Addressing soft-matter questions using quantum many-body physics tools

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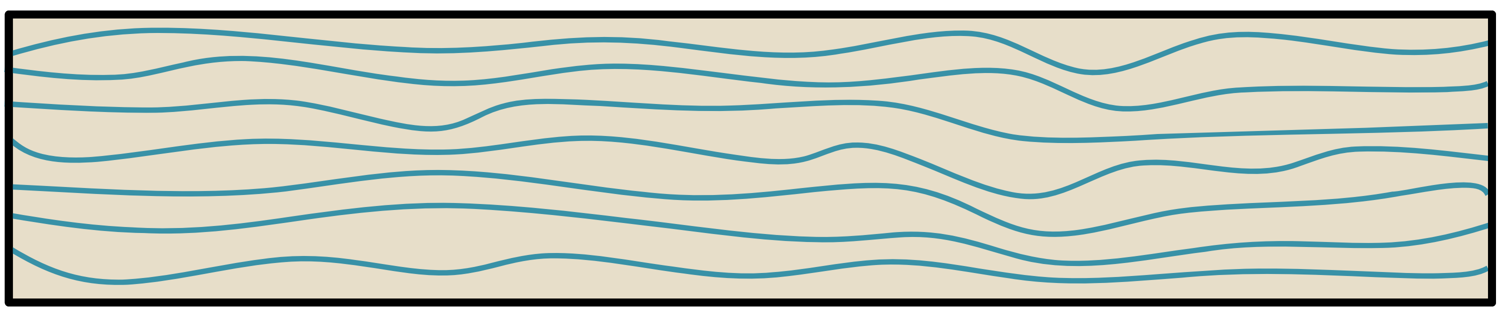
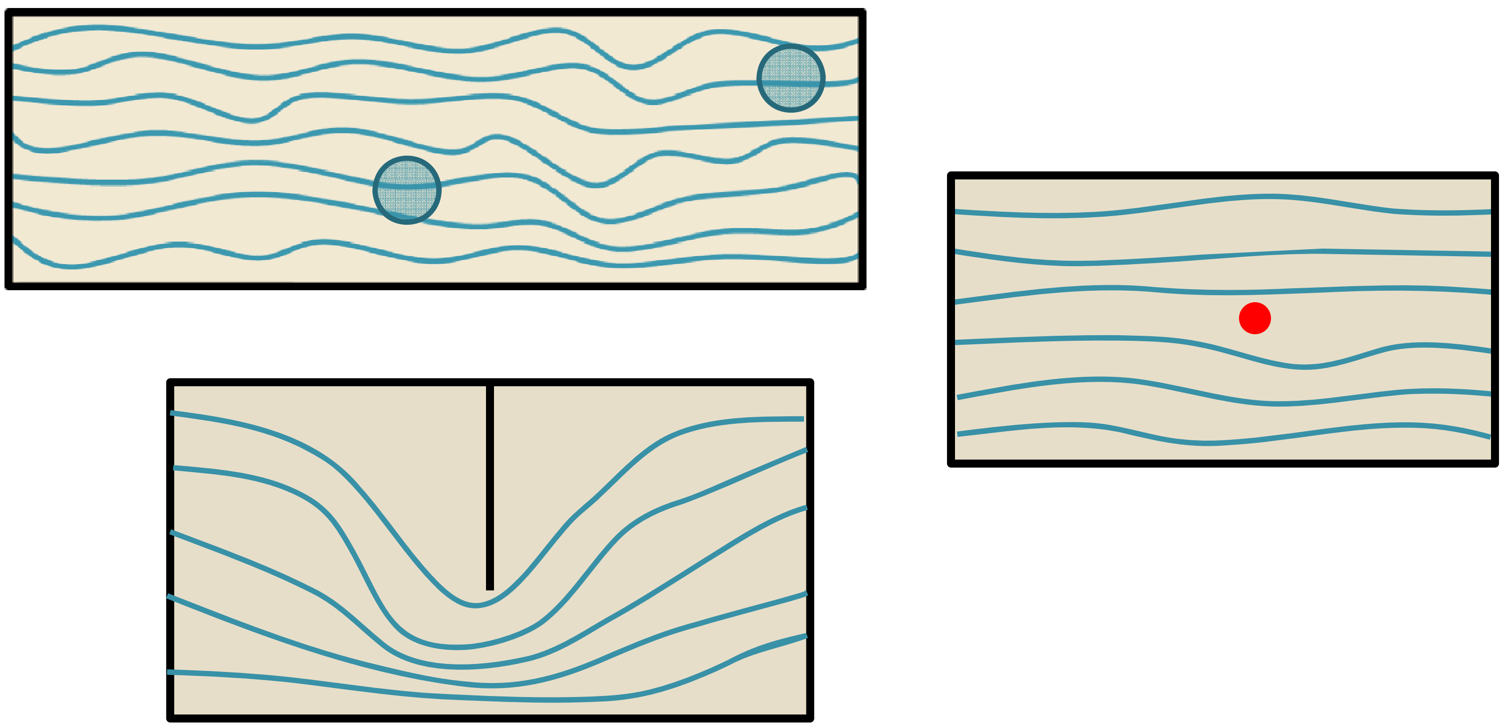
Approach

- Develop analogy between statistical mechanics of directed polymers in two dimensions and quantum one-dimensional systems (cf. de Gennes 1968)
- Apply modern quantum techniques to elucidate behavior of directed polymer systems



Mission

- Characterize density fluctuations, thermodynamics, and effect of geometry and topology in directed polymer system

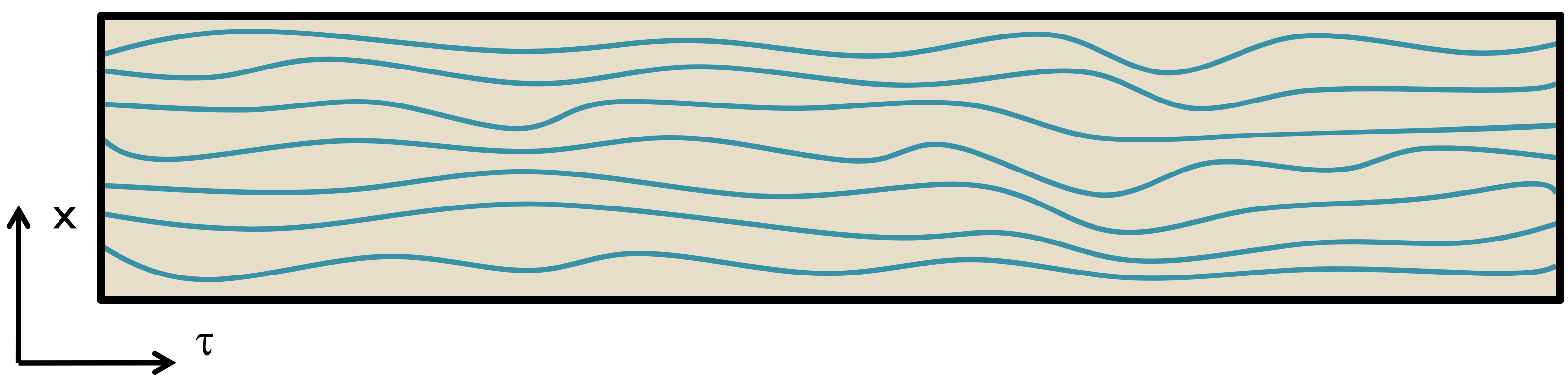


Outline

- Part I: Polymer system and mapping
- Part II: Interactions and density structure and correlations
- Part III: Geometrically and topologically constrained systems

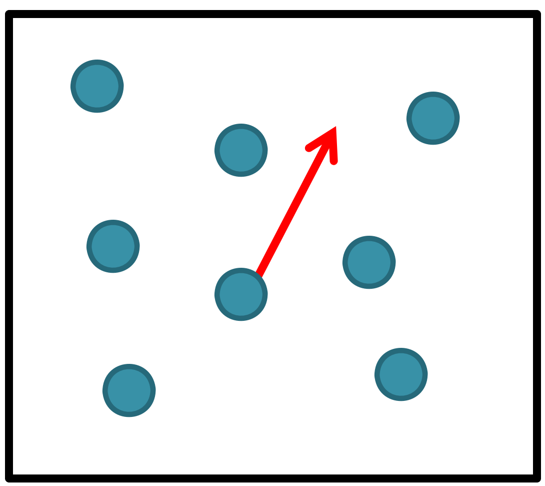
Part I: System

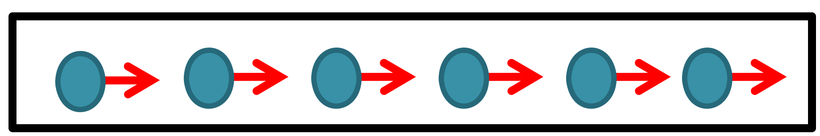
- Clean system of ideal polymers
- 2-dimensional: a substrate or a thin sheet
- Directed via tension or directional potential



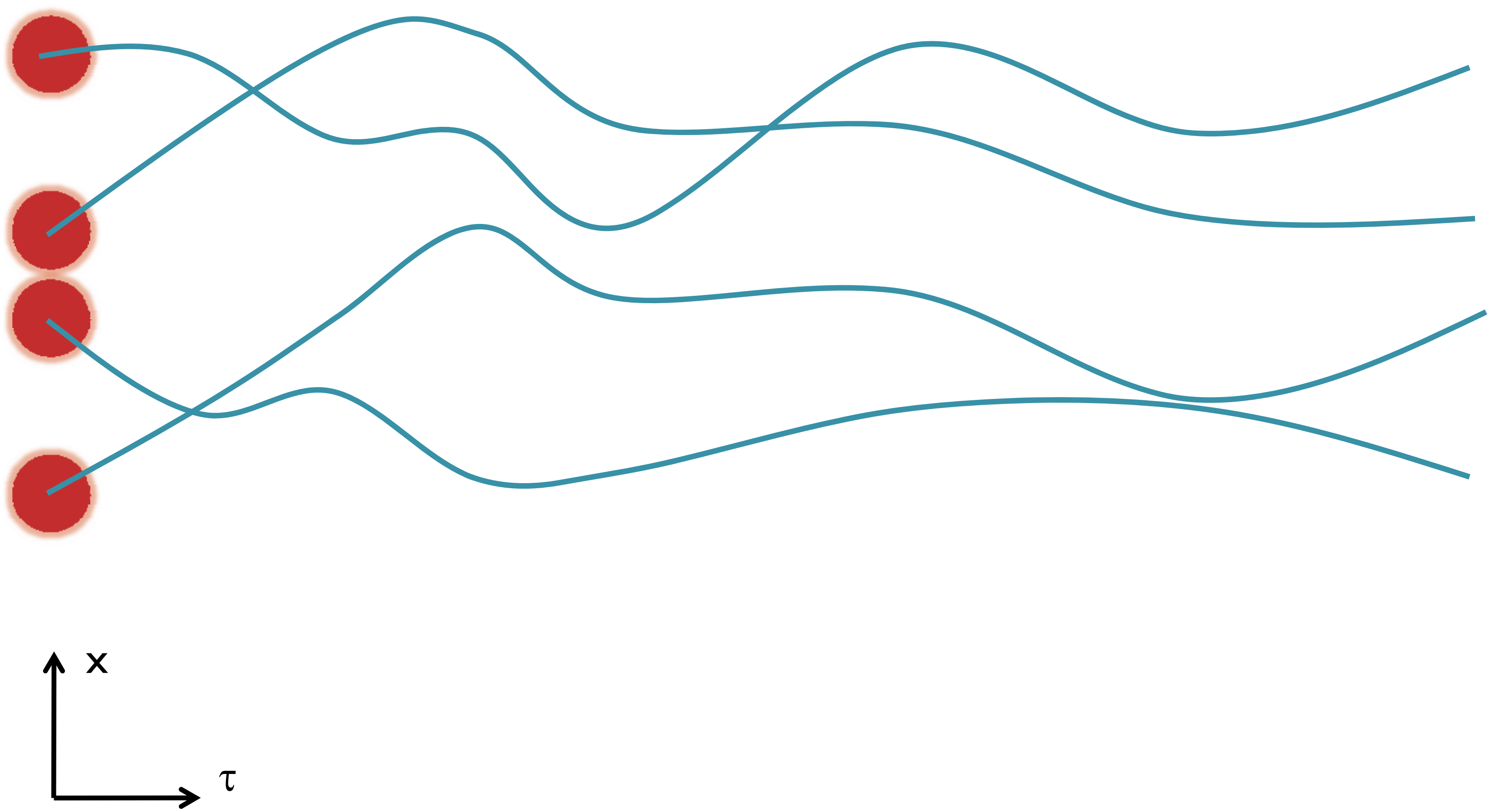
Collective excitations in low dimensions

- Interacting particles in 1D, or lines in 2D, yield only collective excitations
- Single-polymer dynamics suppressed
- Emergent polymer fluid has new properties





Quantum particles to classical lines



From thermal lines to quantum particles

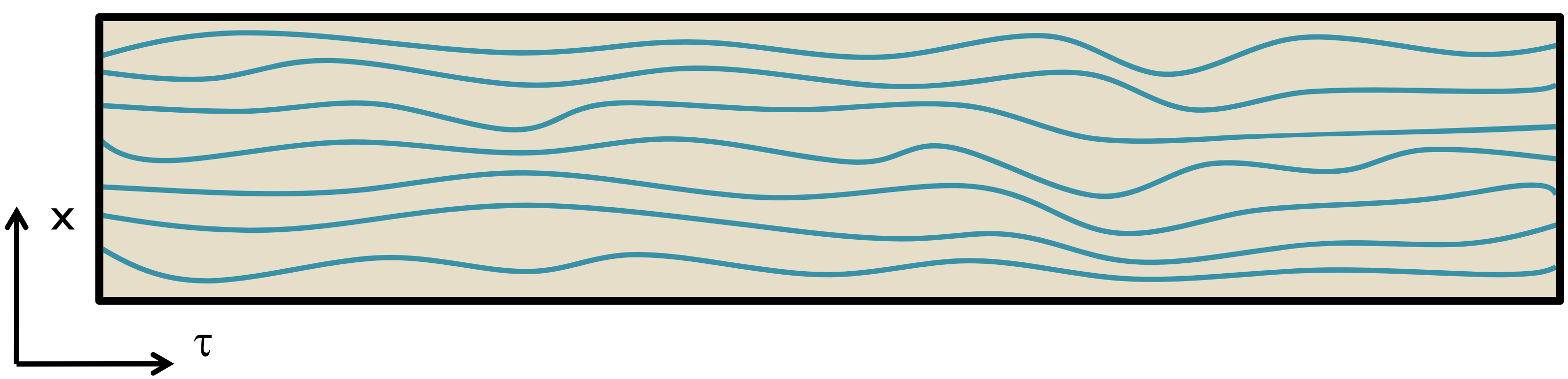
$$\int \mathcal{D}x_i(\tau)\exp\left[-\beta\int_0^{L_\tau} d\tau \sum_i A\dot{x}_i^2(\tau) + U(x_i(\tau)) + \sum_{i<j} V(x_i(\tau), x_j(\tau))\right]$$

$$= \langle\{x_F\}|\exp(-TH/\hbar)|\{x_0\}\rangle$$

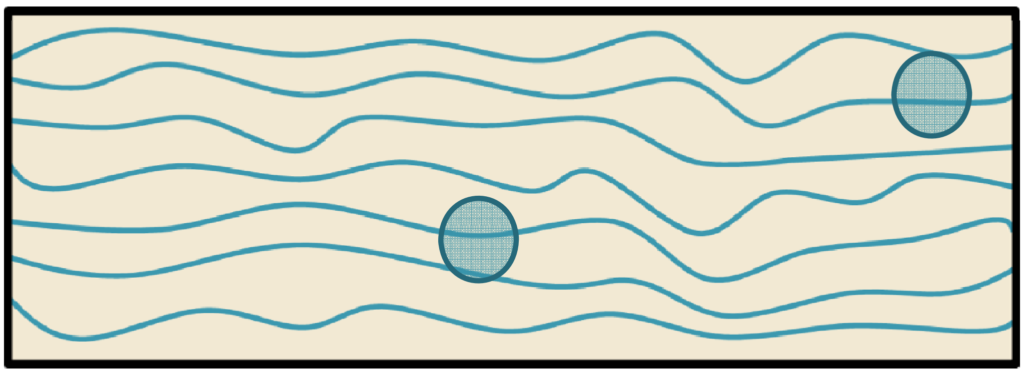
- Partition function for N linelike objects with some interaction
- Imaginary-time matrix element of quantum particles
- Generic quantum system taken to be bosonic: noncrossing polymers are fermionic
- Path integral over polymer conformations $x_i(\tau)$

Parameter relationships

Quantum System	Polymer System
Mass	Tension (units of temperature)
Position	Lateral direction
Time	Longitudinal direction
Inverse temperature	System length
System size	System width

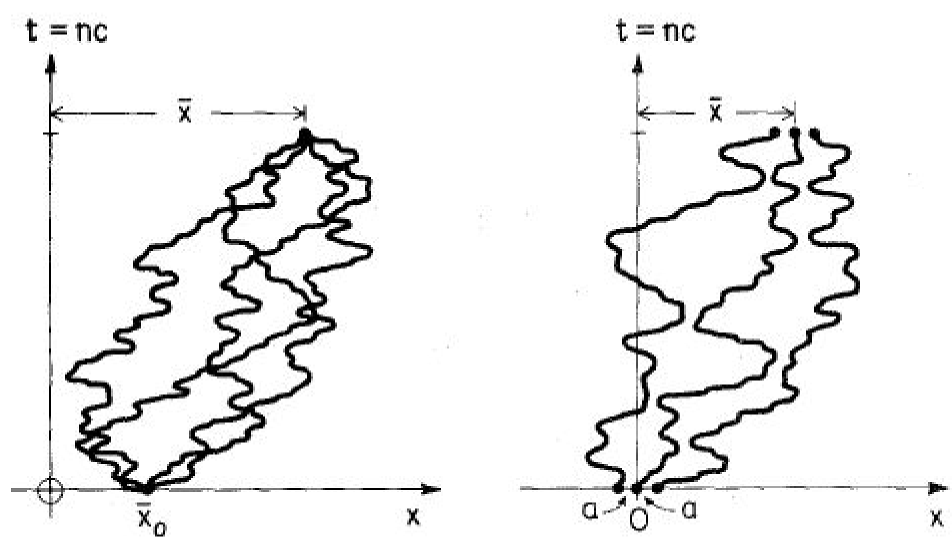


Part II: Interactions and Density Structure and Correlations



de Gennes (1968): noncrossing polymers

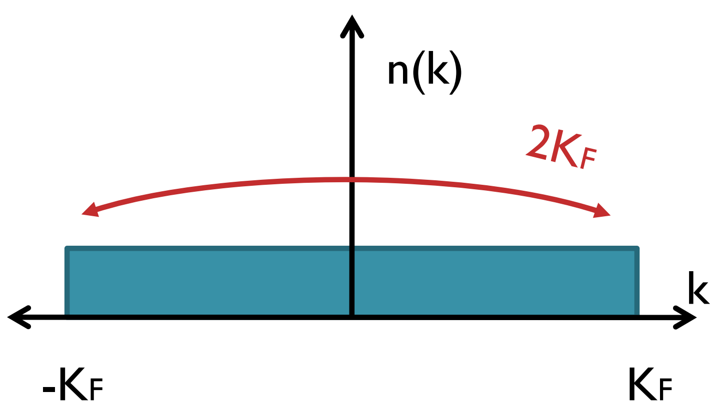
- Noncrossing paths = hardcore bosons
- In 1D, hardcore bosons = free fermions
- Path integrals for free fermions

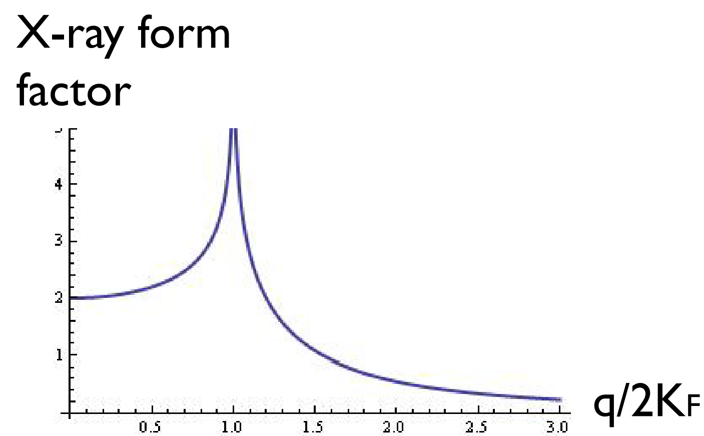


ME Fisher (1984)

de Gennes (1968): noncrossing polymers

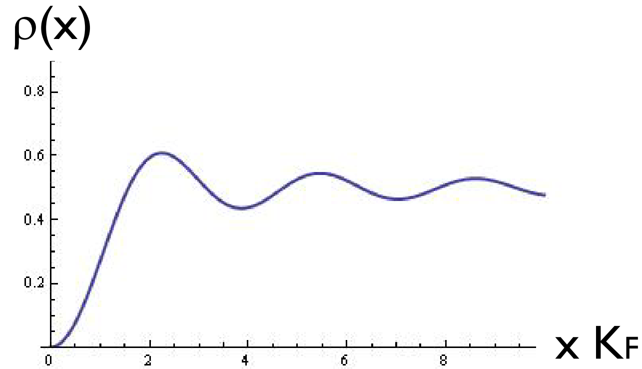
- Ground state dominance far from system boundaries
- Sum over single-particle excitations
- X-ray form factor displays logarithmic divergence corresponding to Kohn anomaly of Fermi gas



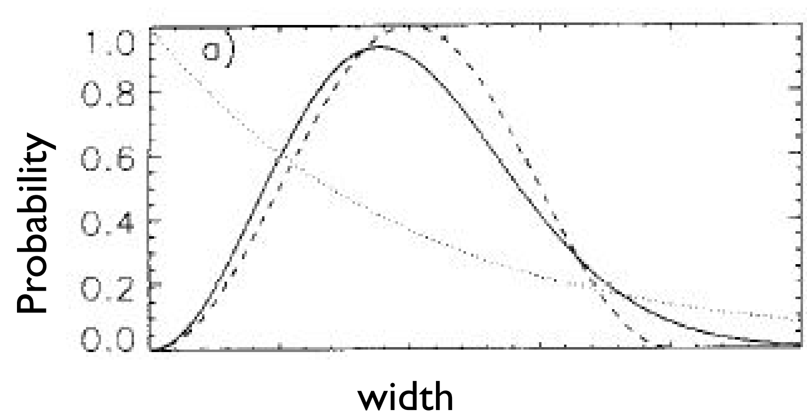


Behavior of noncrossing polymers

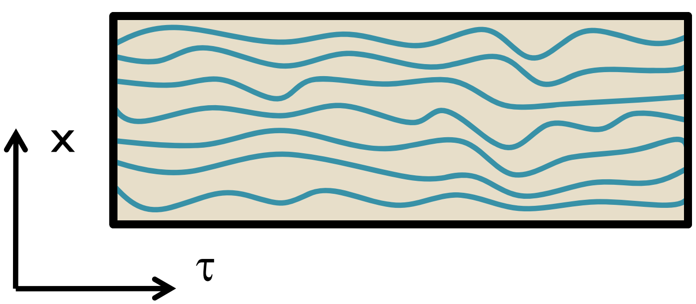
- Friedel oscillations near edges
- Density-density correlations
- Interpolymer width distribution



Width Distribution



Barelt et al. 1990



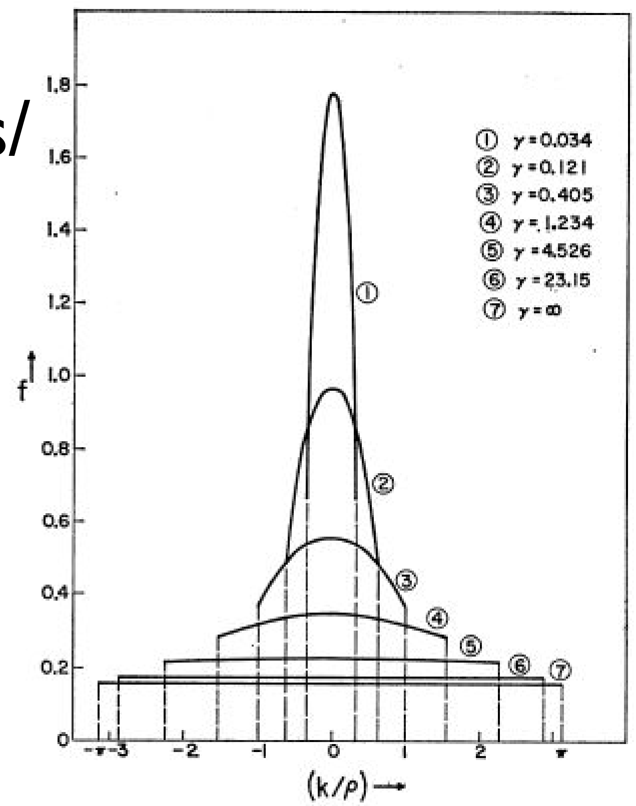
Lieb-Liniger (1963) model

$$H = \sum_i \frac{p_i^2}{2m} + 2c \sum_{i<j} \delta(x_i - x_j)$$

- c = ∞ case: hardcore bosons/ free fermions/noncrossing polymers
- Bethe Ansatz solution:

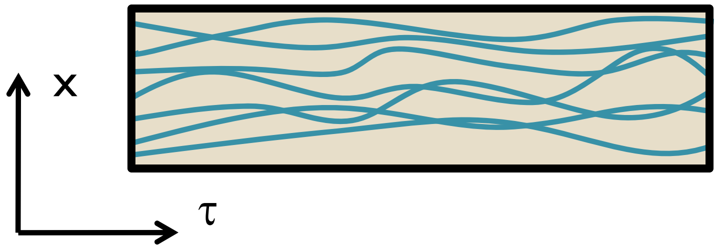
$$\Psi(x_1, x_2 \ldots x_N) = \sum_P e^{i\theta_P} \mathrm{P} \exp(ik_1 x_1 + ik_2 x_2 \ldots)$$

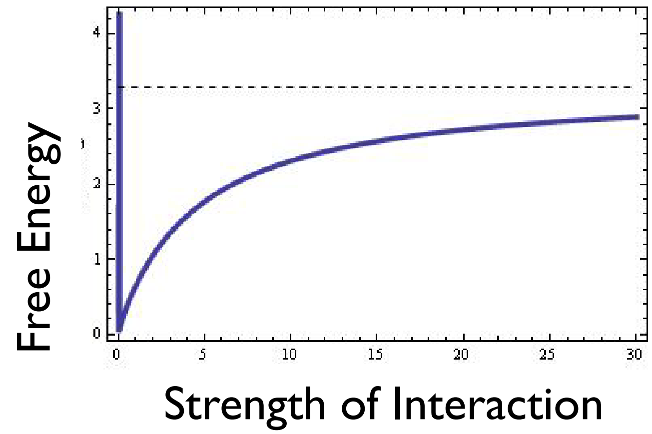
- Single-particle excitations extinguished

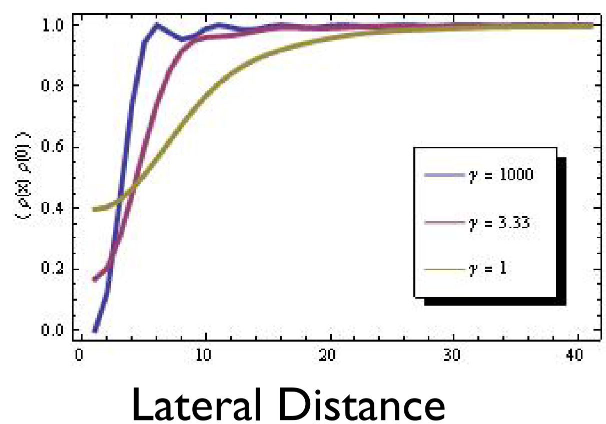


Results via Lieb-Liniger

- System free energy
- Lateral correlations found from Lieb-Liniger ground state
- Friedel oscillations
- More general correlations require Lieb-Liniger excitation spectrum







Alternative technique: bosonization

$$H = \frac{1}{2\pi}\int dx\left[uK\left(\nabla\theta(x)\right)^2 + \frac{u}{K}\left(\nabla\phi(x)\right)^2\right]$$

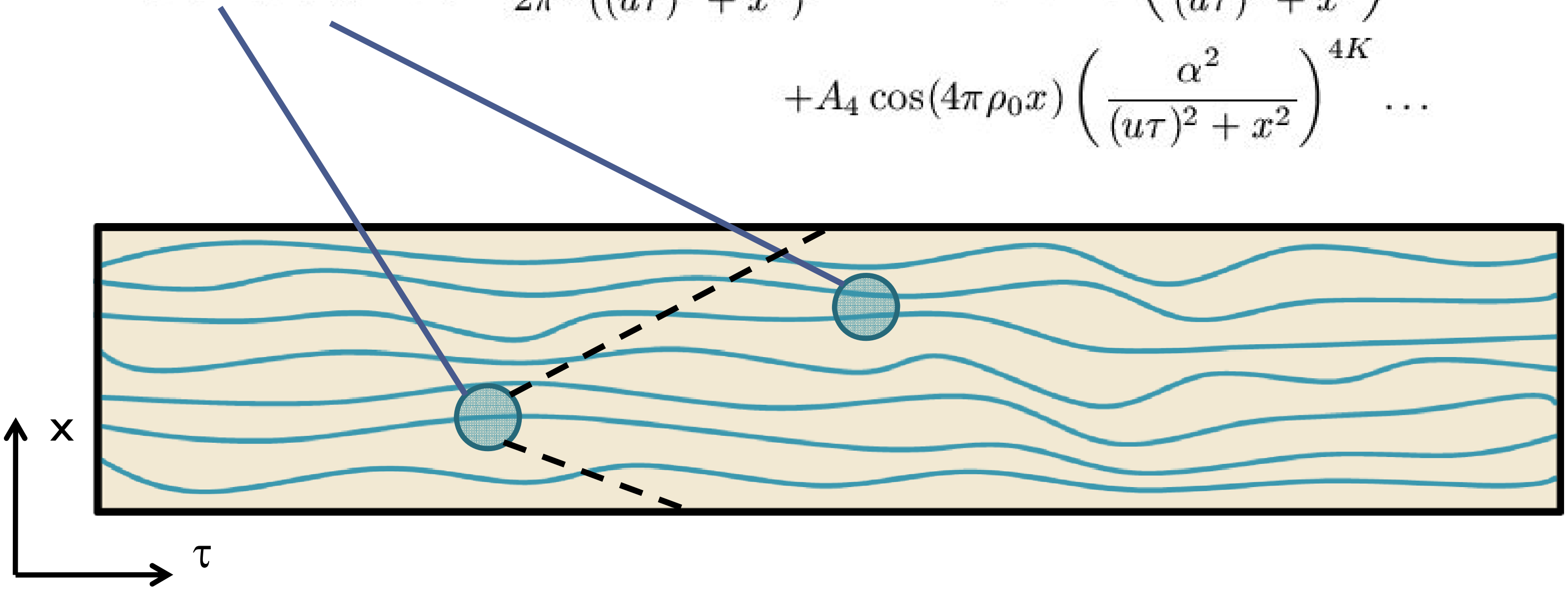
$$[\nabla\phi(x), \theta(x')] = -\pi i\delta(x - x')$$

$$\psi^\dagger = \sqrt{(\rho_0 - \frac{1}{\pi}\nabla\phi(x))}\sum_p \exp\left(2pi\left(\pi\rho_0 x - \phi(x)\right)\right) \quad e^{-i\theta(x)}$$

- Universal field theory for 1D systems
- Characterized by two T-L parameters u, K
- Conjugate fields represent density, phase fluctuations

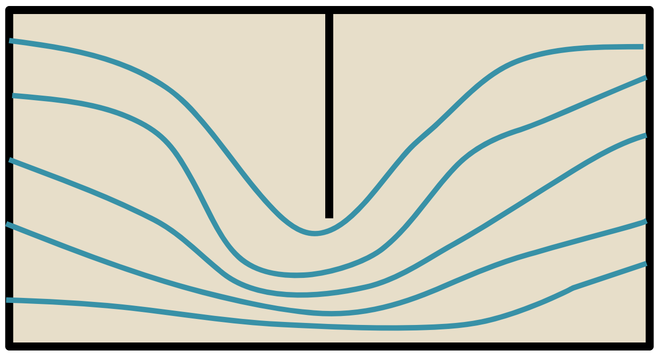
Correlation results via bosonization

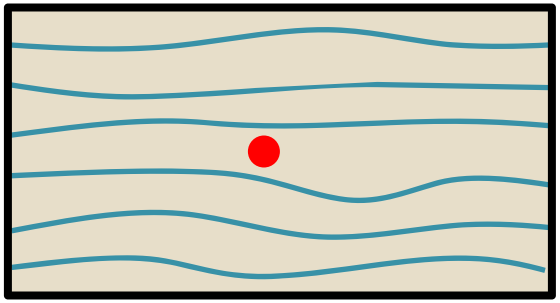
$$\langle \rho(x,\tau)\rho(0)\rangle = \rho_0^2 + \frac{K}{2\pi^2}\frac{(u\tau)^2 - x^2}{((u\tau)^2+x^2)^2} + A_2\cos(2\pi\rho_0 x)\left(\frac{\alpha^2}{(u\tau)^2+x^2}\right)^K + A_4\cos(4\pi\rho_0 x)\left(\frac{\alpha^2}{(u\tau)^2+x^2}\right)^{4K} \dots$$



K=∞	K>1	K=1	K<1
Free bosons	Contact bosons	Hardcore bosons	Long-range bosons
	Attractive fermions	Free fermions	Repulsive fermions

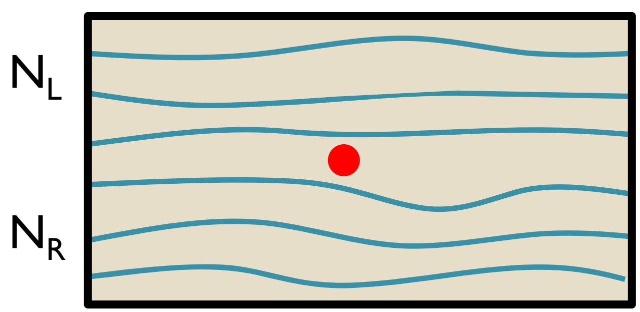
Part II: Geometrical and Topological Restrictions

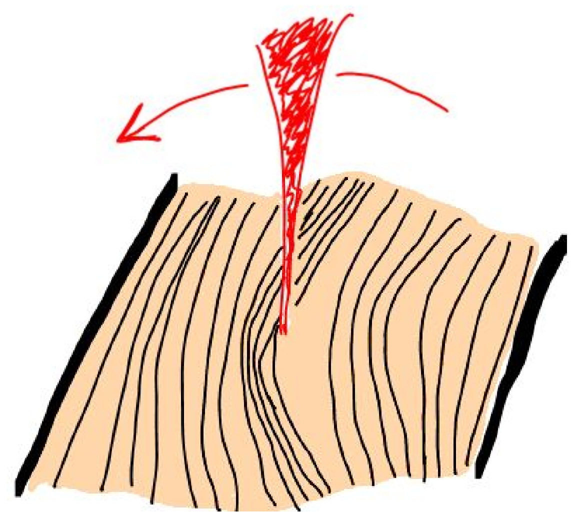




Topological impurities

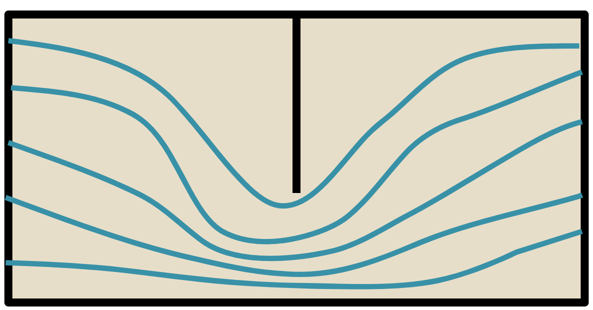
- Weak external potential $V(x,\tau)$ can be handled perturbatively
- Strong potential can restrict number of polymers N_L passing to left, right
- Potential can pull polymers to one side

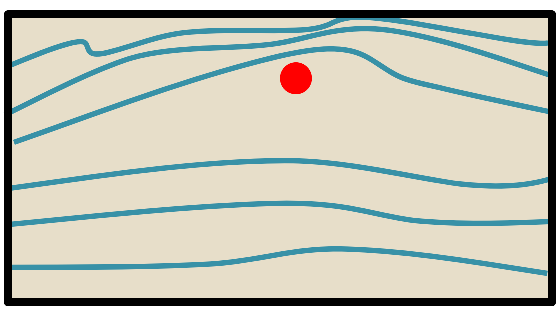




Characterizing the restricted system

- Calculate partition function of system with topological restriction
- Determine polymer density response to constriction
- Connect thermal polymer system to nonequilibrium quantum system



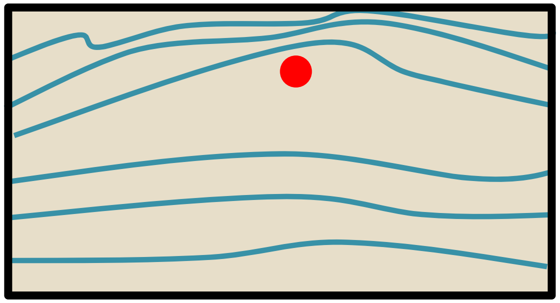


Entropic force

- Ground state of Fermi system:

$$\Psi(x_1, x_2 \ldots x_N) \sim \left(\prod_i \sin \pi x_i / L\right) \prod_{i<j} (\cos \pi x_i / L - \cos \pi x_j / L)$$

- Polymers experience "level repulsion"
- In thermodynamic limit, $O(N^2)$ contribution to free energy is the maximum-probability configuration $\rho(x)$



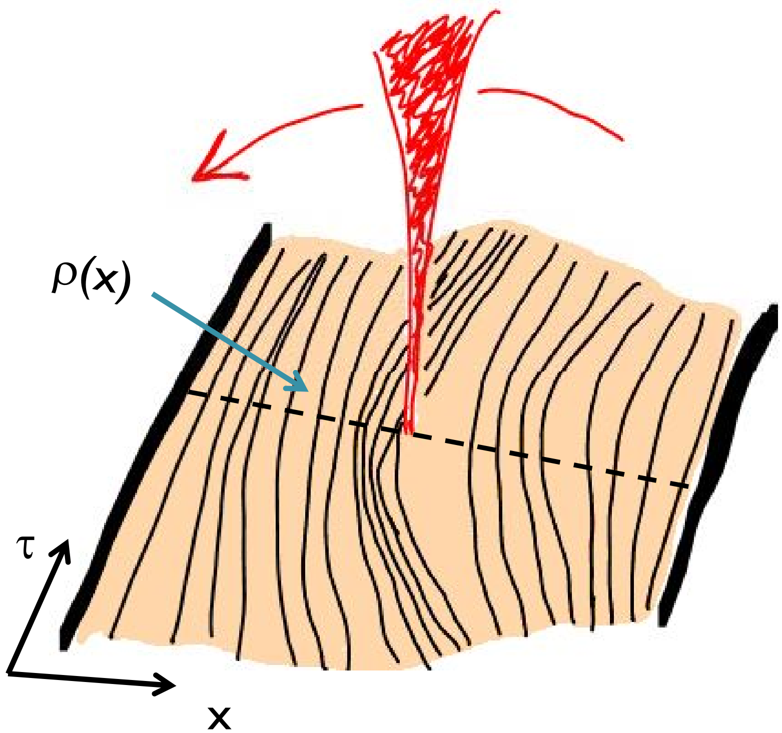
Free energy minimization

$$\text{Free Energy} = N^2 T \int_0^L \int_0^L dx dx' \rho(x)\rho(x') \log\left[(\cos \pi x/L - \cos \pi x'/L)^2\right]$$

$$\text{Normalization:} \quad \int_0^L \rho(x) = 1$$

$$\text{Topological Constraint:} \quad \int_0^a \rho(x) = N_L/N$$

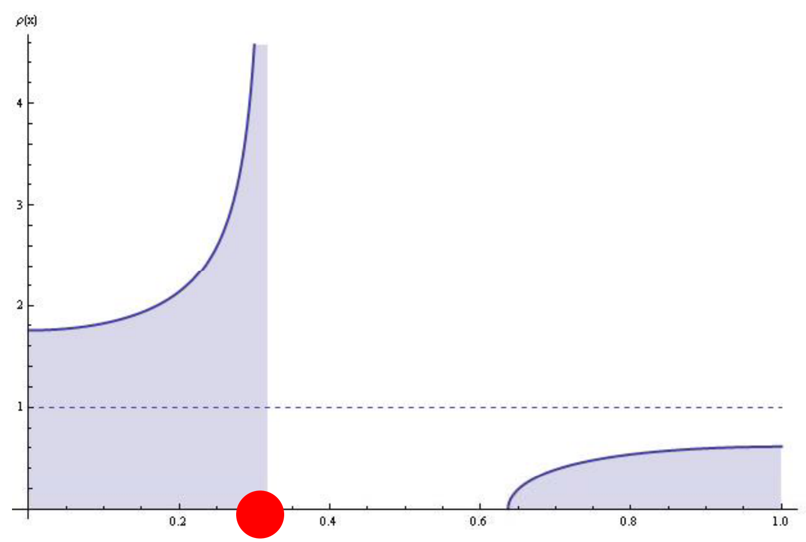
$$\text{Positivity:} \quad \rho(x) \geq 0$$



Polymer density: gaps and singularities

$$\rho(x) = \frac{\theta(a-x)+\theta(x-g)}{\pi}\sqrt{\frac{\cos\pi g/L - \cos\pi x/L}{\cos\pi a/L - \cos\pi x/L}}$$

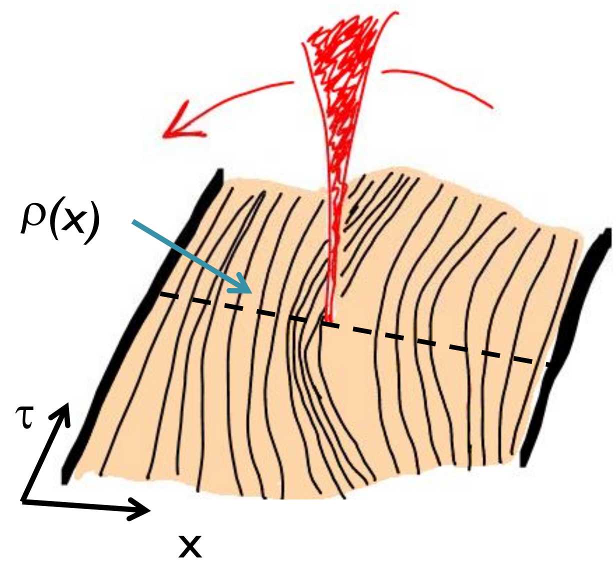
Polymer density



a

g

Lateral position



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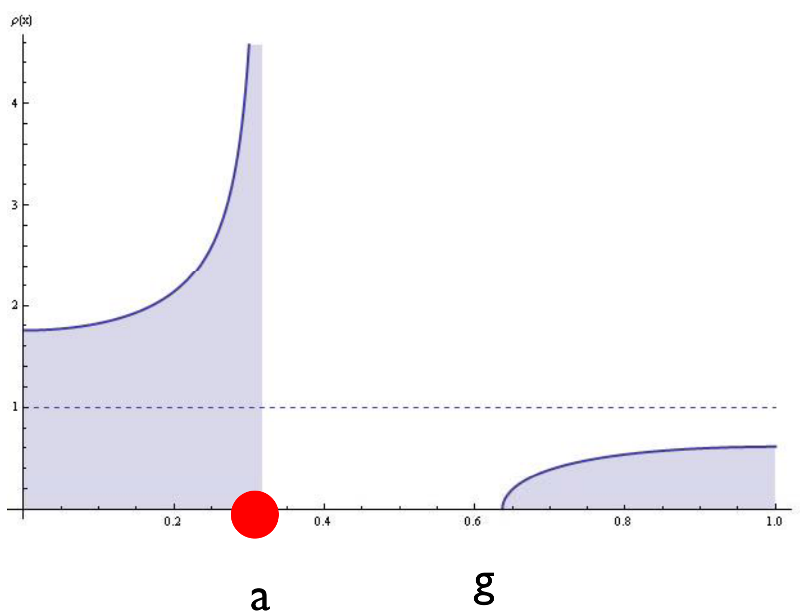
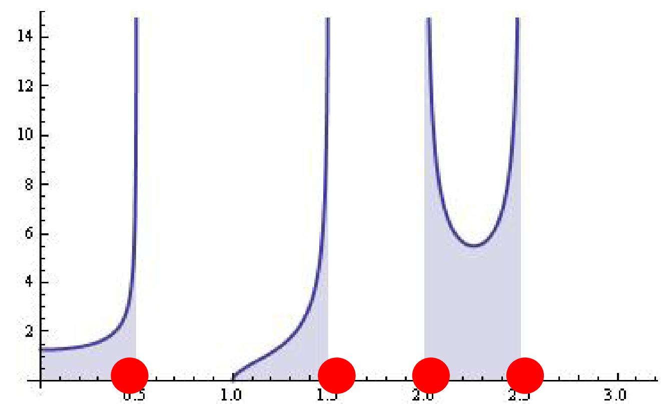
Polymer
density

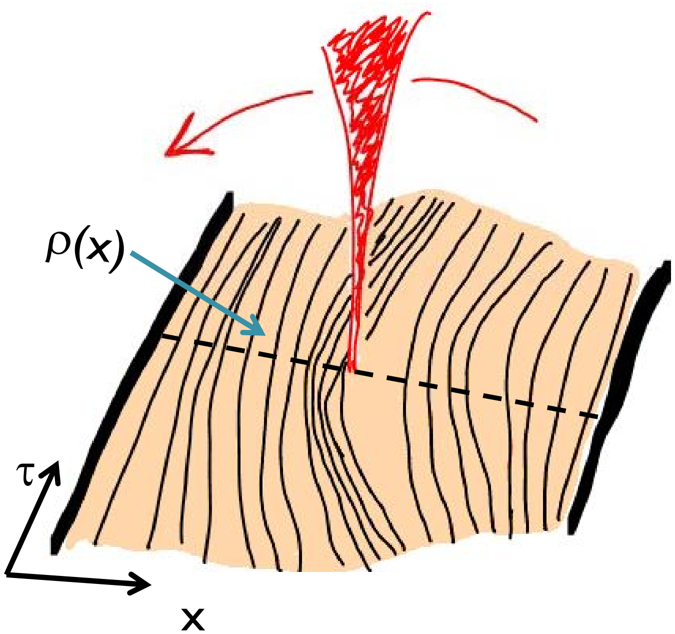


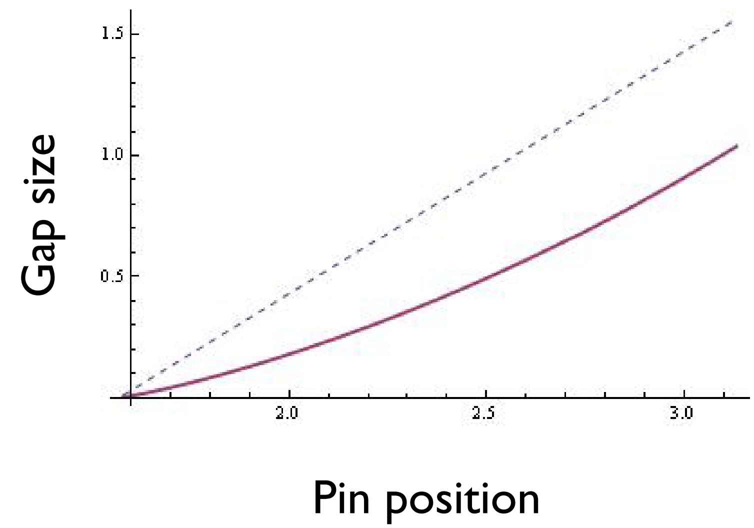


Lateral
position

Why a gap?

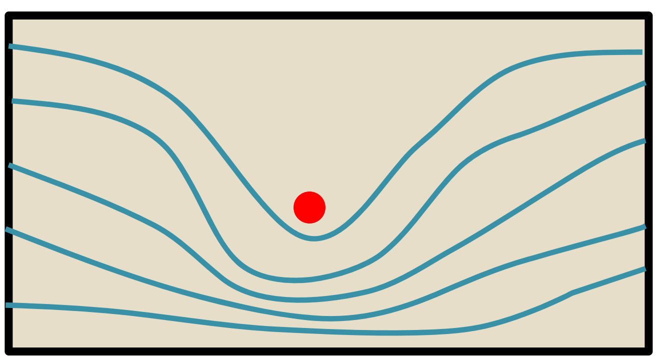
- Emergent long-range force
- Contact between two regions of polymers at later “time”

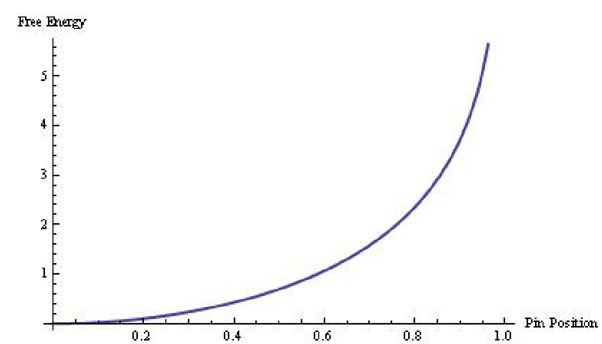




Force law for topological pin

- Force on pin ~ $N^2 T/L$
- For $N_L = 0$, $\text{Free Energy} = -N^2\, T \log\left(1 + \cos \pi a/L\right)$
- Small displacement: Hooke's law
- Tight constriction: logarithmic divergence





Conclusions

- Interactions strongly modify 2D polymer behavior
- Topological constraints can generate long-range effects in polymer system and connect to nonequilibrium quantum systems
- Polymer distributions and correlations can be described using quantum many-body techniques

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