# Nonuniversal Aspects of Anomalous Diffusion with Absorption

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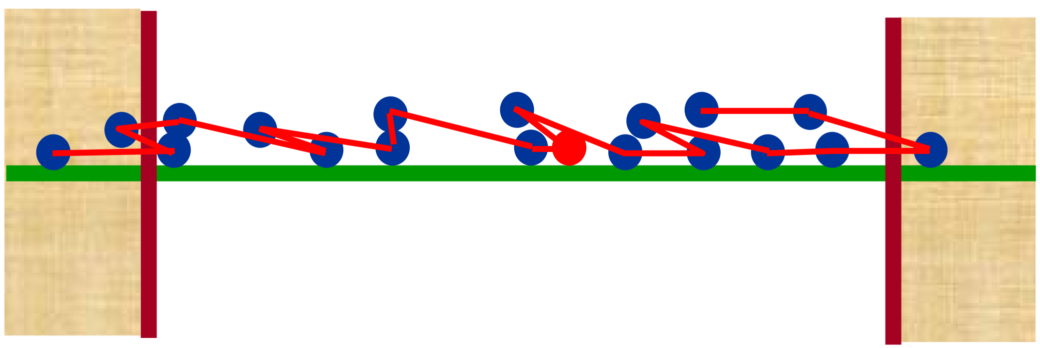
**Tel Aviv University**



with

**Mehran Kardar**, MIT

**Assaf Amitai**, TAU

**Clément Chatelain**, ENS Cachan

**Jeffrey Chuang**, BC

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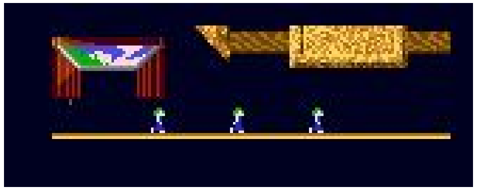
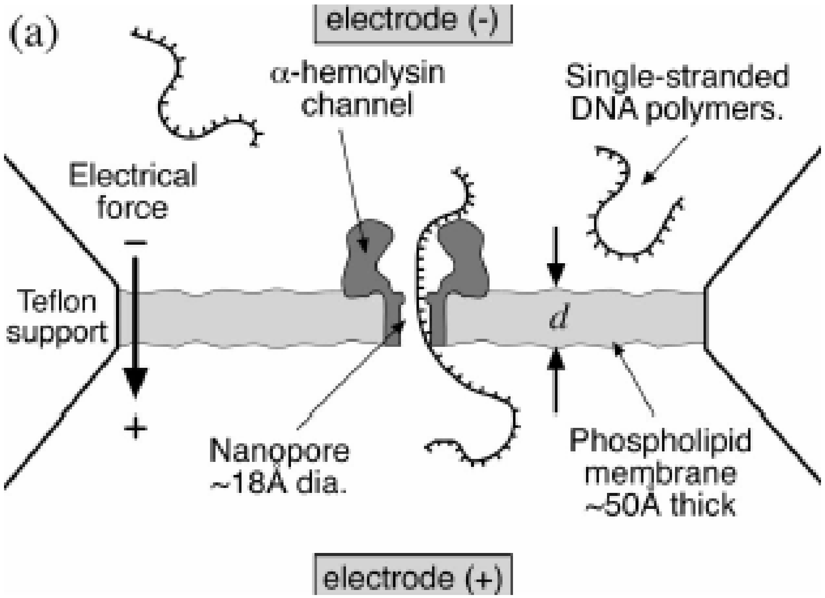
Workshop on "Steady-states, fluctuations and dynamics of non equilibrium systems," June 2009, Weizmann/Technion

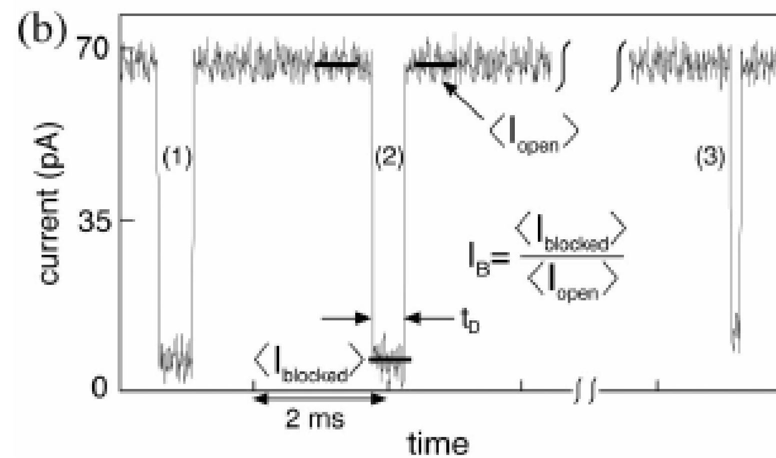
# Outline

- *Translocation of a polymer through a pore*
- *Translocation as an anomalous diffusion*
- *Anomalous dynamics of monomers*
- *Anomalous dynamics with controlled exponent*
- *Absorbing boundaries – translocation vs. monomer diffusion*
- *How (non)universal is anomalous diffusion?*
- *Conclusions*



# *Measuring translocation of a polymer*



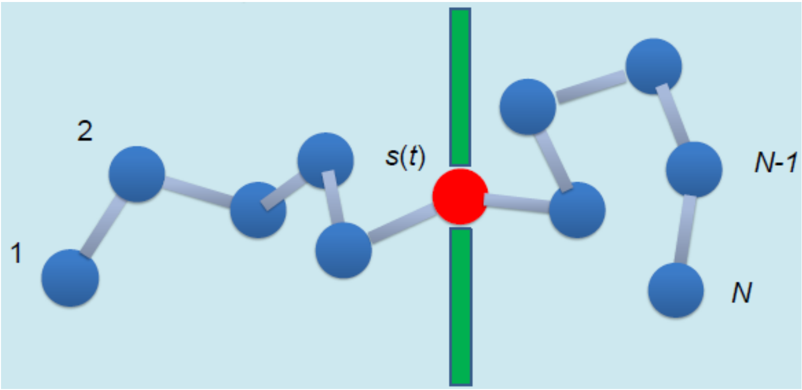

Single-stranded DNA molecules (negatively charged) are electrically driven through a pore

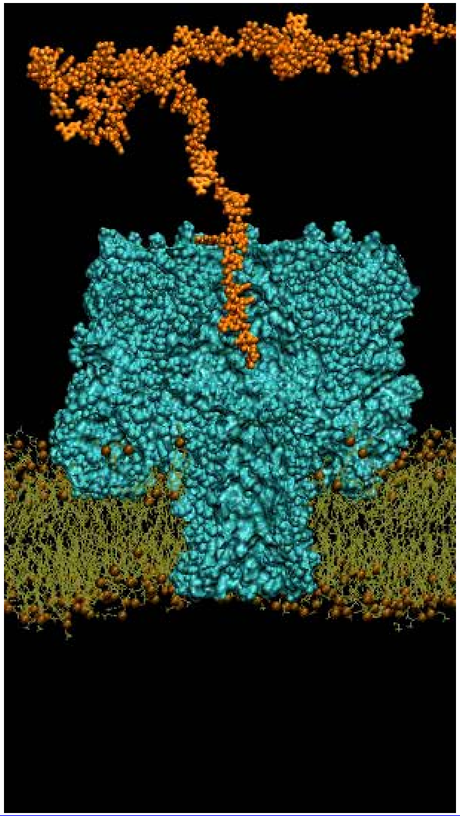
Meller, Nivon, Branton PRL **86**, 3435 (2001)

Bates, Burns, Meller Biophys.J., **84**,2366 (2003)

# *"Translocation" – the simplest problem*

*Find mean translocation time & its distribution as a function of N, forces, properties of the pore*



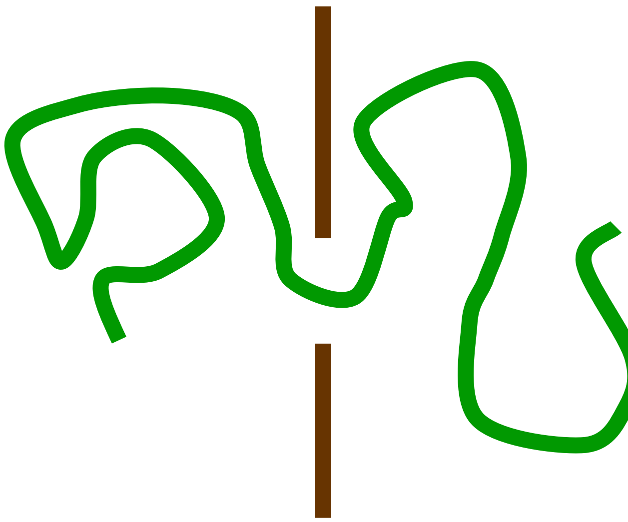



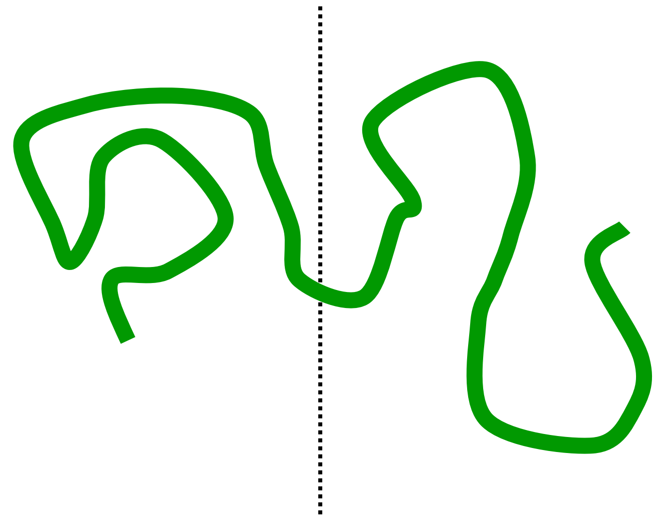
A. Aksimentiev, K. Schulten

Theor.&Comp.Biophys.Group

Urbana-Champaign

# *Translocation vs. free diffusion*





$$\tau \sim N^2$$

$$R_g^2 \approx aN^{2\nu} \quad R_g^2 \approx D_{\text{polymer}}\tau = \frac{D_0}{N}\tau$$

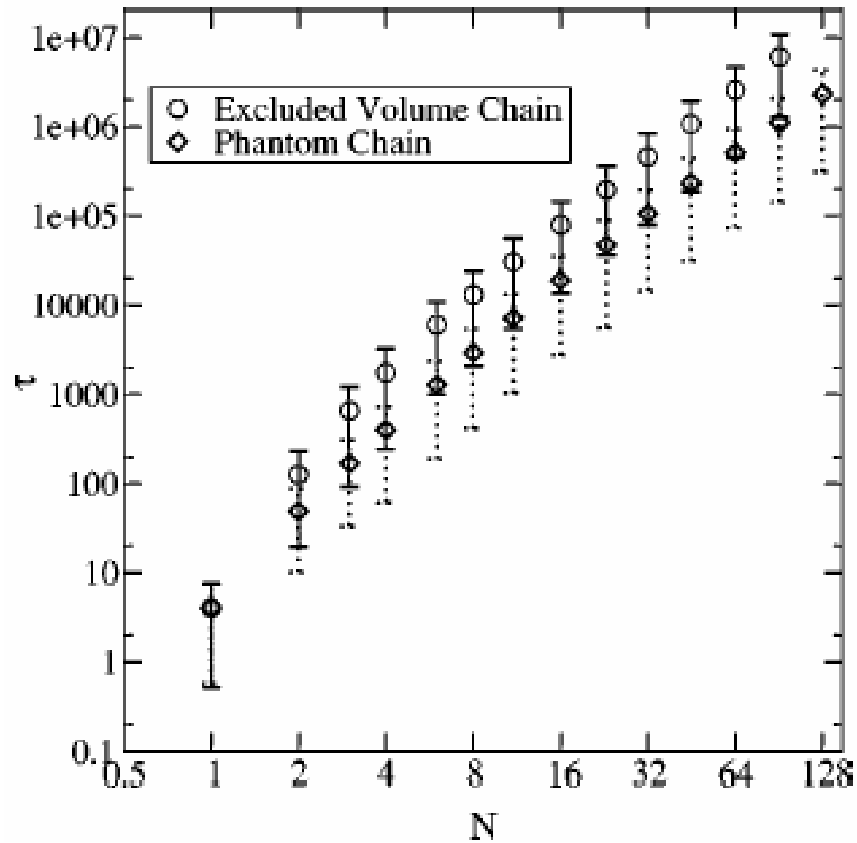
$$\tau \sim N^{1+2\nu} \quad (1+2\nu = 2.5,\, 2.18 \text{ for } d = 2,3)$$

*Translocation is faster than free diffusion!???*

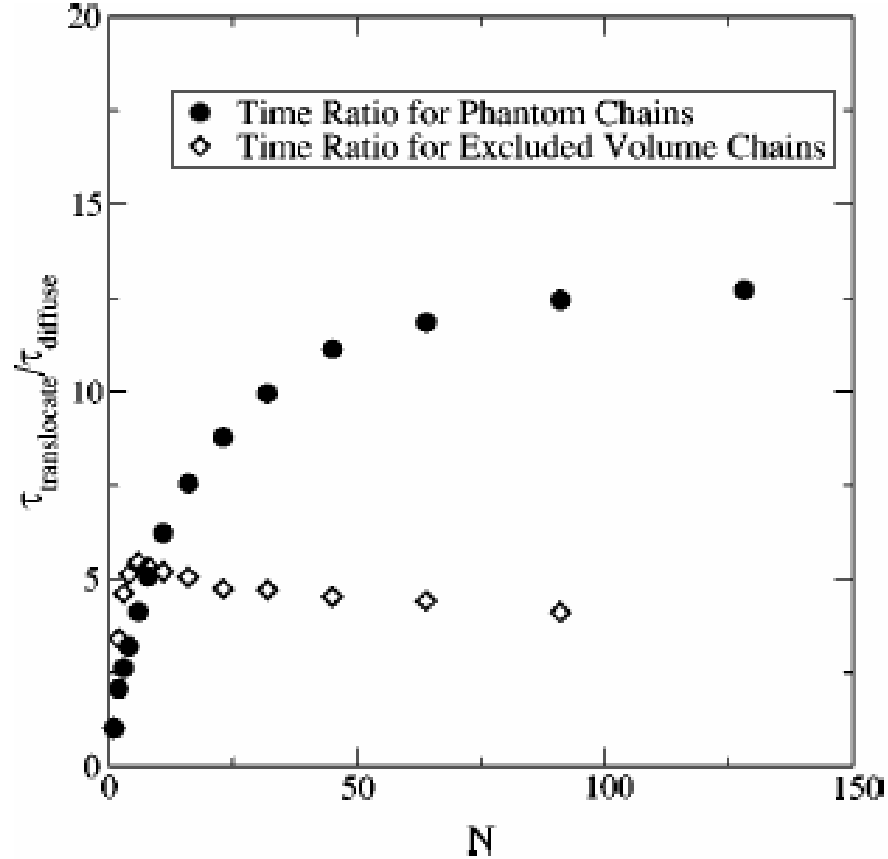
Sung, Park, PRL **77**, 783 (1996);
Muthukumar, JCP **111**, 10371 (1999)

Chuang, Kantor, Kardar,
PRE **65**, 011892 (2001)

# Translocation time of 2D polymer



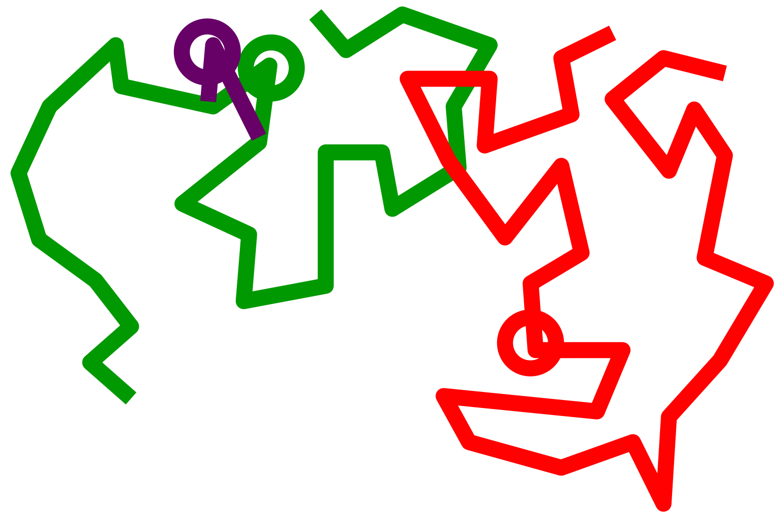

Translocation time of 2D phantom & self-avoiding polymers (averaged over 10,000 cases)




Ratio between translocation times of 2D phantom and self-avoiding polymers with and without membrane

Chuang, Kantor, Kardar, PRE **65**, 011892 (2001)

# *Anomalous diffusion of a monomer*



$$\langle r^2(t)\rangle = 2dD_0 t, \qquad \text{for } t < t_{\text{micro}}$$

$$\langle r^2(t)\rangle = 2dD_{\text{polymer}} t, \quad \text{for } t > \tau$$

$$R_g^2 \approx D_{\text{polymer}}\tau = \frac{D_0}{N}\tau, \text{ in Rouse regime}$$

$$\langle r^2(t)\rangle \approx a^{2-2\alpha}(D_0 t)^\alpha, \text{ for } t_{\text{micro}} < t < \tau$$

$$\alpha = \frac{2\nu}{1+2\nu}$$

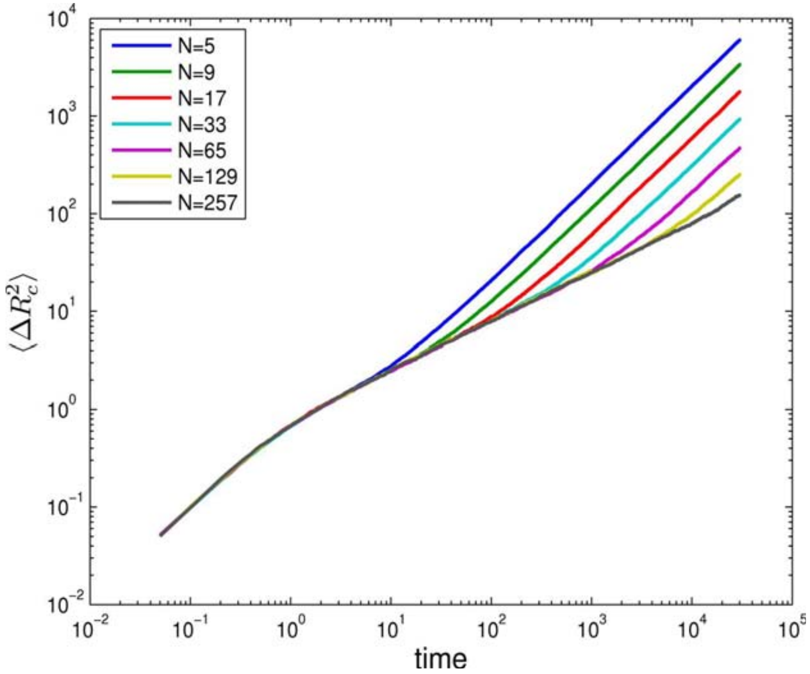
$$\alpha = \tfrac{1}{2}, \qquad \text{for phantom polymer}$$

$$\alpha = \tfrac{3}{5}, \qquad \text{for 2D SAW}$$

$$\alpha = 0.54, \quad \text{for 3D SAW}$$

Kremer, Binder, JCP **81**, 6381 (84);
Grest, Kremer, PR **A33**, 3628 (86);
Carmesin, Kremer, Macromol. **21**, 2819 (88)

# Anomalous diffusion of a monomer (contn'd)




$$\left\langle r^2(t)\right\rangle = 2dD_0 t, \qquad \text{for } t < t_{\text{micro}}$$

$$\left\langle r^2(t)\right\rangle = 2dD_{\text{polymer}} t, \quad \text{for } t > \tau$$

$$R_g^2 \approx D_{\text{polymer}}\tau = \frac{D_0}{N}\tau, \text{ in Rouse regime}$$

$$\left\langle r^2(t)\right\rangle \approx a^{2-2\alpha}(D_0 t)^{\alpha}, \text{ for } t_{\text{micro}} < t < \tau$$

A.Amitai, M.Sc. Thesis (2009)

# Anomalous translocation of a polymer

$$\left\langle \Delta s^2(t=\tau) \right\rangle \approx N^2$$

$$R_g^2 \approx D_{\text{polymer}}\tau = \frac{D_0}{N}\tau, \text{ in Rouse regime}$$

$$\tau \approx N R_g^2 / D_0 \sim N^{1+2\nu}$$

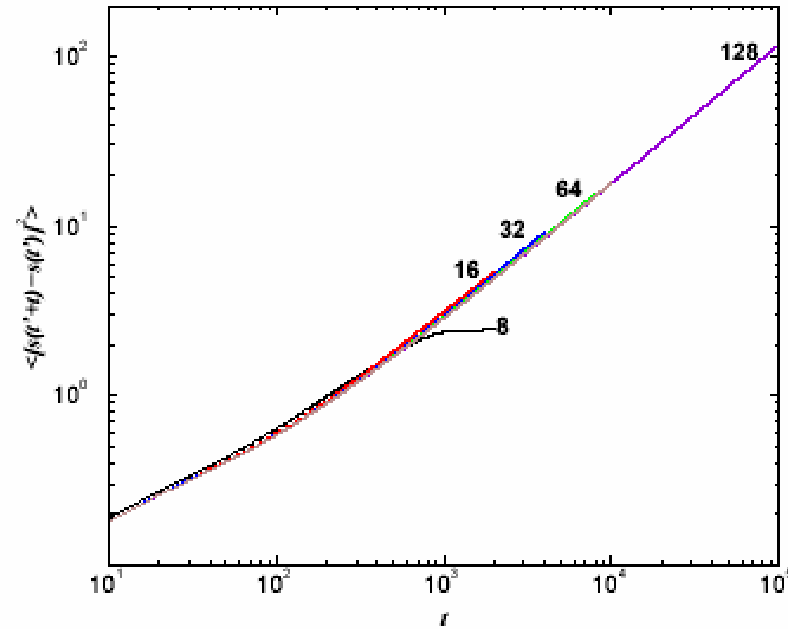
$$\left\langle \Delta s^2(t) \right\rangle \sim t^{\alpha}, \qquad \text{for } t < \tau$$

$$\alpha = \frac{2}{1+2\nu}$$

$$\alpha = 1, \qquad \text{for phantom polymer}$$

$$\alpha = \tfrac{4}{5}, \qquad \text{for 2D self-avoiding polymer}$$

$$\alpha = 0.92, \text{ for 3D self-avoiding polymer}$$



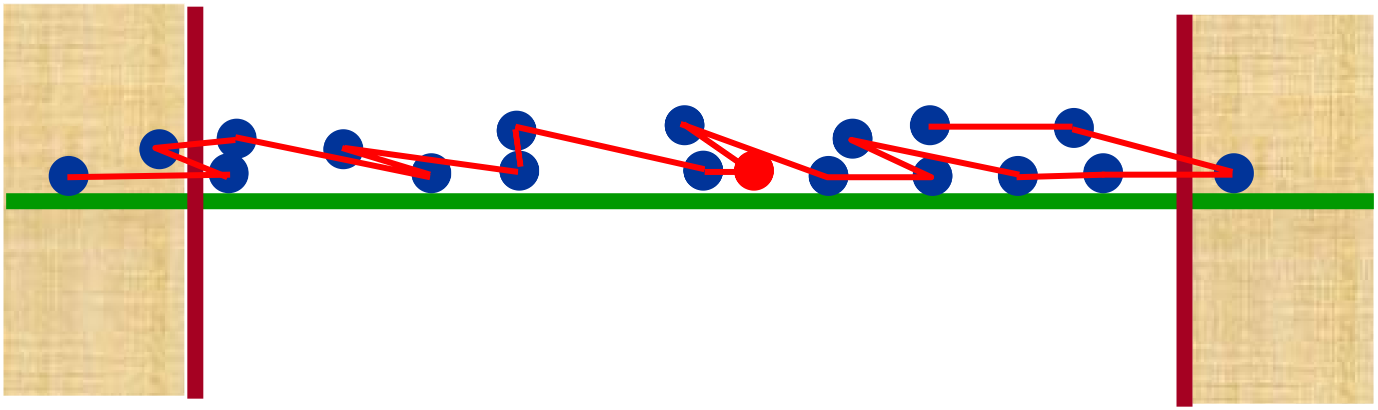

Time dependence of fluctuations in translocation coordinate in 2D self-avoiding polymer. The slope approaches 0.80.

Kantor, Kardar,

PRE **69**, 21806 (2004)

Chuang, Kantor, Kardar,
PRE **65**, 011892 (2001)

# *Diffusion of a monomer in 1D phantom polymer*



$$H = \frac{\kappa}{2}\sum_{n=1}^{N-1}\left(R_{n+1} - R_n\right)^2$$

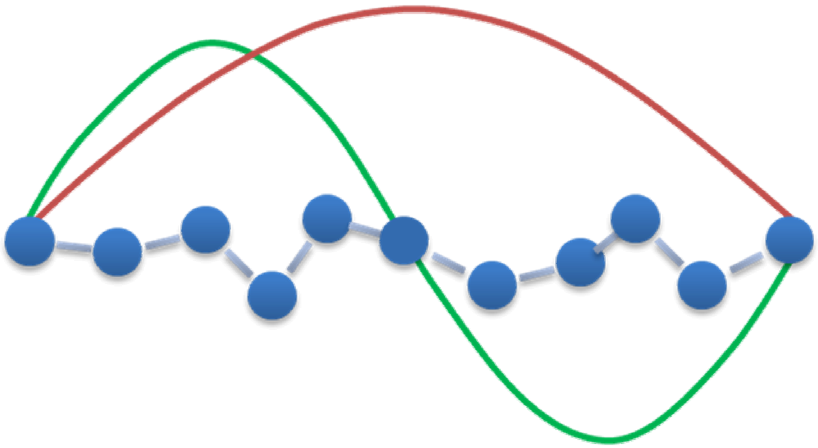
$$\zeta\frac{dR_n}{dt} = -\kappa(2R_n - R_{n+1} - R_{n-1}) + f_n$$

Y. Kantor, M. Kardar, PRE **76**, 61121 (2007)

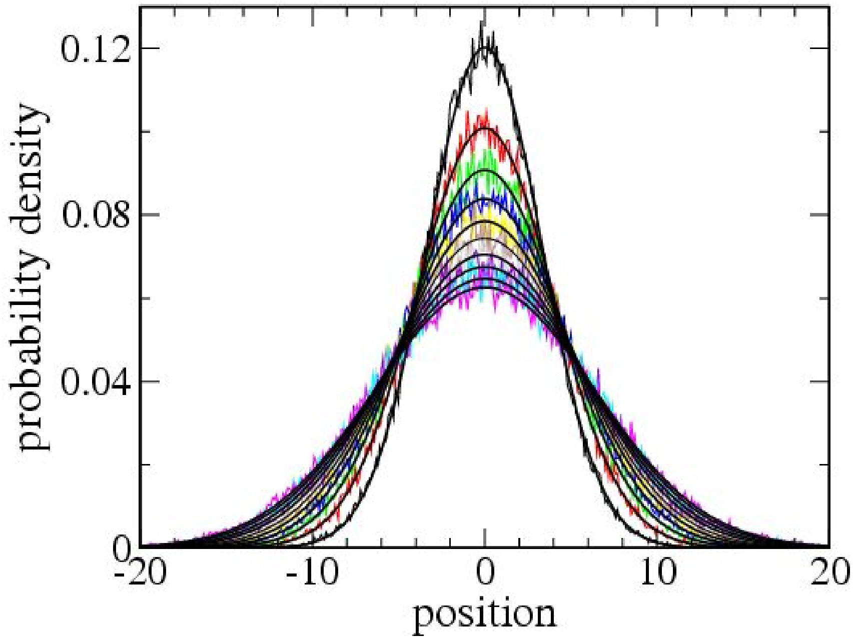
# Rouse (Fourier) modes of polymer

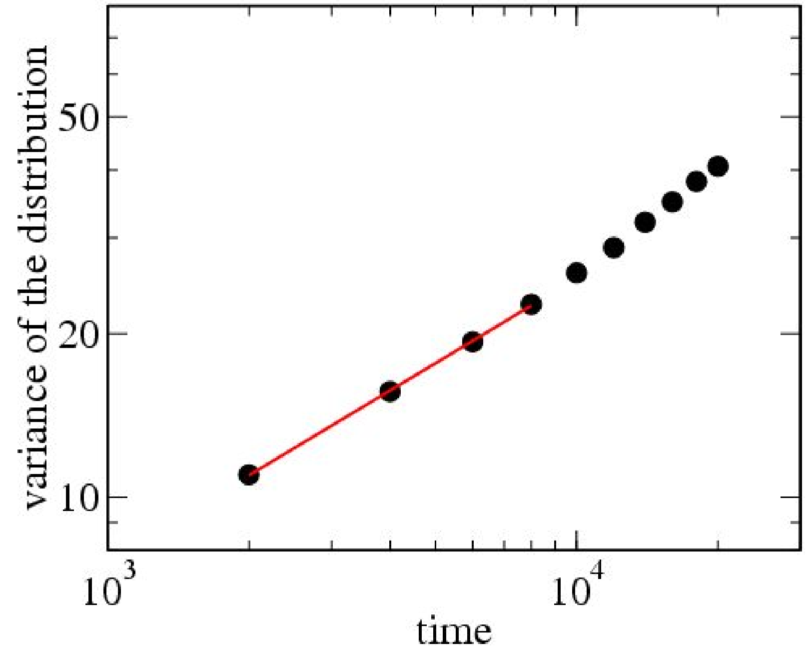
$$\zeta \frac{\partial R_n}{\partial t} = -\kappa\left(2R_n - R_{n+1} - R_{n-1}\right) + f_n(t)$$

$$u_q = \frac{1}{N}\sum_{n=1}^{N} R_n \cos\left(n - \frac{1}{2}\right)\frac{q\pi}{N}$$



# "Normal" anomalous diffusion of a monomer




$$u_q = \frac{1}{N}\sum_{n=1}^{N} R_n \cos[q(n-\tfrac{1}{2})]$$

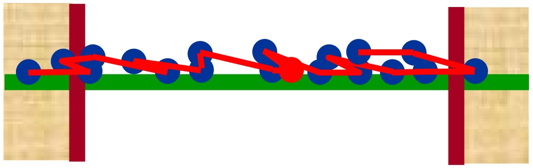
$$\left\langle R_c^2 \right\rangle \sim t^{1/2}$$

$$\zeta_q \frac{\partial u_q}{\partial t} = -\kappa_q u_q + W_q \qquad \kappa_q = 8N\kappa \sin^2\left(\frac{q\pi}{2N}\right) \qquad \zeta_q = 2N\zeta \qquad \zeta_0 = N\zeta$$

$$\left\langle W_q(t)\right\rangle = 0 \qquad \left\langle W_p(t) W_q(t')\right\rangle = 2k_B T \zeta_q \delta(t-t')\delta_{p,q}$$

Y. Kantor, M. Kardar, PRE **76**, 61121 (2007)

# Controlled anomalous diffusion of a monomer

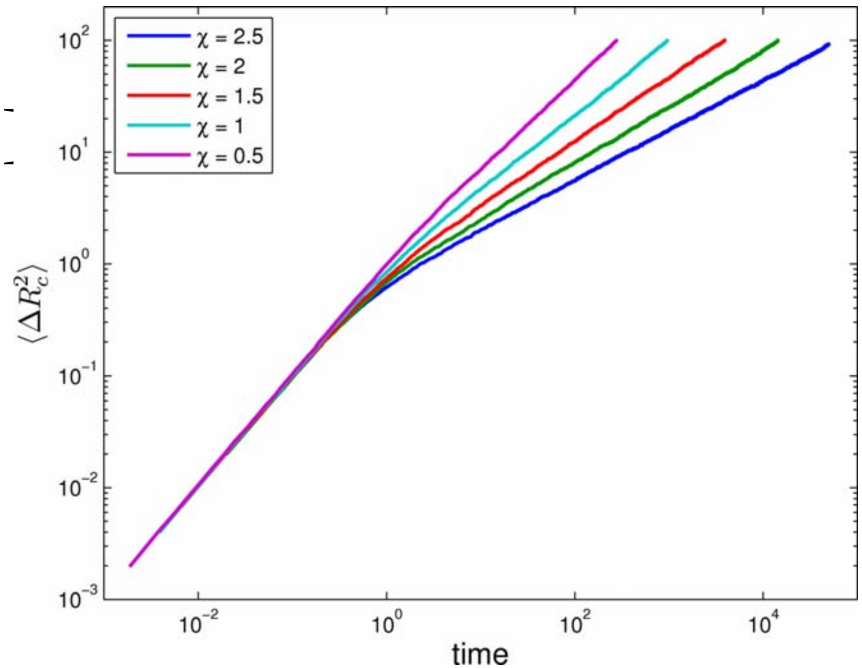


$$\zeta_q \frac{\partial u_q}{\partial t} = -\kappa_q u_q + W_q \qquad \zeta_q = 2CN\zeta\left(\frac{q}{N}\right)^{1-\chi/2} \qquad \zeta_0 = \zeta N^{\chi/2}$$

$$u_q = \frac{1}{N}\sum_{n=1}^{N} R_n \cos[q(n-\tfrac{1}{2})]$$

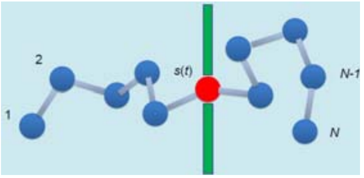
$$\left\langle \Delta R_c^2 \right\rangle \sim t^{\alpha}$$

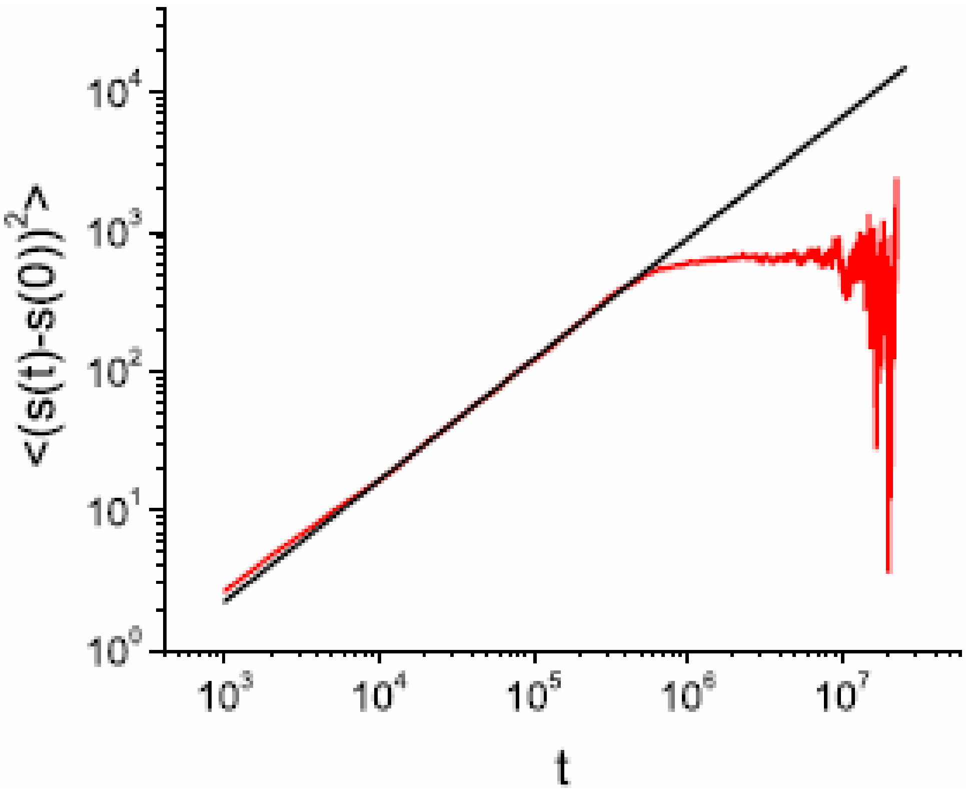
$$\alpha = \frac{2}{2+\chi}$$




A.Amitai, M.Sc. Thesis (2009)

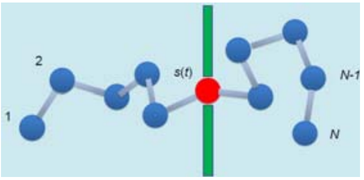
# *Time-dependence of the variance of the translocation coordinate*

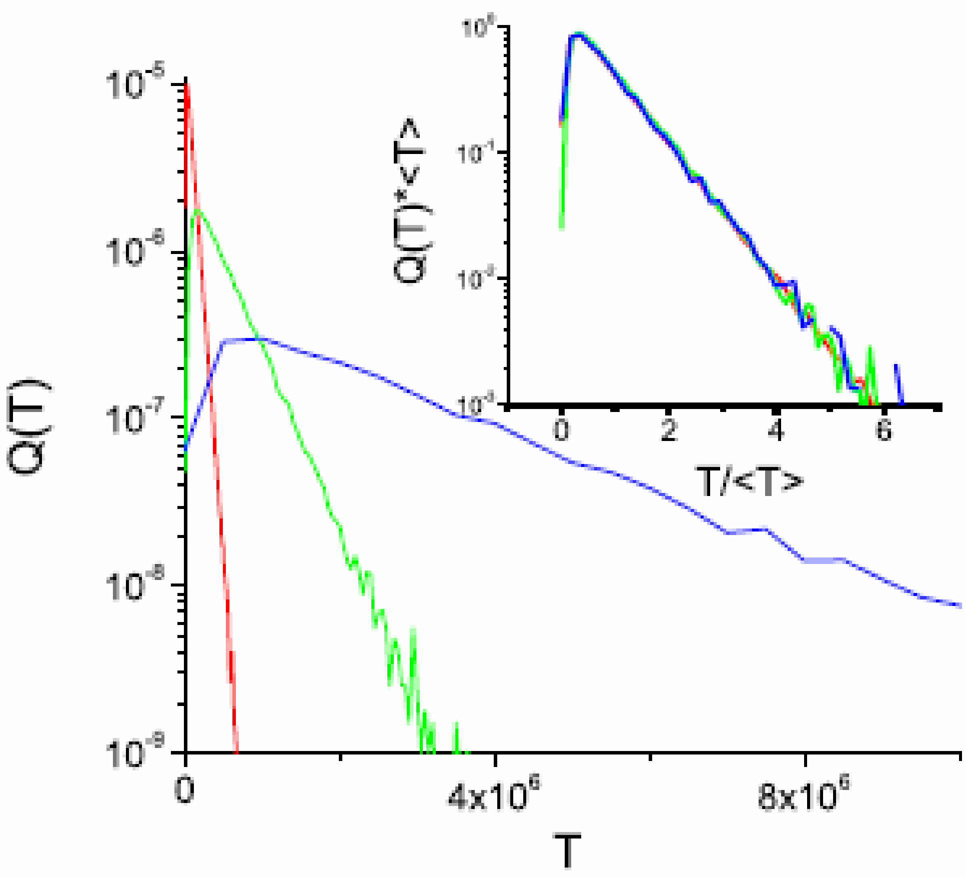



C.Chatelain, Y. Kantor, M. Kardar PRE78, 021129 (2008)

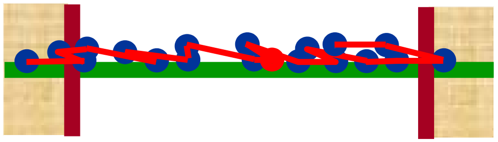
# *Translocation time distribution for self-avoiding polymer in 2D*

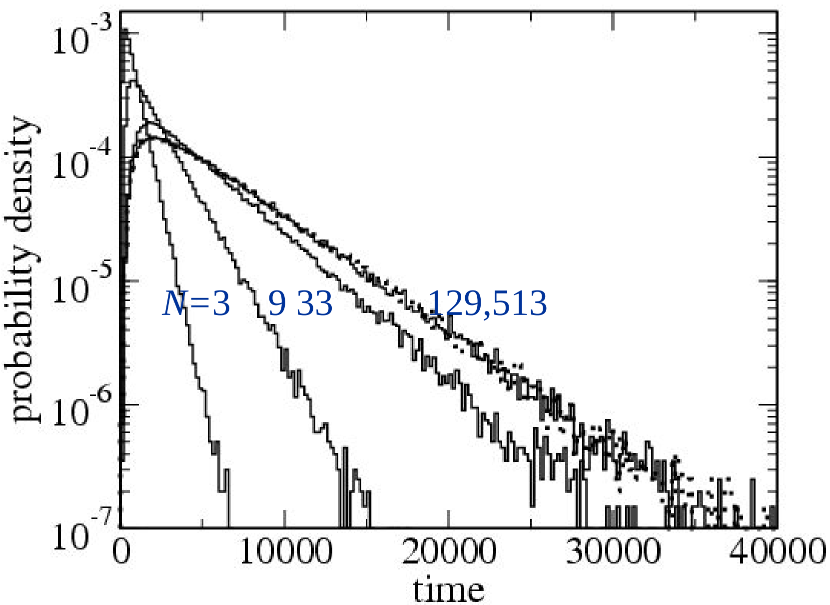


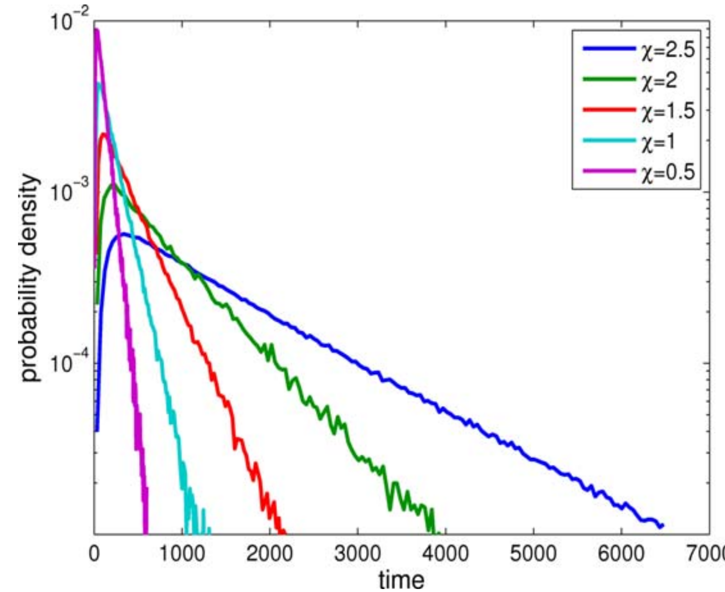

C.Chatelain, Y. Kantor, M. Kardar PRE78, 021129 (2008)

# *Monomer with two absorbing boundaries*






Y. Kantor, M. Kardar, PRE **76**, 61121 (2007)




A.Amitai, M.Sc. Thesis (2009)

$$Q(t) \sim \mathrm{e}^{-At}$$

HOWEVER:

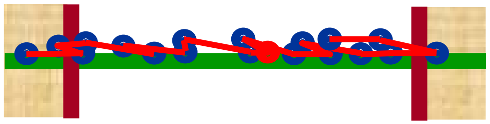
S. Nechaev et al. J.Stat.Phys. **98**, 281 (2000),

G. Oshanin arXiv:0801.0676 & 0801.2914

PREDICTION

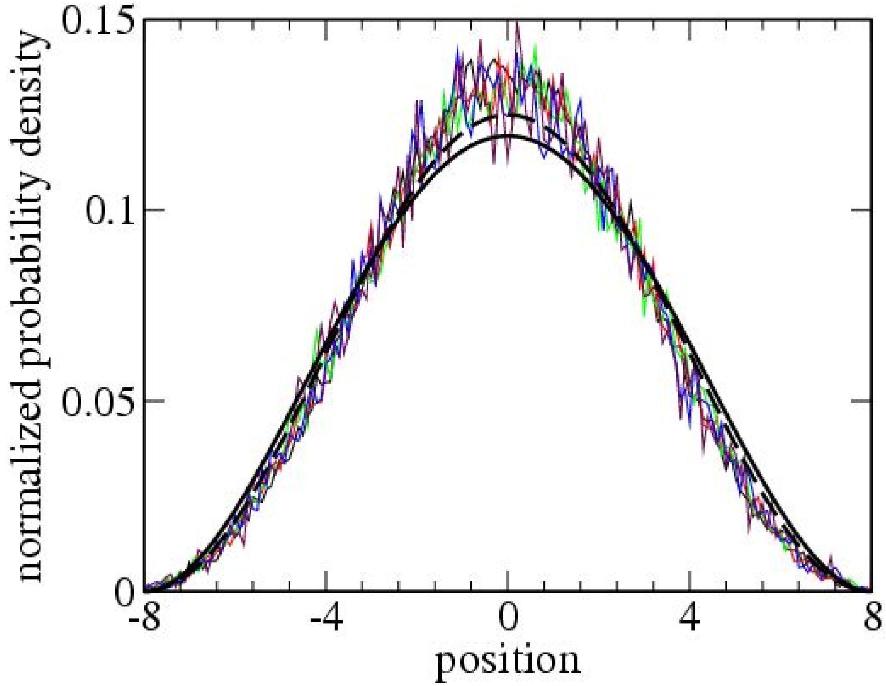
$$Q(t) \sim \mathrm{e}^{-Ct^{1/2}}$$

# *The "slowest mode"*



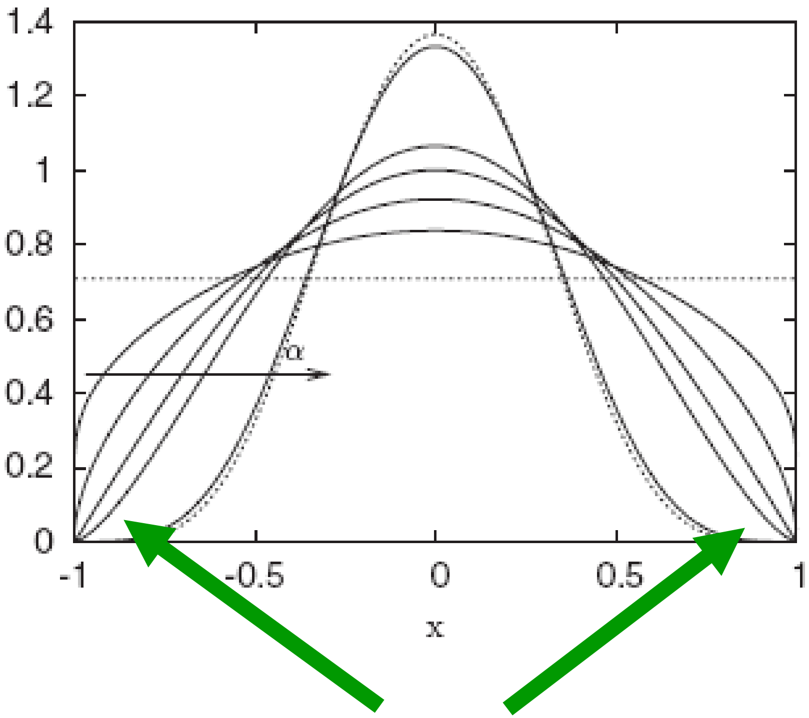
For a normal diffuser

$$P(r,t)=\sum_{n=1}^{\infty}A_n\cos\left(\frac{2n\pi r}{L}\right)\exp\left(-\left(\frac{n\pi}{L}\right)^2 Dt\right)$$




$$\alpha=\frac{1}{2}$$

# *Fractional Laplacian with Absorbing Boundaries*




$$(1-|x|)^{1/\alpha}$$

$$\frac{\partial P(x,t)}{\partial t} = \frac{\partial^{2/\alpha}}{\partial |x|^{2/\alpha}} P(x,t) \equiv -(-\Delta)^{\alpha} P(x,t)$$

$$\frac{\partial^{2/\alpha}}{\partial |x|^{2/\alpha}} \mathrm{e}^{iqx} = -|q|^{2/\alpha}\ \mathrm{e}^{iqx}$$

$$Q(t) \sim \mathrm{e}^{-t/\tau}$$


A. Zoia, A. Rosso, M. Kardar, PRE **76**, 21116 (2007).

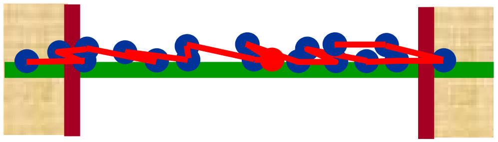
A. Bottcher, H. Widom J.Math.Anal.Appl. **322**, 990 (2006) & Operator Theory: Adv. And Appl. **171**, 73 (2006)

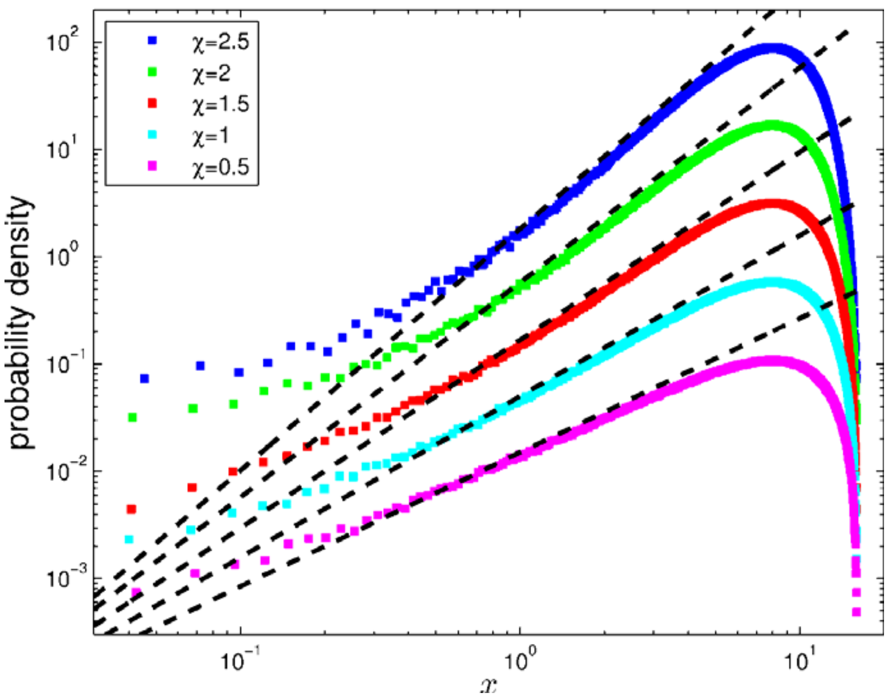
A. Ramani, B. Grammaticos, Y. Pomeau, J.Phys.A**40**, F391 (2007)

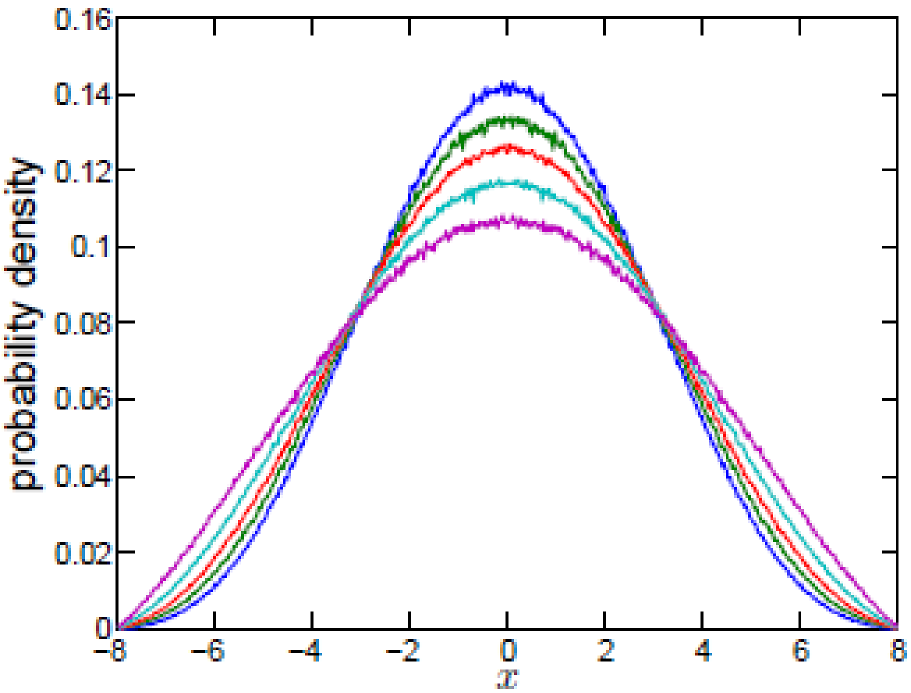
E. Katzav and M. Adda-Bedia, arXiv:0711.2518 (2007)

G. Zumhofen and J. Klafter, Phys. Rev. E**51**, 2805 (1995)

# *Two absorbing boundaries – "the slowest mode"*






$$p \sim (x - x_b)^{\phi}$$

plotted slopes $\phi = 1/\alpha$

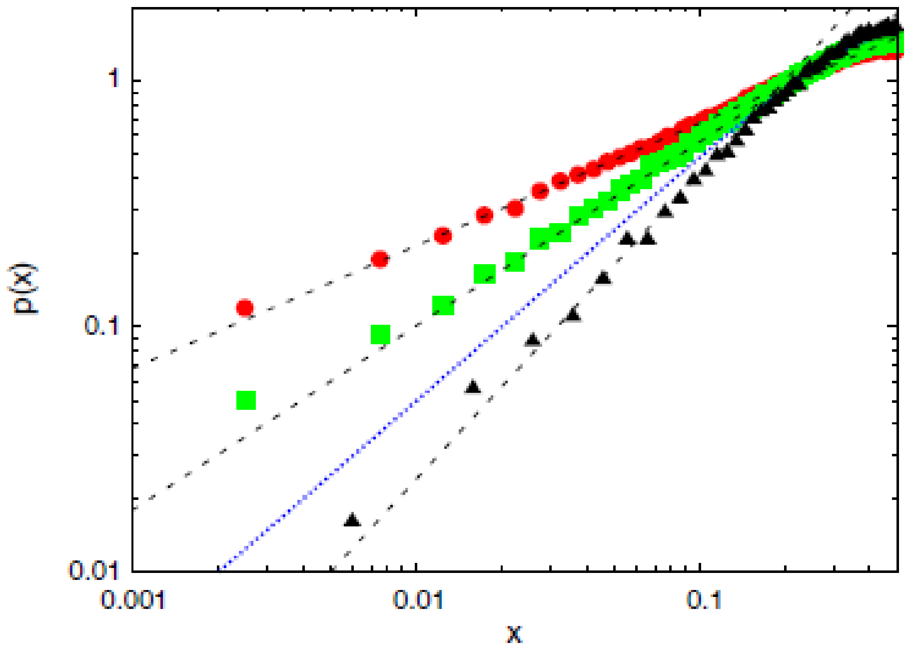
$$\alpha = \frac{2}{2+\chi}$$

Y. Kantor, M. Kardar, PRE **76**, 61121 (2007)

A.Amitai, Y.Kantor, M.Kardar (2009)

# *Anomalous diffusion generated by Langevin equation*

$$\zeta \frac{\Delta R}{\Delta t} = f(t), \quad \langle f \rangle = 0, \quad \langle f(t) f(t+k\Delta t) \rangle \sim |k-1|^{\alpha} + |k+1|^{\alpha} - 2|k|^{\alpha}$$

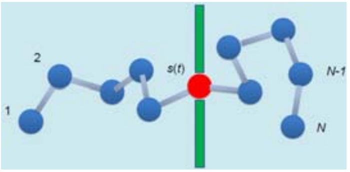


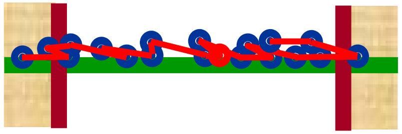

$$p \sim (x - x_b)^{\phi}$$

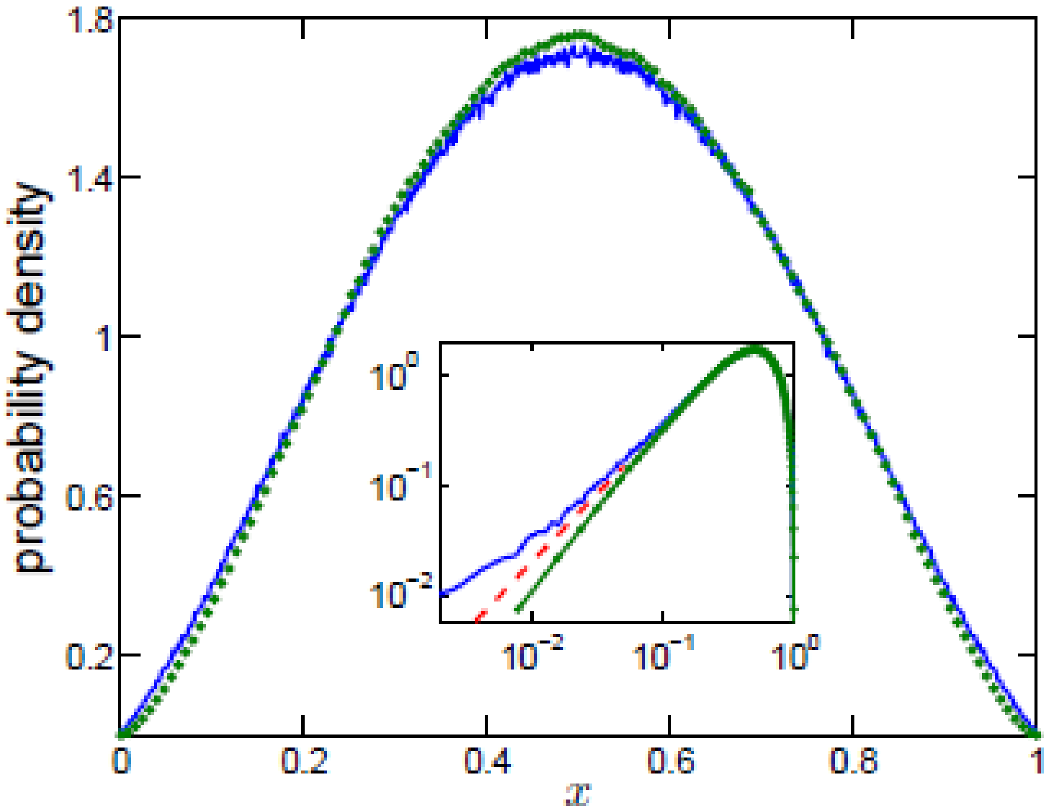
$$\phi = \frac{2-\alpha}{\alpha} \text{(compare with } \phi = 1/\alpha\text{)}$$

A.Zoia,A.Rosson,S.Majumdar, PRL**102**, 120602(2009)

# *Long-time distribution of translocation variable*

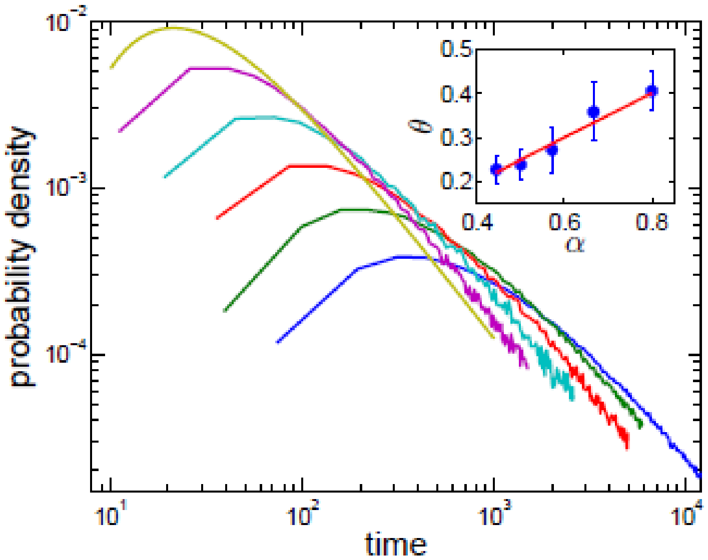


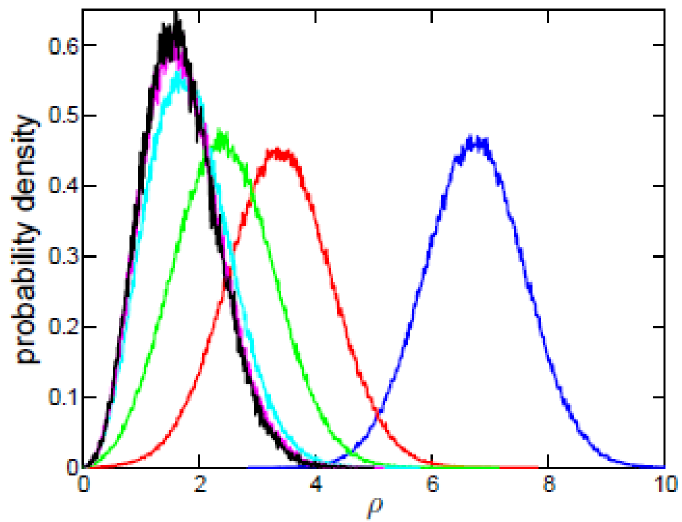






C.Chatelain, Y. Kantor, M. Kardar PRE78, 021129 (2008)

# *One absorbing boundary – the stationary state*




$$Q(t) \sim t^{-1-\theta}$$

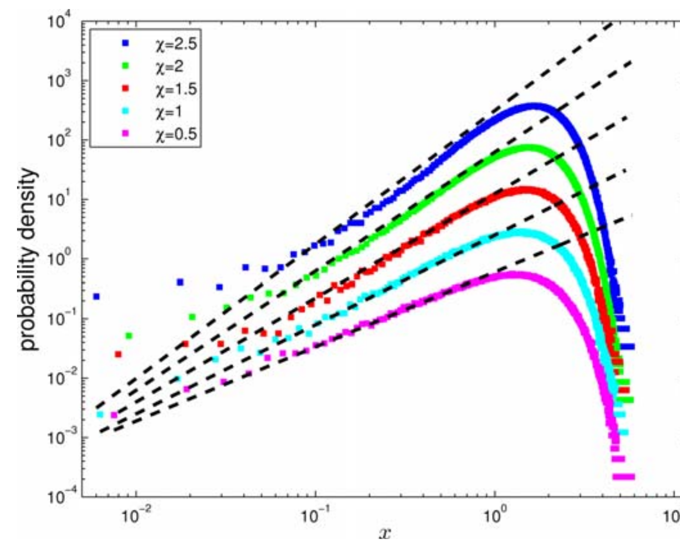
$$\text{(for nomal diffuser } \theta = \frac{1}{2}\text{)}$$

$$\text{we get } \theta \approx \alpha / 2$$

Compare with $\theta = 1 - \alpha / 2$

Krug, Kallabis, Majumdar, Cornell, Bray, Sire, PRE 56, 2702 (1997).

$$\rho = x / t^{\alpha/2}$$




$$p \sim (x - x_b)^{\phi}$$

$$\text{plotted slopes } \phi = 1/\alpha$$

# *Anomalous diffusion generated by Langevin equation*

$$\zeta \frac{\Delta R}{\Delta t} = f(t), \quad \langle f \rangle = 0, \quad \langle f(t) f(t+k\Delta t) \rangle \sim |k-1|^{\alpha} + |k+1|^{\alpha} - 2|k|^{\alpha}$$

$$p \sim (x - x_b)^{\phi}$$

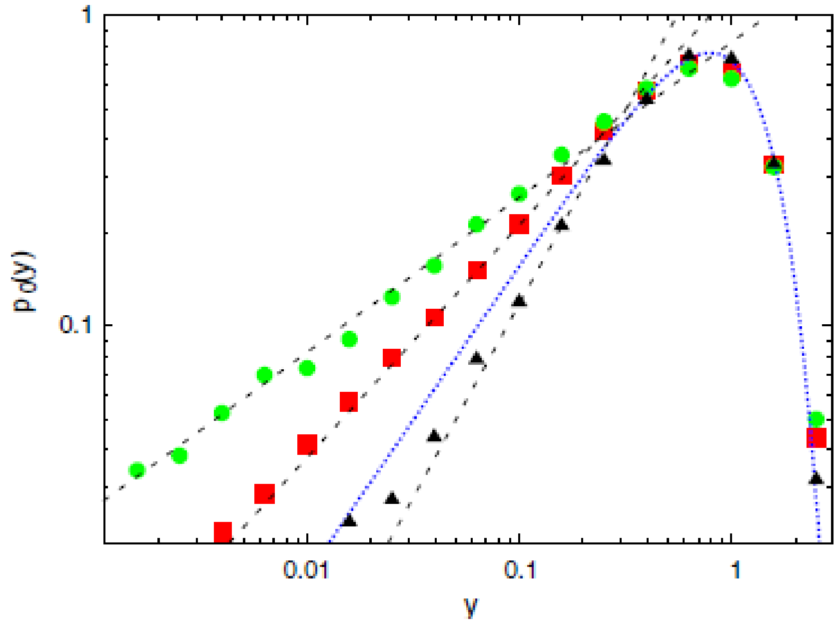
$$\phi = \frac{2-\alpha}{\alpha} \text{ (compare with } \phi = 1/\alpha)$$

For processes with time reversal symmetry

$$\phi = 2\theta/\alpha$$

but we have

$$\phi \approx 1/\alpha, \quad \theta \approx \alpha/2, \quad 2\theta/\alpha \approx 1$$




A.Zoia,A.Rosson,S.Majumdar, PRL102, 120602(2009)

# Conclusions/Perspectives

- *Monomer in a polymer & translocation variable perform similar sub-diffusion processes*
- *Fractional Laplacian provides an approximate shape of the stable long-time distribution*
- *Survival probability decays exponentially*
- *Despite qualitative similarities there is no simple relation between diffusion processes considered in this work*
- *Sub-diffusion generated by Langevin process differs from sub-diffusion generated by Rouse modes (possible resolution of differences in the lack of time-reversibility or stationarity)*

# That's all