特征值问题的多重校正算法的一些研究

摘要

有限元方法是求解科学研究和实际工程问题的重要数值方法, 在流体力学、电磁学、电子结构计算以及其它科学工程研究领域取得了巨大成功. 同时经过众多工程师、力学家和数学家的努力, 有限元方法及其理论已经达到非常完善的地步. 特征值问题有限元方法是有限元理论的重要组成部分, 迄今为止已经出现一些影响较大的结果: 20世纪80年代, I.Babuška和J.Osborn建立了有限元方法求解特征值问题的数学理论框架; 林群、许进超和周爱辉提出两空间和二网格离散技巧求解特征值问题, 为求解特征值问题开辟了一个新的方向; 2011年, 林群和谢和虎提出了求解特征值问题的多重校正算法, 进而构造了多重网格方法, 使求解特征值问题的效率达到最优. 这些工作极大丰富和推动了特征值问题的研究及后续工作.

本文在已有研究工作的基础上, 结合多重校正算法以及多重网格算法的技巧, 提出了求解特征值问题的套迭代多重网格算法. 该方法的思想是把特征值问题转化为一系列细空间上的边值问题以及粗空间上的特征值问题. 同时对边值问题不需要精确求解, 只需要利用多重网格方法得到一个近似解. 这种方法只需要线性计算复杂度即可得到特征值问题的最优误差估计. 同时我们将该方法推广到半线性特征值问题并且也得到了最优的误差估计. 对于有奇性的问题, 自适应加密技术是一种有效的算法. 我们将多重校正的技巧和自适应有限元方法相结合, 提出了多重校正自适应方法, 并将其成功地应用到半线性椭圆问题以及基于密度泛函理论的第一原理电子结构的计算中.

Abstract

The finite element method is one of important numerical methods to solve scientific and engineering problems, which has been widely used in various fields, such as structural fluid dynamics, electromagnetics, electronic structure calculations and other areas of science and engineering. Meanwhile, it has been established a complete theory in mathematics by engineers and mathematicians. Finite element method is also an efficient method for eigenvalue problems. The corresponding history can be tracked back to 1980s when I.Babuška and J.Osborn established the finite element theory for eigenvalue problems. Lin, Xu and Zhou proposed the two-space and two-grid discretization methods to improve the efficiency of solving eigenvalue problems. In 2011, Lin and Xie introduced the multilevel correction method and derived the optimal error estimates. All these work promoted the

development of finite element method for eigenvalue problems.

In this thesis, a full multigrid scheme is proposed to solve the eigenvalue problems by combing the skills of multilevel correction method and multigrid method for boundary value problems. This method transforms the eigenvalue problem into a series of boundary value problems in finer finite element spaces and eigenvalue problems in low dimensional spaces. Besides, these boundary value problems just need to solved by multigird method approximately. Furthermore, we extended this method to semilinear eigenvalue problems and derived optimal error estimates similarly. For problems with singularity, we designed a multilevel correction type adaptive finite element method. This method has already been used to solve semilinear elliptic problems and Kohn-Sham models successfully.