Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Theory of Disk-to-Vesicle Transformation JIANFENG LI, AN-CHANG SHI, Department of Physics and Astronomy, McMaster University — Self-assembled membranes from amphiphilic molecules, such as lipids and block copolymers, can assume a variety of morphologies dictated by energy minimization of system. The membrane energy is characterized by a bending modulus (κ), a Gaussian modulus (κ_G), and the line tension (γ) of the edge. Two basic morphologies of membranes are flat disks that minimize the bending energy at the cost of the edge energy, and enclosed vesicles that minimize the edge energy at the cost of bending energy. In our work, the transition from disk to vesicle is studied theoretically using the string method, which is designed to find the minimum energy path (MEP) or the most probable transition path between two local minima of an energy landscape. Previous studies of disk-to-vesicle transition usually approximate the transitional states by a series of spherical cups, and found that the spherical cups do not correspond to stable or meta-stable states of the system. Our calculation demonstrates that the intermediate shapes along the MEP are very different from spherical cups. Furthermore, some of these transitional states can be meta-stable. The disk-to-vesicle transition pathways are governed by two scaled parameters, $\kappa_{G/}\kappa$ and $\gamma R_0/4\kappa$, where R_0 is the radius of the disk. In particular, a meta-stable intermediate state is predicted, which may correspond to the open morphologies observed in experiments and simulations.

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Date submitted: 20 Nov 2008 Electronic form version 1.4