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：

Numerical Analysis of the Multiple Scattering Method for Quantum Eigenvalue Problems

邀请人：戴小英 研究员

报告时间：2020 年 12 月 22 日（周二）

下午 15:00-16:00

报告地点：数学院南楼

205 教室

摘要：

The multiple scattering theory (MST), also called Korringa-Kohn-Rostoker (KKR) method, is widely used in electronic structure calculations of solid materials. In the MST method, a perfect separation between the atomic potentials and configuration geometries can be achieved. This can be exploited in the simulations to reduce the computational costs for many large-scale systems, including defected and disordered systems. This work studies the MST method by a rigorous numerical analysis and derives a spectral convergence rate for the numerical approximations, which justifies the reliability and efficiency of the MST method.

欢迎大家参加！