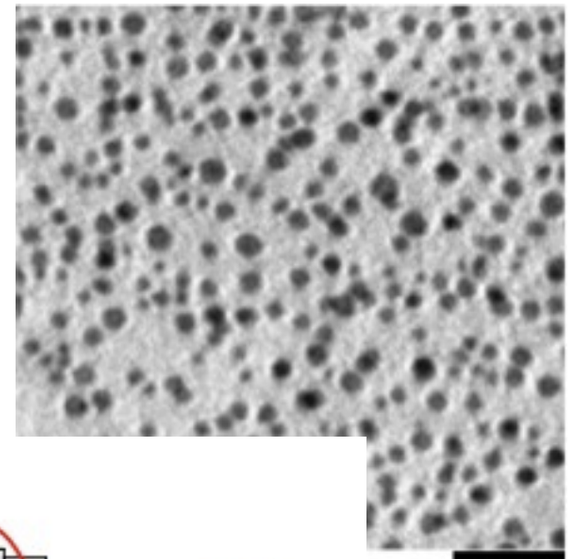
Effect of Size Distribution of Magnetic Nanoparticles on Metastability Across Dynamic Phase Boundary

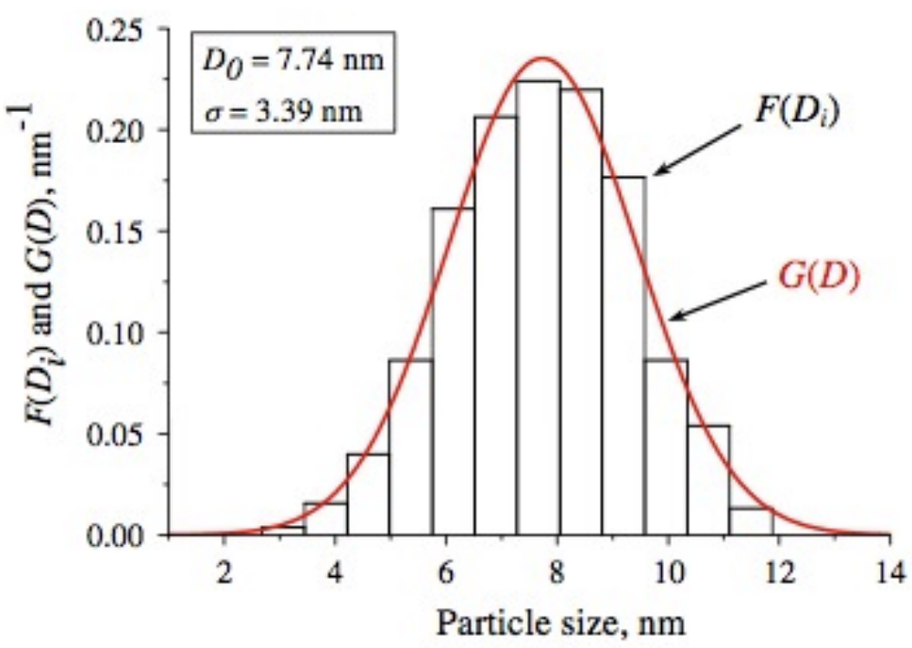
Yoh Yamamoto and Kyungwha Park
Department of Physics, Virginia Tech

Introduction

Introduction

- Experiments: a collection of magnetic nanoparticles have distribution in sizes and shapes and influence properties of the nanoparticles.

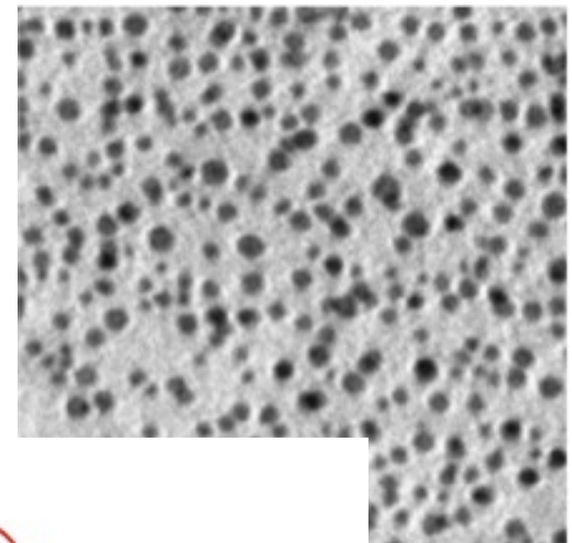


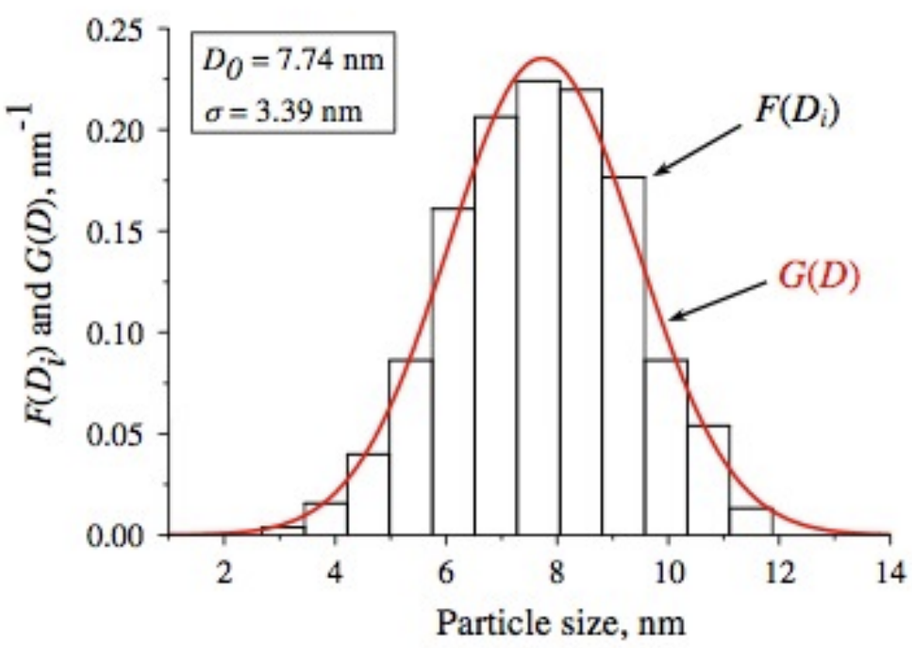


J Nanopart Res, **10** 487, (2008)

Introduction

- Experiments: a collection of magnetic nanoparticles have distribution in sizes and shapes and influence properties of the nanoparticles.
- To simulate the size distribution, we used a Gaussian distribution in magnetic anisotropy parameter.

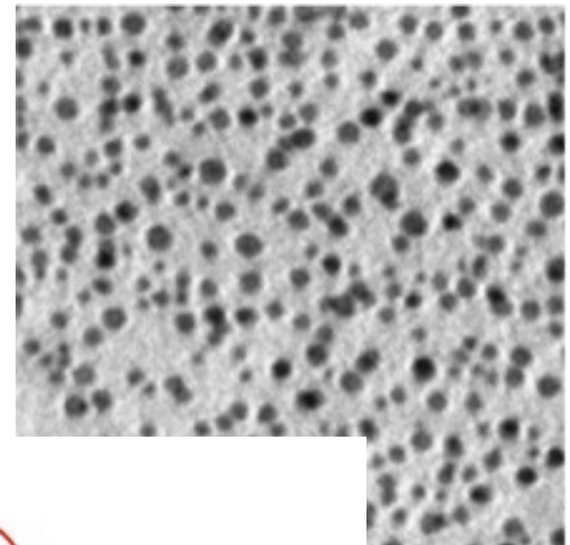


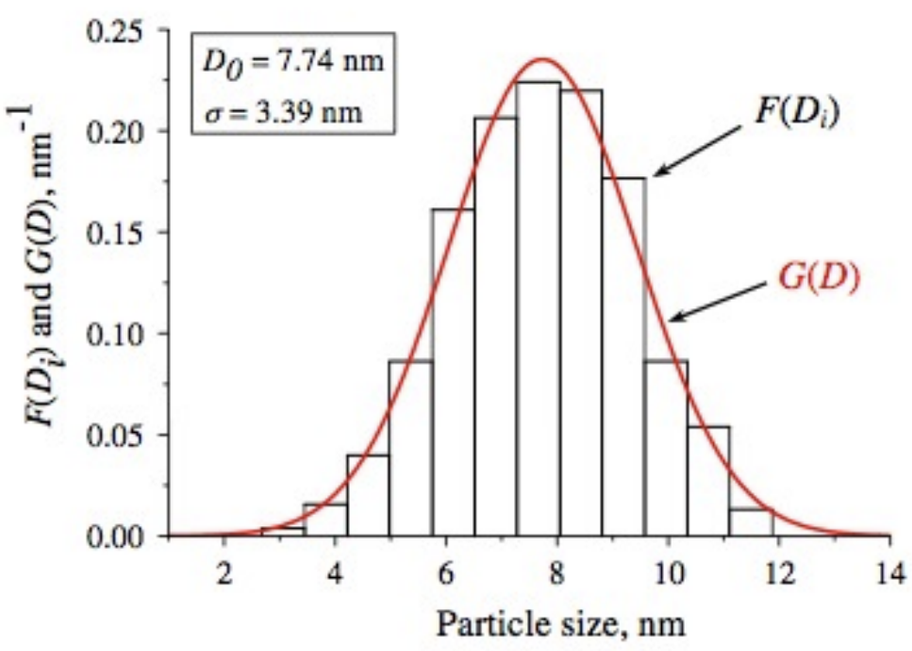


J Nanopart Res, **10** 487, (2008)

Introduction

- Experiments: a collection of magnetic nanoparticles have distribution in sizes and shapes and influence properties of the nanoparticles.
- To simulate the size distribution, we used a Gaussian distribution in magnetic anisotropy parameter.
- We simulate metastability using kinetic Monte Carlo simulations.





J Nanopart Res, **10** 487, (2008)

Spin S=1 Blume-Capel Model for ferromagnets

$$\mathcal{H} = -2J \sum_{\langle i,j \rangle} S_{iz} S_{jz} - H \sum_{i} S_{iz} - D \sum_{i} S_{iz}^2$$

Spin S=1 Blume-Capel Model for ferromagnets

$$\mathcal{H} = -2J \sum_{\langle i,j \rangle} S_{iz} S_{jz} - H \sum_{i} S_{iz} - D \sum_{i} S_{iz}^2$$

- J>0: Ferromagnetic exchange coupling.

Spin S=1 Blume-Capel Model for ferromagnets

$$\mathcal{H} = -2J \sum_{\langle i,j \rangle} S_{iz} S_{jz} - H \sum_{i} S_{iz} - D \sum_{i} S_{iz}^2$$

- J>0: Ferromagnetic exchange coupling.
- Spin S=1 can have a state of $M_z = \pm 1, 0$.

Spin S=1 Blume-Capel Model for ferromagnets

$$\mathcal{H} = -2J \sum_{\langle i,j \rangle} S_{iz} S_{jz} - H \sum_{i} S_{iz} - D \sum_{i} S_{iz}^2$$

- J>0: Ferromagnetic exchange coupling.
- Spin S=1 can have a state of $M_z = \pm 1, 0$.

Spin S=1 Blume-Capel Model for ferromagnets

$$\mathcal{H} = -2J \sum_{\langle i,j \rangle} S_{iz} S_{jz} - H \sum_{i} S_{iz} - D \sum_{i} S_{iz}^2$$

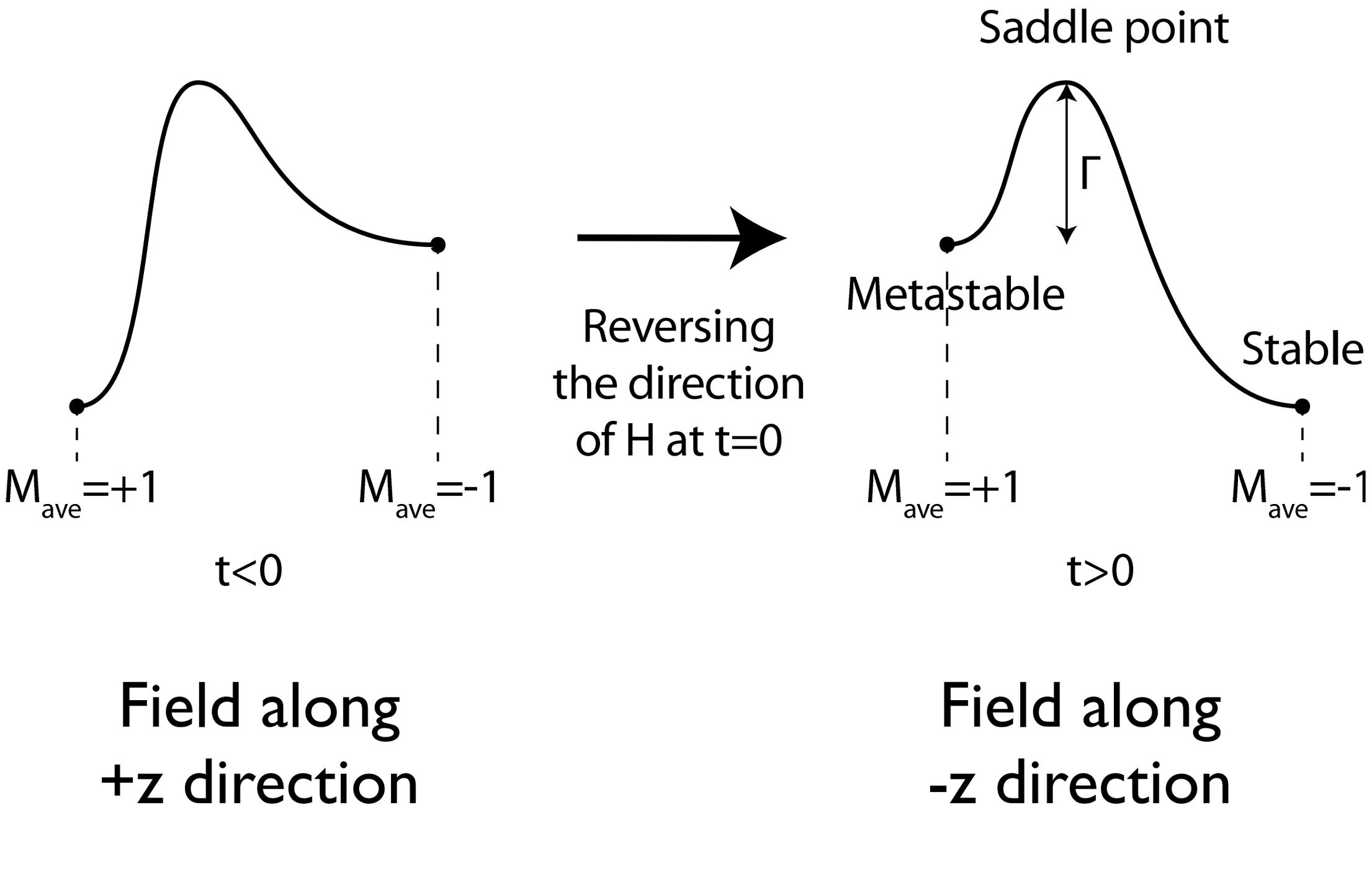
- J>0: Ferromagnetic exchange coupling.
- Spin S=1 can have a state of $M_z = \pm 1, 0$.
- D: Magnetic anisotropy parameter.

Spin S=1 Blume-Capel Model for ferromagnets

$$\mathcal{H} = -2J \sum_{\langle i,j \rangle} S_{iz} S_{jz} - H \sum_{i} S_{iz} \boxed{- D \sum_{i} S_{iz}^2}$$

- J>0: Ferromagnetic exchange coupling.
- Spin S=1 can have a state of $M_z = \pm 1, 0$.
- D: Magnetic anisotropy parameter.
- D>0 and we introduce Gaussian distribution.

Metastability



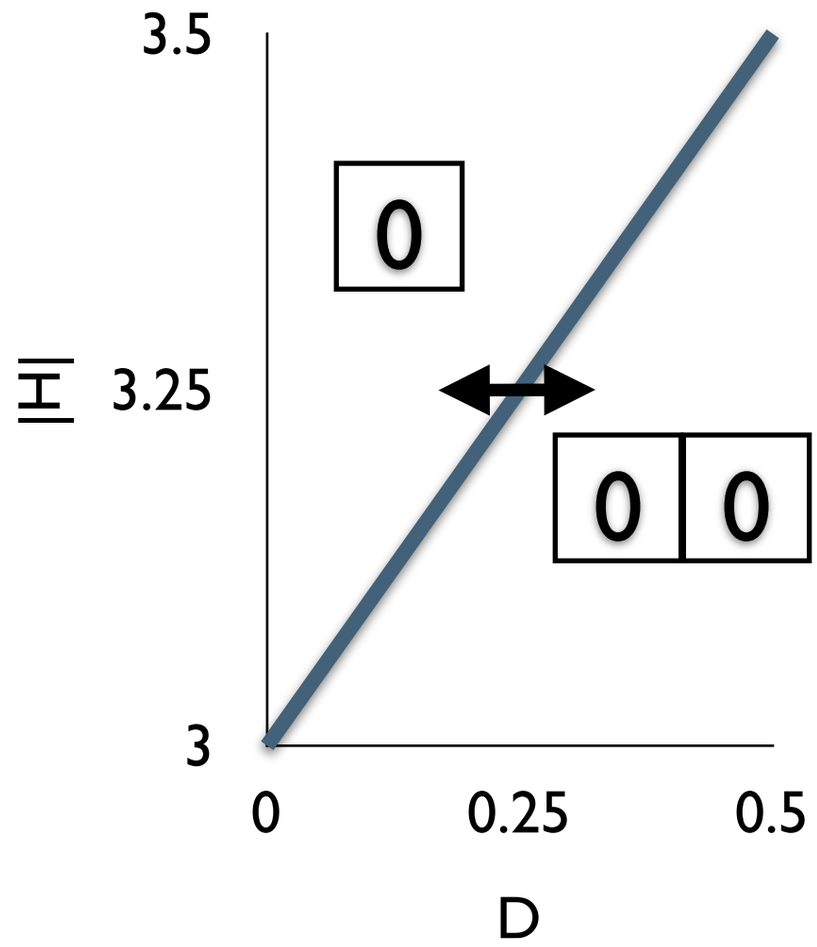
Field along
+z direction

Field along
-z direction

- We are interested in the single-droplet (SD) regime where the metastable decay is driven by a single critical droplet.

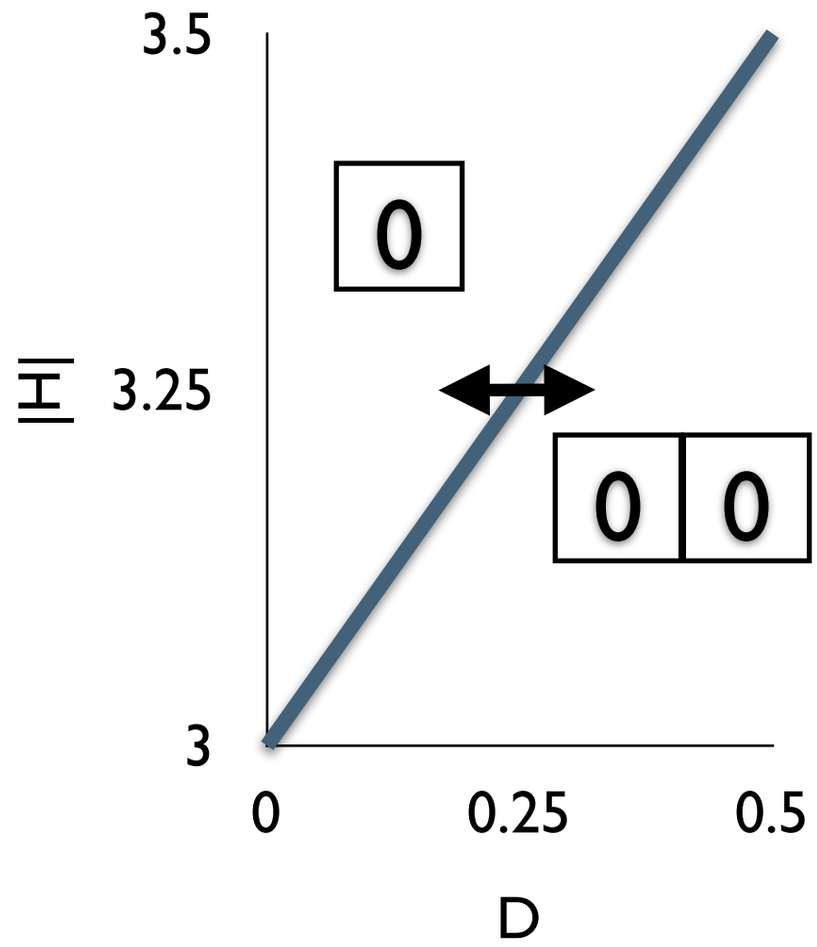
- We are interested in the single-droplet (SD) regime where the metastable decay is driven by a single critical droplet.
- For our model, SD regime appears when $|H|<D+4$ and $T \to 0$. L>droplet size.

Kinetic Monte Carlo Simulation



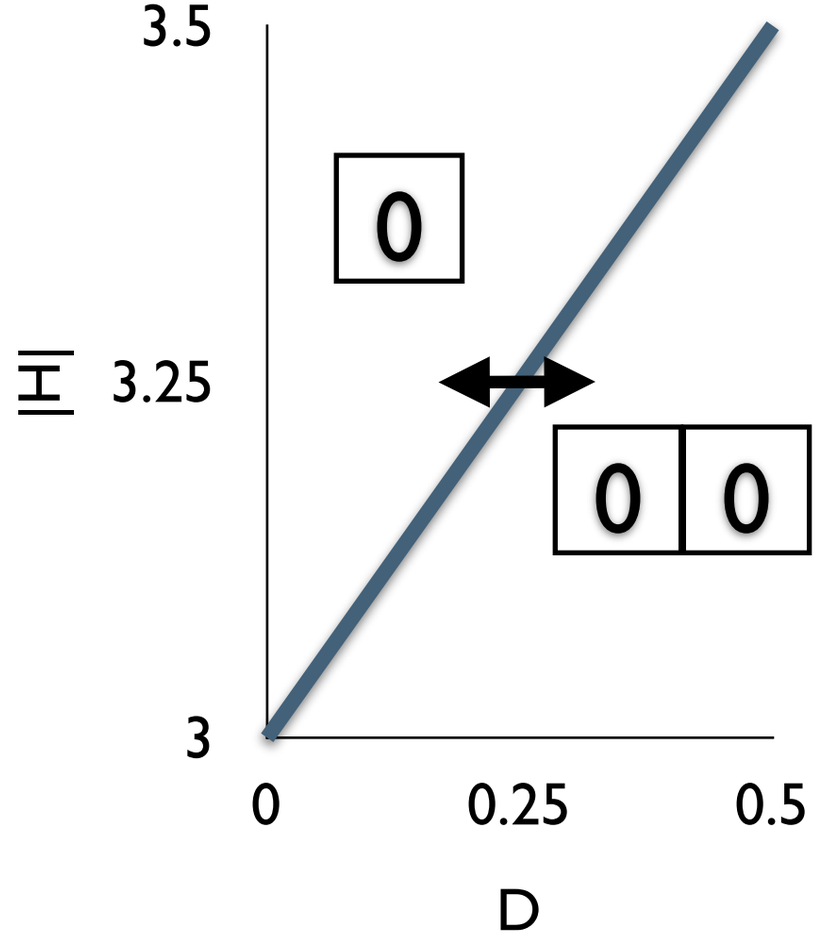
Kinetic Monte Carlo Simulation

- 2D square lattice (L×L) with periodic boundary condition.



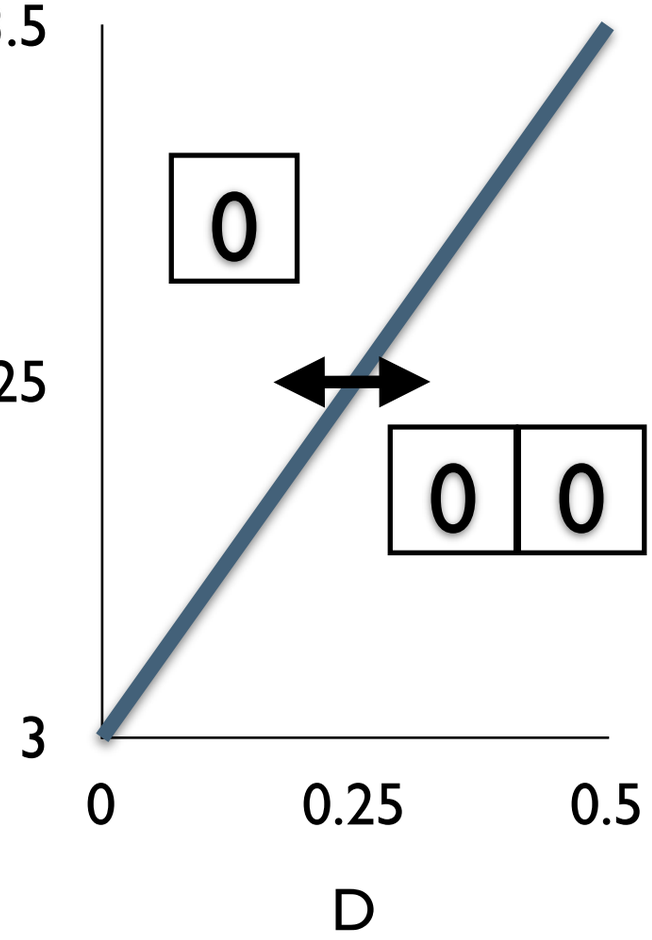
Kinetic Monte Carlo Simulation

- 2D square lattice (L×L) with periodic boundary condition.
- 2000 thermal escapes.



Kinetic Monte Carlo Simulation

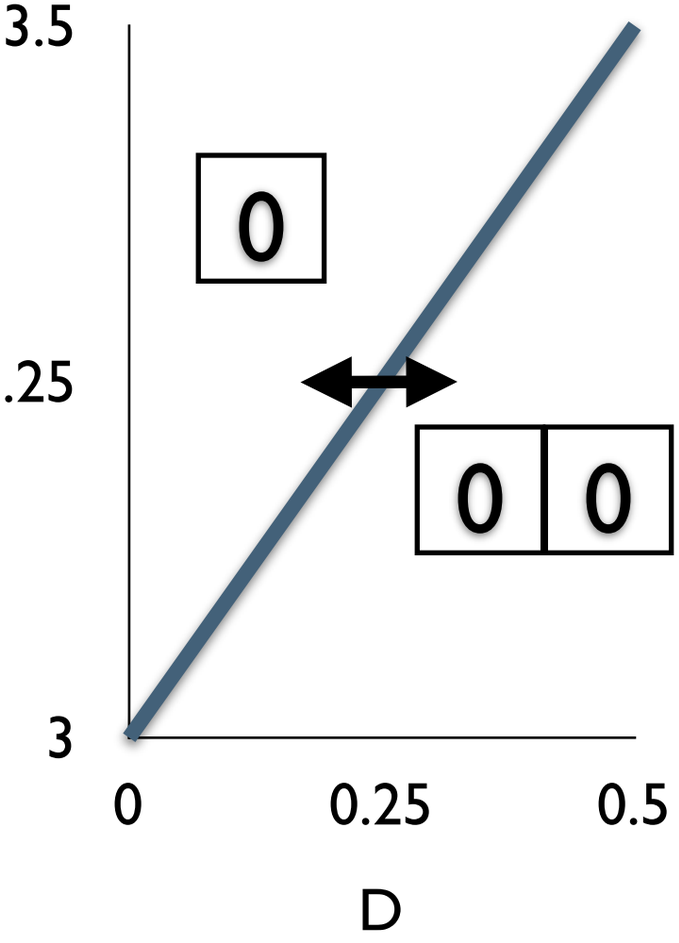
- 2D square lattice (L×L) with periodic boundary condition.
- 2000 thermal escapes.
- A distribution across phase boundary at H=-3.25 (fixed) and D_0=0.25



Kinetic Monte Carlo Simulation

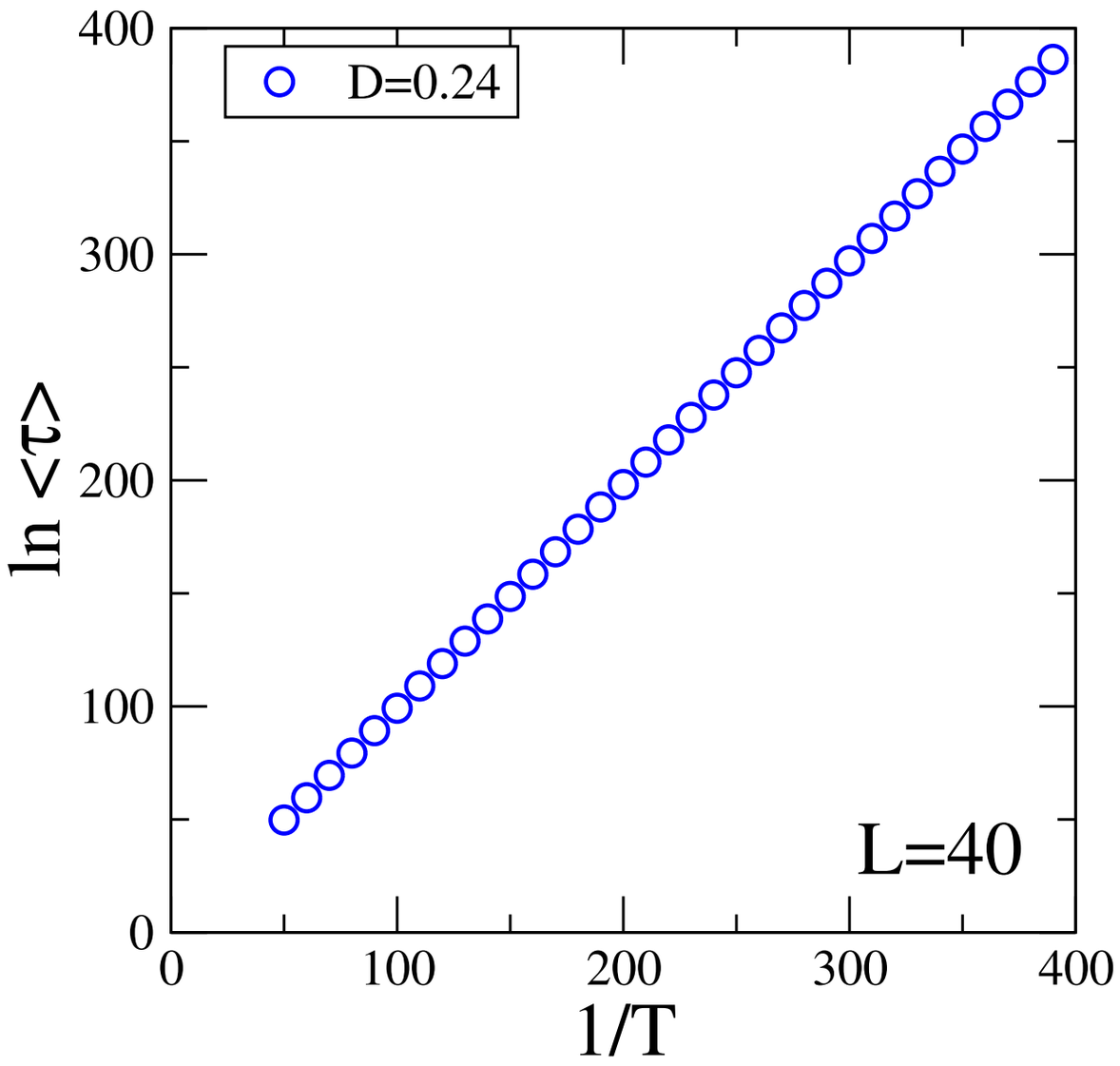
- 2D square lattice (L×L) with periodic boundary condition.
- 2000 thermal escapes.
- A distribution across phase boundary at H=-3.25 (fixed) and D_0=0.25
- Glauber transition rate:

$$W = \frac{1}{1 + e^{(E_{new} - E_{old})/T}}$$



Constant D

|H|=3.25 D=0.24

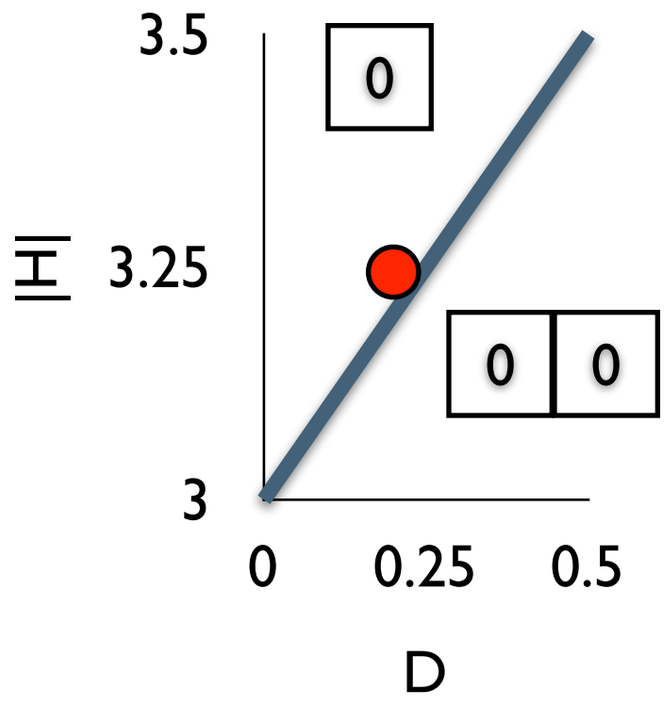


- Average lifetime follows Arrhenius Law

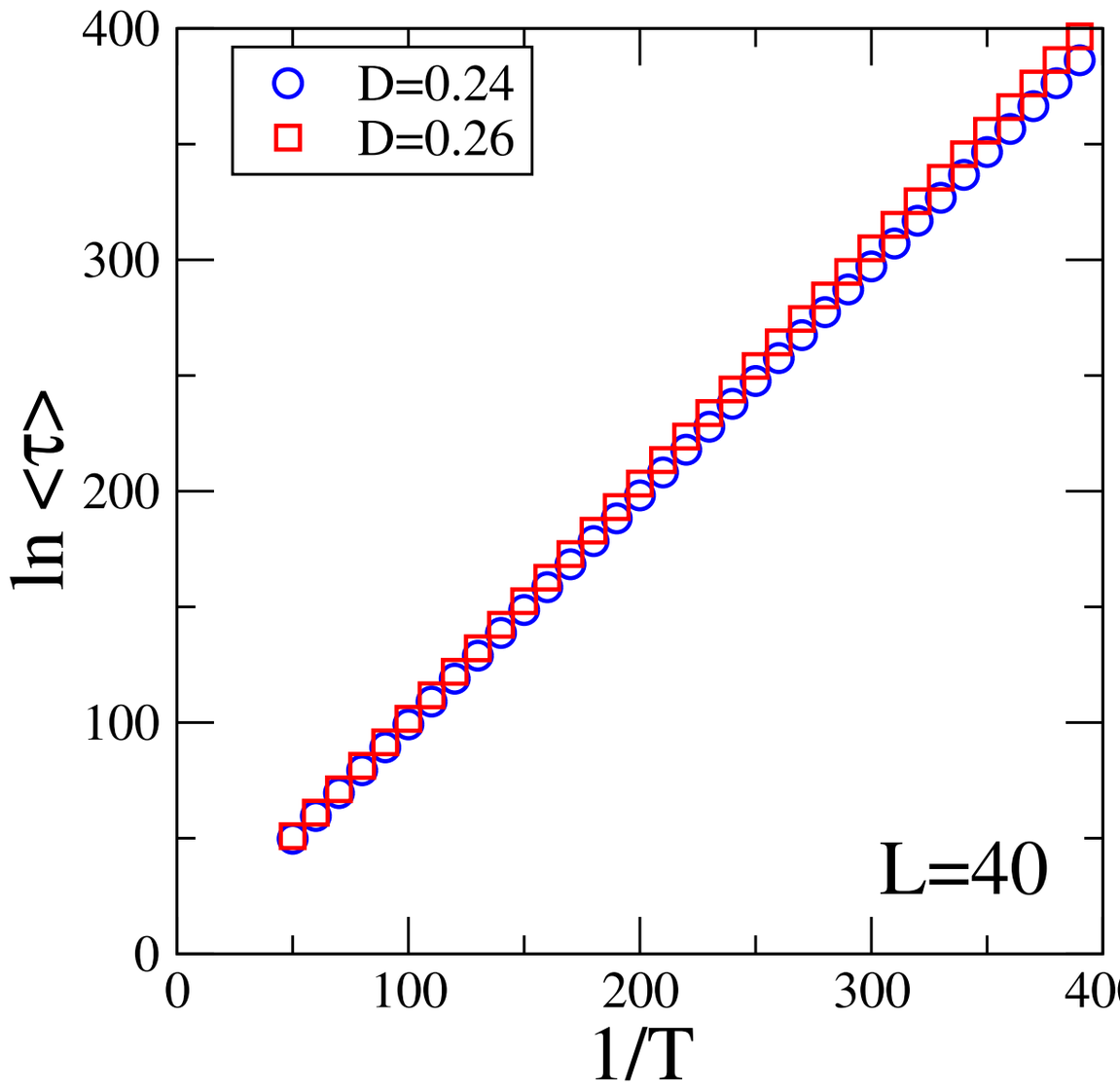
$$\langle \tau \rangle = A e^{\Gamma/T}$$

- Energy barrier Γ=4-|H|+D

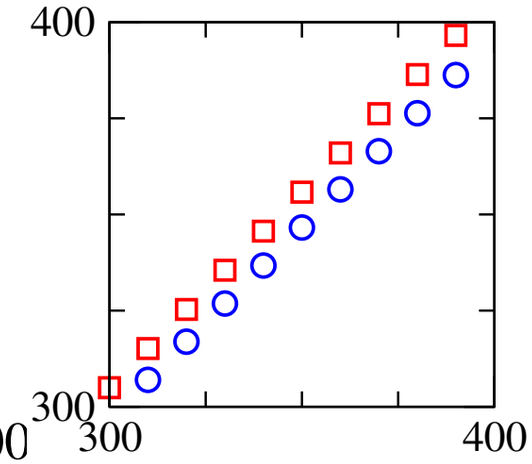
A=9/8

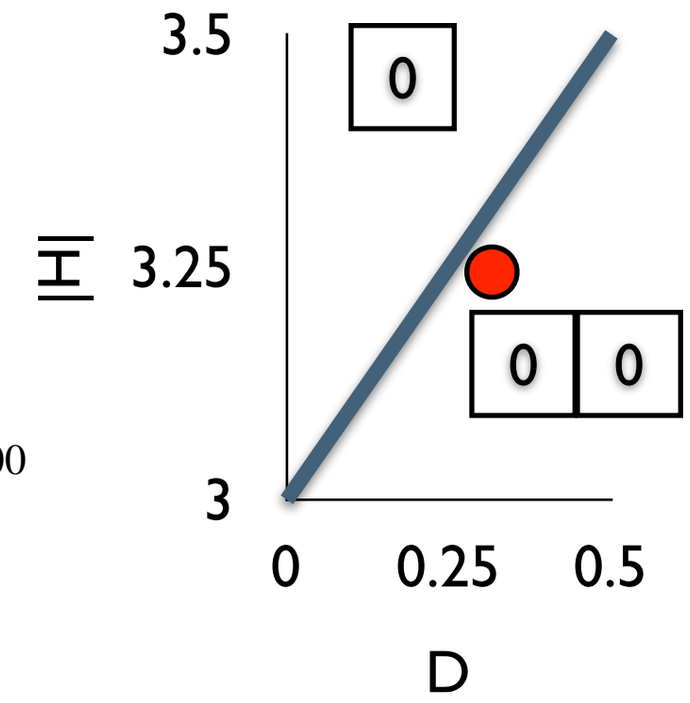


Constant D
|H|=3.25 D=0.26



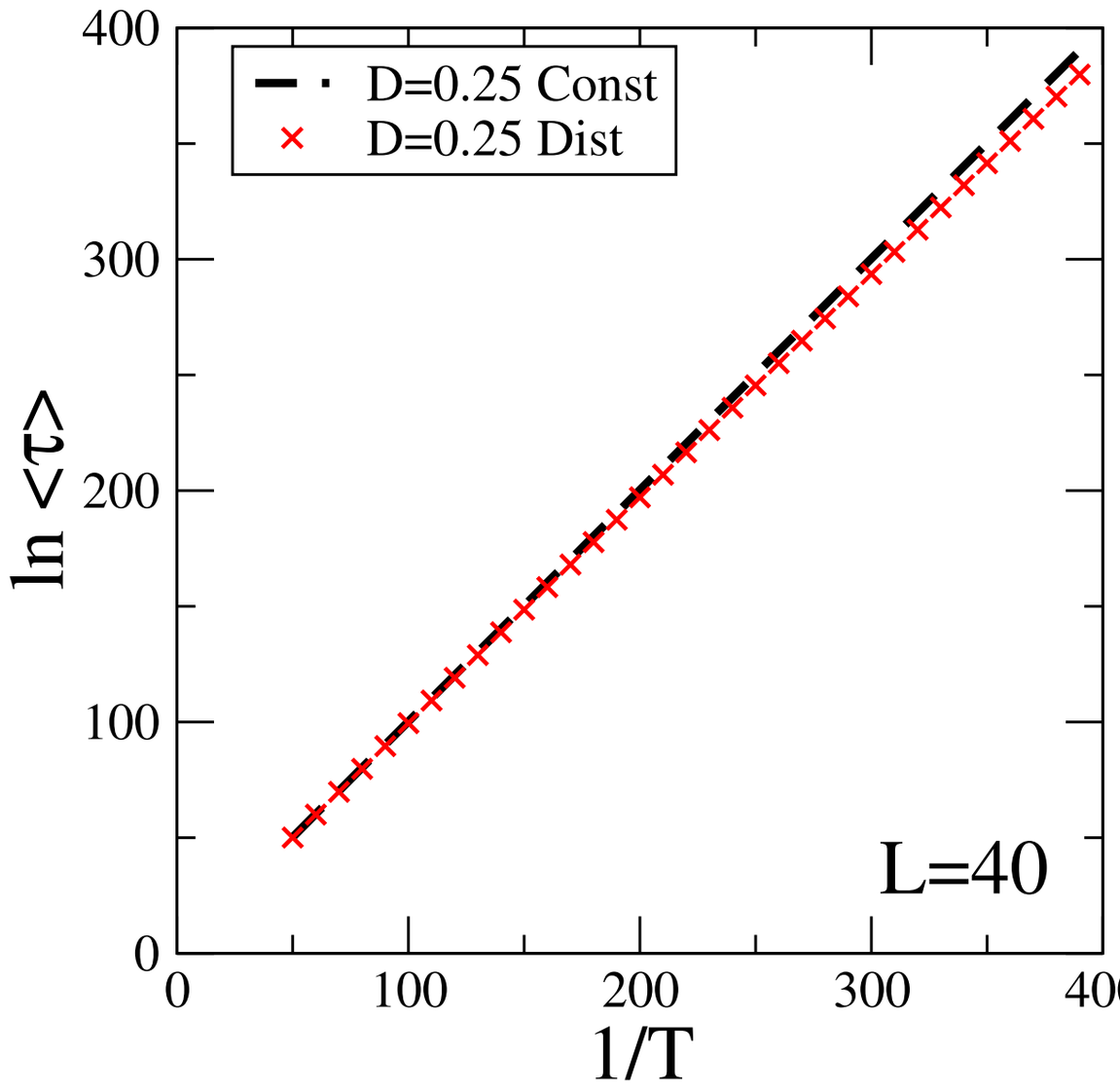
- Larger energy barrier: Γ=7-2|H| +2D

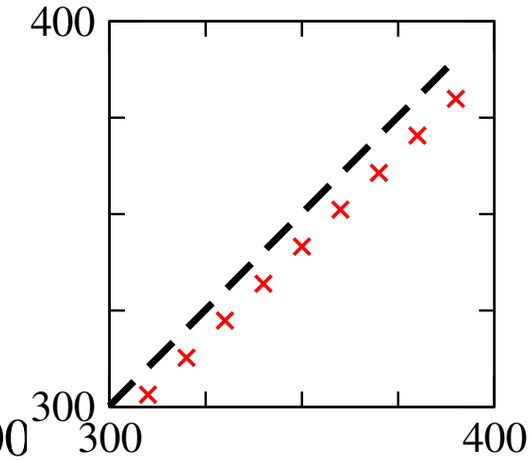




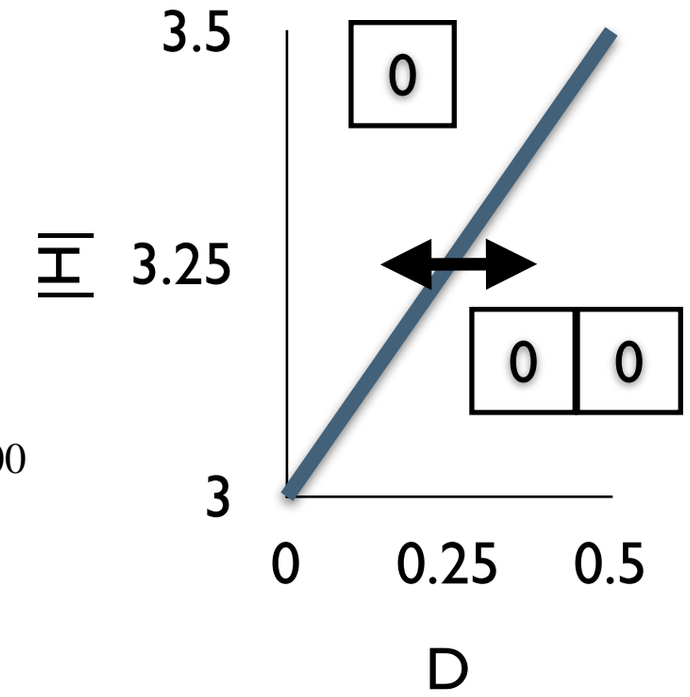
Gaussian Distribution in D

$|H|=3.25$ $D_0=0.25$ $\sigma_D=0.0125$



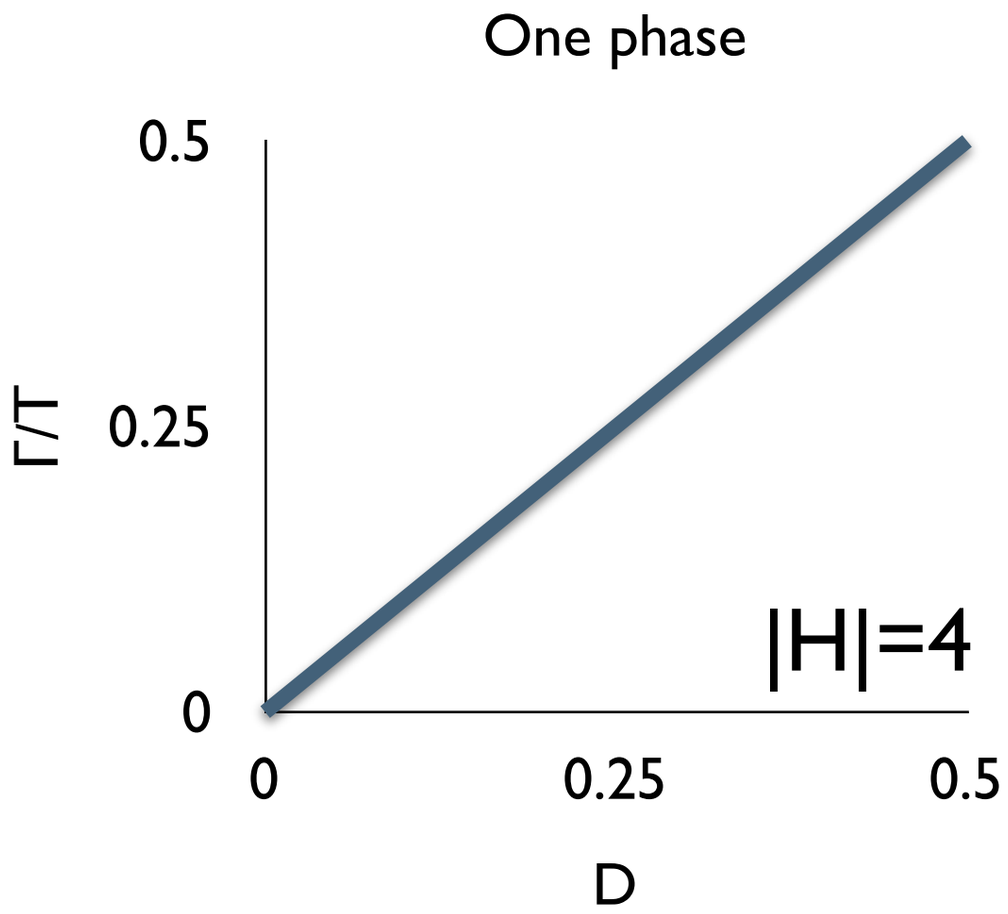


- : Decrease in lifetime with a distribution in D.



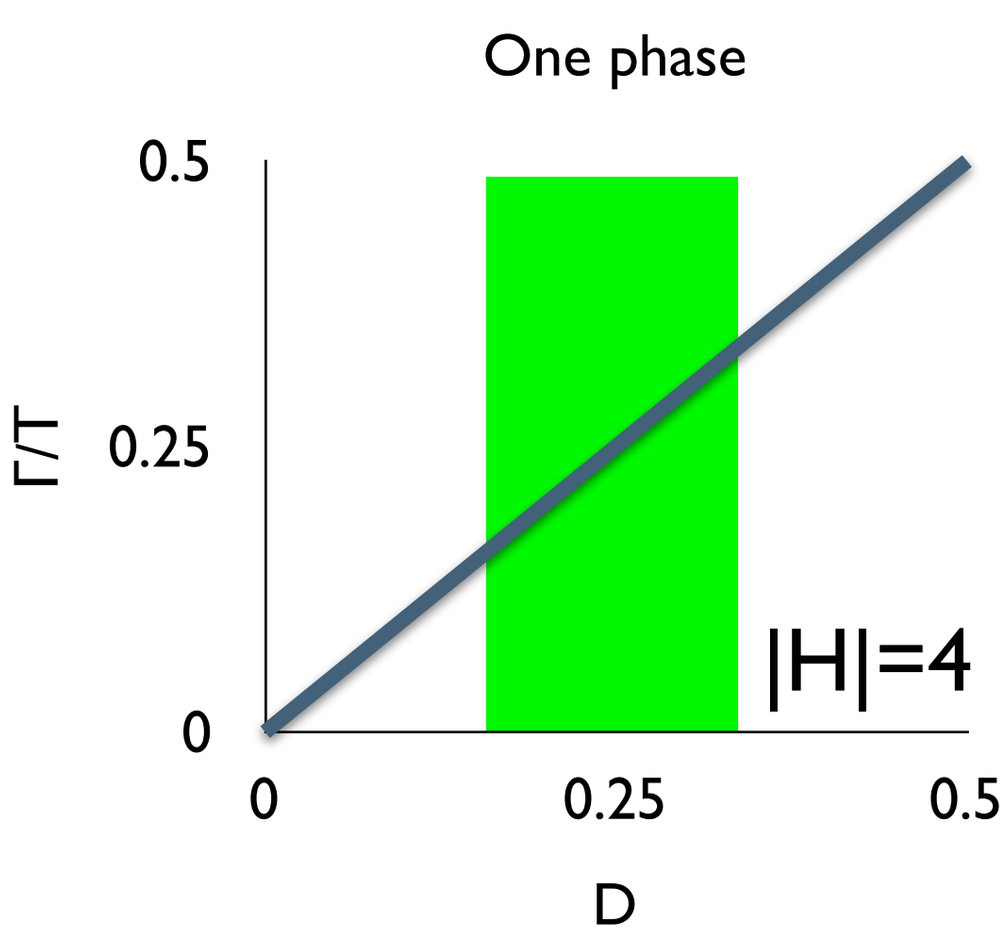
Comparison to Our Previous Study

- Previously, we studied $\boxed{0}$ phase with a distribution in D with fixed |H|=4. (Y.Y. and Park PRB **84**, 094415 (2011))
- Avoid high Γ and prefer low Γ especially in low temperature scenario



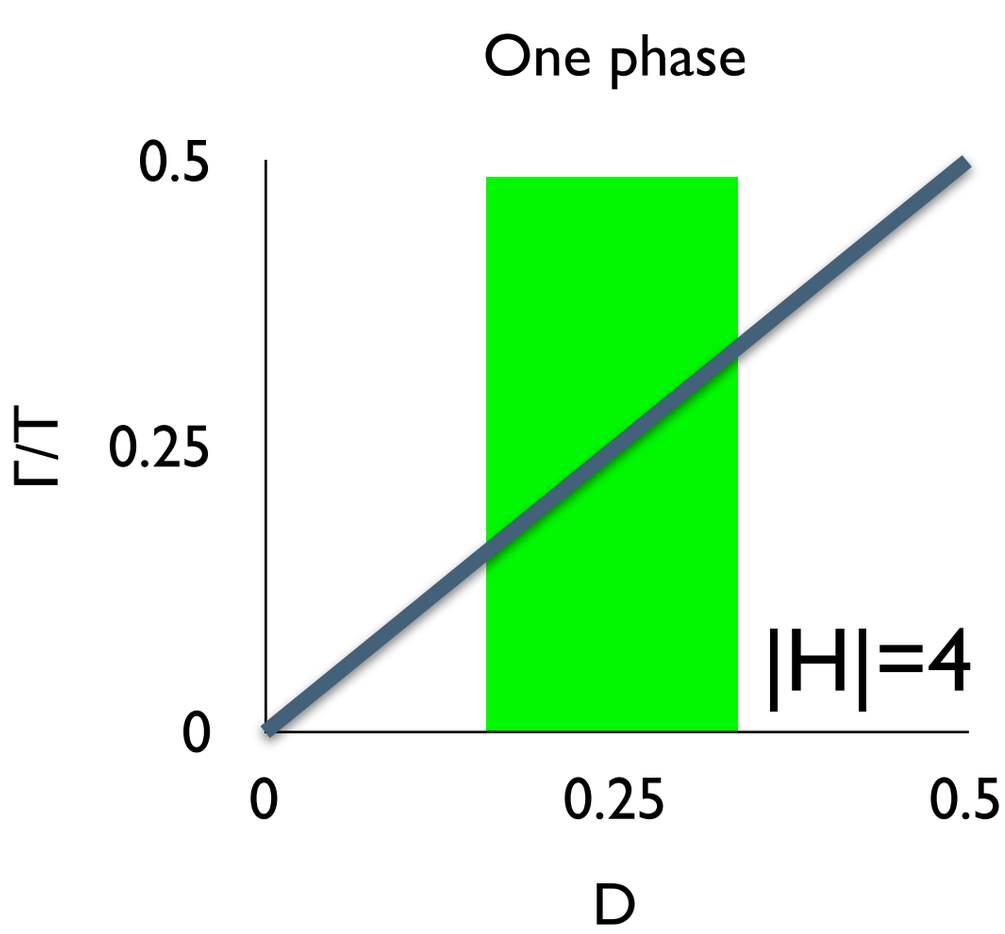
Comparison to Our Previous Study

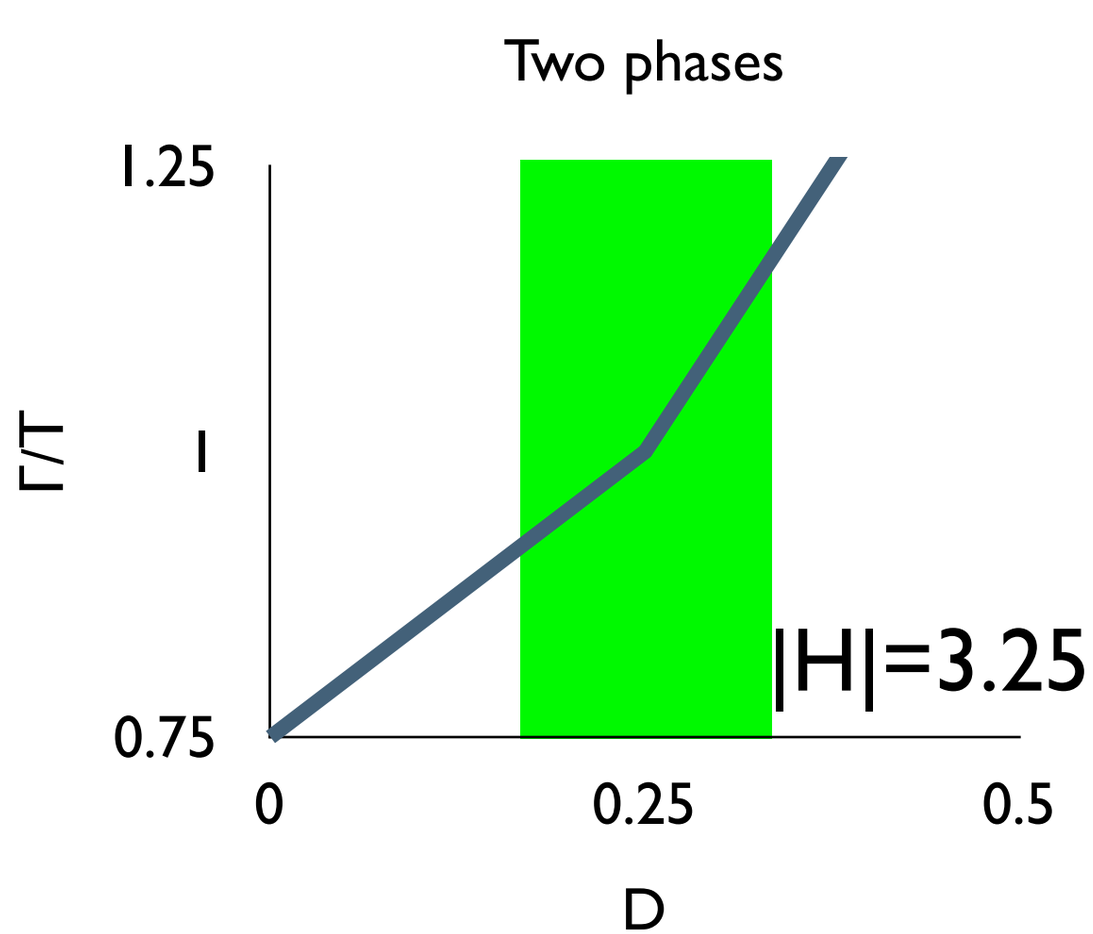
- Previously, we studied $\boxed{0}$ phase with a distribution in D with fixed |H|=4. (Y.Y. and Park PRB **84**, 094415 (2011))
- Avoid high Γ and prefer low Γ especially in low temperature scenario



Comparison to Our Previous Study

- Previously, we studied $\boxed{0}$ phase with a distribution in D with fixed |H|=4. (Y.Y. and Park PRB **84**, 094415 (2011))
- Avoid high Γ and prefer low Γ especially in low temperature scenario





Conclusion

- We find that the average lifetime of the metastable state decreases with distribution in D.
- The phase with smaller critical droplet size (smaller energy barrier) has the most contribution to the lifetime.
- Analytical expression - work in progress.