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ScienceDirect
Journal of Computational and Applied Mathematics 205 (2007) 509–532
JOURNAL OF COMPUTATIONAL AND APPLIED MATHEMATICS
www.elsevier.com/locate/cam

An efficient algorithm for the Schrödinger–Poisson eigenvalue problem

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Received 15 August 2005; received in revised form 24 May 2006

Abstract

We present a new implementation of the two-grid method for computing extremum eigenpairs of self-adjoint partial differential operators with periodic boundary conditions. A novel two-grid centered difference method is proposed for the numerical solutions of the nonlinear Schrödinger–Poisson (SP) eigenvalue problem.We solve the Poisson equation to obtain the nonlinear potential for the nonlinear Schrödinger eigenvalue problem, and use the block Lanczos method to compute the first k eigenpairs of the Schrödinger eigenvalue problem until they converge on the coarse grid. Then we perform a few conjugate gradient iterations to solve each symmetric positive definite linear system for the approximate eigenvector on the fine grid. The Rayleigh quotient iteration is exploited to improve the accuracy of the eigenpairs on the fine grid. Our numerical results show how the first few eigenpairs of the Schrödinger eigenvalue problem are affected by the dopant in the Schrödinger–Poisson (SP) system. Moreover, the convergence rate of eigenvalue computations on the fine grid is $O(h^3)$.

Keywords: Schrödinger eigenvalue problem; Schrödinger–Poisson system; Wave functions; Two-grid method; RQI

1. Introduction

In recent years, some numerical methods have been proposed for computing the first few eigenpairs of the Schrödinger eigenvalue problem. See e.g., [8,18,19]. In particular, the homotopy continuation method [19] was exploited to solve the Schrödinger eigenvalue problem with Dirichlet boundary conditions, where various linear potentials were numerically tested. However, in the case of Dirichlet boundary conditions most of the multiple eigenvalues are double. Livne and Brandt [18] design linear-complexity multiscale algorithms for computing, storing, and manipulating eigenfunctions of the 1D periodic Schrödinger eigenvalue problem and other related differential operators. Recent research articles concerning the computations of interior eigenpairs of the Schrödinger equation can be found in [14,27].

Xu and Zhou [28] developed a two-grid finite element discretization scheme for second order linear elliptic eigenvalue problems. Let $\tilde{h}$ and h be the uniform meshsizes on the coarse and the fine grids, and (u, λ) and (u_h, λ_h) be the corresponding exact and the approximate eigenpairs on the fine grid, respectively. They show that $\|\nabla(u - u_h)\|_{L^2} =$

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[1] Supported by the National Science Council of R.O.C. (Taiwan) through Project NSC 93-2115-M-005-005.

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doi:10.1016/j.cam.2006.05.013

$O(h + \widetilde{h}^2)$ and $|\lambda - \lambda_h| = O(h^2 + \widetilde{h}^4)$. These estimates mean that one can obtain asymptotic optimal errors by taking $\widetilde{h} = O(h^{\frac{1}{2}})$. Recently the authors [5] developed a two-grid finite element discretization scheme for semilinear elliptic eigenvalue problems.

In this paper we modify the two-grid finite element scheme in [5], and propose a new implementation of the two-grid method for computing extremum eigenpairs of self-adjoint partial differential operators with periodic boundary conditions. The problem can be expressed as

$$F(u, \lambda) = 0, \tag{1}$$

where $F : \mathbf{B} \times \mathbb{R} \to \mathbf{B}$ is a smooth mapping with $u \in \mathbf{B}$, $\lambda \in \mathbb{R}$, $\mathbf{B}$ is some Banach space, and $\mathbb{R}$ is the real line. For the Schrödinger eigenvalue problem

$$L(\phi, \omega) = -\Delta\phi + \widetilde{V}\phi - \omega\phi = 0, \tag{2}$$

where $(\phi, \omega) = (0, \omega)$ is a trivial solution, where $\widetilde{V}$ is the linear potential. Therefore, we can treat an eigenpair of the operator equation as a solution curve branching from the trivial solution curve at the eigenvalue [26, Chapter 9, p. 572]. We will combine the ideas of the two-grid discretization scheme together with the predictor–corrector method and develop a new algorithm for computing the extremum eigenpairs of the discrete Schrödinger eigenvalue problem.

To start, we discretize the operator equation (1) on the coarse grid by the centered difference approximations. Then we use the block Lanczos method to compute extremum eigenpairs on the coarse grid, which also can handle multiple and clustered eigenpairs as well. The implementations are inexpensive since the order of the coefficient matrix on the coarse grid is relatively small compared to the one on the fine grid. An alternative is to use the function `eig` in MATLAB to compute the first few eigenpairs. The extremum eigenpairs we obtained on the coarse grid will be used as predicted points to compute their counterparts on the fine grid. To obtain the target eigenpairs on the fine grid, we consider the first order approximation of the operator equation. Instead of solving symmetric positive definite (SPD) linear systems with multiple-right-hand sides for the eigenvectors, we propose to use the conjugate gradient (CG) method [11, Chapter 10] to solve each SPD linear system using a few iterations. The approximate eigenvalues on the fine grid are obtained by computing the corresponding Rayleigh quotients. Our main concern here is that the fine grid solutions only serve as starting initial guesses for the Rayleigh quotient iteration (RQI). Therefore, it is unnecessary to compute eigenvectors on the fine grid to the desired accuracy for solving linear systems. Our numerical experience shows that performing one CG iteration for each linear system would suffice to supply an acceptable initial guess for the RQI. We emphasize here that it is the RQI which give us accurate solutions in the two-grid method.

Three issues remain to be addressed concerning the two-grid method described above. First, how many extremal eigenpairs on the coarse grid can be used as initial guesses for computing their counterparts on the fine grid? Next, do multiple and clustered eigenvalues on the coarse grid suffice to approximate their counterparts on the fine grid? That is, the multiplicity of eigenvalues between these two grids must be consistent. Finally, we must choose a proper number of eigenvalues to compute so that the multiplicity of eigenvalues is never missed. The answers to these questions are based on some basic analysis as well as the numerical performance of the two-grid method on the linear eigenvalue problem

$$\Delta u + \lambda u = 0 \quad \text{in } \Omega = (0, 1)^n,$$

with periodic boundary conditions, and $n = 2, 3$.

Next, to study how the first few eigenpairs of the linear Schrödinger eigenvalue problem will be affected by a dopant, we consider the Schrödinger–Poisson (SP) system. We apply the two-grid method described above, and develop a two-grid method for computing numerical solutions of the SP system [15]. The system describes a quantum mechanical model of extremely small devices in semiconductor nanostructures where the quantum structure has to be taken into account. We also use the block Lanczos method to compute the first few, say k eigenpairs on the coarse grid. Then we consider the nonlinear Schrödinger eigenvalue problem as a parameter-dependent problem

$$L(\phi, \omega) + \alpha N(\phi) = 0, \quad \alpha \in [0, 1], \tag{3}$$

where $N(\phi) = V\phi$ denotes the effect of the nonlinear potential V. We choose an initial step size α_0 with $j\alpha_0 = 1$, $j \in \mathbb{N}$, for the continuation method, and solve the Poisson equation to obtain V for (3). Then we go back to (3) and use the block Lanczos method to find the first k eigenpairs. This process is repeated until $j\alpha_0 = 1$ is reached.