数学与系统科学研究院

计算数学所学术报告

报告人：　**Prof. Weiguo Gao**

（ ***Fudan University*** ）

报告题目：

NLEP in KS-DFT: The derivation and a little theory

邀请人：　　周爱辉研究员

报告时间：**2011** 年 **8** 月 **2** 日（周二）

上午 **9：00-10：00**

报告地点：　　科技综合楼三层 **301**

计算数学所小报告厅

Abstract:

First I will show the form of the nonlinear eigenvalue problems (NLEP) arising from Kohn-Sham density functional theory (KS-DFT) through a simple 3D model problem and summarize some known results about the existence of the minima. Then I will talk about the convergence of the self-consistent field (SCF) iteration. We show that for the class of problems considered (which is a simplification of the nonlinear eigenvalue problems in KS-DFT), the SCF iteration produces a sequence of approximate solutions that contain two convergent subsequences. We identify the condition under which the SCF iteration becomes a contractive fixed point iteration that guarantees its convergence.

欢迎大家参加！