Linear Algebra and its Applications 488 (2016) 148–167

Contents lists available at ScienceDirect

Linear Algebra and its Applications

www.elsevier.com/locate/laa

Structure preserving parallel algorithms for solving the Bethe–Salpeter eigenvalue problem

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ARTICLE INFO

Article history:
Received 2 January 2015
Accepted 18 September 2015
Available online 2 October 2015
Submitted by V. Mehrmann

MSC:
65F15

Keywords:
Bethe–Salpeter equation
Tamm–Dancoff approximation
Hamiltonian eigenvalue problems
Structure preserving algorithms
Parallel algorithms

ABSTRACT

The Bethe–Salpeter eigenvalue problem is a dense structured eigenvalue problem arising from discretized Bethe–Salpeter equation in the context of computing exciton energies and states. A computational challenge is that at least half of the eigenvalues and the associated eigenvectors are desired in practice. We establish the equivalence between Bethe–Salpeter eigenvalue problems and real Hamiltonian eigenvalue problems. Based on theoretical analysis, structure preserving algorithms for a class of Bethe–Salpeter eigenvalue problems are proposed. We also show that for this class of problems all eigenvalues obtained from the Tamm–Dancoff approximation are overestimated. In order to solve large scale problems of practical interest, we discuss parallel implementations of our algorithms targeting distributed memory systems. Several numerical examples are presented to demonstrate the efficiency and accuracy of our algorithms.

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http://dx.doi.org/10.1016/j.laa.2015.09.036
0024-3795/

1. Introduction

The absorption of a photon by a molecular system or solid can promote an electron in an occupied single-particle state (or orbital) to an unoccupied state while keeping the charge neutrality. In the physics community, this process is often described as the simultaneous creation of a negatively charged quasielectron (or simply electron) and a positively charged quasihole (or hole) in the material that was originally in the lowest energy electronic configuration (the ground state). Upon absorbing a photon, the entire molecular or extended system is in an excited state that contains a correlated electron–hole pair, which is referred to as an *exciton*. The amount of energy required to trigger this excitation gives an important characterization of the material. In many-body physics, a two-particle collective excitation is often described by a two-particle Green's function, with the excitation energy level being a pole of this function. It has been shown that the two-particle Green's function satisfies an equation often known as the *Bethe–Salpeter equation* (BSE) [28].

The poles of the two-particle Green's function can be obtained by computing the eigenvalues of a Hamiltonian operator $\mathcal{H}$ associated with this Green's function. It can be shown that, with an appropriate discretization scheme, the finite dimensional representation of the Bethe–Salpeter Hamiltonian has the following block structure

$$H = \begin{bmatrix} A & B \\ -\overline{B} & -\overline{A} \end{bmatrix}, \tag{1}$$

where $A, B \in \mathbb{C}^{n\times n}$, with

$$A = A^{\mathsf{H}}, \qquad B = B^{\mathsf{T}}. \tag{2}$$

Here we use A^{H} to denote the conjugate transpose of A and B^{T} to denote the transpose of B. We will refer to an eigenvalue problem of the form (1) with the additional symmetry given by Equation (2) as a *Bethe–Salpeter eigenvalue problem*.

In principle, we are interested in all possible excitation energies, although some excitations are more likely to occur than others. Such likelihood can often be measured in term of what is known as the *spectral density* or *density of states* of H, which is defined to be the number of eigenvalues per unit energy interval [19], that is,

$$\phi(\omega) = \frac{1}{2n}\sum_{j=1}^{2n} \delta(\omega - \lambda_j), \tag{3}$$

where λ_j's denote the eigenvalues of H. This formulation requires all eigenvalues of H to be real, which is the case for most physical systems. In addition, the optical absorption