Dynamics of a tagged monomer: Effects of elastic pinning and harmonic absorption

Shamik Gupta

Laboratoire de Physique Théorique et Modèles Statistiques,
Université Paris-Sud, France

Joint work with

Alberto Rosso
Christophe Texier

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Bounds on human demeanour.

- Upper bound: To bring in happiness wherever you go.

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The model

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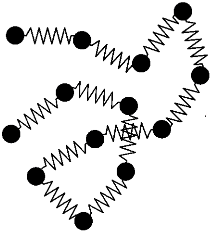

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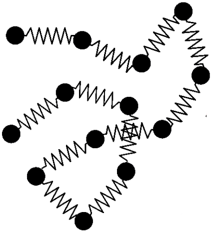

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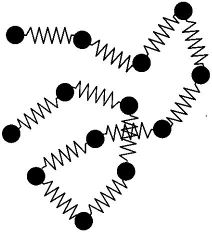

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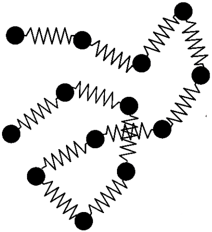

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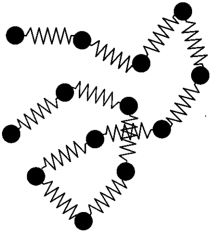

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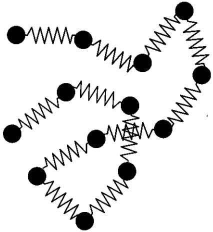

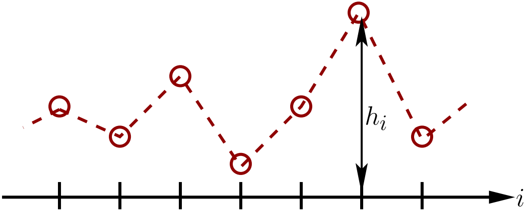

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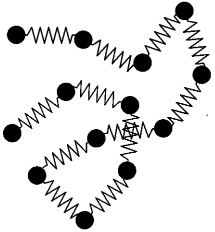

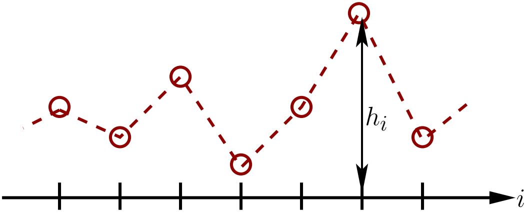

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6. Set $T = 1$.

Diffusion and Subdiffusion

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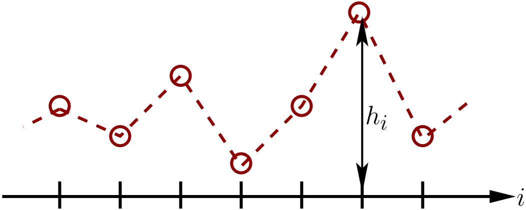

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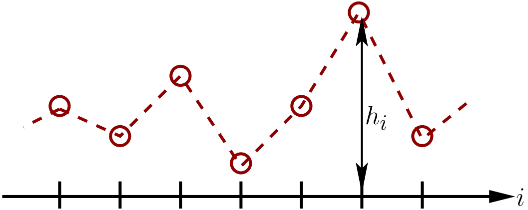

2. Centre of mass $(1/L)\sum_{i=1}^{L} h_i(t) \to$ Markovian dynamics, normal diffusion:

   Mean-squared displacement $\sim 2(1/L)t$.

Rouse polymer: Diffusion and Subdiffusion

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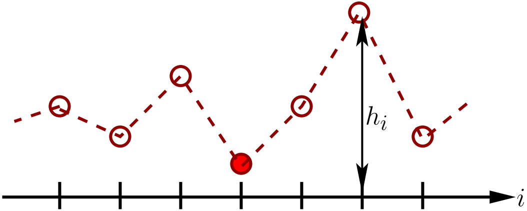

2. Tagged monomer $\rightarrow$ Non-Markovian dynamics, anomalous diffusion: Mean-squared displacement $\sim \sqrt{\frac{2}{\pi}} b_0 \sqrt{t}$.

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   - b_0 encodes memory of polymer configuration at $t = 0$.
   - Equilibrium at $t = 0$
     $\rightarrow$ Tagged monomer exhibits fractional Brownian motion (correlated increments), $b_0 = \sqrt{2}$.
   - Out of equilibrium flat configuration at $t = 0$
     $\rightarrow$ Correlated increments drawn from a Gaussian distribution with a time-dependent variance, $b_0 = 1$ *(Krug* et al. (1997)*)*.

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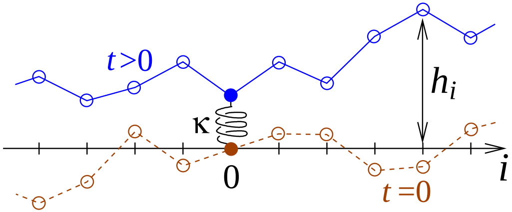

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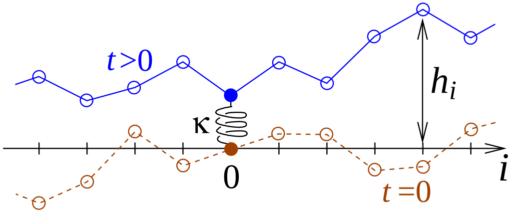

  2. Absorption of the tagged monomer on an interval. Example: Reactant attached to a monomer encounters an external reactive site fixed in space.

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- Questions:
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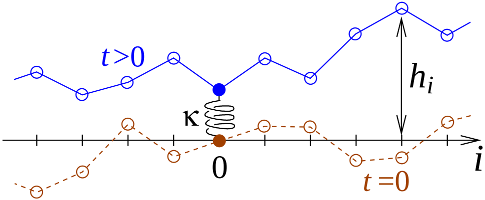
- Our work:
  Exact analytical results for elastic pinning and harmonic absorption.
  In particular, *strong* memory effects in the relaxation to the steady state.

Elastic pinning

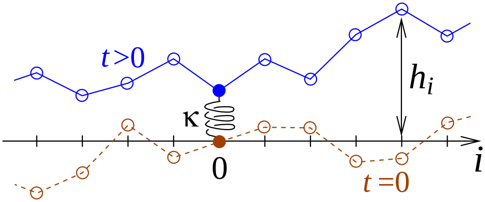


$$\frac{\partial \mathcal{W}_t[h|h^0]}{\partial t} = \Big[\sum_i \frac{\partial^2}{\partial h_i^2} + \sum_{i,j} \frac{\partial}{\partial h_i}\Lambda_{ij} h_j\Big]\mathcal{W}_t[h|h^0];$$

$$-\Lambda_{ij} = \Delta_{ij} - \kappa\,\delta_{i,j}\delta_{i,0}.$$

Langevin approach *(Viñales and Despósito (2006,2009), Grebenkov (2011))*

Elastic pinning



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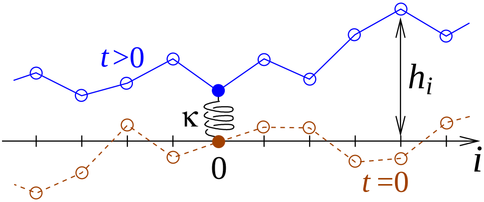

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2. $\mathcal{W}_t[h|h^0] = \sqrt{\det\left(\frac{\Lambda}{2\pi(1-e^{-2\Lambda t})}\right)}\exp\left[-\frac{1}{2}(h-e^{-\Lambda t}h^0)^{\mathrm{T}}\frac{\Lambda}{1-e^{-2\Lambda t}}(h-e^{-\Lambda t}h^0)\right].$

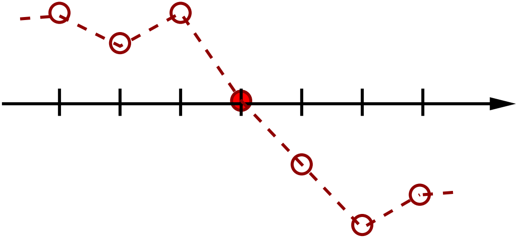
Flat initial condition

$t = 0:$

$t > 0: T = 1$ $+$ elastic pinning with spring constant κ.

Equilibrated initial condition

$t = 0$: Equilibrated at temp. T_0



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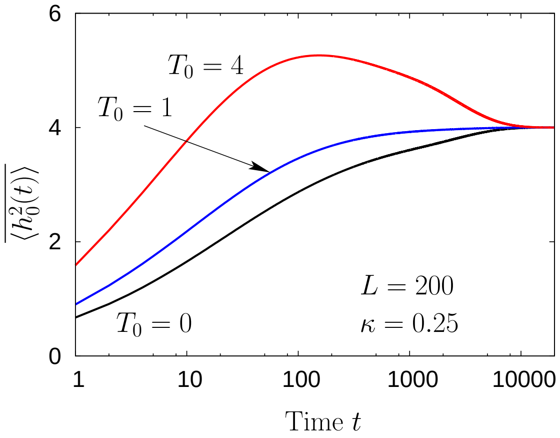
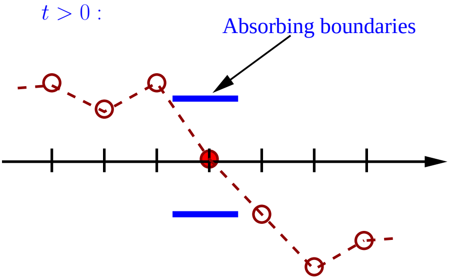
Elastic pinning: Exact results



$$\overline{\langle h_0^2(t) \rangle} \simeq \frac{1}{\kappa}\left[1 + \frac{T_0 - 1}{\kappa}\sqrt{\frac{2}{\pi t}} - \frac{T_0 c_1}{\kappa^2 t} + \cdots\right].$$

Absorption in an interval



- $\frac{\partial \mathcal{W}_t[h|h^0]}{\partial t} = \left[\sum_i \frac{\partial^2}{\partial h_i^2} - \sum_{i,j} \left(\frac{\partial}{\partial h_i} \Delta_{ij} h_j \right) \right] \mathcal{W}_t[h|h^0]$.

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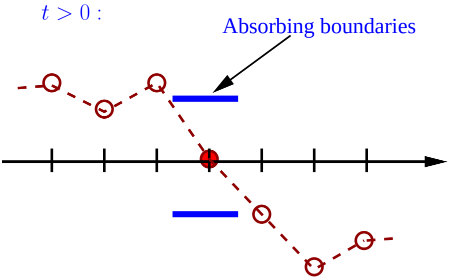

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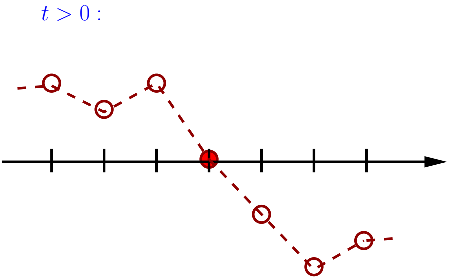
- Absorbing boundary conds. for the tagged monomer.

Harmonic absorption

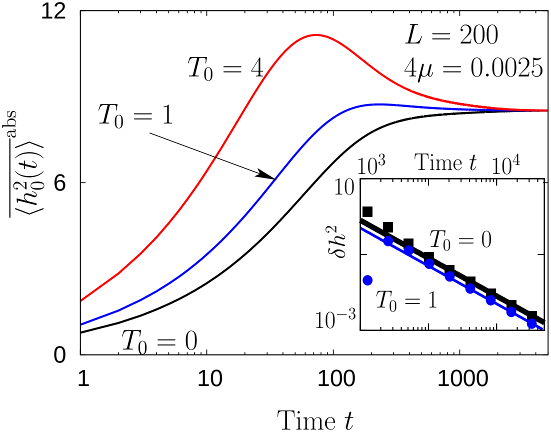


Absorption probability $\propto \mu h_0^2(t)$.

- $\frac{\partial \mathcal{W}_t[h|h^0]}{\partial t} = \Big[\sum_i \frac{\partial^2}{\partial h_i^2} - \sum_{i,j} \Big(\frac{\partial}{\partial h_i} \Delta_{ij} h_j + h_i A_{ij} h_j \Big) \Big] \mathcal{W}_t[h|h^0]$;

$A_{ij} = \mu \, \delta_{i,j} \, \delta_{i,0}$.

Harmonic absorption: Exact results



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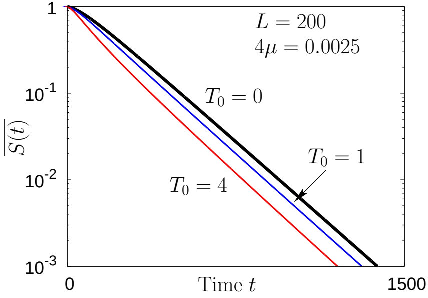
3. $\partial_t S(t) = -\mu \, \langle h_0^2(t) \rangle \, S(t)$.
4. $S(t) = \exp\Big(-\mu \int_0^t d\tau \, \langle h_0^2(\tau) \rangle \Big)$.



Consistent with simulations *(Kantor and Kardar (2004))*.

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4. Hydrodynamic effects for the chain or long-range elastic interactions for the interface may be included by replacing Δ with the corresponding fractional Laplacian $-(-\Delta)^{z/2}$.