# Stretched Exponential to Power Law Relaxation in Kinetically Constrained Models

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# Stretched Exponential to Power Law Relaxation
# in
# Kinetically Constrained Models

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## Collaborators


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- Saroj Nandi


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# Slow Decays

Slow decays such as

- Stretched exponential $\varphi(t) \sim \exp\left[-\left(\frac{t}{\tau}\right)^{\beta}\right]$
- Power law $\sim t^{-\alpha}$

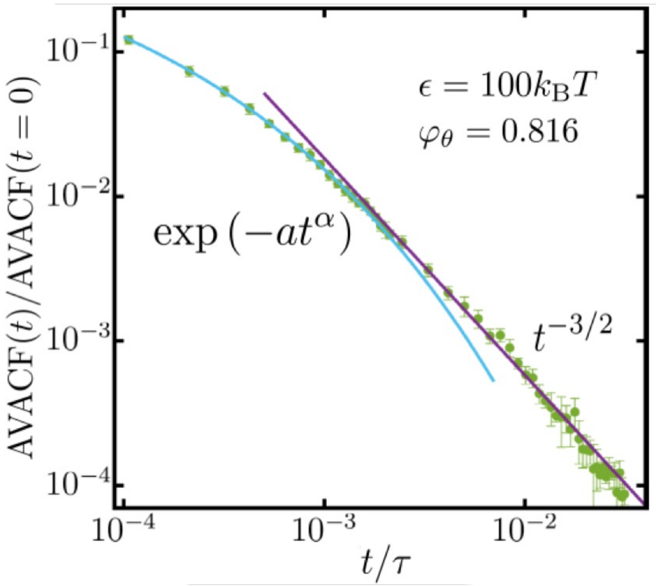
can arise from a variety of mechanisms, e.g.

- Conservation laws, Criticality,
  Hierarchical relaxation, Kinetic constraints, FDPO ...

Crossovers between the two forms occur in some cases.

Can we understand why?

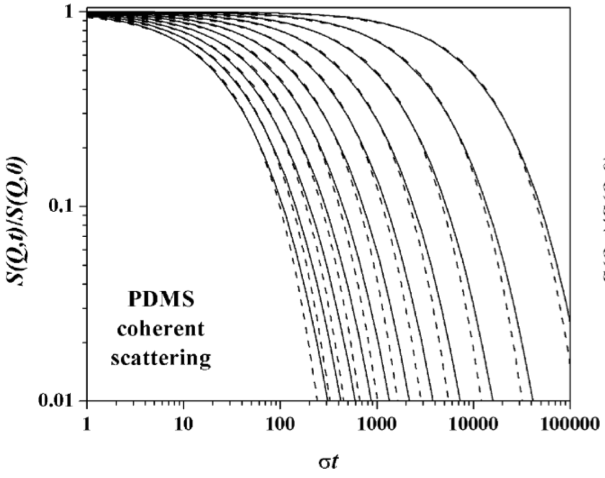
# Stretched Exponential to Power Law : Examples

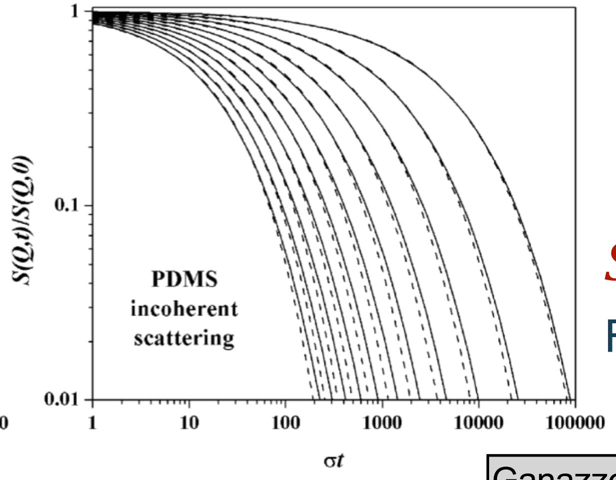



Simulation studies for colloidal glasses of active particles in 3d

AVACF: Angular Velocity Auto-Correlation Function

Clara Abaurrea-Velasco, Lozano, Bechinger, and de Graaf
Phys. Rev. Lett. **125**, 258002 (2020)




Simulation studies for the dynamics of polymer chains

$S(Q,t)$: Dynamic Structure Factor at wave vector $Q$

Ganazzoli, Raffaini, and Arrighi
Phys. Chem. Chem. Phys., 2002, **4**, 3734 (2002)

# Stretched Exponential to Power Law : Models

We investigate the crossover in two models with kinetic constraints, and elucidate why it occurs.

- Domain walls to doublons

  Bound states emerge as a function of time and change the pattern of decay

  S. Mukherjee, P. Pareek, M. Barma, S. K. Nandi, arXiv:2307.01801

- Domain walls in arrested states of a frustrated system

  Domain wall dynamics generates stretched exponentials.

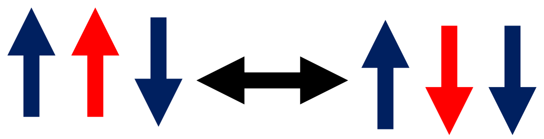
  Ensemble averages generate power laws.

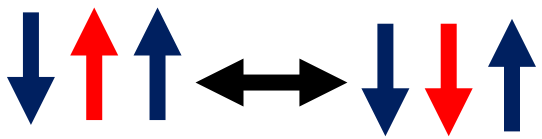
  V. Gupta, S. K. Nandi, M. Barma, Phys. Rev. E (2020).

# Domain Wall Dynamics

## Kinetic constraint:

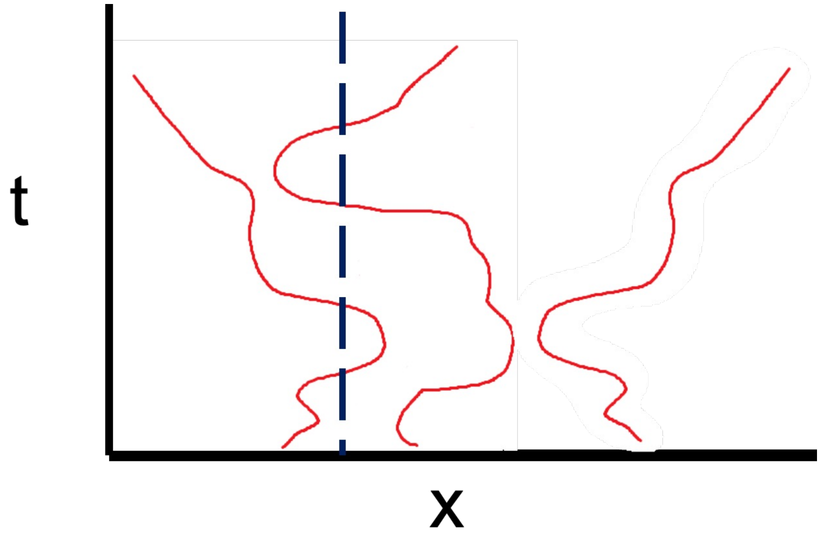
A spin can flip only if its neighbours are oriented oppositely





Spin flip $\Longrightarrow$ A domain wall (DW) steps right or left

DWs perform random walks with a hard core constraint: A simple exclusion process




What is the implication for the spin-spin autocorrelation function?

# Spin Autocorrelation Functions with Conserved DWs

[J. L. Skinner, J. Chem. Phys, 1983;     H. Spohn, Comm. Math. Phys.,1989]

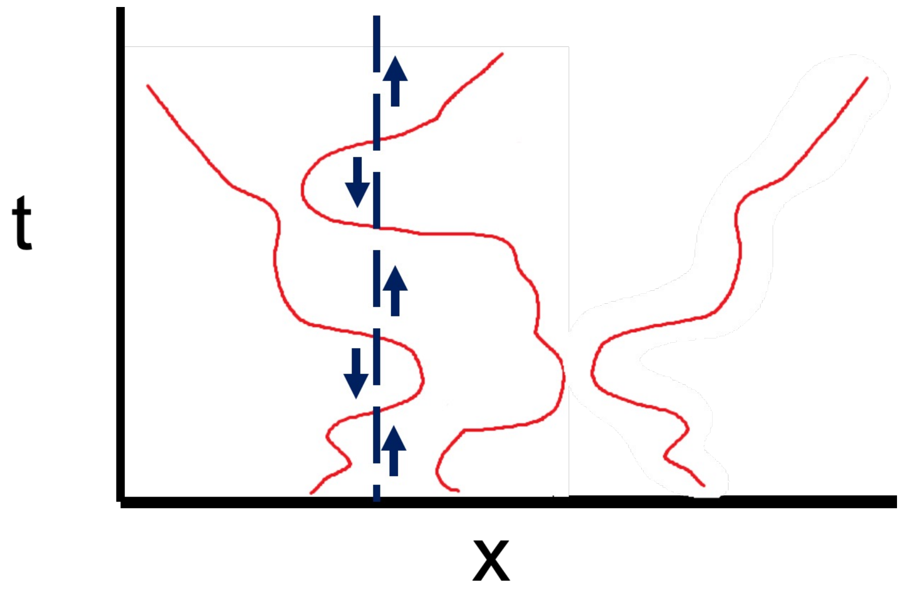
A spin flips only if a DW crosses it.

How long does that take?

$Prob$ (Domain length $l$)$\sim \exp(-\,l/\xi)$

Diffusion of DWs $\;\Longrightarrow\;$ $t \sim l^2$.

Thus expect $C(t) \sim exp\, -(t/\tau)^{1/2}$




Bounds on $1/\tau$     [H. Spohn, 1989]

Upper Bound     $\frac{1}{\tau} \leq 2[\sqrt{\pi}\,(1+\cosh\beta)]^{-1}$.

The Lower Bound is obtained through a variational process.

# The DWD Model and the XOR-FA Model

DWD ≡ Domain Wall to Doublon

[S. Mukherjee, P. Pareek, M. Barma, S. K. Nandi, ArXiv 2023]

XOR-FA ≡ XOR Fredrickson-Andersen

[L. Causer, I. Lesanovsky, M. C. Banuls, J. P. Garrahan, PRE (2020)]


Both refer to the conserved DW model in the presence of a field $\sum S_i$.

The XOR-FA is model motivated by Rydberg atoms in their "facilitated" state:
An atom changes its state only if a single neighbour is in the excited state.

The XOR-FA analysis focuses on DW trajectories and whether they bunch up.

The DWD analysis focuses on the spin autocorrelation function.

# Doublons

Dynamics:

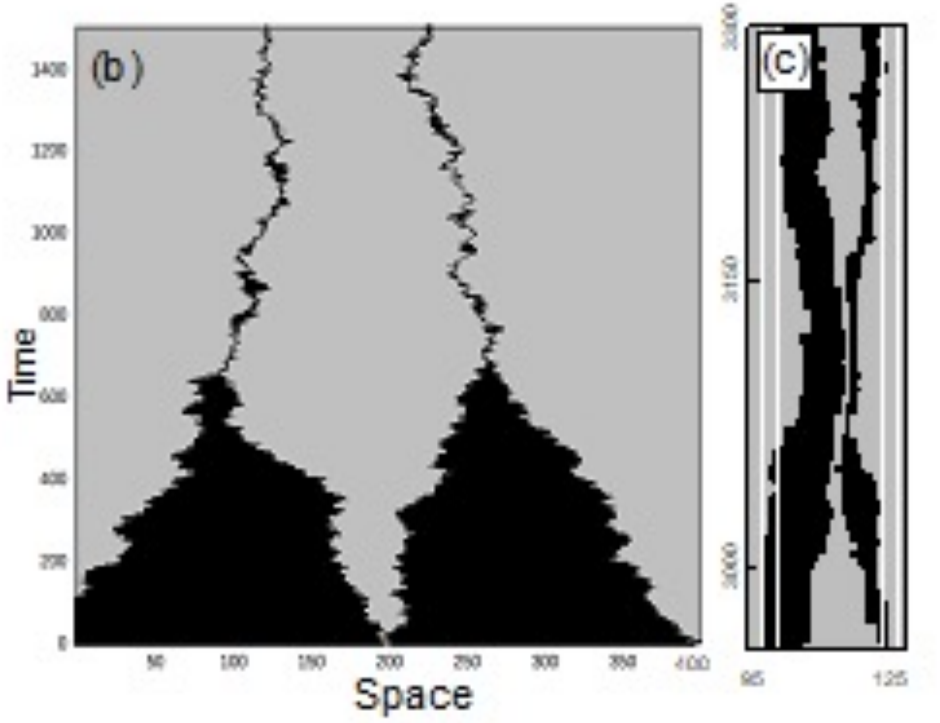

DWs perform biased random walks, with alternating easy directions.

Up-spin domains tend to shrink

$\Longrightarrow$

Effective attraction between alternating pairs of DWs

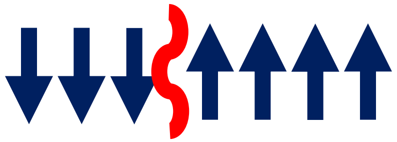
--- leads to the formation of doublons.




The change in the nature of excitation
(DW to doublon) induces a change
in the dynamics.

# Diffusion of DWs and Doublons

Domain Walls perform biased random walks, with alternating easy directions.



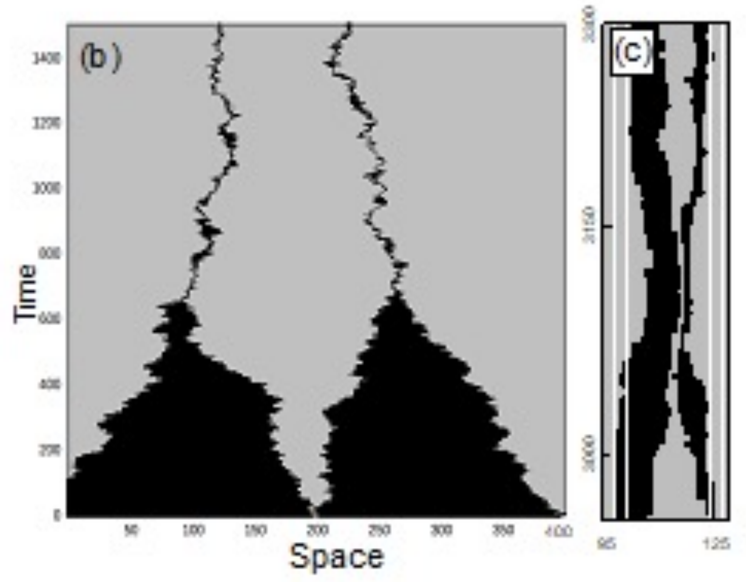
$$v_{DW} = 1 - c$$

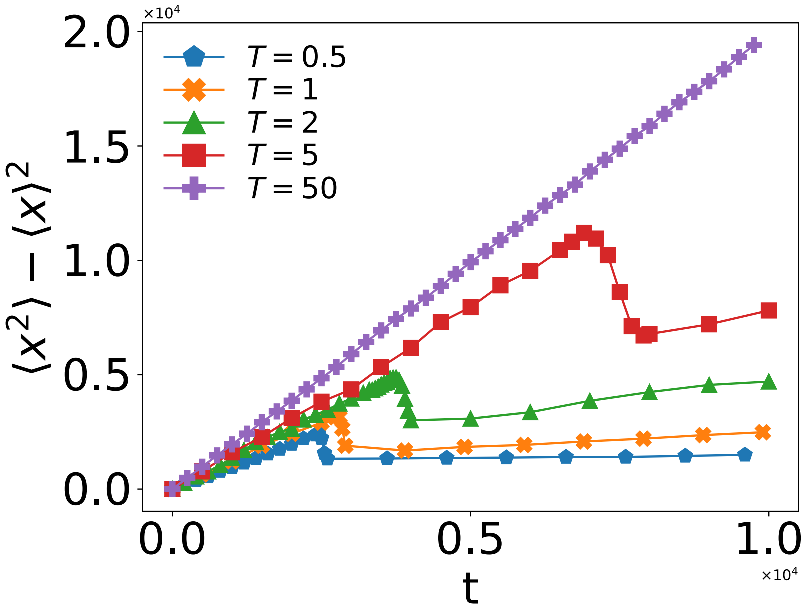
$$D_{DW} = \frac{1+c}{2}$$

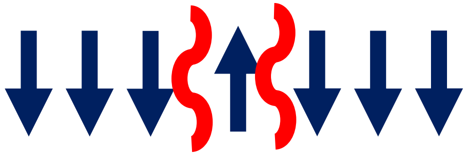
$$with \;\; c = \exp(-2/T)$$

Doublons perform unbiased random walks, with a hard core constraint.

Size fluctuations decrease as $T \to 0$.

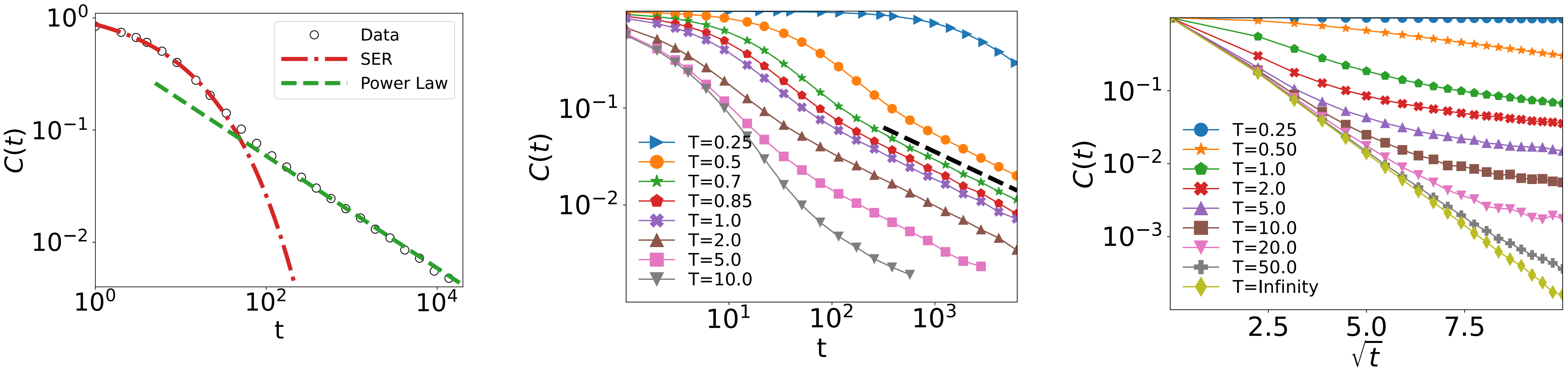


$$D_{doublon} = \frac{c}{2}$$

# Macroscopic Number of Domain Walls



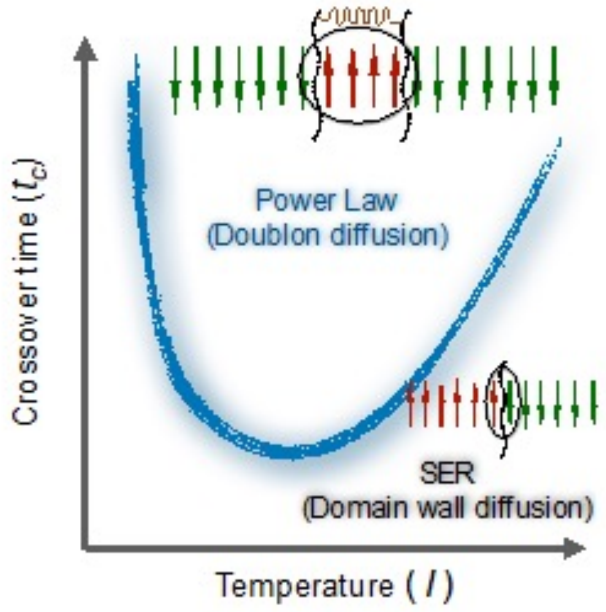

Observe a crossover to an asymptotic power law decay $\sim t^{-1/2}$ .

*At high $T$* : The power-law decay is preceded by a stretched exponential.

$$C(t) \sim exp\,-(t/\tau)^{1/2} \quad \text{for } t < \ t_{cross}$$

*At low $T$* : The power-law decay is preceded by a faster relaxation.

# The Crossover Time



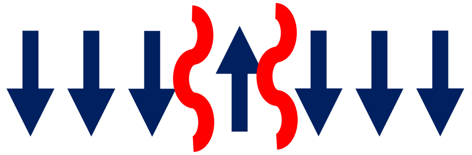

$t_{cross}$ is a non-monotonic function of temperature

As $T$ increases, $t_{cross}$ goes up as the bias vanishes.

As $T$ decreases, $t_{cross}$ goes up as most microscopic update attempts are unsuccessful.

# Doublon - Dimer Mapping

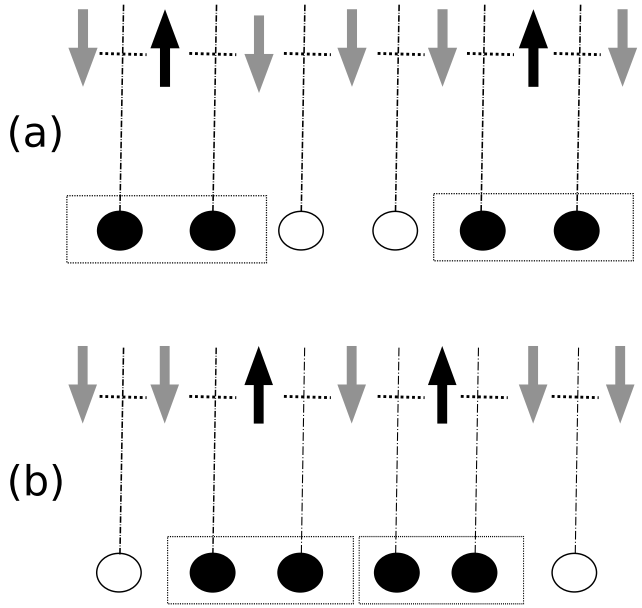
In the low-temperature limit, a doublon → a single up spin.



Hard core constraint of DWs $\Longrightarrow$ Minimum spacing of doublon spins= 2

This enables a mapping to dimer diffusion in 1D.

Autocorrelation function $\sim t^{-1/2}$



# Quenching Frustrated Systems → Arrested States

The Axial Next Nearest Neighbor (ANNNI) model involves competing n.n. and n.n.n. interactions

$$\mathcal{H} = -J_1 \sum_i S_i S_{i+1} + J_2 \sum_i S_i S_{i+2}$$

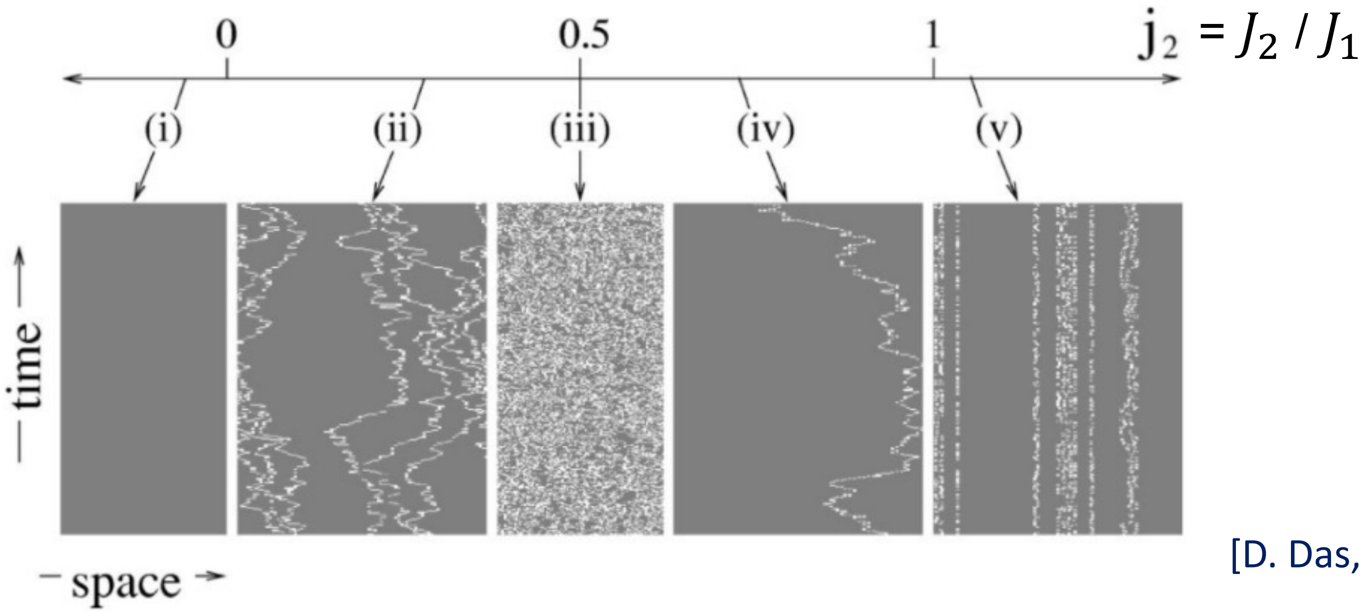
Frustration + Rapid cooling towards T=0 ⇒ Arrested states

Conserved dynamics

Moves: ↑↑ ↔ ↓↓ ↔ ↑↓ ↔ ↓↑ if the sign of $J_1$ is flipped

Allow only energy-lowering or equal-energy moves

Dynamics in arrested states




[D. Das, MB (1999)]

# Dynamics in an Arrested State

Interestingly, several of the arrested states are dynamically alive.

## Dynamics

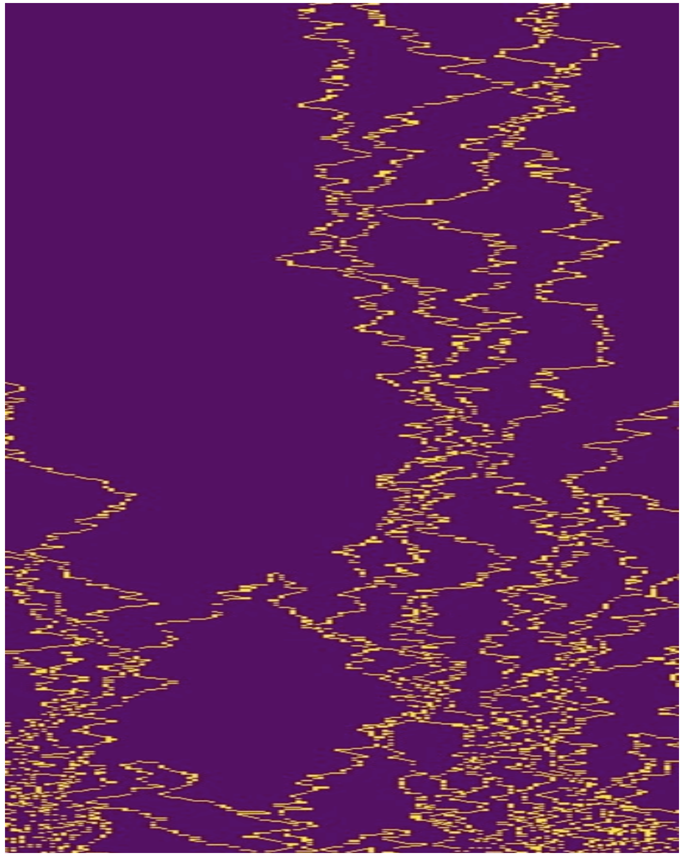
T=0 ⇒ Energy-raising moves are not allowed

Find:
Domain walls perform random walks with interesting interactions

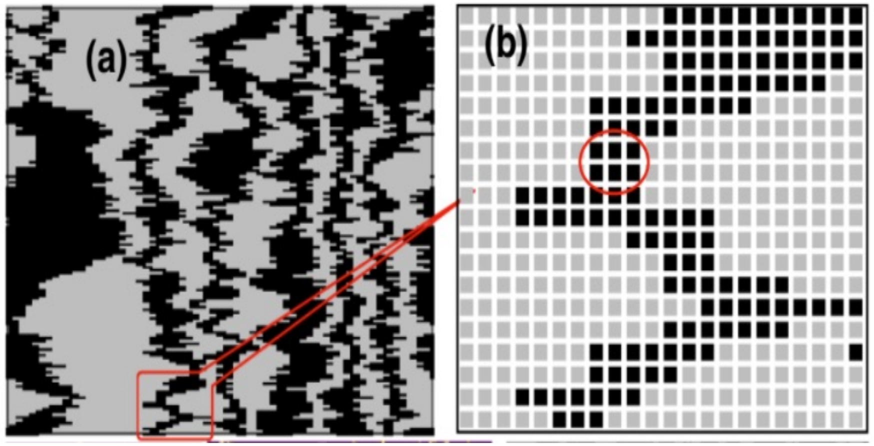
- Annihilation of domains with an even separation of DWs
- In steady state, only odd-separation domains remain
- Distance of closest approach = 3

Thus the *approach to steady state* involves *annihilation* of DWs

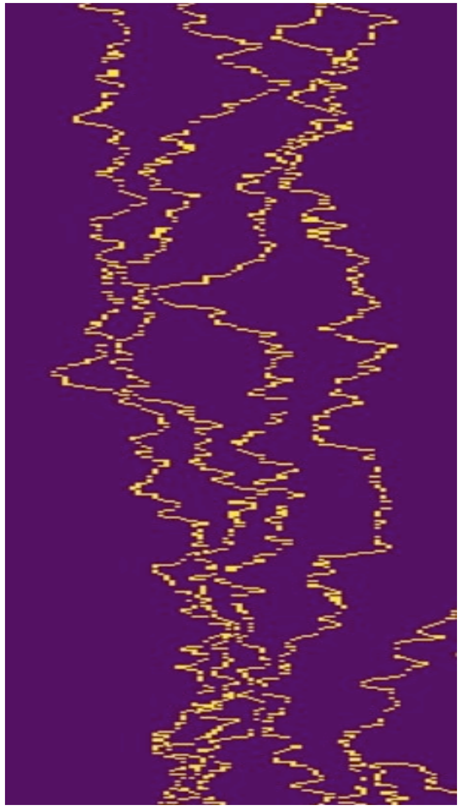
The *dynamics in steady state* involves conserved DWs with *exclusion*



Domain wall evolution



# The Steady State



How many domain walls are there?

- Conservation law:

  $\uparrow\uparrow \leftrightarrow \downarrow\downarrow \Rightarrow$ Sublattice magnetization $M_{sub} = M_A - M_B$ invariant

- Random initial condition:

  $\Rightarrow N_{DW} = M_{sub} \sim O(\sqrt{L})$ where $L$ is the system size

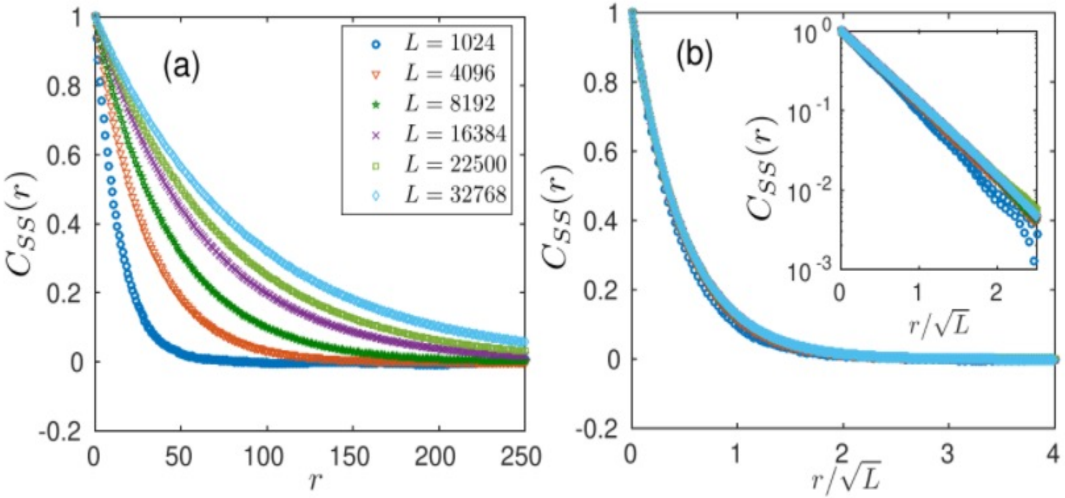
Sub-extensive number of RWs $\Rightarrow$ Important consequences

Correspondence to simple exclusion process:

Every allowed configuration is equally likely

Steady state static correlation

$$C_{SS}(r) \equiv < S_i S_{i+r} >= \exp(-\frac{2r}{\sqrt{L}})$$

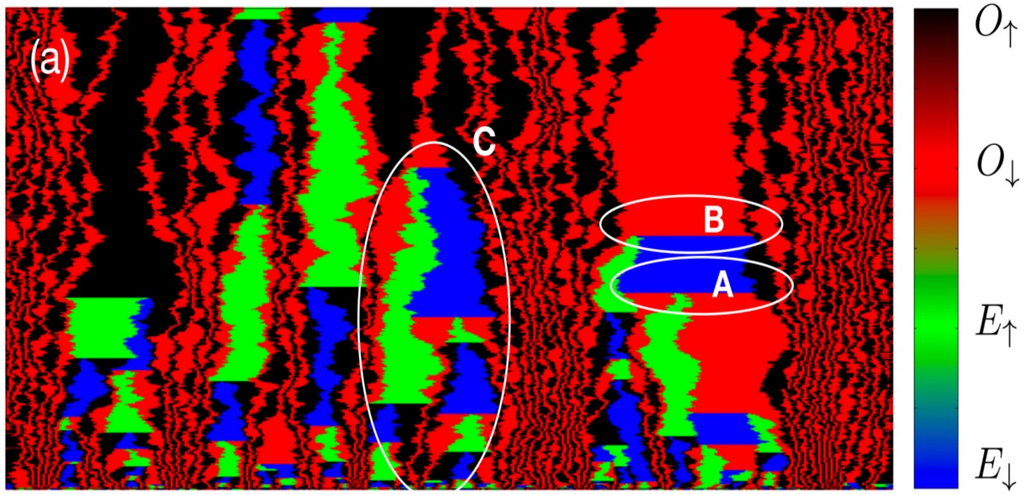


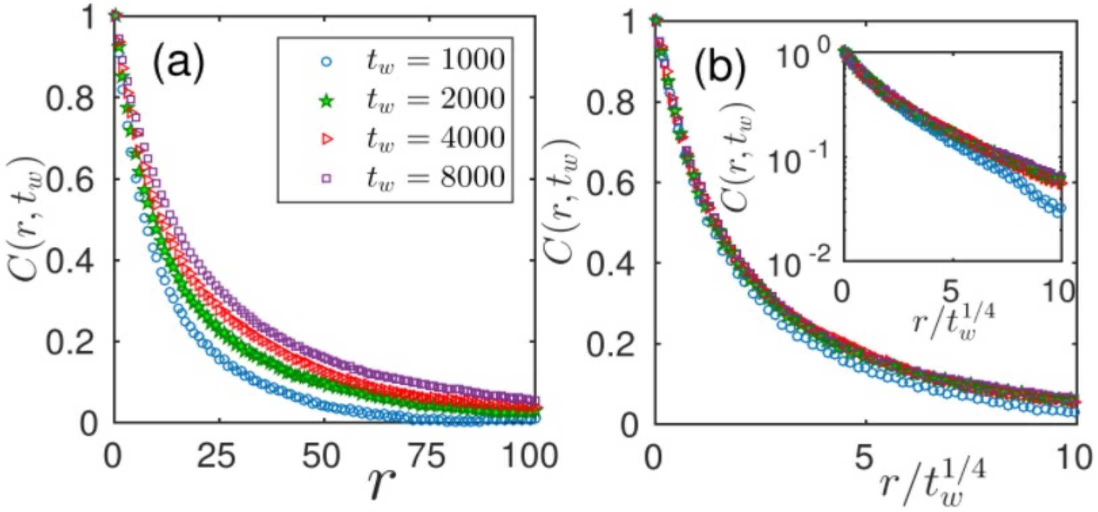
# Approach to the Steady State

## Coarsening

- After time $t_w$, equilibrium within patches of size $\mathcal{L}(t_w)$
- $C(r, t_w)$ obtained from $C_{SS}(r) = \exp(-\frac{2r}{\sqrt{L}})$ by replacing $L \rightarrow \mathcal{L}(t_w)$
- Even-domain disappearance is governed by diffusing, annihilating DWs $\Rightarrow \quad \mathcal{L}(t_w) \sim {t_w}^{1/2}$

Conclude $\quad C(r, t_w) = \exp(-\frac{Br}{{t_w}^{1/4}})$



# Dynamics in the steady state

## Autocorrelation function

$$\varphi(t) \equiv < S_i(t_0) S_i(t_0+t) > \; - < S_i\;(t_0) >^2$$

Considered earlier for the exclusion process with a finite density of DWs

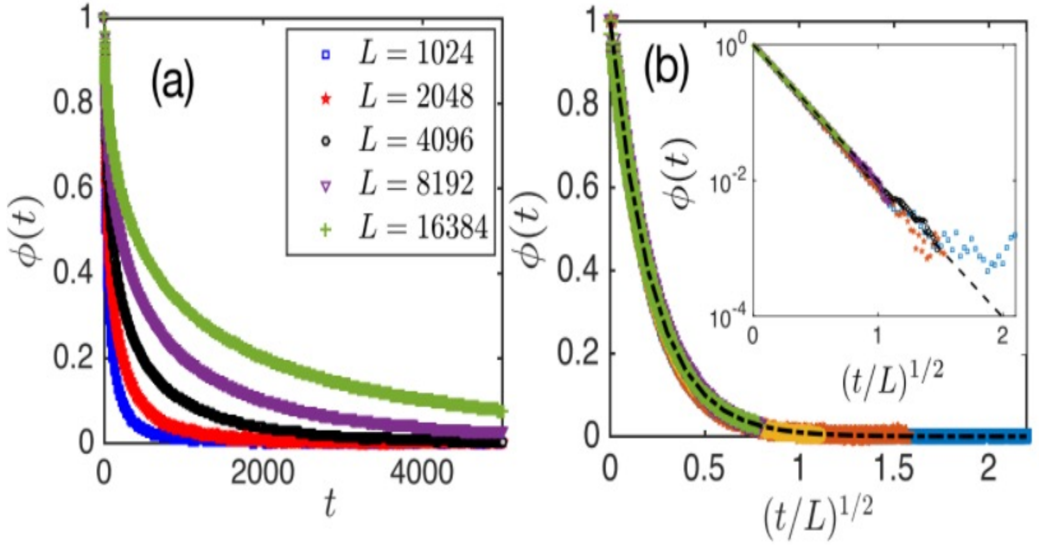
[J. L. Skinner (1983), H. Spohn (1989)]

Taking $\rho \sim \frac{1}{\sqrt{L}}$, obtain

. $\varphi(t) = \exp[-A\left(\frac{t}{L}\right)^{\frac{1}{2}}]$

An ultra-long $L$-dependent relaxation time

-- a “size-stretched exponential”



# Ensemble Average

Consider performing quenches from completely disordered states, with differing $N$.

Ensemble average

$$q(t) = \left\{ \frac{1}{L} \sum_i < S_i(t_0) S_i(t_0 + t) > - < S_i(t_0) >^2 \right\}$$

The distribution of $N$ follows

$$P(N) = \sqrt{\frac{2}{\pi L}} \exp\left[\frac{-N^2}{2L}\right] \quad \Rightarrow \quad q(t) = \sqrt{\frac{2}{\pi L}} \int_0^\infty exp\left[\frac{-N^2}{2L}\right] exp\left[\frac{-A_0 N t^{1/2}}{L}\right]$$

Result:

$$q(t) = \exp\left[\frac{{A_0}^2 t}{2L}\right] erfc\left(A_0 \sqrt{\frac{t}{2L}}\right)$$

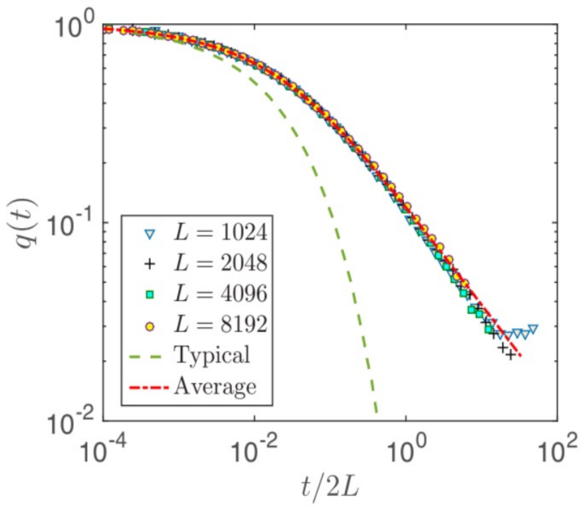
--- a Mittag-Leffler function with index $^1/_2$

Short times:

$$q(t) \approx [1 - A_0 \sqrt{\frac{2}{\pi}} (t/L)^{\frac{1}{2}}]$$

Long times:

$$q(t) \approx \sqrt{2/\pi {A_0}^2} \; (t/L)^{-1/2}$$



# Conclusions

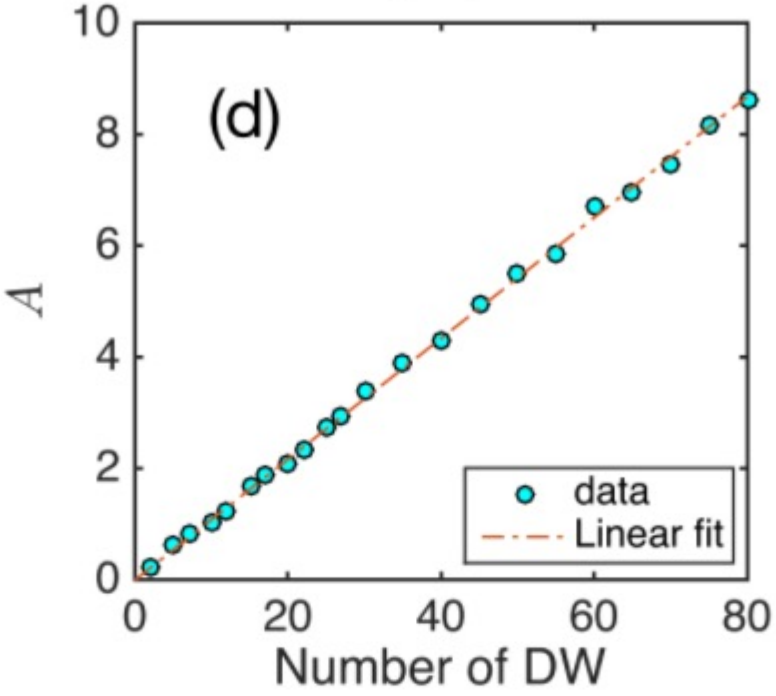
Kinetically constrained models with a conserved number of domain walls sometimes show a crossover from stretched exponential to power law decay.

In the Domain wall to Doublon model

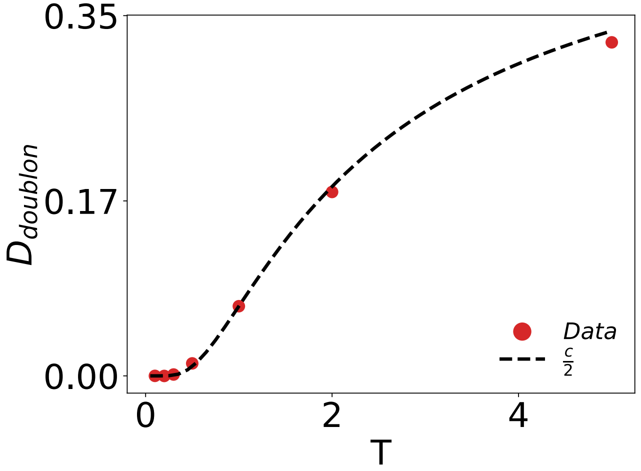
An effective attraction between alternating pairs of domain walls $\Longrightarrow$ Doublons
Once they form, they change the pattern of decay

In the Arrested state obtained by quenching from an ANNNI model

Single samples show a size-stretched exponential decay
Averaging over the ensemble of initial conditions
$\Longrightarrow$ A Mittag-Leffler function, which embodies the crossover



(d)
A
Number of DW
data
Linear fit

$D_{doublon}$
T
Data
$\frac{c}{2}$