

Computation of saddle point and its application on nucleation

Lei Zhang¹, Qiang Du² and Zhenzhen Zheng³

¹ Beijing International Center for Mathematical Research, Peking University, Beijing 100871,
zhangl@math.pku.edu.cn

² Department of Mathematics, Pennsylvania State University, PA 16802, USA, qdu@math.psu.edu

³ Department of Mathematics, Beijing University of Posts and Telecommunications, Beijing 100876,
China, zhengzz@gmail.com

Key Words: *Saddle point, critical nucleus, nucleation, solid state, phase field, phase transformation*

Abstract: *Saddle point search on an energy surface has attracted much attention in various areas. In this talk, I will first introduce efficient numerical methods for finding saddle points. Then I will combine the developed methods with the phase field model to study the nucleation during phase transition in solids and predict the morphologies of critical nuclei. Numerical simulations reveal many interesting results of nucleation in solid state phase transformation.*