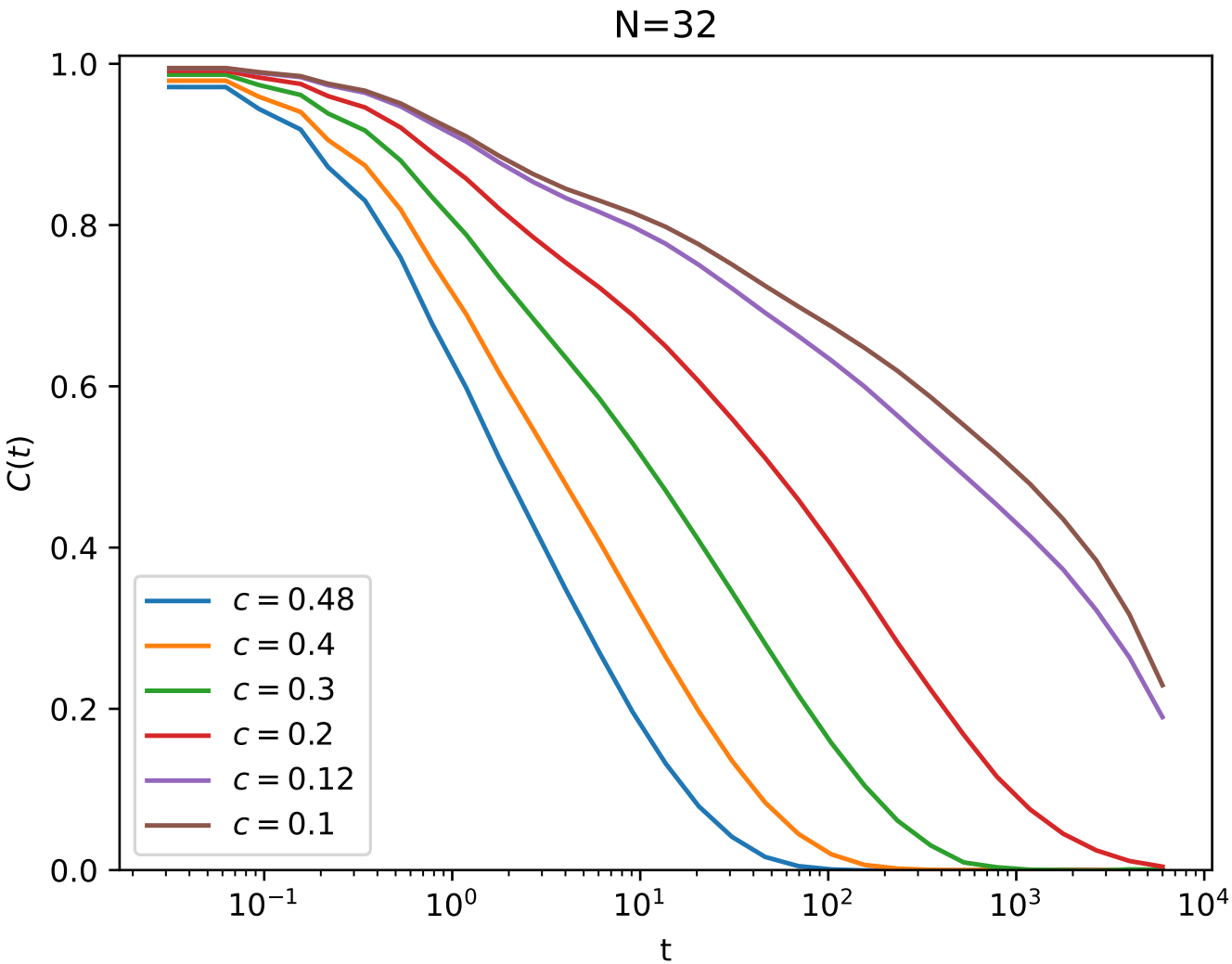
Compare $C(t)$ of $N = 64$ and 128 for different concentrations c. From MC simulations of finite 1D East model (PBC).

Exact $C(t)$ for 1-dimensional East model



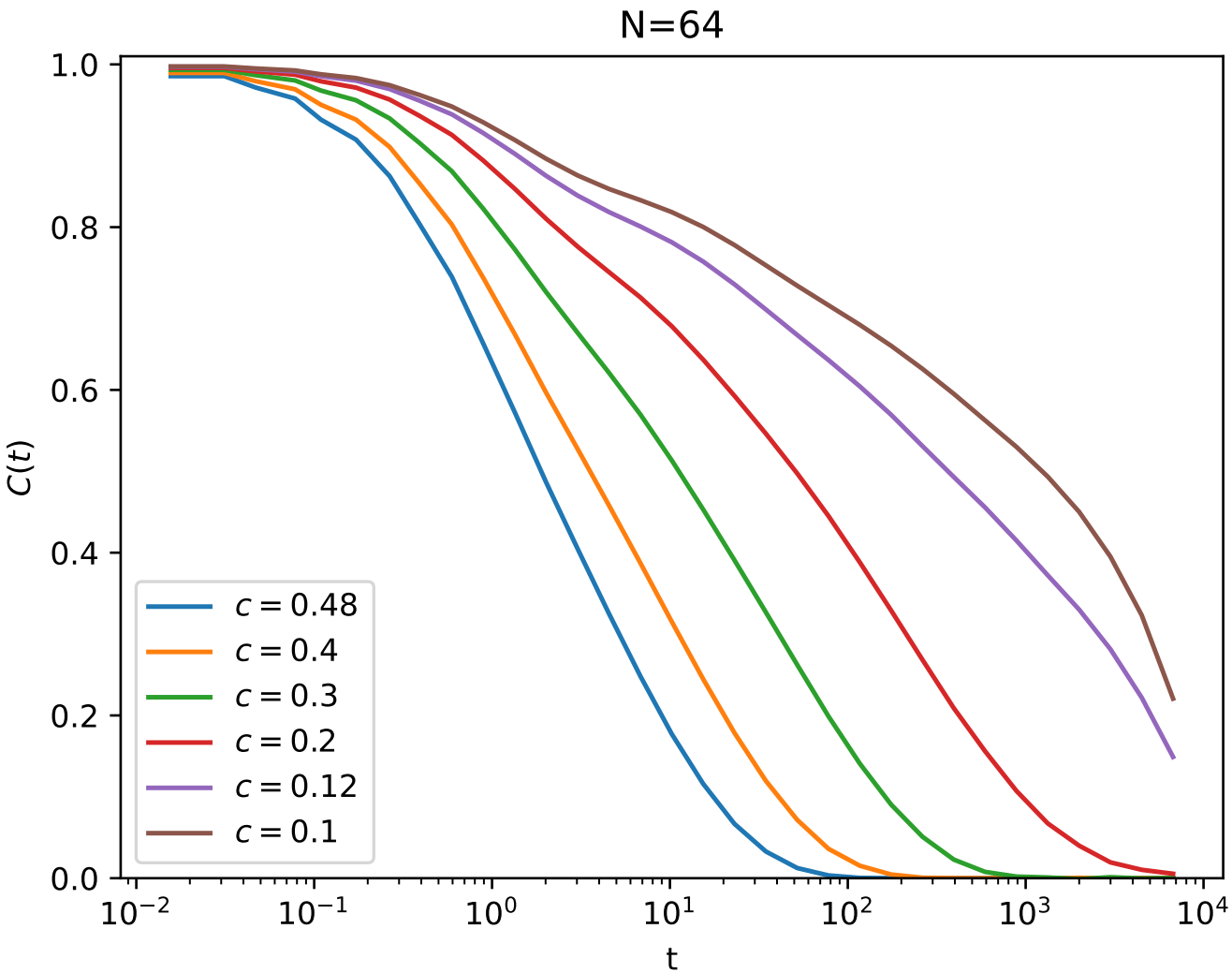
Exact $C(t)$ (solid lines) from **numerical results** for finite chains (**Eisinger and Jaeckle, 1991**).

β-dependence of $C(t)$ (semi-log plot)



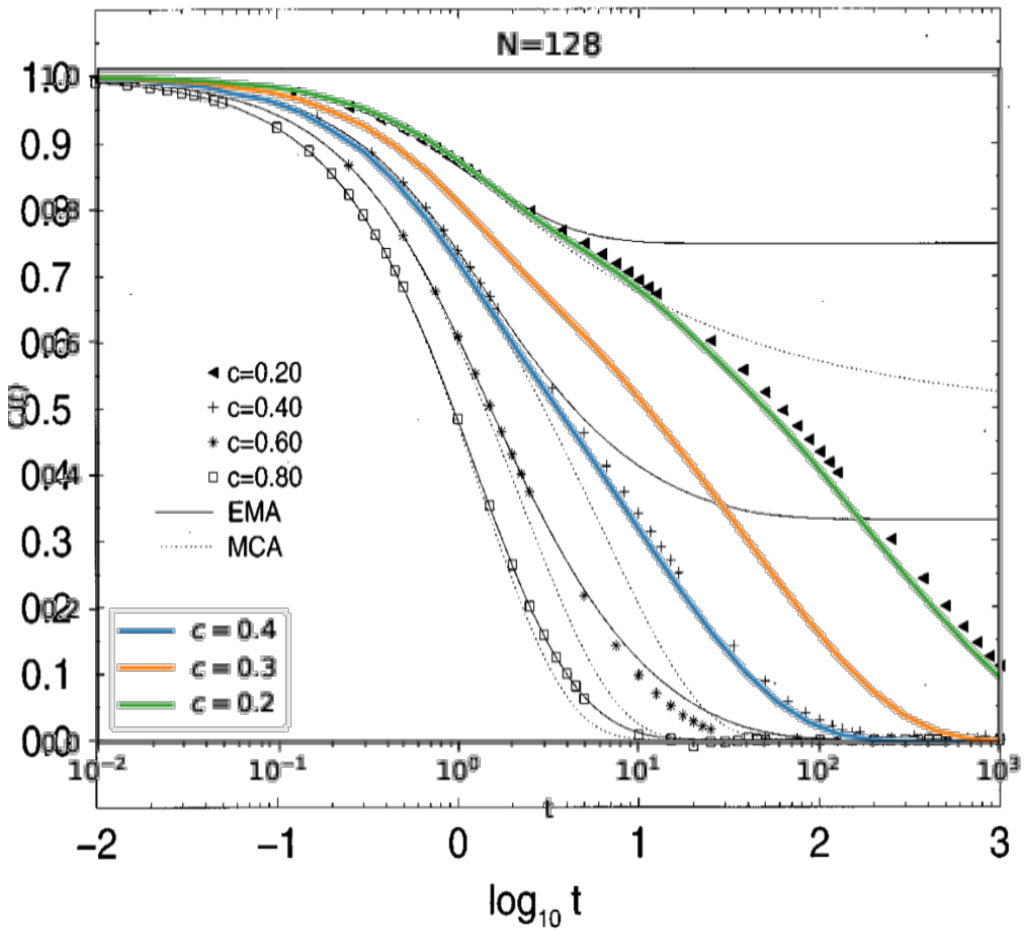
t-dependence and β-dependence of $C(t)$

β-dependence of $C(t)$ (semi-log plot)



t-dependence and β-dependence of $C(t)$

β-dependence of $C(t)$ (semi-log plot)



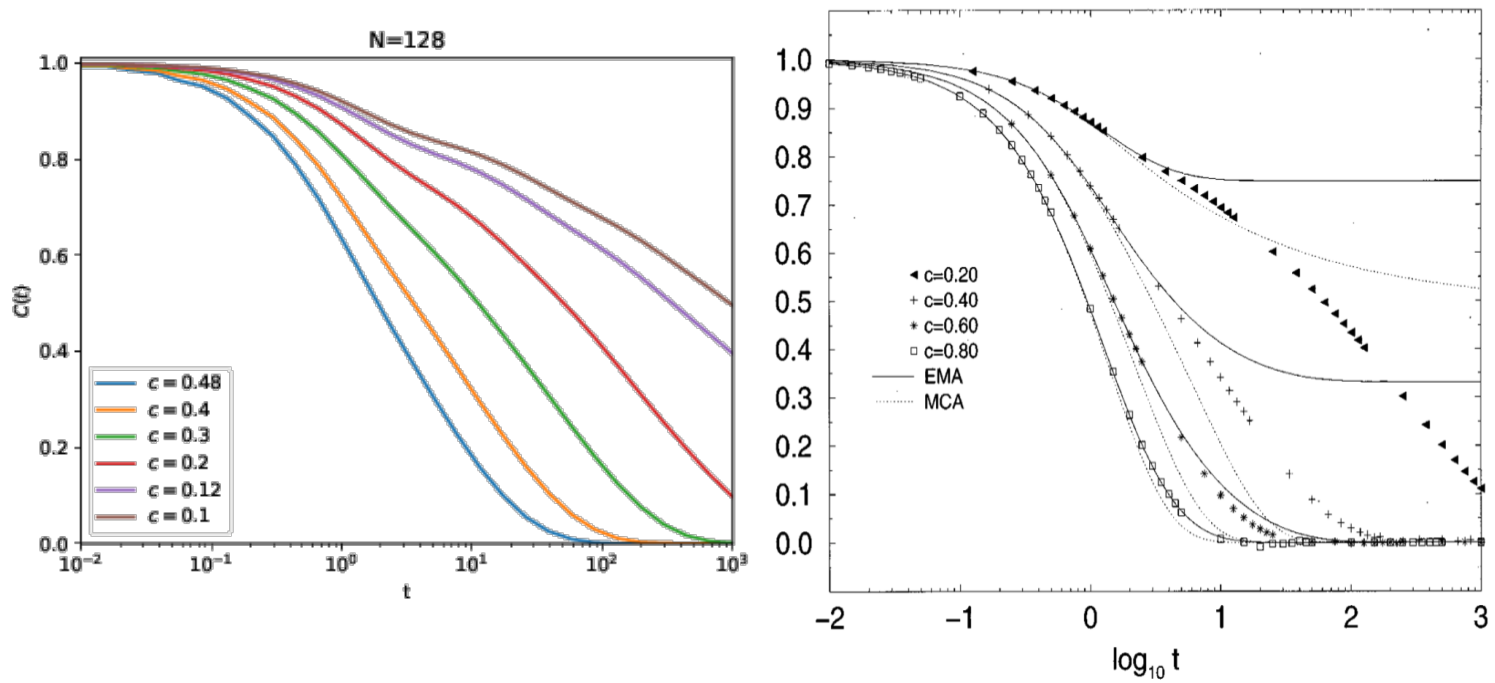
$C(t)$ for $c = 0.2$(green) and $c = 0.4$(blue) in our simulations are agree with the simulation results in **Pitts, Young and Andersen,2000**.

$\rightarrow$ For $c < 0.5$, our MC simulations are correct!
Question: Why we can not generate $c > 0.5$ in the MC simulations?

β-dependence of $C(t)$ (semi-log plot): Test 1

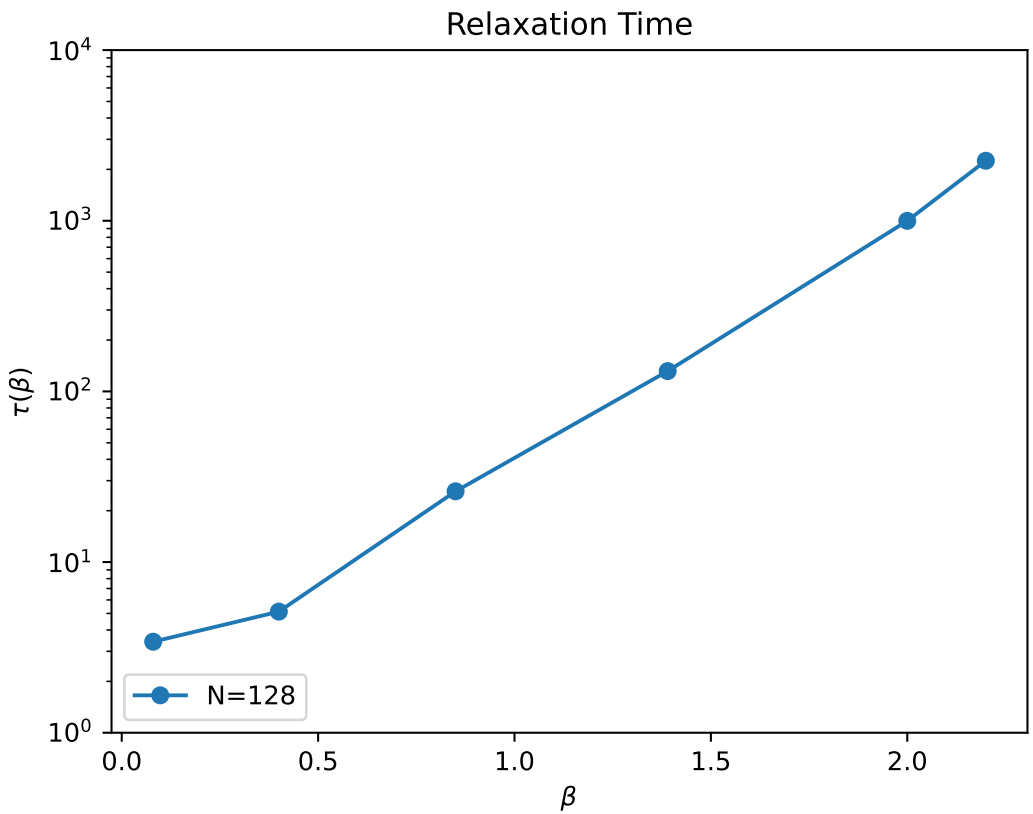
J-E (EMA) theory provides an excellent fit to the data at higher c and **fits short time data well at lower** c's, but ultimately fails because the EMA correlator dost not decay to 0 for $c < 0.5$

Kawasaki (MCA) theory is less accurate at all c's, predicting relaxation that is **too rapid at short times** at all c's and then predicting **a failure to relax to 0 at long times for low** c**'s**. (**Pitts, Young, and Andersen,2000**)



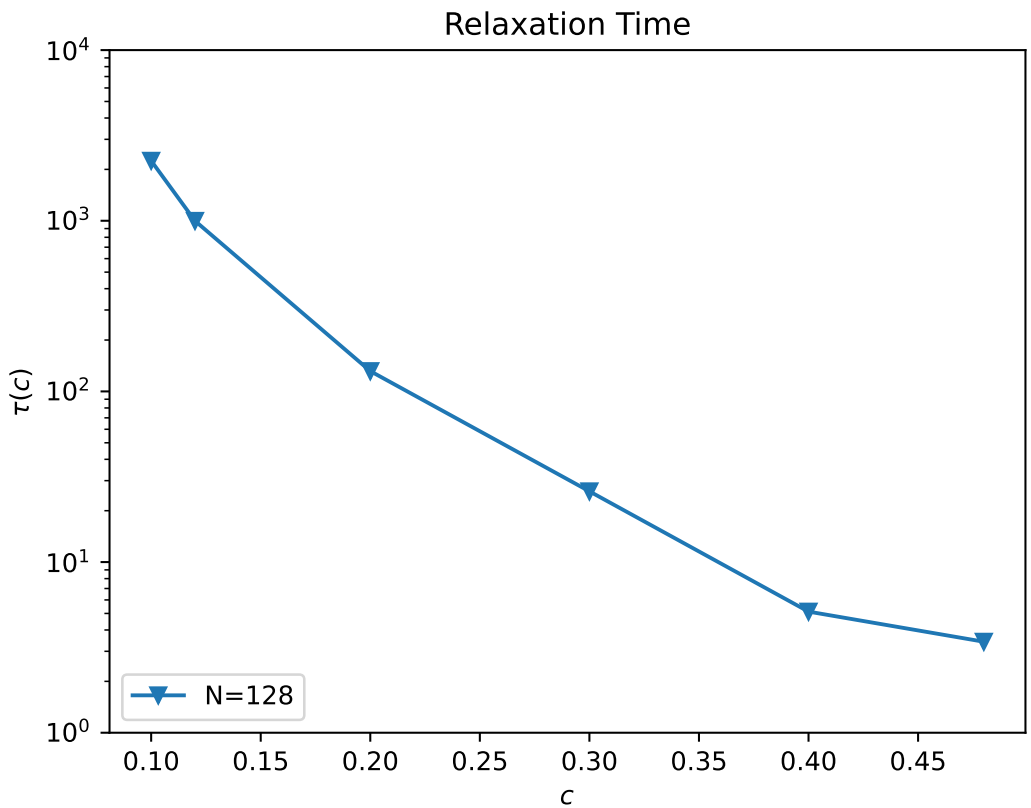
(Left) $C(t)$ for different c's in our simulations and (Right) the simulation results in **Pitts, Young and Andersen,2000**, **EJ** (solid), and **Kawasaki** (dotted).

β-dependence of relaxation time τ



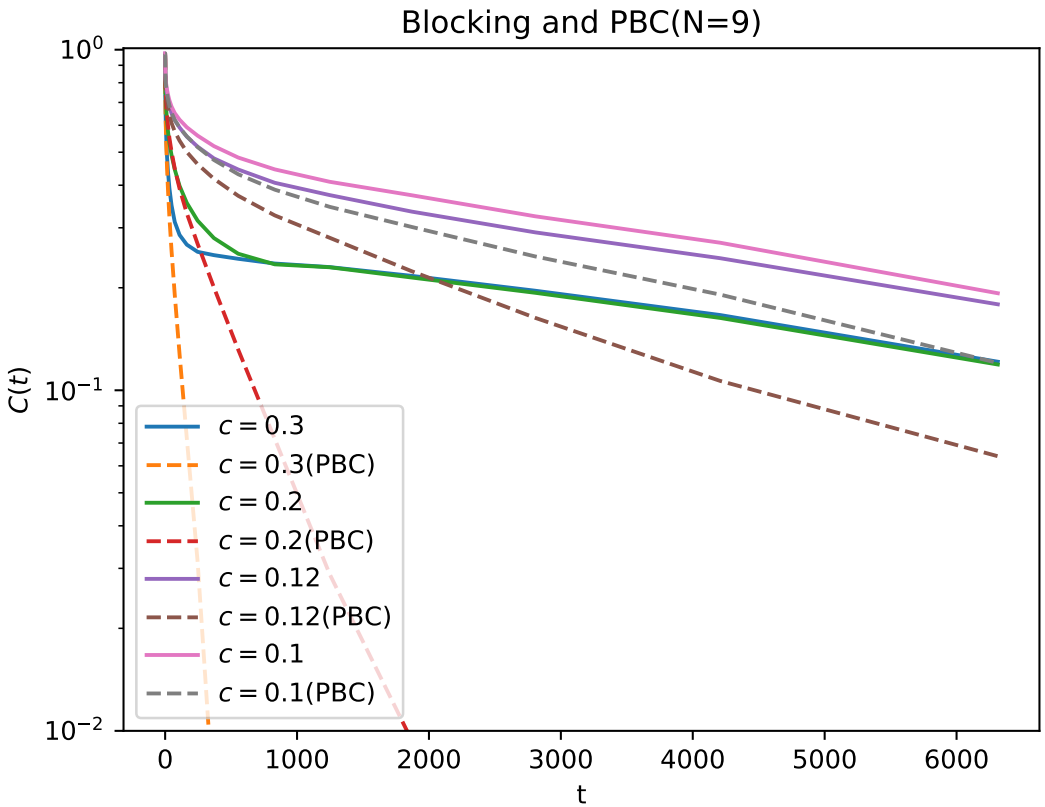
β-dependence of $C(t)$. $N = 128$.

c-dependence of relaxation time τ



c-dependence of $C(t)$. $N = 128$.

For $C(t)$: Test the program



The relaxation of $C(t)$ for 1D East chain with blocking boundary ($N = 9$) is slower than that with PBC. While, $C(500) = 0.06$ in **Jaeckle1991**. We get different values $C(500) = 0.25$, Why? (Here we use $N = 9$ for this blocking boundary. The result also different from that in **Jaeckle1991**.)

Concepts: Definition of the East model

- There are no static interactions between spins, but there is an energy difference between the spin up and spin down states for each spin: $\Delta E = E_1 - E_{-1}$.
- The energy difference $\Delta E/T$ determines c (c is the equilibrium concentration of up spins at any temperature). ΔE is a constant in the East model, so the energy difference can be written as $1/T$, or β.
- β is the ratio of energy difference $\Delta E = 1$ and $k_B T = T$.
- The thermodynamic state is specified by a single state variable c.
- c is also the probability that any particular spin is up.

Concepts: Facilitating set

- In each model, for each site i there is a set of f neighboring sites $S(i)$ s.t. the spin on site i can flip only if all the spins on the sites $S(i)$ are up.
- **Facilitating set** $S(i)$ of site i for the East model: spin $i+1$.

A simplifying case

Definitions:

- The **state** Γ of a system of N spins is specified by $n_1, \cdots, n_N$;
- The possible transitions of the system are those in which a single spin flips;
- The flip rate for spin i depends on the state of spin $i+1$.

Assumptions:

- The spins are statistically independent at equilibrium;
- All **sites** have the **same distribution function** for the occupation number, ie, $\forall i, t = \infty, p(n_i = 0) = 1 - c, p(n_i = 1) = c$;
- $\rho_0(\Gamma) = \prod_{i=1}^{N} p(n_i)$.

For $C(t)$:

- $\phi(t) = \frac{\langle \delta n_i(t) \delta n_i(0) \rangle}{c(1-c)}$ (**Eisinger and Jaeckle, 1991**, where $\sigma_i = \pm 1$).
- $C(t) = \frac{\langle \delta n_i(t) \delta n_i(0) \rangle}{\langle \delta n_i(0)^2 \rangle}$. What is the difference between $C(t)$ and $\phi(t)$?
  $C(t) = \phi(t)$. ($n_i = 0$ or 1)
- $C(t)$ can also be written as $\frac{P(s_i(t=1)|s_i(t=1)) - c}{1-c}$.
- $c = \langle n_i \rangle = 0.9, 0.8$ (CHECK THIS PROBLEM! ?)
- At low T, c is small (**Sollich 2003**).
- For $N \to \infty$, all boundary conditions (free BC, blocking BC (**JCP, 113,8671**) and PBC) gives the **same** result of $C(t)$! (**Pitts, Young, Andersen, 2000, JCP, 113,8671**)

The up-spin persistence function $P_1(t)$

- In $[0, t]$, s_{i-1} has been up a fraction m of the time, and the evolution of s_i has been that (evolution) of a single spin over time mt.
- $P(m, t)$: The distribution of m for a given t by $P(m; t)$. What's does $P(m, t)$ mean? A: There are two possible answers. **(1)** Perform one MC simulation, spin s_{i-1}, $i = 0, \cdots, N-1$, has been up m_i times. The distribution of m_i is $P_{\text{space}}(m; t)$; **(2)** Perform X times simulations, for site i, the spin s_{i-1} have m_x times up state. The distribution of m_x is $P_{\text{time}}(m; t)$. (**Sollich 2003**).
- **Question**: Is the $P_{\text{time}}(m; t)$ identical to $P_{\text{space}}(m; t)$? Answer and prove.

Theoretical object: to derive an equation of $C(t)$ (kinetic theory of $C(t)$)

In general,

$$\frac{dC(t)}{dt} + \omega C(t) + \omega^{-1} \int_0^t d\tau M^{\text{irr}}(t-\tau)\frac{dC(\tau)}{d\tau} = 0, \tag{5}$$

where $\omega = k(0)$, $k(t) = -\frac{dC(t)}{dt}$, M^{irr} is irreducible memory function. (**Pitts, Andersen 2000**)
In MCT, assume that

$$M^{\text{irr}}(t) = \sum_n a_n(c)[C(t)]^n. \tag{6}$$

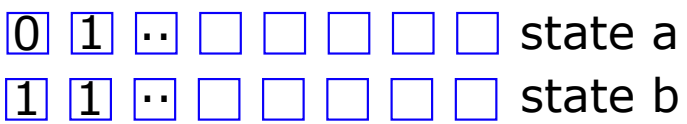
Some approximations:

- $M^{\text{irr}}_{\text{K}}(t) = c(1-c)[C(t)]^2$ (**Kawasaki1995**)
- $M^{\text{irr}}_{\text{EJ}}(t) = c(1-c)C(t)$ (**Eisinger and Jaeckle 1993**)
- diagrammatic representations of the irreducible memory function $\rightarrow$ obtained the irreducible memory kernel from a set of irreducible diagrams: $M^{\text{irr}} = c(1-c)C(t)$ for $(c < 0.5)$ (**Pitts, Young, Andersen, J. Chem. Phys. 2000, 113, 8671**) (**Pitts and Andersen, 2001**)
- A matrix formalism defined in the complete dynamic phase space (**Wu, Cao, J. Phys. Chem. B 2004, 108, 6796**).

More about $C(t)$: Detailed balance

Let the state $\alpha = (s_1, s_2, \cdots, s_N)$. In equilibrium, $\frac{\partial P_\alpha(t)}{\partial t} = 0 \Rightarrow P_\alpha(t) W_{\alpha\to\beta} = P_\beta(t) W_{\beta\to\alpha}$, where

- $P_\alpha(t)$ is the probability of the chain being in state α.
- From detailed balance, $W_{a\to b} = e^{-\beta}$; $W_{b\to a} = 1 \Rightarrow$ $P_b(t)/P_a(t) = e^{-\beta}$ (see Figure).



Two states of the 1-D finite East model with N sites.

More about $C(t)$: Detailed balance condition (In general)

We now restrict attention to systems for which there is a stationary distribution function $\rho_0(\Gamma)$ s.t. the transition probabilities obey the DBC (**Pitts and Andersen, 2001**):

$$W(\Gamma', \Gamma)\rho_0(\Gamma) = W(\Gamma, \Gamma')\rho_0(\Gamma'). \tag{7}$$