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：

Sparse Cubature Grids, Boys' Theorem, and the Local Schrödinger Equation Method

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下午 **15:30-16:30**

报告地点：　科技综合楼三层 **311**

计算数学所报告厅

Abstract:

The local Schrödinger equation (LSE) method is a very accurate method for solving the electronic Schrödinger equation. It works by creating an analytic basis set through iteratively applying the Hamiltonian on some initial basis function. The coefficients of these functions are then determined by solving the electronic Schrödinger equation at a set of points. The LSE method does not have the limitation of requiring that the basis be analytically integrable. The current strategy for this method is to sample points using Monte-Carlo. Using Boys' theorem we see that the LSE method can be reformulated as a numerical integration problem, i.e. the Monte-Carlo sampling is actually numerical integration where the points have uniform weights. Using Monte-Carlo provides satisfactory results, however Monte-Carlo does not take into account the smoothness of the integrand. Recent results from Griebel and others in the mathematics of complexity literature show how one may construct accurate grids for performing efficient integration where the number of points only increase polynomially with respect to dimension. In this presentation the mechanics of the approach will be explained and preliminary results will be shown.

欢迎大家参加！