# 数学与系统科学研究院

# 计算数学所学术报告

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报告题目：

**Nucleation of Quasicrystals**

邀请人：　张硕 副研究员

报告时间：**2021** 年 **12** 月 **7** 日（周二）

上午 **10:00-11:00**

报告地点：科技综合楼

**311** 教室

# Abstract:

**Despite the fact that tremendous efforts have been made on the study of quasicrystals since their discovery in 1984, nucleation of quasicrystals, viz. the emergence of a quasicrystal from a crystalline phase, still presents an unsolved and challenging problem. The difficulties lie in that quasicrystals and crystals are incommensurate structures in general, so there are no obvious epitaxial relations between them. In this talk, we proposed a saddle dynamics method to solve this problem by applying the Landau theory of phase transitions. We obtained the accurate critical nuclei and transition pathways connecting crystalline and quasicrystalline phases. The results reveal that phase transitions between the crystalline and quasicrystalline phases could follow two possible pathways, corresponding to a one-stage phase transition and a two-stage phase transition involving a metastable lamellar quasicrystalline state, respectively. The proposed computational methodology not only reveals the mechanism of nucleation of quasicrystals, but also paves the way to investigate a wide range of physical problems undergoing the first-order phase transitions.**


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