Commun. Comput. Phys.
doi: 10.4208/cicp.2018.hh80.08

Vol. **24**, No. 4, pp. 1073-1100
October 2018

# Computing Eigenvalues and Eigenfunctions of Schrödinger Equations Using a Model Reduction Approach

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Received 30 June 2017; Accepted (in revised version) 8 November 2017

**Abstract.** We present a model reduction approach to construct problem dependent basis functions and compute eigenvalues and eigenfunctions of stationary Schrödinger equations. The basis functions are defined on coarse meshes and obtained through solving an optimization problem. We shall show that the basis functions span a low-dimensional generalized finite element space that accurately preserves the lowermost eigenvalues and eigenfunctions of the stationary Schrödinger equations. Therefore, our method avoids the application of eigenvalue solver on fine-scale discretization and offers considerable savings in solving eigenvalues and eigenfunctions of Schrödinger equations. The construction of the basis functions are independent of each other; thus our method is perfectly parallel. We also provide error estimates for the eigenvalues obtained by our new method. Numerical results are presented to demonstrate the accuracy and efficiency of the proposed method, especially Schrödinger equations with double well potentials are tested.

**AMS subject classifications**: 35J10, 65F15, 65N25, 65N30

**Key words**: Schrödinger equation, eigenvalue problems, model reduction, two-level techniques, problem dependent basis functions, computational chemistry.

## 1 Introduction

In this paper, we construct a set of problem dependent basis functions to compute eigenvalues and eigenfunctions of Schrödinger equations. To be more specific, we consider the eigenvalue problem of the stationary Schrödinger equation with a potential $V(x)$ of the

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following form

$$\mathcal{H}u(x) := -\Delta u(x) + V(x)u(x) = \lambda u(x), \quad x \in \Omega \subseteq R^d, \tag{1.1}$$

$$u(x) = 0, \quad x \in \partial\Omega \subseteq R^d, \tag{1.2}$$

where $\Omega$ is a bounded domain in $\mathbb{R}^d$ and $V(x): R^d \to R$ is a real-valued function. $\lambda$ and $u(x)$ are the corresponding eigenvalues and eigenfunctions of the Hamiltonian operator $\mathcal{H} = -\Delta + V(x)$. We should emphasize that the spectrum of the Hamiltonian operator $\mathcal{H}$ can have negative values and physically the negative part of the spectrum corresponding to bound states and they have many important applications in computational chemistry [6, 17, 18, 29].

The eigenvalue problem of (1.1) in variational form reads: find an eigenvalue $\lambda$ and its associated eigenfunction $u(x) \in W := H_0^1(\Omega)$ such that

$$a(u,v) := \int_\Omega \big(\nabla u(x) \cdot \nabla v(x) + V(x)u(x)v(x)\big)dx = \lambda \int_\Omega u(x)v(x)dx = \lambda(u,v), \tag{1.3}$$

for all $v \in W$. By using the finite element method (FEM), we obtained the discretized problem of the eigenvalue problem (1.3): find $\lambda_h$ and associated eigenfunctions $u_h(x) \in V_h \subseteq W$ such that

$$a(u_h, v_h) = \lambda_h(u_h, v_h), \quad \text{for all} \quad v_h \in V_h, \tag{1.4}$$

where $V_h$ is a conforming finite element space spanned by $N_h$ nodal basis functions on some regular finite element mesh $\mathcal{T}_h$ with mesh size $h$. After the FEM discretization, one could apply eigenvalue algorithms, including QR-algorithm, Lanczos algorithm, and Arnoldi iteration, directly to the $N_h$-dimensional finite element matrices to obtain the eigen-pairs $\{\lambda_h, u_h\}$, see [10] and references therein. We remark that it is extremely expensive to compute eigenvalues and eigenfunctions of (1.4) when $N_h$ becomes big. For example, finding all eigenvalues and eigenvectors of the matrix corresponding to the FEM discretization of (1.4) using QR-algorithm costs $6N_h^3 + \mathcal{O}(N_h^2)$ flops.

In practice, however, we are mainly interested in the first few lowermost eigenvalues and eigenfunctions as they have important meanings in computational chemistry [19]. In addition, when we use the FEM to approximate eigenvalues of (1.4), the number of reliable numerical eigenvalues takes up only a tiny portion of the total degrees of freedom $N_h$ in the resulting discrete system. See [2, 30–32, 35] for the discussion of second-order elliptic eigenvalue problems.

This motivates us to avoid the application of eigenvalue algorithms for the fine-scale FEM discretization (1.4) and build a low-dimensional generalized finite element space so that we can accurately and efficiently compute the lowermost eigenvalues and eigenfunctions. Specifically, we introduce a coarse discretization of the physical space $\Omega$ into mesh $\mathcal{T}_H$ with mesh size $H \gg h$. On the coarse mesh $\mathcal{T}_H$, we build a set of basis functions $\{\Psi_i(x)\}_{i=1}^{N_H}$ that generate a low-dimensional generalized finite element space $V_c$. The dimension of $V_c$ is $N_H$ and it is much smaller than $N_h$. In the low-dimensional space $V_c$,