Auto-correlations of spins in 1D East Model

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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:

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

$\langle \cdots \rangle$: 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 (Theory)	$c(N = 64)$	$c(N = 128)$	$c(N = 256)$
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

The values of c obtained by the MC simulation are too large at high β.
$\leftarrow$ The system does not in equilibrium when the configurations are recorded.

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

To make sure the system is in equilibrium, We set

$$\text{total steps} = \text{INT}[N_{\text{step}}(1+\beta)^2], (\beta > 0) \tag{4}$$

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 (Theory)	$c(N = 64)$
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

As β increase, we need longer trajectory (more samples) to make sure the c from simulated data.

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

Besides producing long trajectory, we use longer trajectory for analyzing data: 3000 $\rightarrow$ 10000.

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

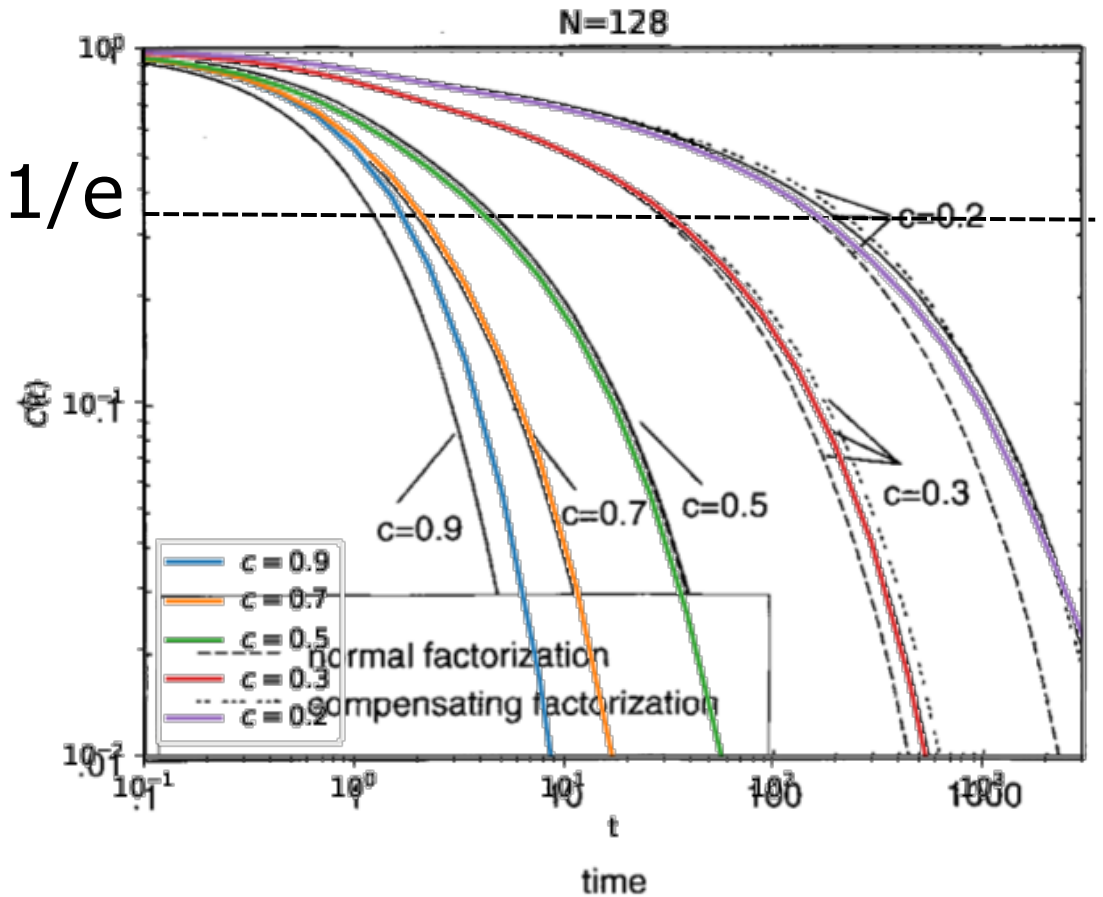
β	c (Theo.)	$c(N = 32)$	$c(N = 64)$	$c(N = 128)$
0.08	0.4800	0.4798	0.4801	0.4799
0.40	0.4013	0.4014	0.4009	0.4012
0.85	0.2994	0.2999	0.2999	0.2998
1.39	0.1994	0.1983	0.2006	0.1993
2.00	0.1192	0.1117	0.1194	0.1214
2.20	0.0997	0.1074	0.0981	0.1030

The total steps (10000) is large enough for high β (eg.,$\beta = 2.2$)! Therefore, the trajectories are from system in equilibrium.

MC Move Scheme for 1-dimensional East model

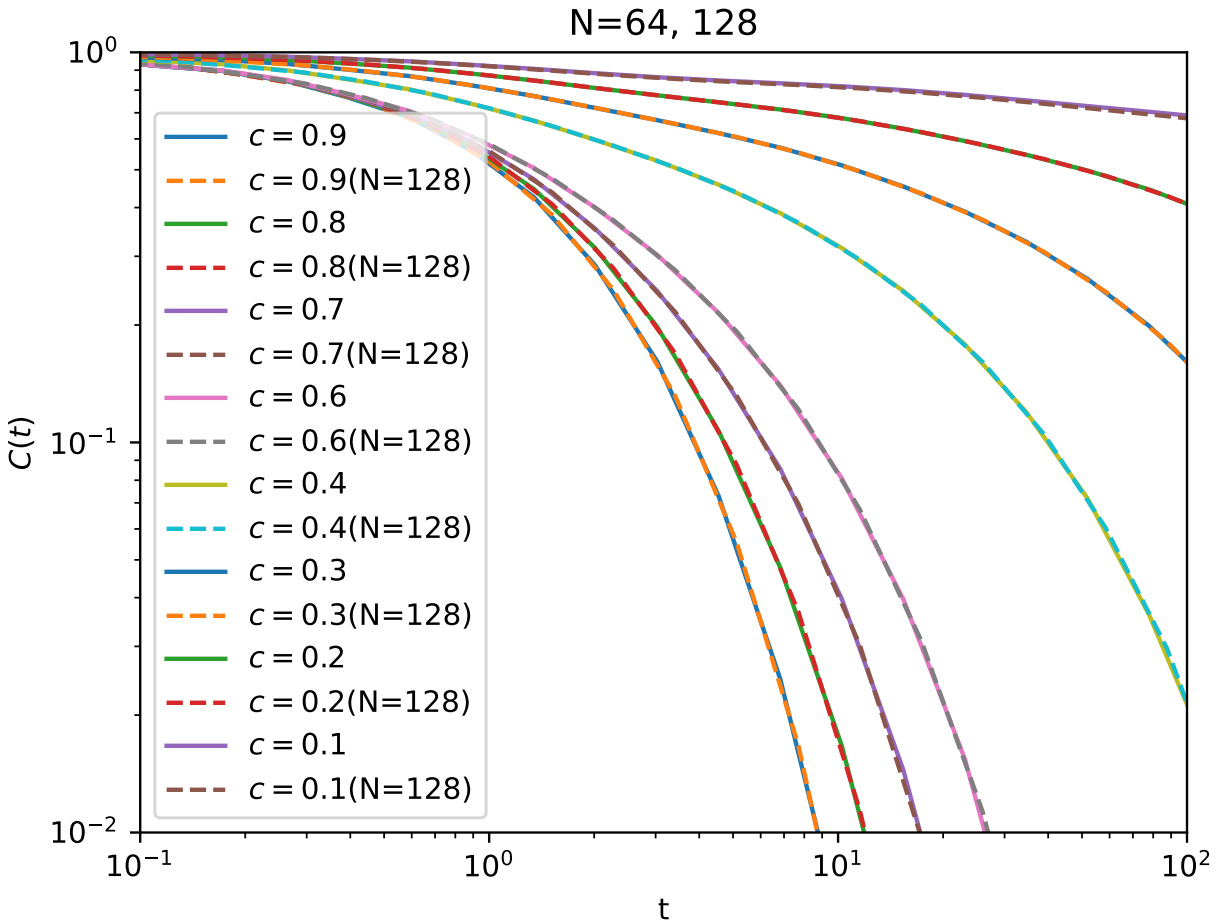
- N randomly chosen sites update one by one. Each update is labeled by index (time) i, $i = 1, 2, \cdots$. At each step i, we record the configuration.
- We only calculated the correlation function at the time (i) in the set $\{1, 2, 3, 5, 7, 11, 17, 25, 38, \cdots\}$, $\mathrm{INT}((3/2)^n)$, for $n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



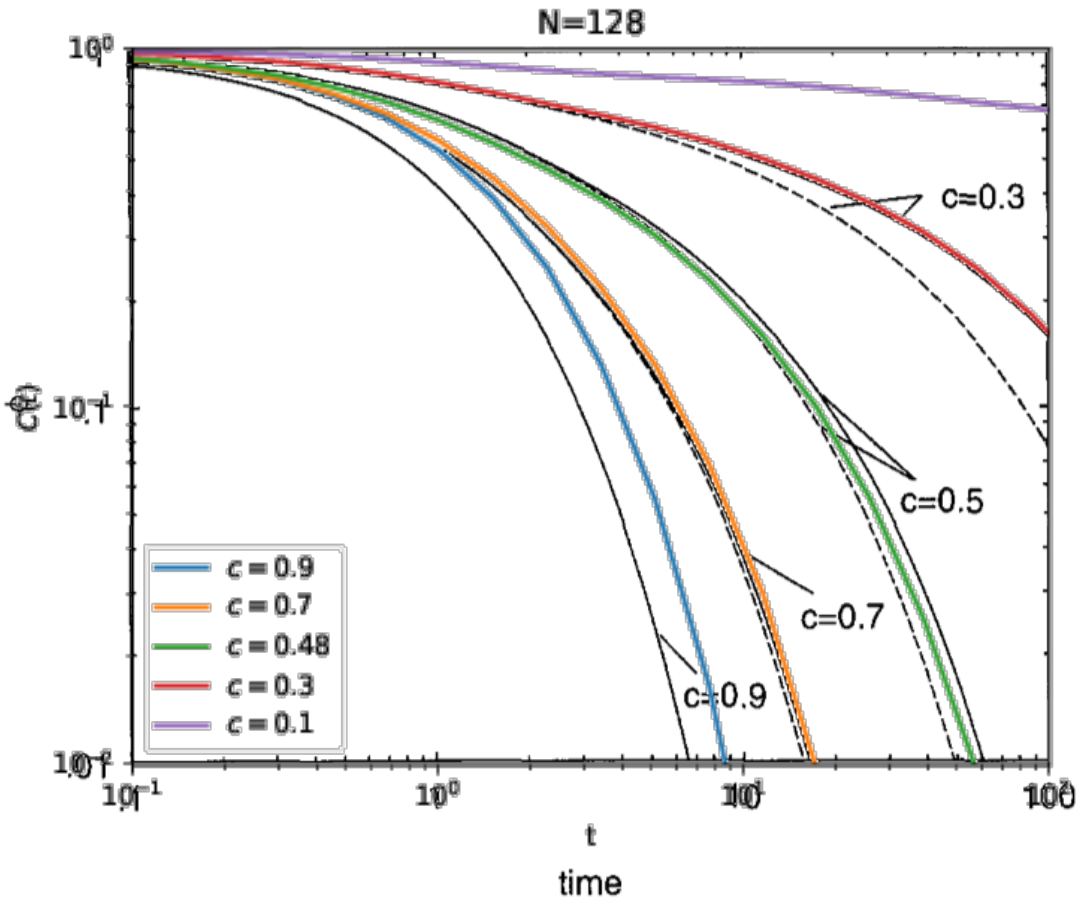
$C(t)$ from MC simulations of finite 1D East model (PBC) and from **Eisinger and Jaeckle (1993)** (semi-infinite chain).

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



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

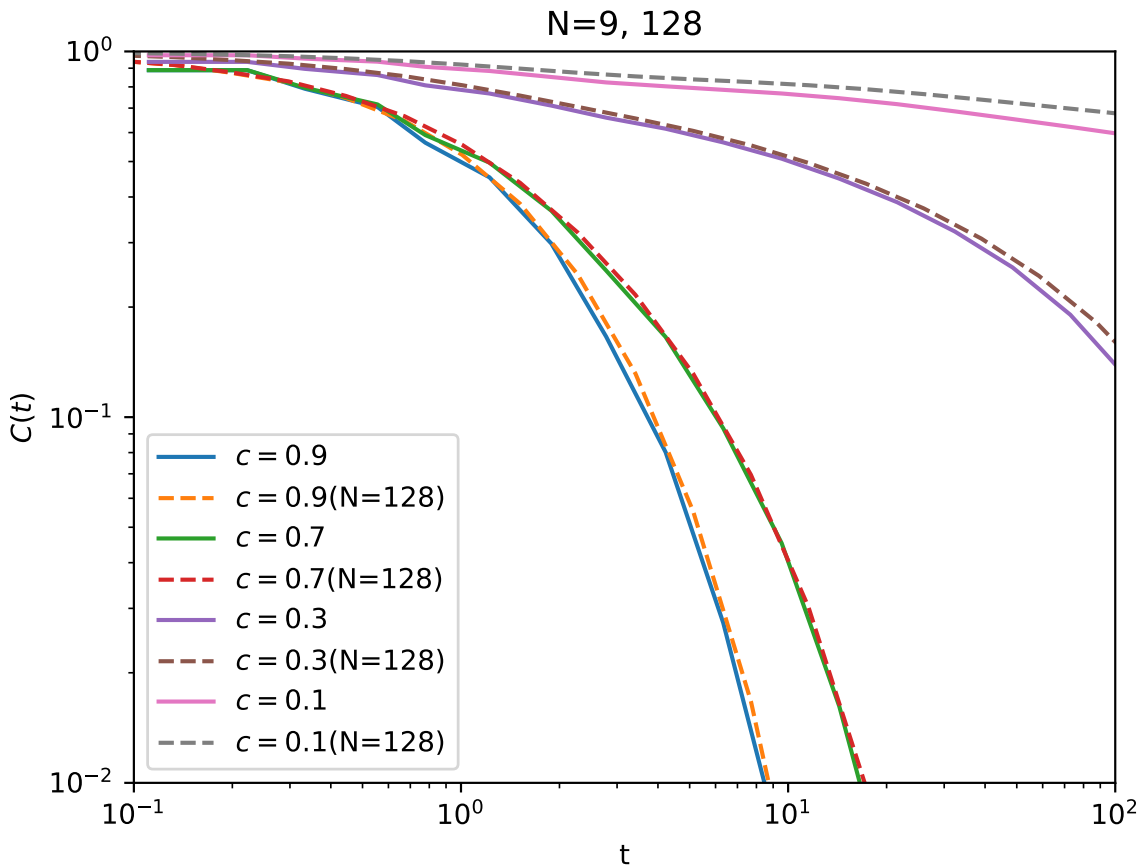
$C(t)$ for 1-dimensional East model: Ours v.s. Eisinger-Jackle(1991)



Our simulation results (color solid lines) of $C(t)$ for c= 0.3, 0.5, 0.7, 0.9, and the exact $C(t)$ (black solid lines) from **numerical results** for finite chains (**Eisinger and Jaeckle, 1991**).

For $c = 0.9$, our simulation result is different from that of Eisinger-Jackle's numerical result.

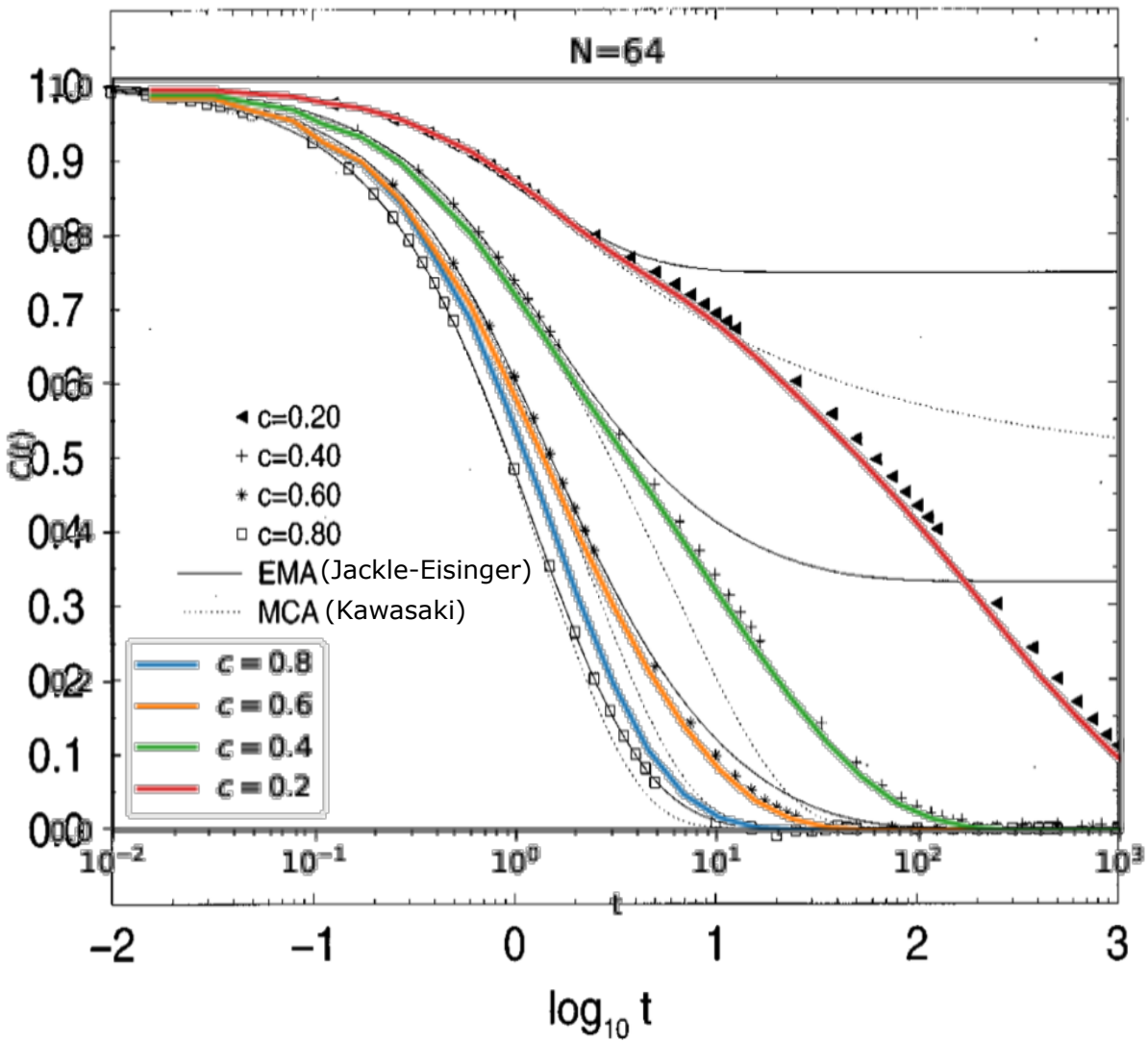
The difference of $C(t)$ for $c = 0.9$ comes from the finite size?



$C(t)$ of $N = 9$ decays faster than that of $N = 128$, but they are close when c is 0.9.

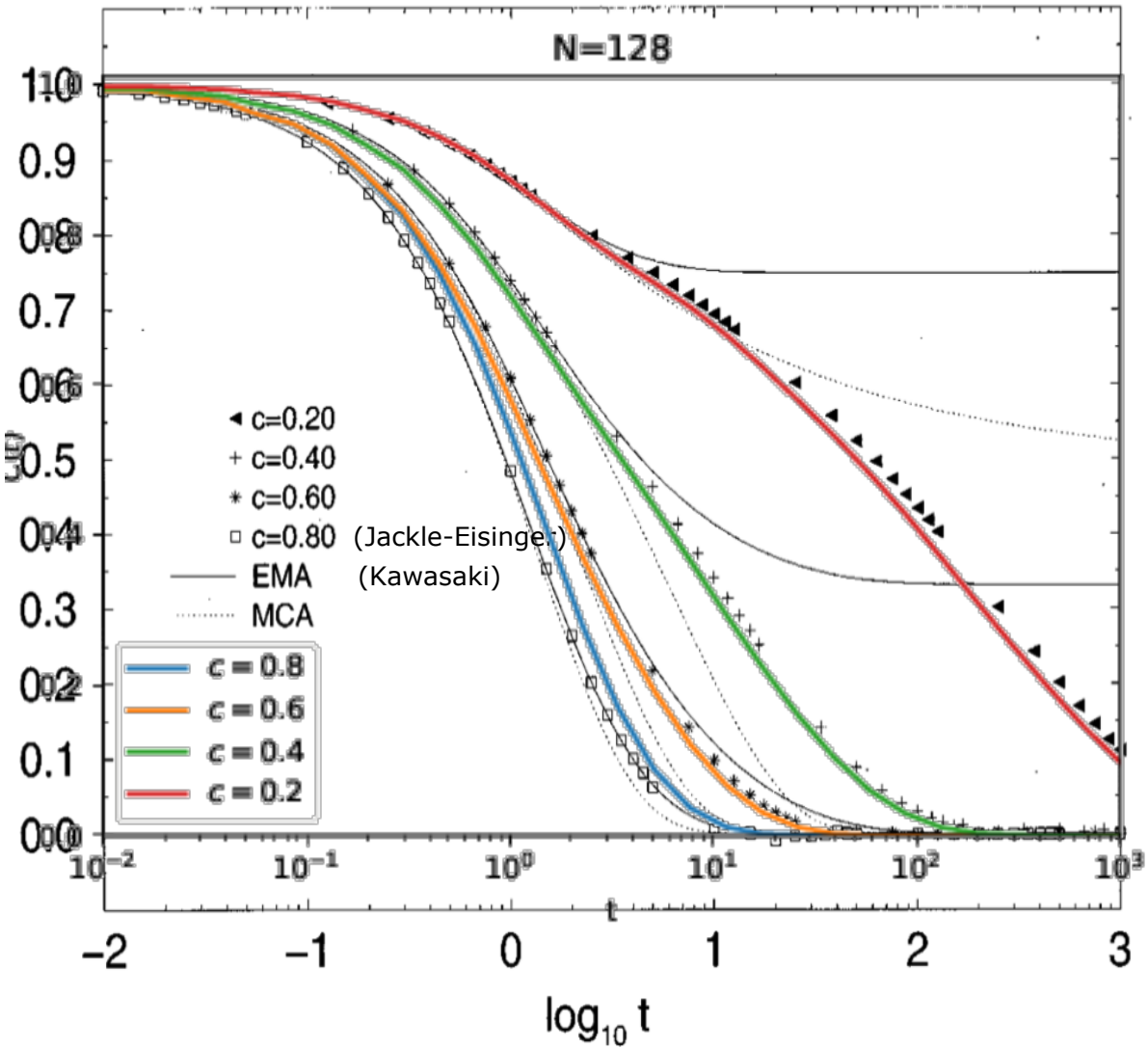
Therefore, the difference between ours and Eisinger-Jackle1991's simulation results does not come from the different of size N.

β-dependence of $C(t)$ (N=64)



$C(t)$ for $c = 0.2$(red), $c = 0.4$(green), $c = 0.6$ (orange) and $c = 0.8$ (blue?) in our simulations are agree with the simulation results in **Pitts, Young and Andersen,2000**.

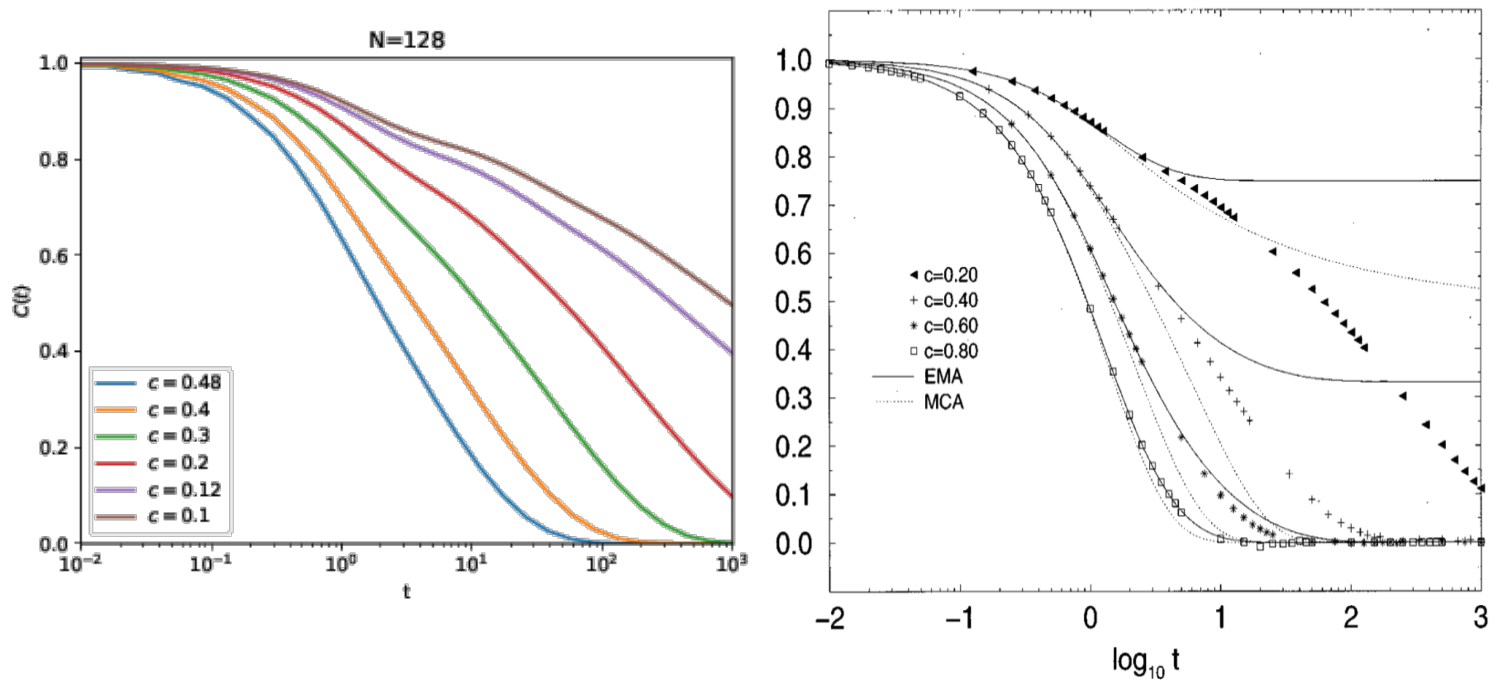
β-dependence of $C(t)$ (N=128)



$C(t)$ for $c = 0.2$(red), $c = 0.4$(green), $c = 0.6$ (orange) and $c = 0.8$ (blue) in our simulations are agree with the simulation results in **Pitts, Young and Andersen,2000**.

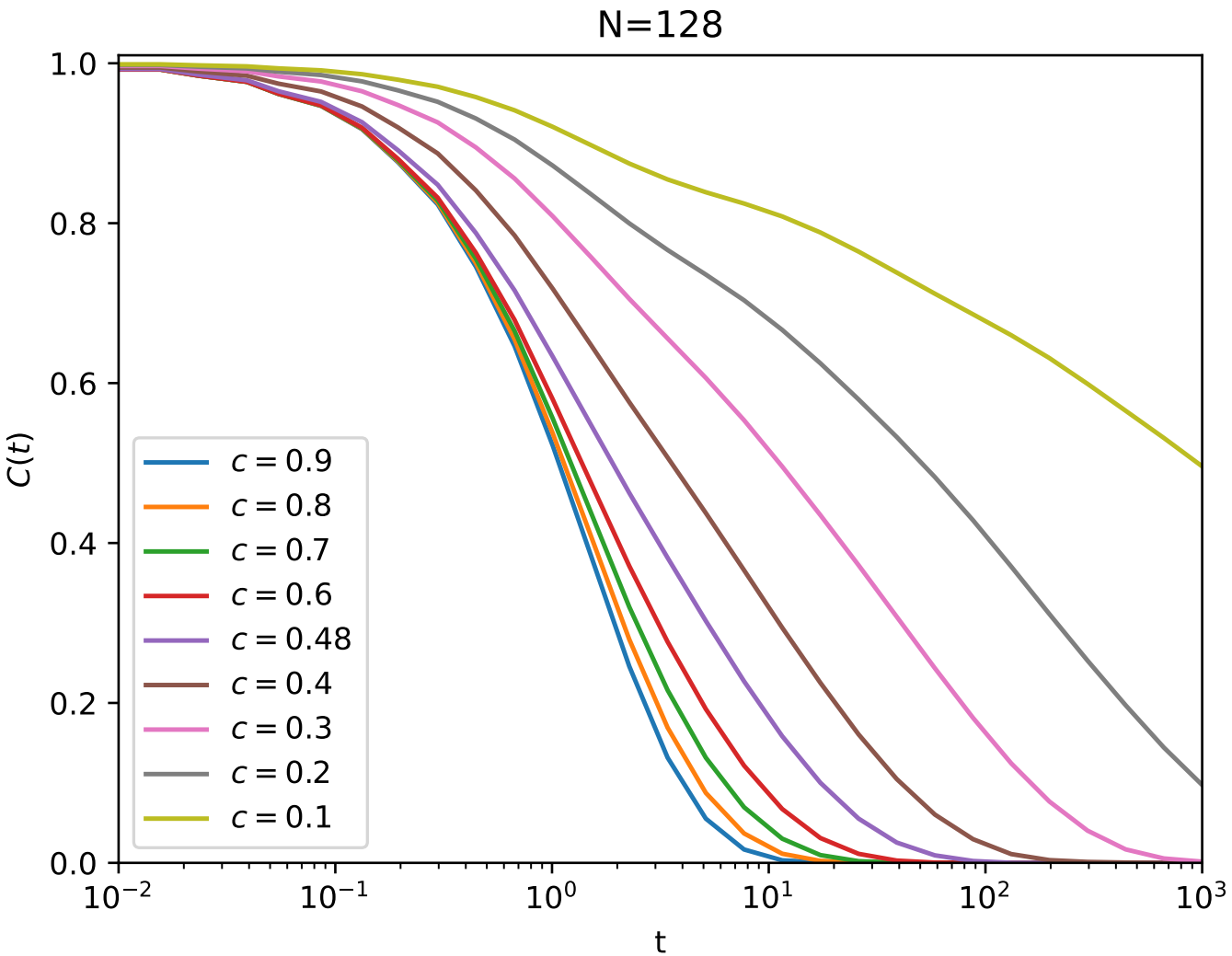
β-dependence of $C(t)$

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**)



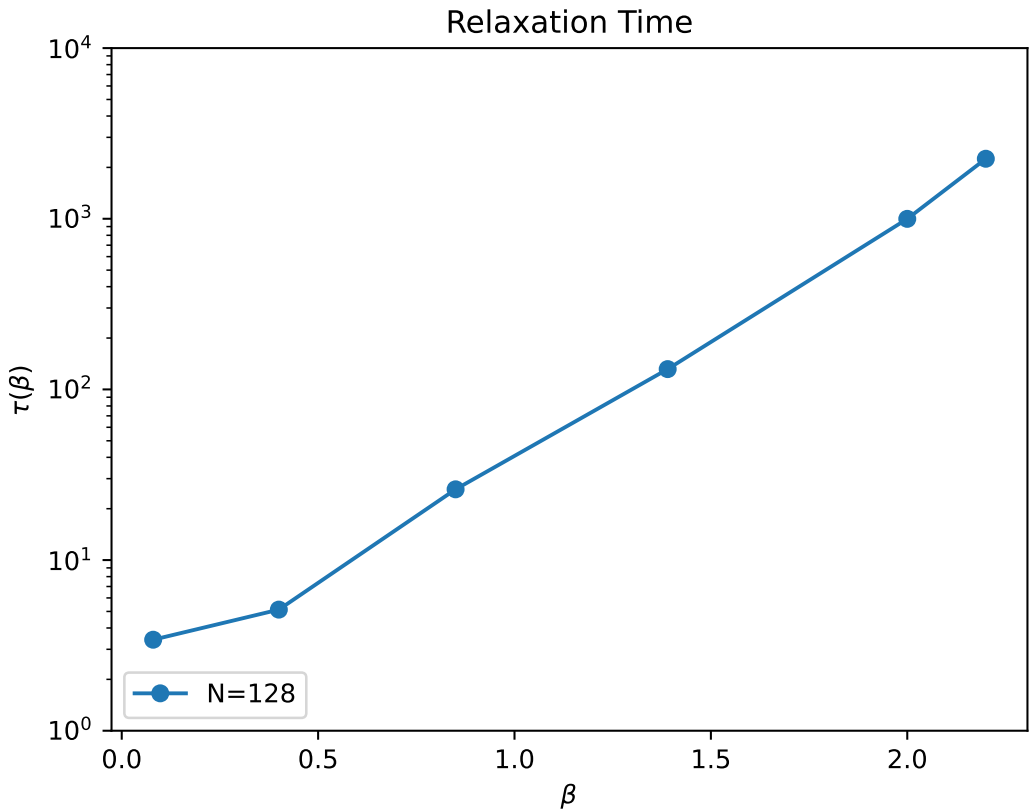
(Left) $C(t)$ for different c's in our simulations and (Right) the simulation results in **Pitts, Young and Andersen,2000**, **EJ** (solid), and **Kawasaki** (dotted).

β-dependence of $C(t)$: Simulation results



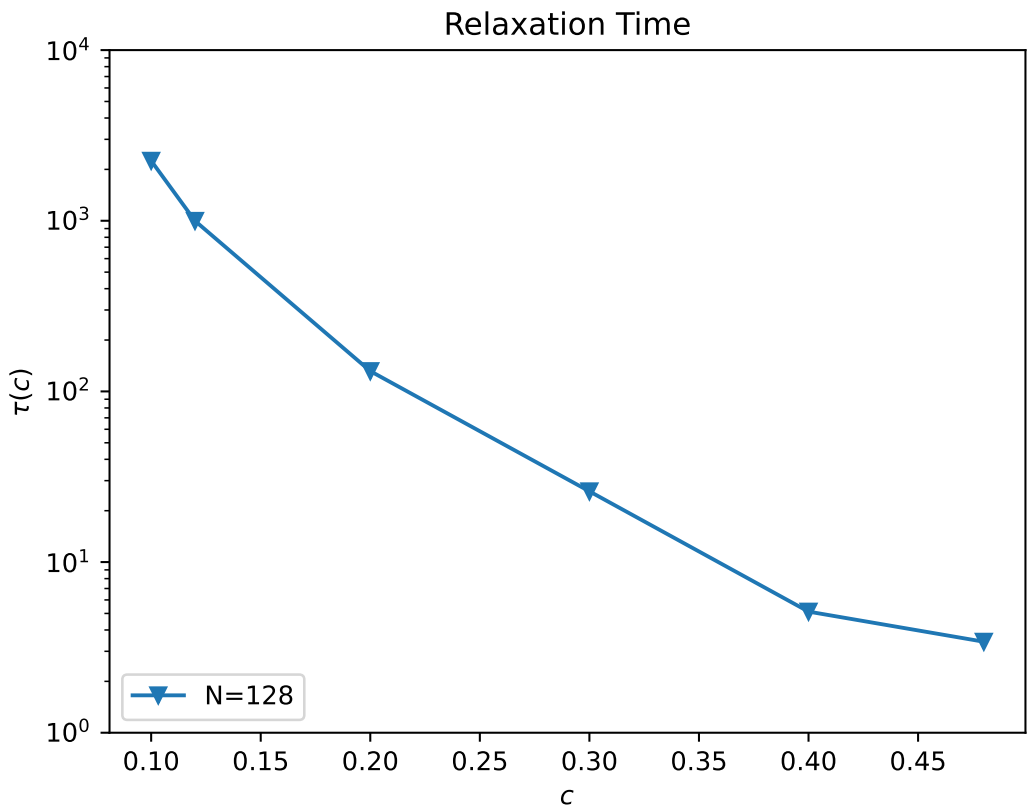
$C(t)$ for different c's in our simulations.

β-dependence of relaxation time τ



β-dependence of $C(t)$. $N = 128$.

c-dependence of relaxation time τ



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

1(1) 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.

1 (2) $C(t)$:

- $\phi(t) = \frac{\langle \delta n_i(t) \delta n_i(0) \rangle}{c(1-c)}$ (**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 relation between $C(t)$ and $\phi(t)$?

$$C(t) = \frac{\langle \delta n_i(t) \delta n_i(0) \rangle}{\langle \delta n_i(0)^2 \rangle} = \frac{\langle n_i(t) n_i(0) \rangle - c^2}{c - c^2} = \frac{\langle \delta n_i(t) \delta n_i(0) \rangle}{c(1-c)}. \quad (5)$$

  $C(t) = \phi(t)$ (Because $n_i = 0$ or 1).
- $C(t)$ can also be written as $\frac{P(s_i(t=1)|s_i(t=1)) - c}{1-c}$.
- $c = \langle n_i \rangle = 0.9, 0.8, \cdots$ is the up spin concentration for the state at **negative temperature**.
- 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**)

1 (3) For $\beta < 0$

For $\beta < 0$, similar to formula 4, we set

$$\text{total steps} = \text{INT}[N_{\text{step}}(1-\beta)^2](\beta < 0), \tag{6}$$

where $N_{\text{step}} = 10000$.
A given spin may only flip if the neighboring spin to the right is up, with an acceptance ratio A,

$$A = \begin{cases} 1, \text{ for } 01 \to 11 \\ e^{\beta}, \text{ for } 11 \to 01. \end{cases} \tag{7}$$

1 (4) For $\beta < 0$, to check if the system reach equilibrium

Q3: Besides using long trajectory, how to know that the system is in equilibrium?
A3: Need longer trajectory for analyzing data: 10000.

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

β	c (Theory)	$c(N = 32)$	$c(N = 64)$	$c(N = 128)$
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
-0.40	**0.5987**	0.5987	0.5987	0.5985
-0.85	**0.7006**	0.7010	0.7006	0.7005
-1.39	**0.8006**	0.8005	0.8005	0.8006
-2.20	**0.9002**	0.9003	0.9002	**0.9002**

2 (1) For $\beta < 0$, if we sample earlier $\cdots$

To find the reason for not consist correlations at $c = 0.9$, we ask a Question1: For $\beta < 0$, if we sample earlier, will the correlation function decay faster?
For $\beta < 0$, instead of formula 6, we set

$$\text{total steps} = N_{\text{step}} \ (\beta < 0), \tag{8}$$

where $N_{\text{step}} = 10000$.
A given spin may only flip if the neighboring spin to the right is up, with an acceptance ratio A,

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

2 (2) Calculate c

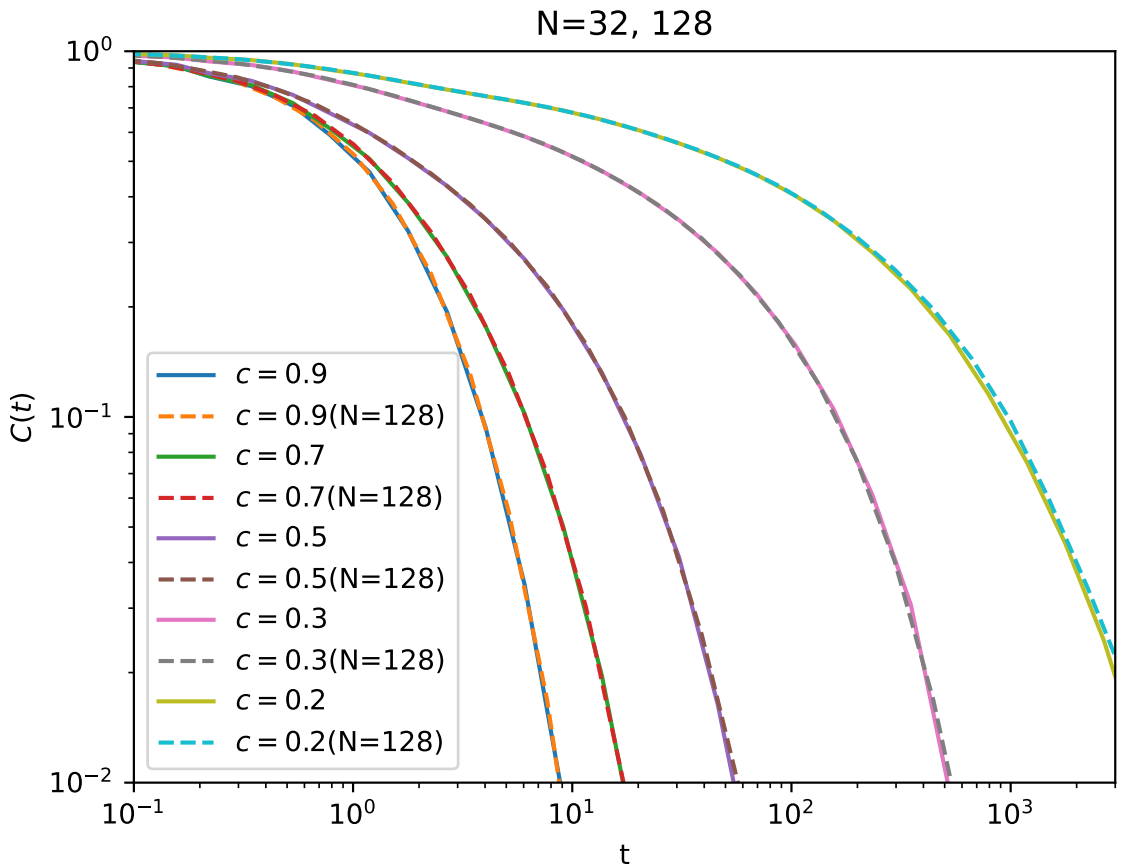
Based on formula 8, we calculated the c for different β's for the model of $N = 32$.

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

β	c (Theory)	$c(N = 32)$
-0.40	**0.5987**	0.5988
-0.85	**0.7006**	0.7006
-1.39	**0.8006**	0.8009
-2.20	**0.9002**	0.9002

Since when $\beta < 0$, system relaxes faster than it at any $\beta > 0$, formula 8 is good.

2 (3) $C(t)$ from formula 8 and 6 is the same.



$C(t)$ of $N = 32$ still does not relax faster (Here, the data $N = 128$ is those calculated from formula 6 for $\beta < 0$.)

Answer1: Because the system is in equilibrium when we record the configurations, for $\beta < 0$, when we sample with formula 8, the correlation function is the same.

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

In general,

$$\frac{dC(t)}{dt} + \omega C(t) + \omega^{-1} \int_0^t d\tau M^{\text{irr}}(t-\tau)\frac{dC(\tau)}{d\tau} = 0, \tag{9}$$

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

$$M^{\text{irr}}(t) = \sum_n a_n(c)[C(t)]^n. \tag{10}$$

Some approximations:

- $M^{\text{irr}}_{\text{K}}(t) = c(1-c)[C(t)]^2$ (**Kawasaki1995**) [**PROBLEM5:** This equation is not consistent in dimension. Check and give the correct form!]
- $M^{\text{irr}}_{\text{EJ}}(t) = c(1-c)C(t)$ (**Eisinger and Jaeckle 1993**) [**PROBLEM5':** This equation is not consistent in dimension. Check and give the correct form!]
- 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**).

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

Problem 3: Derive the dynamical Eq. of $C(t)$

$$\frac{dC(t)}{dt} + \omega C(t) + \omega^{-1} \int_0^t d\tau M^{\text{irr}}(t-\tau) \frac{dC(\tau)}{d\tau} = 0, \tag{11}$$

where $\omega = k(0)$, $k(t) = -\frac{dC(t)}{dt}$, M^{irr} is irreducible memory function.
Solution: (Ref. Pitts2000, JCP,113, 8671) From

$$C(z) = \frac{1}{z + \omega + M(z)}; M(z) = -\frac{M^{irr}(z)}{1 + \omega^{-1} M^{irr}(z)}, \tag{12}$$

One obtain $C(z) + \frac{1}{\omega}(zC(z) - C(t=0)) + \frac{1}{\omega^2} M^{irr}(z)(zC(z) - C(t=0)) = 0$. Then perform inverse Laplace transform, one obtain Eq.11 (The initial condition $C(t=0) = 1$ is used).

3 (2b) Theoretical object: to derive an equation of $C(t)$ (kinetic theory of $C(t)$)

Problem 3: Derive the dynamical Eq. of $C(t)$.

J.C.P. 113, 8671 (2000, PRE)

$$\tilde{C}(z) = \frac{1}{z+\alpha+\tilde{M}(z)} \quad (2.1)$$

$$\tilde{M}(z) = -\frac{\tilde{M}^{irr}(z)}{1+\alpha^{-1}\tilde{M}^{irr}(z)} \quad (*)$$

$$\Rightarrow \tilde{C}(z)(z+\alpha)+\tilde{C}(z)\tilde{M}(z)=1$$

$$\Rightarrow \tilde{M}(z) = \frac{1-\tilde{C}(z)(z+\alpha)}{\tilde{C}(z)} \quad (*2)$$

$$(*) \text{ and } (*2) \Rightarrow \frac{\tilde{M}^{irr}(z)}{1+\alpha^{-1}M^{irr}(z)} = \frac{\tilde{C}(z)(z+\alpha)-1}{\tilde{C}(z)}$$

$$\tilde{C}(z)(z+\alpha)+\tilde{C}(z)\tilde{M}(z)=1 \Rightarrow M(z) = \frac{1-C(z)(z+\alpha)}{C(z)}$$

$$\Rightarrow \frac{M^{irr}(z)}{1+\alpha^{-1}M^{irr}(z)} = \frac{C(z)(z+\alpha)-1}{C(z)} \qquad \alpha = -\dot{C}(0) \equiv \omega$$

$$\Rightarrow M^{irr}(z)C(z) = C(z)z + C(z)\alpha - 1 + \alpha^{-1}M^{irr}(z)C(z)z + \alpha^{-1}M^{irr}(z)C(z)\alpha - \alpha^{-1}M^{irr}(z)$$

$$\Rightarrow 0 = zC(z) + \omega C(z) - 1 + \frac{1}{\omega}M^{irr}(z)zC(z) - \frac{1}{\omega}M^{irr}(z)$$

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

$$\Rightarrow \boxed{\frac{dC(t)}{dt} + \omega C(t) + \frac{1}{\omega}\int_0^t M^{irr}(t-\tau)\frac{dC(\tau)}{d\tau}d\tau = 0} \quad (94)$$

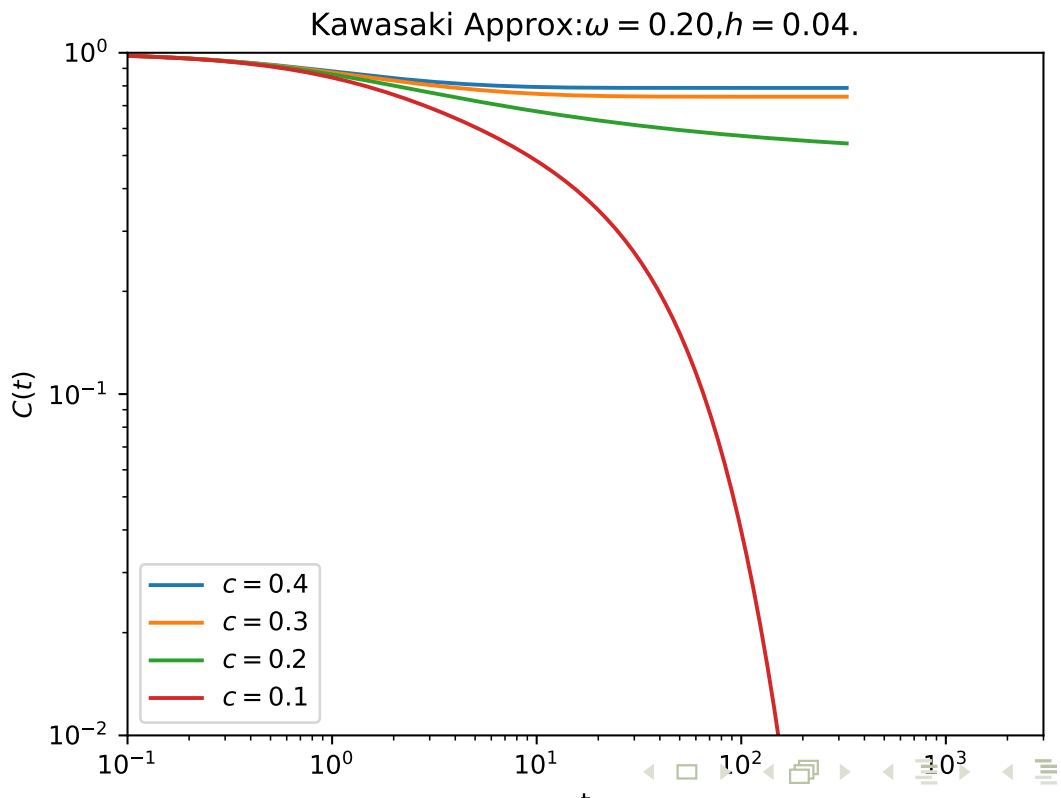
The dynamical eqn of the $C(t)$.

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

Problem 4: Solve the dynamical Eq. of $C(t)$

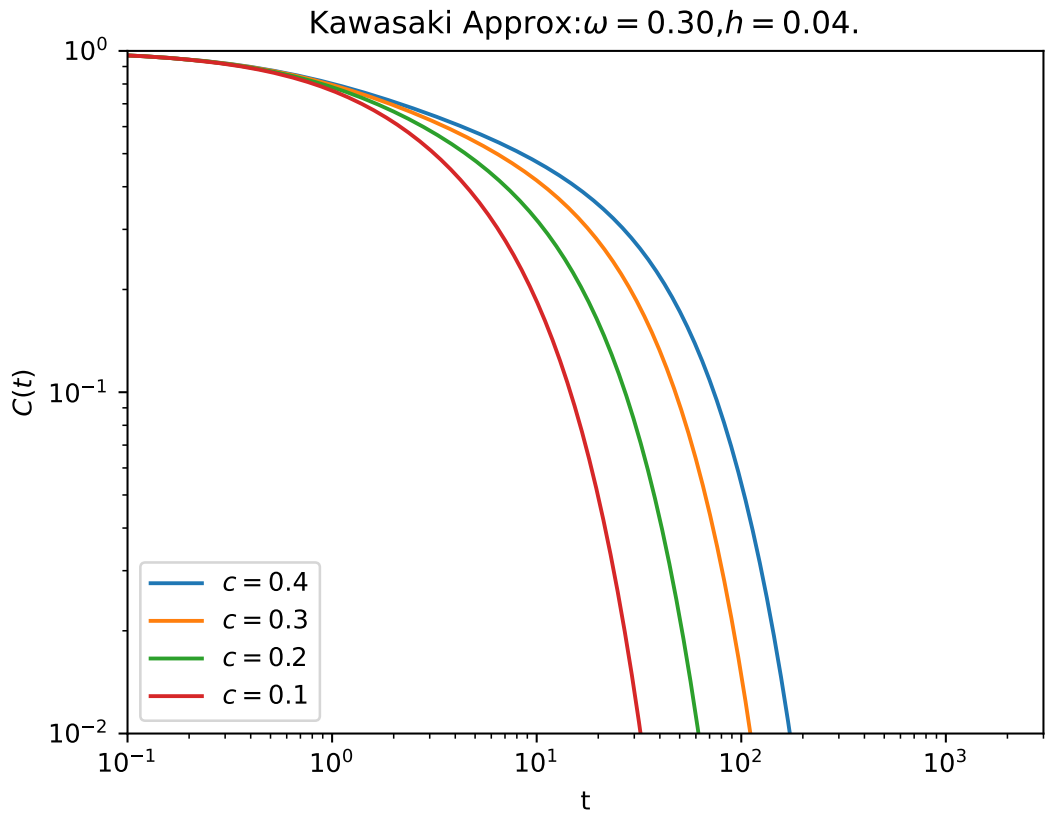
$$\frac{dC(t)}{dt} + \omega C(t) + \omega^{-1} \int_0^t d\tau M^{\text{irr}}(t-\tau) \frac{dC(\tau)}{d\tau} = 0,$$

where $\omega = k(0)$, $k(t) = -\frac{dC(t)}{dt}$, M^{irr} is irreducible memory function.
Solution: From Kawasaki approximation: We set ω in $[0.1, 0.3, 0.5, 0.7, 0.9, 1.0, 2.0]$, respectively. The calculated $C(t)$ is shown in the Fig.s.



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

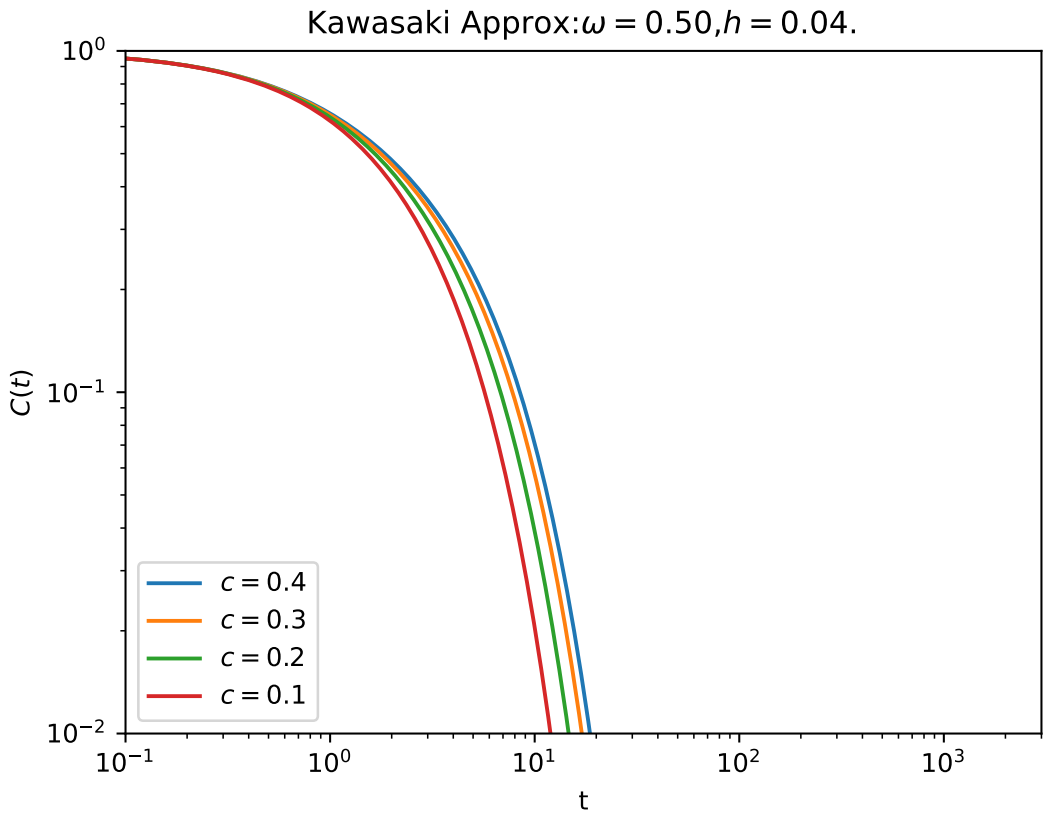
Solution: From Kawasaki approximation: We set ω in $[0.1, 0.3, 0.5, 0.7, 0.9, 1.0, 2.0]$, respectively. The calculated $C(t)$ is shown in the Fig.s.



Calculated $C(t)$ from kawasaki approximation. ($\omega = 0.3$)

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

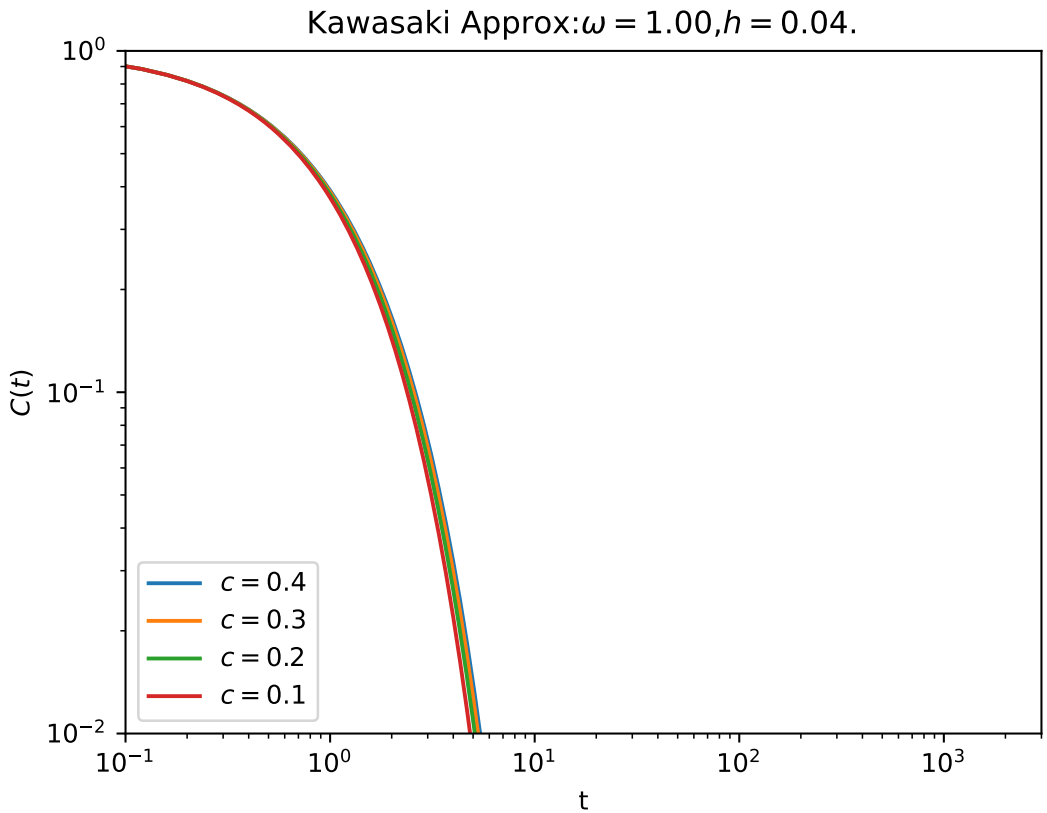
Solution: From Kawasaki approximation: We set ω in $[0.1, 0.3, 0.5, 0.7, 0.9, 1.0, 2.0]$, respectively. The calculated $C(t)$ is shown in the Fig.s.



Calculated $C(t)$ from kawasaki approximation. ($\omega = 0.5$)

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

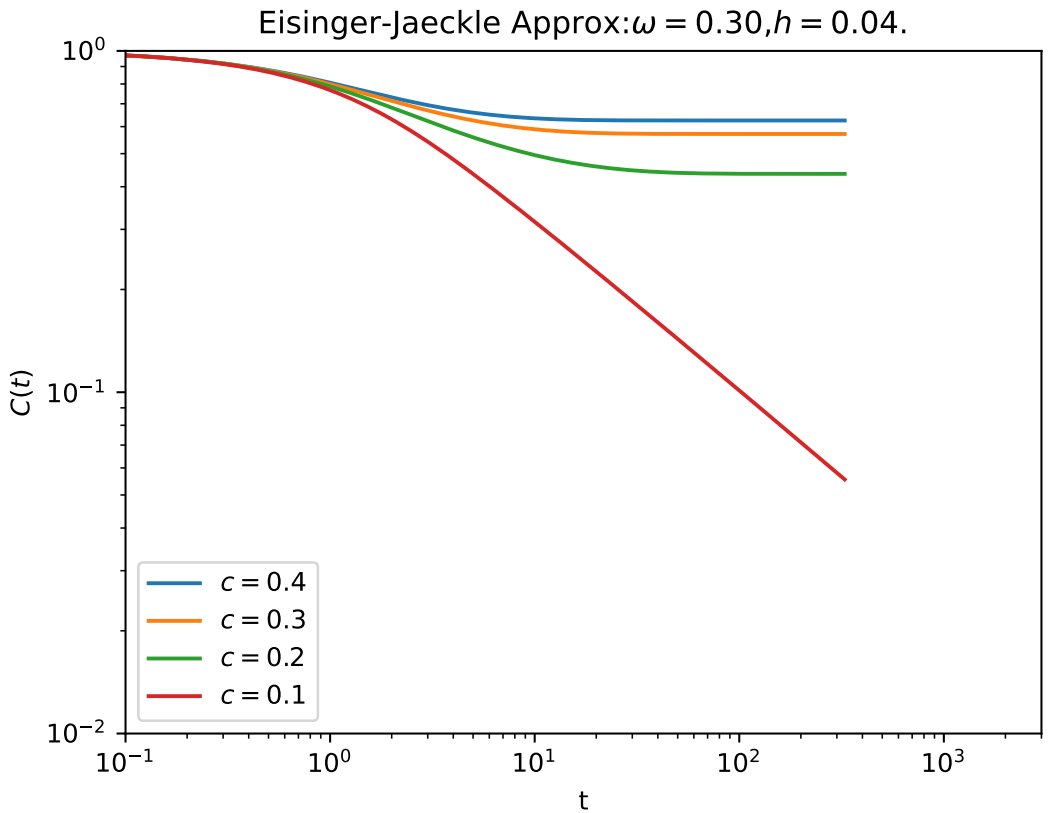
Solution: From Kawasaki approximation: We set ω in $[0.1, 0.3, 0.5, 0.7, 0.9, 1.0, 2.0]$, respectively. The calculated $C(t)$ is shown in the Fig.s.



Calculated $C(t)$ from kawasaki approximation. ($\omega = 1.0$)

3 (7) Theoretical object: Solve an equation of $C(t)$ (kinetic theory of $C(t)$):— EJ approximation

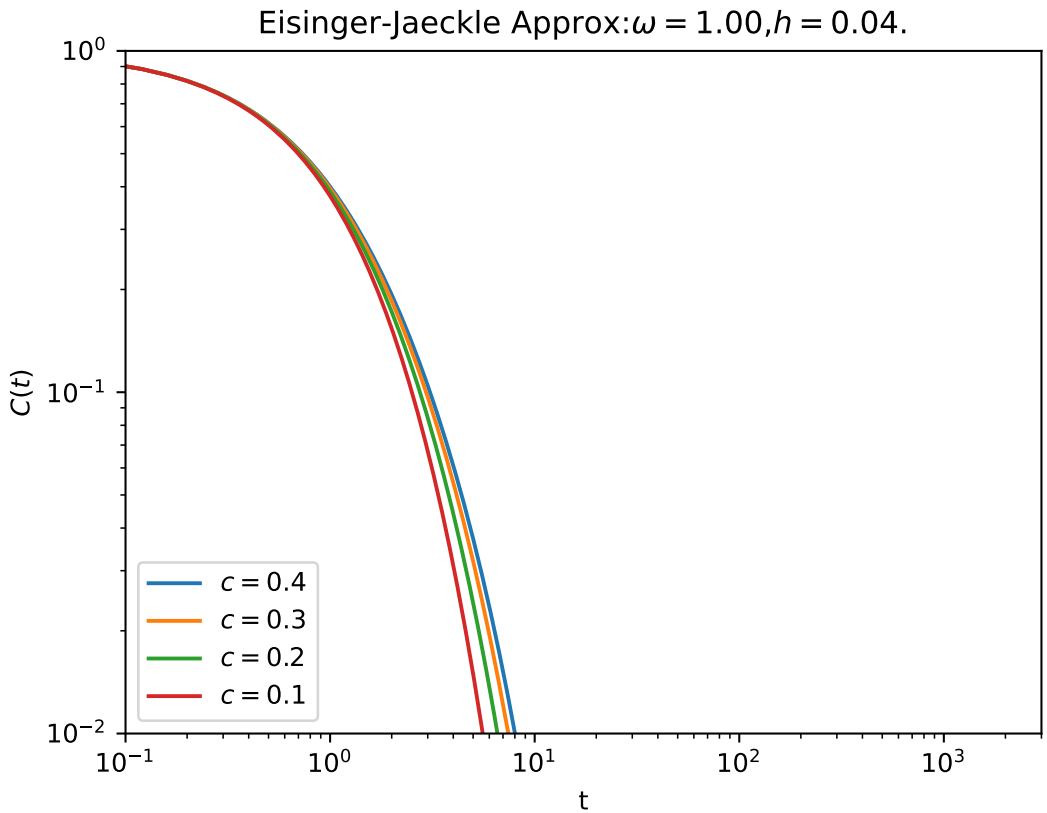
Solution: From EJ approximation: We set ω in $[0.1, 0.3, 0.5, 0.7, 0.9, 1.0, 2.0]$, respectively. The calculated $C(t)$ is shown in the Fig.s.



Calculated $C(t)$ from EJ approximation. ($\omega = 0.3$)

3 (7) Theoretical object: Solve an equation of $C(t)$ (kinetic theory of $C(t)$):— EJ approximation

Solution: From EJ approximation: We set ω in $[0.1, 0.3, 0.5, 0.7, 0.9, 1.0, 2.0]$, respectively. The calculated $C(t)$ is shown in the Fig.s.



Calculated $C(t)$ from EJ approximation. ($\omega = 1.0$)