# 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：**

**A Posteriori Error Estimates for Nonlinear Schr odinger Equations**

**邀请人：　戴小英 副研究员**

**报告时间：2016 年 11 月 28 日（周一）**

**下午 16:00-17:00**

**报告地点：　数学院南楼二层**

**202 教室**

# Abstract:

**The determination of electronic structures often requires to solve nonlinear eigenvalue problems. These problems are computationally very costly, and therefore approximations have to be resorted to, among which the chosen model, the chosen discretization, and the chosen (possibly iterative) algorithm. The a priori analysis for the discretization of such problems is quite recent (see e.g. [1]). It proves the convergence and the optimality of the method used. For a given approximation, the a posteriori analysis, once it is performed, provides a guaranteed upper bound on the total error. It may also enable to separate error components stemming from the different sources of approximation and control each of them. This makes possible to iteratively t the approximation parameters leading to small errors at low computational cost.**

**In this talk, we shall present an a posteriori analysis for a one-dimensional Gross-Pitaevskii type equation in a periodic setting using a planewave discretization [3]. We will provide a computable bound of the error between the exact and approximate solutions. This bound will then be decomposed into two components, each of them depending mainly on one approximation parameter, which are here the number of degrees of freedom and the number of iterations in this iterative algorithm used to solve the problem numerically. Numerical simulations will be presented to illustrate the possibility of balancing the different error components. We shall also present a post-processing on the eigenvalues and eigenfunctions, using a linear perturbation theory based on residual computation [2]. This theoretically and numerically reduces the error signicantly both for eigenfunctions and for the energy.**

**References**

**[1] E. Canc es, R. Chakir and Y. Maday, Numerical analysis of the planewave discretization of orbital-free and Kohn-Sham models, M2AN (highlight article) 46 (2012) 341-388.**

**[2] E. Canc es, G. Dusson, Y. Maday, B. Stamm, and M. Vohral k, A perturbation-method-based post-processing for the planewave discretization of Kohn{Sham models, Journal of Computational Physics 307 (2016) 446-459.**

**[3] G. Dusson, and Y. Maday, A posteriori analysis of a nonlinear GrossPitaevskii-type eigenvalue problem, IMA Journal of Numerical Analysis (2016), drw001.**

欢迎大家参加！