

数学与系统科学研究院

计算数学所学术报告

报告人: 周愈之

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报告题目:

**Plane Wave Methods for Quantum  
Eigenvalue Problems of  
Incommensurate Systems**

邀请人: 戴小英 研究员

报告时间: 2019 年 3 月 26 日 (周二)

下午 15:00-16:00

报告地点: 数学院南楼九层

902 教室

## **Abstract:**

**We propose a novel numerical algorithm for computing the electronic structure related eigenvalue problems of incommensurate systems. Unlike the conventional practice that approximates the system by a large commensurate supercell, our algorithm directly discretizes the eigenvalue problems under the framework of a plane wave method. The emerging ergodicity and the interpretation from higher dimensions give rise to many unique features compared to what we have been familiar with in the periodic systems. The numerical results of 1D and 2D quantum eigenvalue problems are presented to show the reliability and efficiency of our algorithm. Furthermore, the extension of our algorithm to full Kohn-Sham density functional theory calculations is discussed.**

**欢迎大家参加！**