

# Mechanics explains coiled protein polymers in bacteria

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## Abstract

Several cytoskeletal protein polymers in *E. coli*, *B. subtilis*, and other model bacteria have been shown to form coils or rings on the inside of the cell membrane. Some of these structures extend the whole length of the cell (e.g. the proteins MreB and Mbl), some are localized primarily to a pole (e.g. MinD), and some form rings (e.g. FtsZ). We believe that these structures arise from the interaction of the inherent mechanical properties of the protein polymers with the constraints imposed by the curved cell membrane. Stochastic mechanical simulations and analytical theory show that this hypothesis is sufficient to explain all of the structures that have been observed. It also provides a simple explanation for the Z-ring in a sporulating *B. subtilis* to transform from a ring to a coil, to 2 rings, and to finally constrict. In contrast, alternate hypotheses are unable to explain the observed structures and dynamics.

## The research question

Many bacterial proteins form polymers that are bound to the cell membrane in helical or ring shapes. Where do these shapes come from?

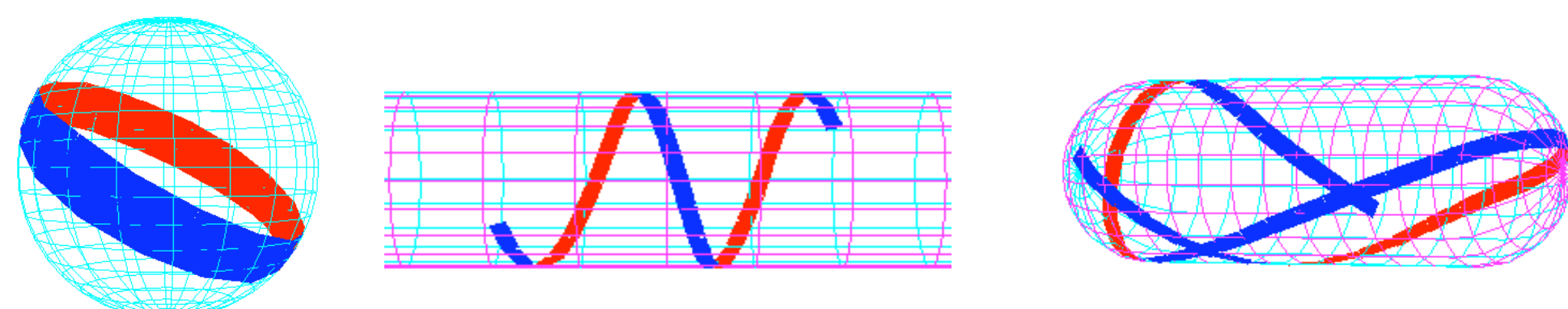
## My hypothesis

They are the low energy structures of stiff polymers that are constrained by the cell membrane.

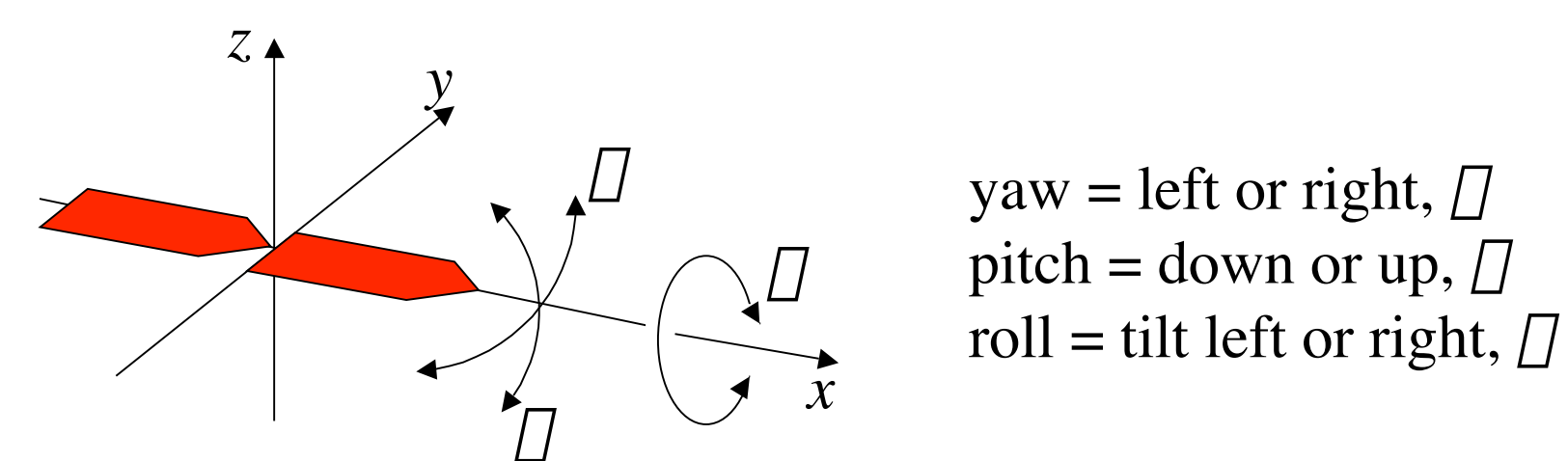
## Modeling a protein polymer

- The polymer is constrained to the surface – sphere, cylinder, or rod
- Each monomer has a single binding face (the “bottom”)

■ = bottom (near side)    ■ = top (far side)



- Bending angles are defined with yaw, pitch, and roll values



- Polymers are stiff because of a bending energy

$$E_{bend} = \sum_{j=1}^n \left[ \frac{k_{\psi}}{2} (\Delta_j \psi)^2 + \frac{k_{\theta}}{2} (\Delta_j \theta)^2 + \frac{k_{\phi}}{2} (\Delta_j \phi)^2 \right]$$

- Based on actin measurements, all bending force constants were set to the same values, so that the polymer behaves mechanically like a solid cylinder.



## Simulation methods

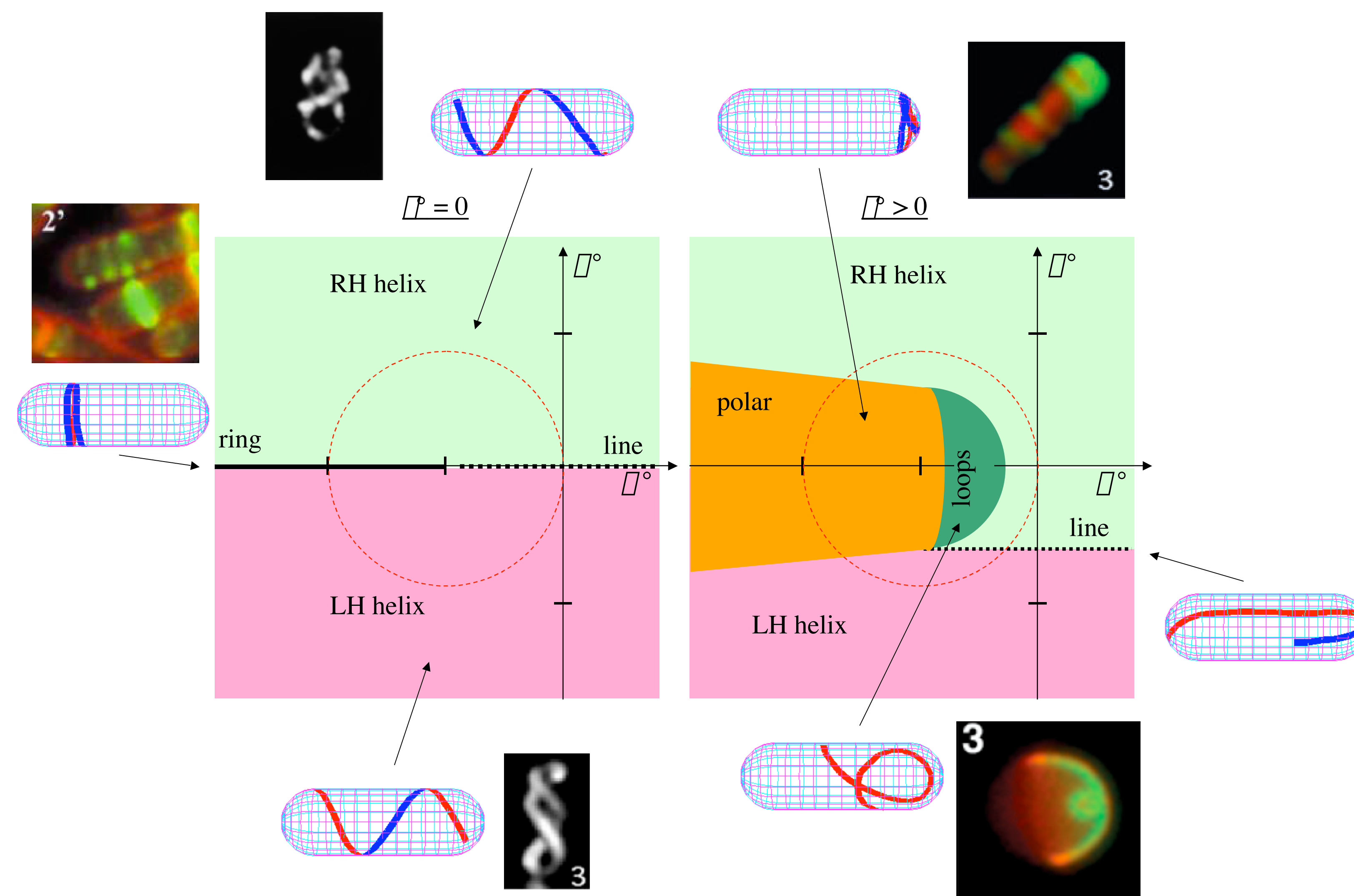
- Used the Metropolis algorithm and simulated annealing (and my own C code)
- Metropolis trial moves chose with equal probability either: (i) displacement of a random internal bend by a random amount, or (ii) treadmilling of the polymer forward or backward by one monomer.

## Results

We see 5 morphologies:

- helices that are left- and right-handed
- rings around the cylinder portion
- polar-targeted circles
- loops on the cylinder portion
- lines that are parallel to the bacterial axis

These morphologies depend on the preferred bending angles:  $\psi$ ,  $\theta$ ,  $\phi$   
They also agree well with fluorescence images



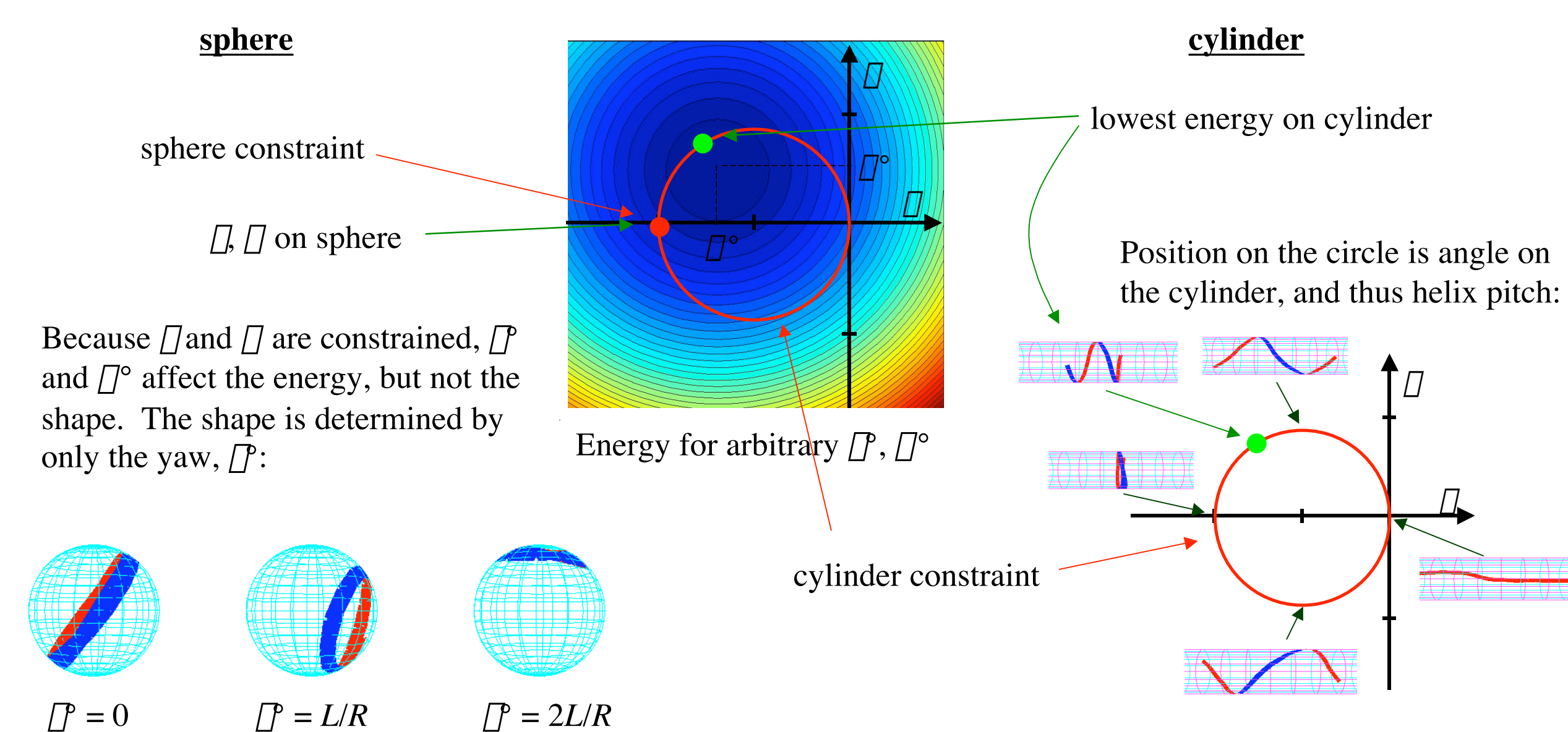
## Explanation of the phase diagram

On a sphere, polymer bends are constrained to:  $\psi = -L/R$ ,  $\theta = 0$ .

On a cylinder, bends are constrained to:  $(\psi - L/2R)^2 + \theta^2 = (L/2R)^2$

$L$  = monomer length,  $R$  = bacterium radius

The potential energy well minimum is at  $(\psi, \theta, \phi)$ , so the resulting yaw, pitch, and roll minimize the energy, while obeying the bending constraints.



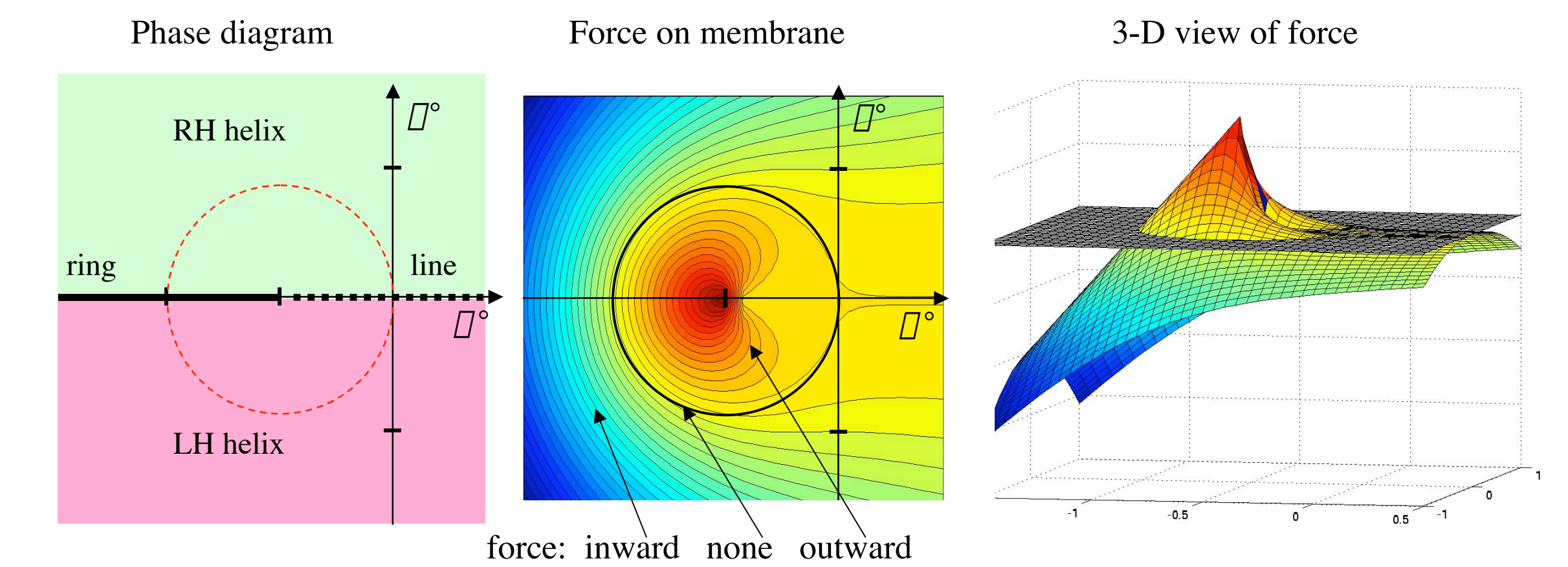
## Prediction: Mechanical forces

Several of the proteins investigated are cytoskeletal.

Question: what does our model predict about polymer forces on the membrane?

Answer:  $\partial E / \partial R$  is the net radial force (ignoring membrane deformation).

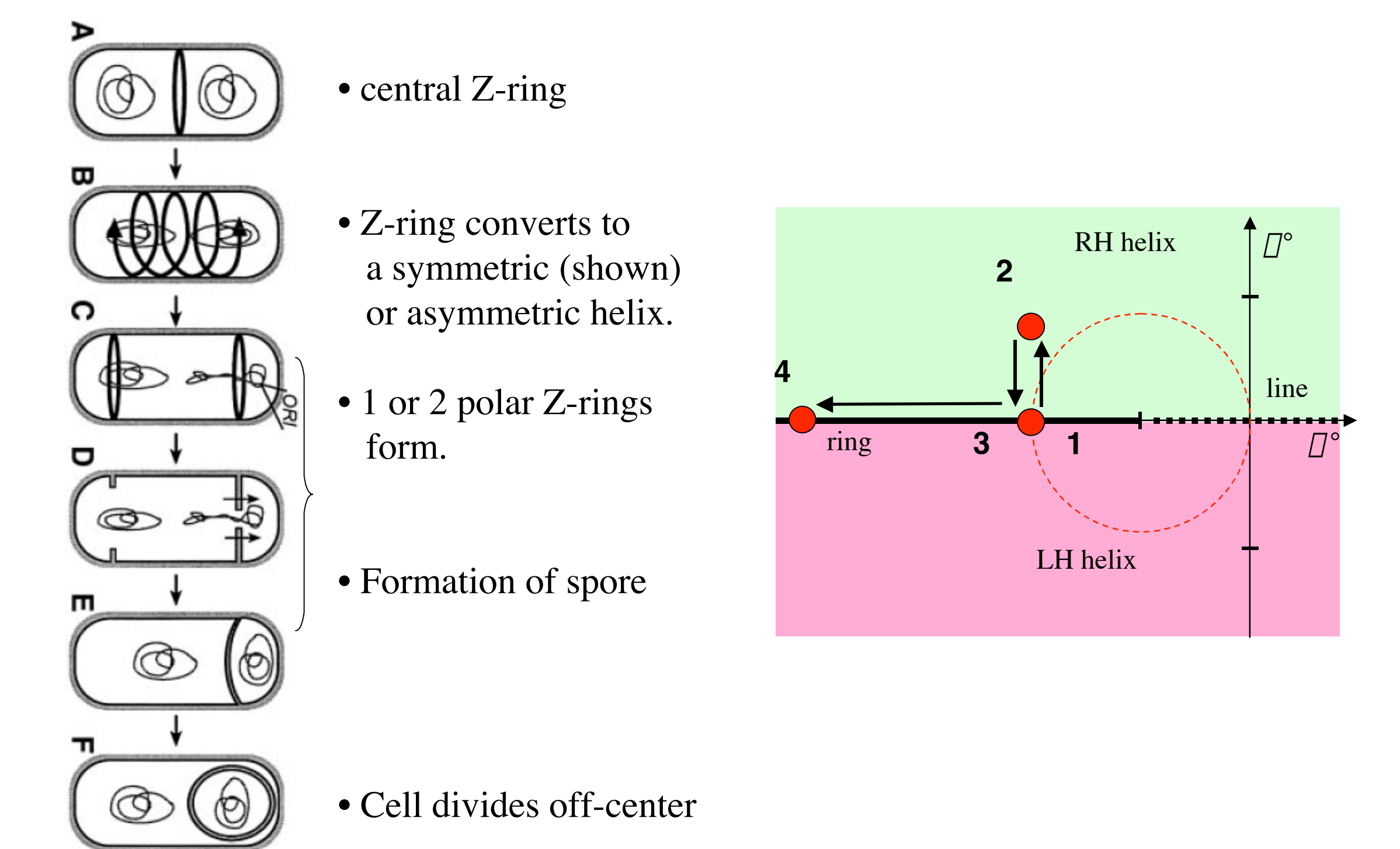
### Results for $\psi = 0$



Conclusion: rings (e.g. FtsZ) can exert strong outward or inward forces, lengthwise polymers exert neither, and helices are intermediate.

## Prediction: *B. subtilis* Z-ring

*B. subtilis* exhibits interesting Z-ring dynamics during sporulation (left). Our guess is that the sporulating cell changes the Z-ring protein composition in a controlled way, which changes the preferred bending angles of the monomers, and thus the morphology of the structure. A pattern of changes that is consistent with observations is shown (right).



## References

- Images in phase diagram  
Shih, Y., T. Le, and L. Rothfield, *Proc. Natl. Acad. Sci. USA*, 100:7865-70, 2003  
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- Image in *B. subtilis* prediction  
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## Acknowledgements

We thank Yu-Ling Shih, Larry Rothfield, and Jay Groves for helpful discussions. This project was funded by an NSF postdoctoral fellowship in biological informatics awarded to SSA and by the DOE GTL project.