# Bubble generation by dipole twisting

Peter Vingaard Larsen

Informatics and Mathematical Modelling
Technical University of Denmark
DK-2800 Kgs. Lyngby
Email: pvl@imm.dtu.dk

Collaborators:

- Peter Leth Christiansen and Ole Bang, Lyngby
- Yuri Gaididei, Kiev
- Juan Archilla, Sevilla

# Overview

- Introduction
  - Previous work
- Model setup
- Analytical results
- Simulation results
  - Bubble generation
- Conclusion and outlook

# Previous work

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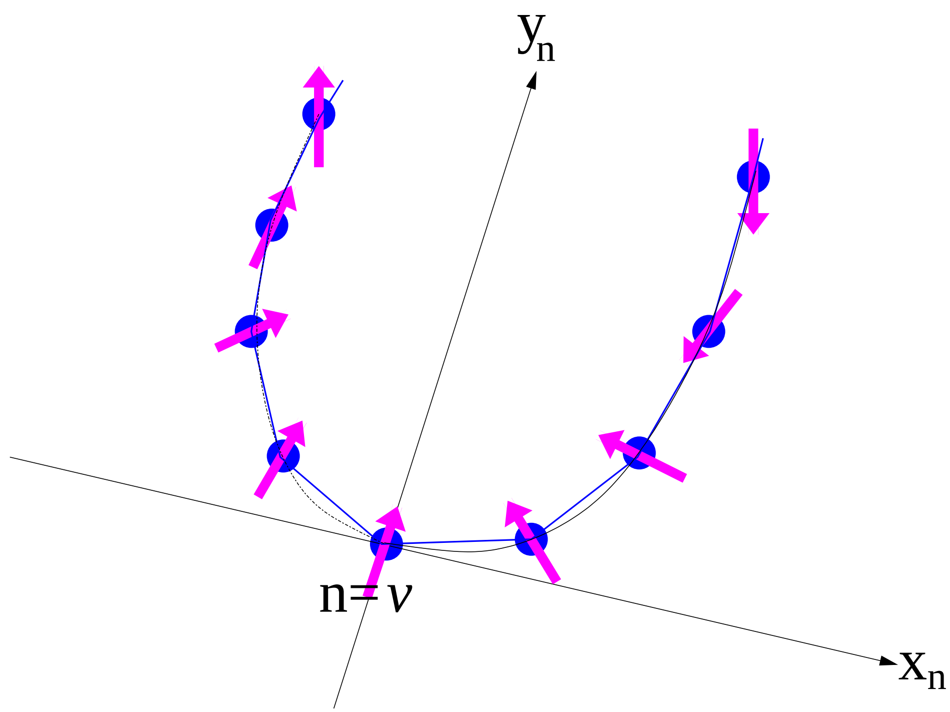
*In this work we will consider both LRI, Morse potential and dipole twisting on a curved chain*

[1] *Peyrard and Bishop*, PRL, **62**, 23, pp. 2755–2758 (1989).
[2] *Mingaleev et. al.*, J. of Phy.: Cond. Mat., vol. **13**, pp. 1181–1192,
[3] *Barbi et. al.*, Phys. Let. A, **253**, pp. 358–369 (1999).

# System setup




Dipole moments (magenta) shown on sites (blue) on a parabola embedded chain in the $xy$-plane.

# The Hamiltonian

In dimensionless variables, the total Hamiltonian for the infinite chain is:

$$H = \sum_n \Big\{ \overbrace{\frac{1}{2}\dot{u}_n^2}^{Kinetic} + \overbrace{\frac{C}{2}\left(u_{n+1}-u_n\right)^2}^{Stacking} + \overbrace{\left(e^{-u_n}-1\right)^2}^{Morse} + \underbrace{\frac{1}{2}\sum_{m\neq n} J_{nm}u_n u_m}_{Dipole} \Big\}.$$

# The Equations of motion

The Hamiltonian gives rise to the following equations of motion

$$\ddot{u}_n - C\left(u_{n-1} - 2u_n + u_{n+1}\right) - 2e^{-u_n}\left(e^{-u_n} - 1\right) + \sum_{m \neq n} J_{nm} u_m = 0.$$

# The dipole interaction

The coefficient, $J_{nm}$, is defined as

$$J_{nm} = \frac{J_0}{|\mathbf{r}_n - \mathbf{r}_m|^3} \left\{ \mathbf{d}_n \cdot \mathbf{d}_m - 3 \left( \mathbf{d}_n \cdot \mathbf{r}_{nm} \right) \left( \mathbf{d}_m \cdot \mathbf{r}_{mn} \right) \right\},$$

where $\mathbf{d}_n$ is the dipole at the $n$'th site and $\mathbf{r}_{nm}$ is a unit vector from the $n$'th to the $m$'th site:

$$\mathbf{r}_{nm} = \frac{\mathbf{r}_n - \mathbf{r}_m}{|\mathbf{r}_n - \mathbf{r}_m|}.$$

# Unit dipole moments, $\mathbf{d}_n$

Dipole moments becomes through geometry

$$\mathbf{d}_n = \left( -\frac{\kappa x_n}{\sqrt{1+\kappa^2 x_n^2}} \sin\phi_n, \quad \frac{1}{\sqrt{1+\kappa^2 x_n^2}} \sin\phi_n, \quad \cos\phi_n \right)$$

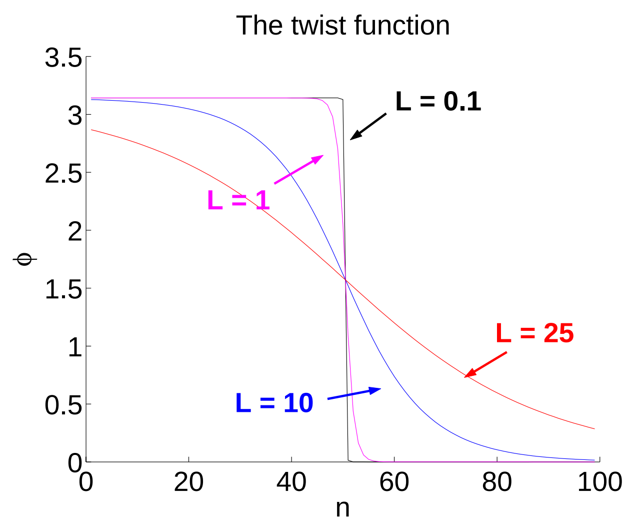
on the parabola embedded chain, $y_n = \frac{\kappa}{2} x_n^2$.

# The twist function, $\phi_n$

The *twist function* is defined as

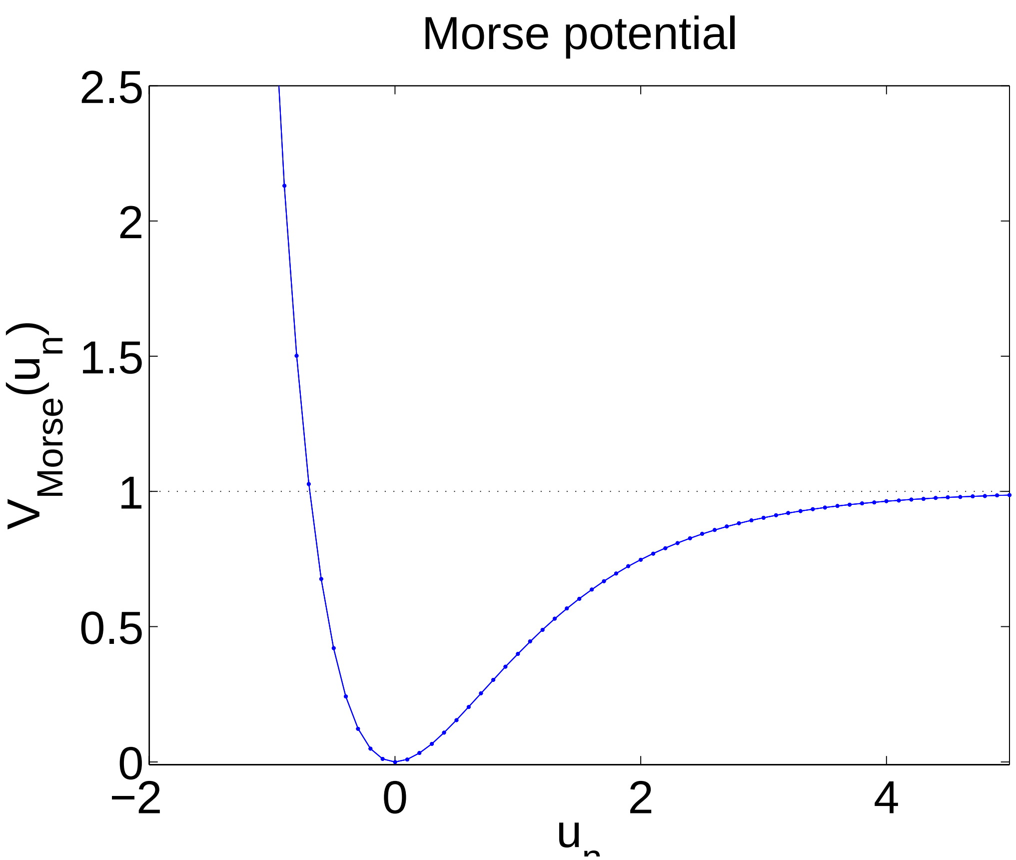
$$\phi_n = 2\arctan\left[\exp\left(-\frac{n-\nu-\frac{1}{2}}{L}\right)\right].$$

with $\nu$ as the site number of the vertex of the parabola and $L$ as the twisting width.

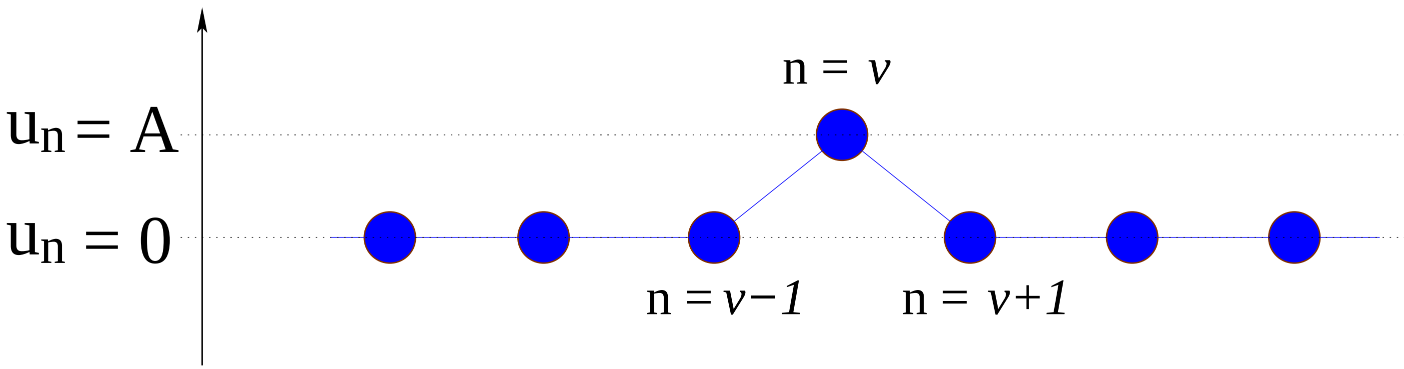



*The twist function for various values of L.*

# The Morse potential



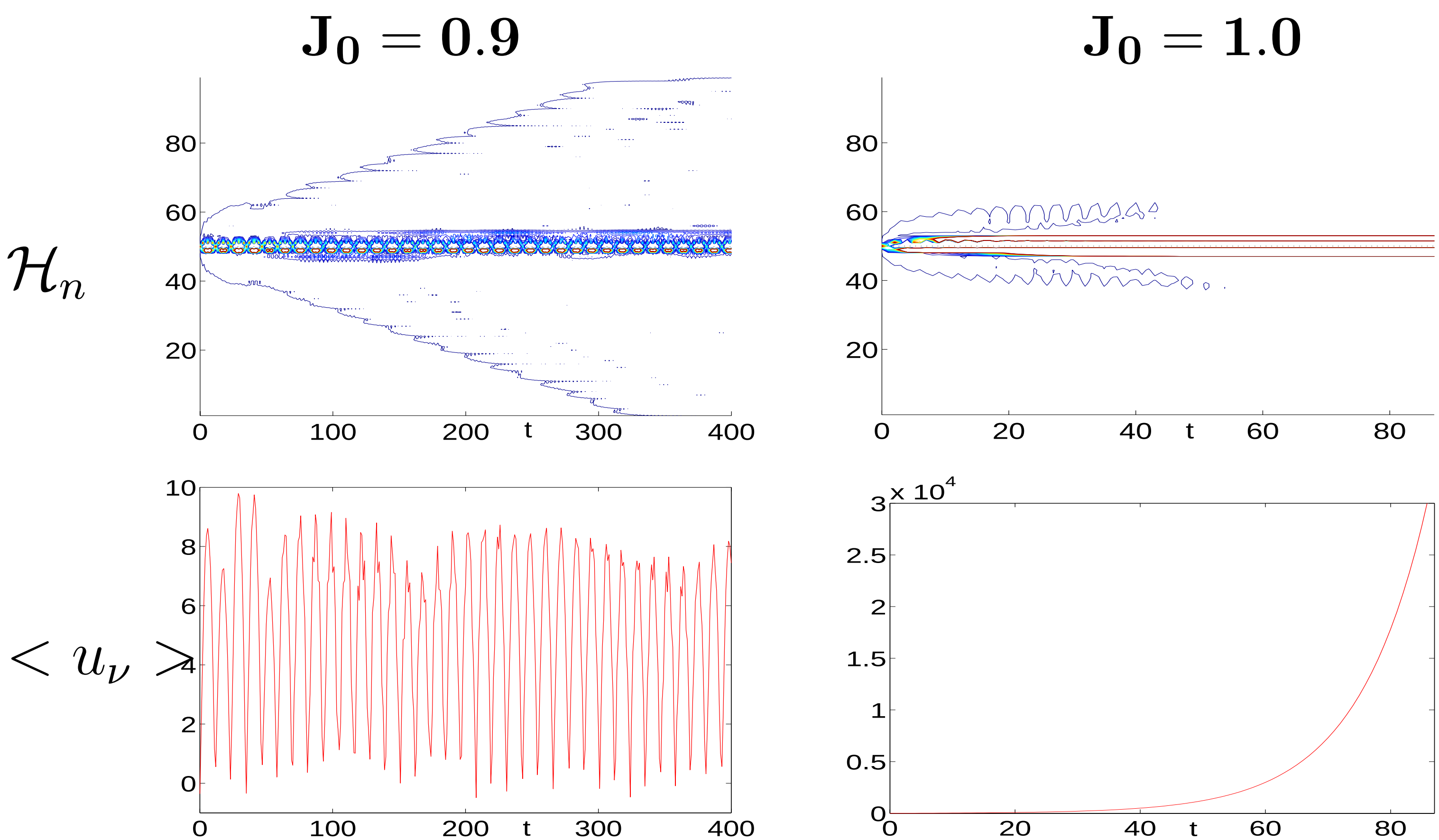
# Initial Conditions




$$u_\nu = A; \quad u_n = 0, \quad n \neq \nu$$

$$\dot{u}_n = 0 \quad \forall n$$

# Bubble example




$$A = -2.5,\ C = 1,\ L \approx 0 \text{ and } \kappa = 0.$$

BUBBLE: A localized unbounded increase of the amplitude.

# Analytical approximation - I

Considering only sites $n = \nu$ and $n = \nu + 1$ with $C = 0$, we are in effect looking at the *dimer*. Hamiltonian is

$$H = \dot{u}^2 + \left(e^{-u} - 1\right)^2 - Ju^2 = T + V,$$

with $J = |J_{\nu,\nu+1}| = |J_{\nu+1,\nu}|$. IC's give a value, H(0), for the Hamiltonian, which now can be integrated:

$$t - t_0 = \int_{u_0}^{u} \frac{d\bar{u}}{\sqrt{H(0) - \left(e^{-\bar{u}} - 1\right)^2 + J\bar{u}^2}}$$

# Analytical approximation - II

For $u \gg 1$ the last term dominates, so

$$t - t_0 = \int_{u_0}^{u} \frac{d\bar{u}}{\sqrt{J\bar{u}^2}},$$

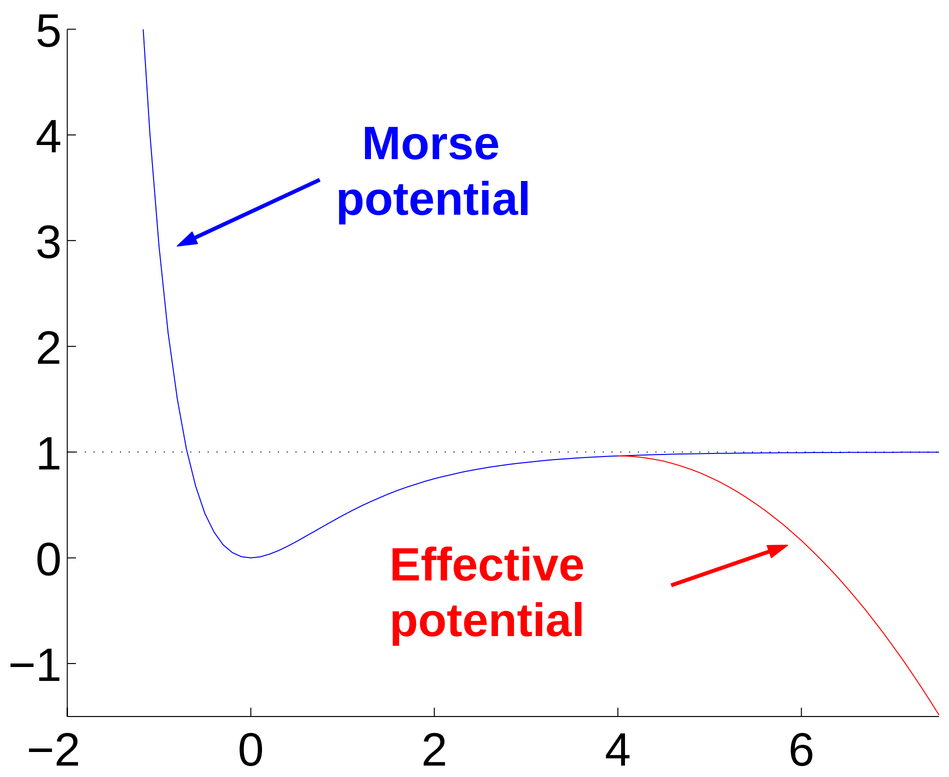
solving to

$$u \approx K \exp\left(\sqrt{J}(t - t_0)\right)$$

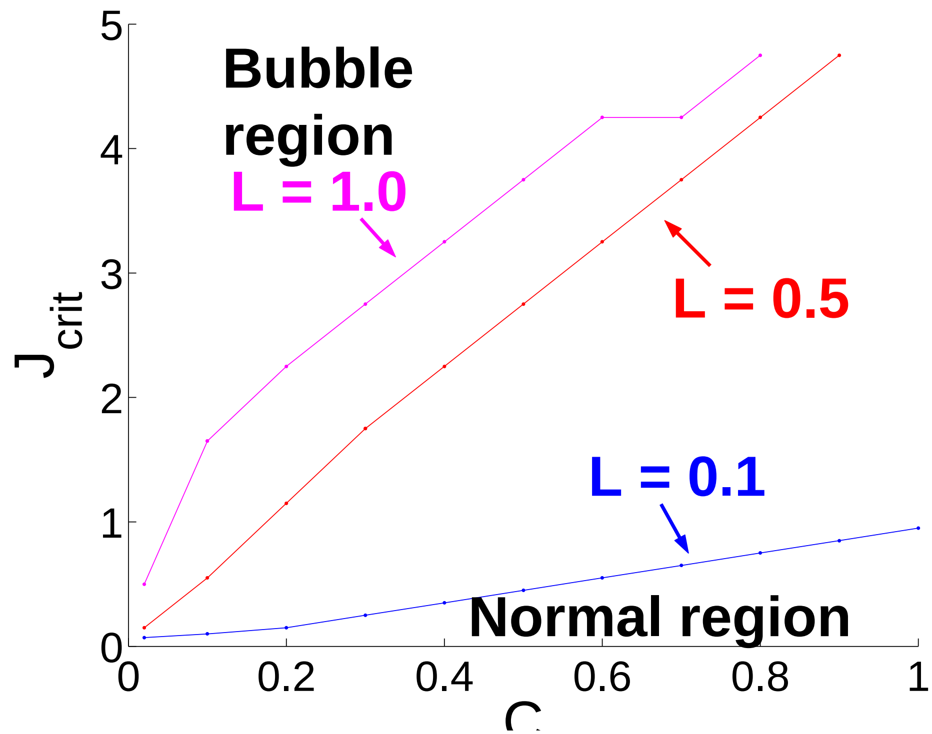
# Analytical approximation - III

The effective potential is thus

$$V(u) = \left(e^{-u} - 1\right)^2 - Ju^2.$$



# Straight chain




*Critical values of $J_0$*
*for $A = -2.5$ and $\kappa = 0.0$.*

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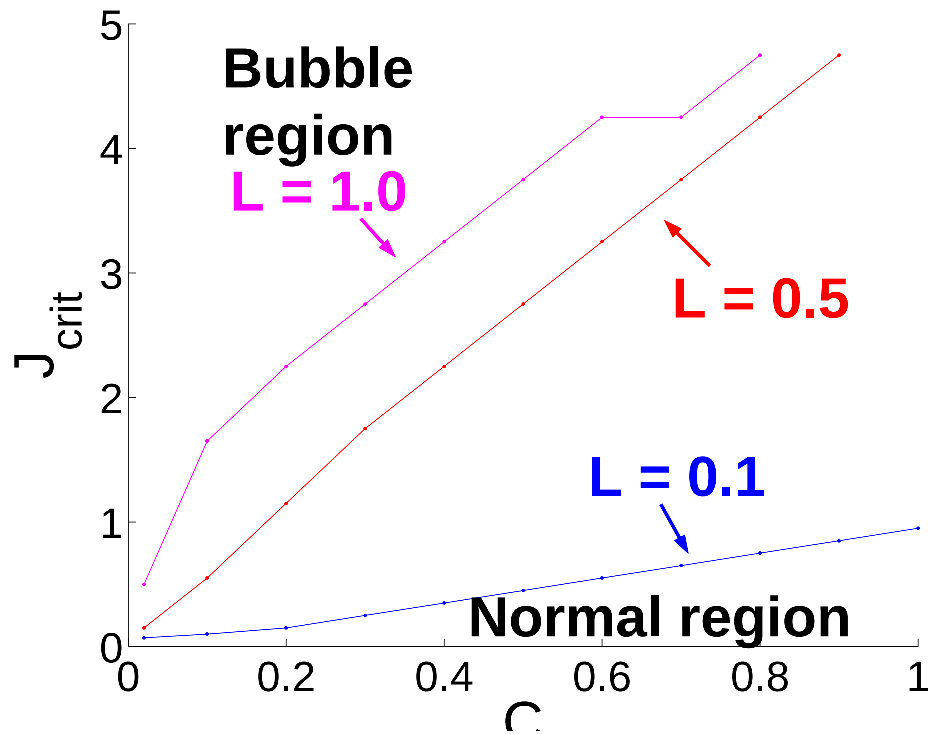


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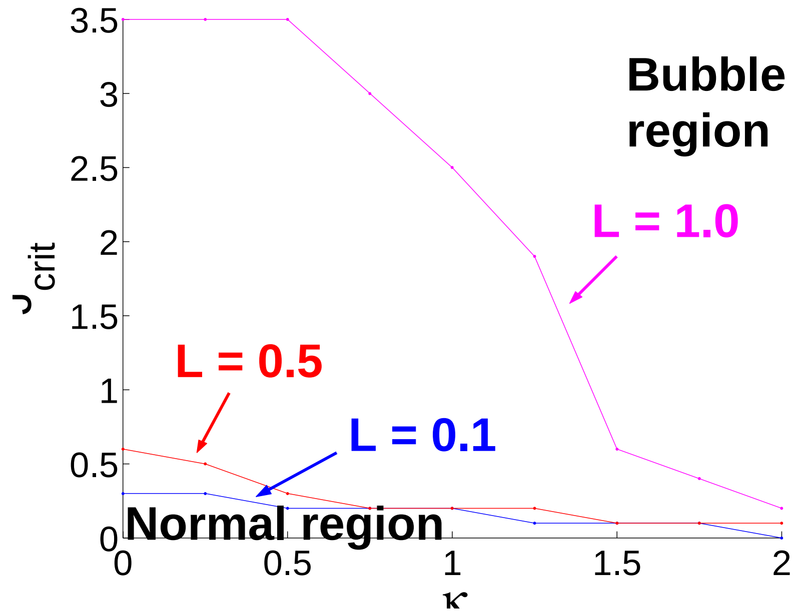
- Larger stacking, $C$, requires larger $J_0$ for bubbling.
- Larger twist width, $L$, requires larger $J_0$ for bubbling.

# Curved chain




*Critical values of* $J_0$ *for* $A = -2.5$ *and* $C = 0.1$.

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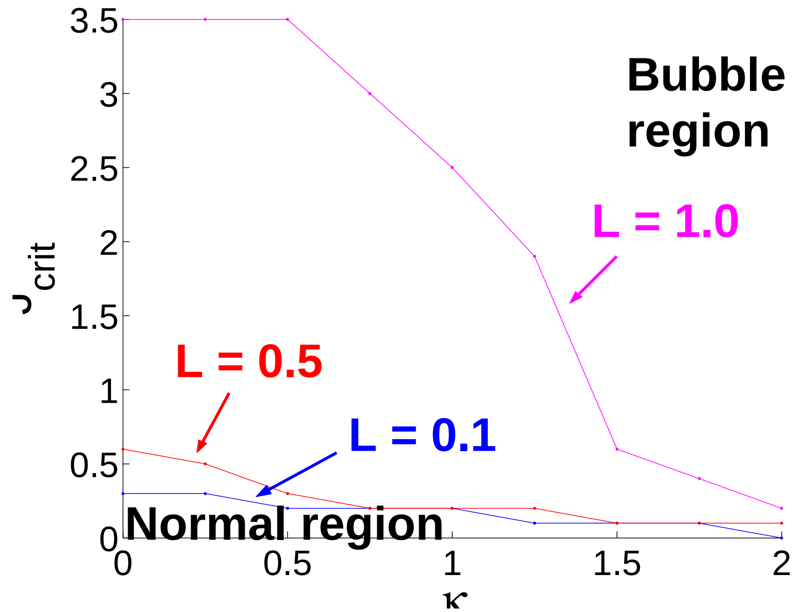


*Critical values of* $J_0$ *for* $A = -2.5$ *and* $C = 0.1$.

- Larger curvature, $\kappa$, can do with smaller $J_0$ for bubbling.
- Larger twist width, $L$, requires larger $J_0$ for bubbling (again).

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- Dipole interaction, twisting and curvature shown to be of importance.
- Work currently on determining physically reasonable parameter values.
- May in turn include temperature in model.