数学与系统科学研究院

计算数学所学术报告

报告人： **Prof. Zhaojun Bai**

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报告题目:

Minimization principles of the linear response eigenvalue problem

邀请人： 袁亚湘 院士

报告时间: **2012 年 6 月 19 日（周二）**

下午 15：30-16：30

报告地点： 科技综合楼三层 **301**

计算数学所小报告厅

Abstract：

The linear response (LR) eigenvalue problem arises from excitation state (energies) caluclations in the study of collective motion of many particle systems. There are a great deal of interests in developing efficient simulation techniques for excitation state calculations of molecules for materials design in energy science.

The first part of this talk is to present theoretical results for the LR eigenvalue problem, which include a minimization principle for the sum of the smallest positive eigenvalues and Cauchy-like interlacing inequalities. Although the LR eigenvalue problem is a nonsymmetric eigenvalue problem, these results mirror the well-known trace minimization principle and Cauchy's inequalities for the symmetric eigenvalue problem. The second part of the talk is to present the best approximation of the few smallest postive eigenvalues via a structure-preserving projection, and a four-dimensional subspace search conjugate gradient-like algorithms for simultaneously computing these eigenvalues and their associated eigenvectors. We will also present numerical examples to illustrate convergence behaviors of the proposed methods with and without preconditioning.

This is a joint work with Ren-cang Li, Dario Rocca and Giulia Galli.

欢迎大家参加！