



# Efficient and accurate algorithms for solving the Bethe–Salpeter eigenvalue problem for crystalline systems

Peter Benner, Carolin Penke\*

Computational Methods in Systems and Control Theory, Max Planck Institute for Dynamics of Complex Technical Systems, Germany

## ARTICLE INFO

### Article history:

Received 19 August 2020

Received in revised form 19 March 2021

### Keywords:

Bethe–Salpeter

Structured eigenvalue problem

Efficient algorithms

Matrix square root

Cholesky factorization

Singular value decomposition

## ABSTRACT

Optical properties of materials related to light absorption and scattering are explained by the excitation of electrons. The Bethe–Salpeter equation is the state-of-the-art approach to describe these processes from first principles (*ab initio*), i.e. without the need for empirical data in the model. To harness the predictive power of the equation, it is mapped to an eigenvalue problem via an appropriate discretization scheme. The eigenpairs of the resulting large, dense, structured matrix can be used to compute dielectric properties of the considered crystalline or molecular system. The matrix always shows a  $2 \times 2$  block structure. Depending on exact circumstances and discretization schemes, one ends up with a matrix structure such as

$$H_1 = \begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \in \mathbb{C}^{2n \times 2n}, \quad A = A^H, \quad B = B^H,$$

$$\text{or } H_2 = \begin{bmatrix} A & B \\ -B^H & -A^T \end{bmatrix} \in \mathbb{C}^{2n \times 2n} \text{ or } \mathbb{R}^{2n \times 2n}, \quad A = A^H, \quad B = B^T.$$

$H_1$  can be acquired for crystalline systems (see Sander et al. (2015)),  $H_2$  is a more general form found e.g. in Shao et al. (2016) and Penke et al. (2020), which can for example be used to study molecules. Additionally, certain definiteness properties may hold. In this work, we compile theoretical results characterizing the structure of  $H_1$  and  $H_2$  in the language of non-standard scalar products. These results enable us to develop a generalized perspective on the currently used direct solution approach for matrices of form  $H_1$ . This new viewpoint is used to develop two alternative methods for solving the eigenvalue problem. Both have advantages over the method currently in use and are well suited for high performance environments and only rely on basic numerical linear algebra building blocks. The results are extended to hold even without the mentioned definiteness property, showing the usefulness of our new perspective.

© 2021 Elsevier B.V. All rights reserved.

## 1. Introduction and preliminaries

The accurate and efficient computation of optical properties of molecules and condensed matter has been an objective actively pursued in recent years [1–4]. In particular, the increasing importance of renewable energies reinforces the interest in the *in silico* prediction of optical properties of novel composite materials and nanostructures.

\* Corresponding author.

E-mail address: [penke@mpi-magdeburg.mpg.de](mailto:penke@mpi-magdeburg.mpg.de) (C. Penke).

New theoretical and algorithmic developments need to go hand in hand with the ever advancing computer technology. In view of the ongoing massive increase in parallel computing power [5], the solution of problems that were considered almost impossible just a few years ago comes within reach. In order to unlock the full potential of a supercomputer, great attention must be paid to the development of parallelizable and reliable methods.

*Ab initio* spectroscopy aims to compute optical properties of materials from first principles, without the need for empirical parameters. A state-of-the-art approach is derived from many-body perturbation theory and relies on solving the Bethe–Salpeter equation for the *density fluctuation response function*  $P(\omega)$ . This function describes the propagation of an electron-hole pair and is used to compute optical properties such as the optical absorption spectrum. Its poles give the excitation energies of the given system (for details see [1]). Restricting the number of considered occupied and unoccupied orbitals, the propagator can be represented in (frequency-dependent) matrix form with respect to a set of resonant and antiresonant two-orbital states. The Bethe–Salpeter equation can be rewritten to show that the inverse of the matrix form of  $P(\omega)$  is approximated by the matrix pencil

$$\mathcal{H} - \omega K, \quad (1)$$

where  $K = \begin{bmatrix} I_n & 0 \\ 0 & -I_n \end{bmatrix}$  contains a positive and a negative identity matrix on its diagonal.  $\mathcal{H} \in \mathbb{C}^{2n \times 2n}$  is a Hermitian matrix. It is computed from the Coulomb interaction and the screened interaction in matrix form (familiar from Hedin's equations [6]) and scalar energy differences between occupied and unoccupied orbitals. The periodicity of crystalline systems implies a time-inversion symmetry in the basis functions used for the discretization. This leads to  $\mathcal{H}$  having the following form:

$$\mathcal{H} = \mathcal{H}_1 = \begin{bmatrix} A & B \\ B & A \end{bmatrix}, \quad A = A^H, \quad B = B^H,$$

where  $^H$  denotes the Hermitian transpose. Throughout the paper  $^T$  denotes the regular transpose without complex conjugation.

In this paper we do not consider the generalized eigenvalue problem given in (1). Instead, we focus on the corresponding standard eigenvalue problem of the matrix

$$H_1 := K^{-1} \mathcal{H}_1 = K \mathcal{H}_1 = \begin{bmatrix} A & B \\ -B & -A \end{bmatrix}, \quad A = A^H, \quad B = B^H, \quad (2)$$

to which we refer as a *BSE matrix of form I*.

An eigenvalue problem of this form is also called linear response eigenvalue problem [7–11], appears in the Casida formalism of time-dependent density functional theory [12] and in the random phase approximation concerning the excitations of atomic nuclei [13].

If the time-inversion symmetry in the basis functions is not exploited or not available in the discretization process of the Bethe–Salpeter approach, the resulting structure is slightly different. The matrix considered for a standard eigenvalue problem then turns out to have the form

$$H_2 := K \mathcal{H}_2 = \begin{bmatrix} A & B \\ -B^H & -A^T \end{bmatrix} \in \mathbb{C}^{2n \times 2n} \text{ or } \mathbb{R}^{2n \times 2n}, \quad A = A^H, \quad B = B^T. \quad (3)$$

We call matrices of this form *BSE matrix of form II*.

In this paper, we present a concise overview of direct methods that exploit the structure given in (2) and improve upon a currently used approach in terms of performance and accuracy. Results and algorithms may partly be known but have not yet been derived in a unified fashion as presented in this paper. This contribution is particularly valuable because the eigenvalue problem appears in many loosely connected fields, spanning nuclear physics, various strands of electronic structure theory and quantum chemistry. Our unified framework shows how techniques that have been developed multiple times in different fields are all based on the same principles. This eases the switch from one technique to a better suited one in the context of complex high performance implementations. The proposed methods are well-suited for high performance computing as they rely on basic linear algebra building blocks for which high performance implementations are readily available. Furthermore, we used the new perspective to generalize the approaches in a setting where certain definiteness properties typically assumed do not hold.

Iterative methods [8–11,14,15] are certainly attractive in the context of large, possibly sparse matrices and when only the few smallest eigenpairs are sought. It is however worthwhile not to neglect direct approaches leading to full diagonalization. When all eigenpairs are of interest, or when it is not clear how many eigenpairs are needed a-priori, a direct method is expected to have a favorable performance. Other reasons include ease of implementation, testing and benchmark purposes. Typically, a direct approach is established first and iterative methods are compared to this baseline in terms of performance and accuracy. In order to guarantee a fair comparison, the direct approach should not be needlessly laborious. This can, however, be said about current implementations [1,2,12], which employ an expensive matrix square root. One of the aims of this paper is to make it clear that a cheaper Cholesky factorization works just as well and points out the mathematical structure underlying these algorithms.

We characterize the structure of the BSE matrices (2) and (3) by employing the concept of non-standard scalar products. We introduce the notation and concepts following [16].

A nonsingular matrix  $M$  defines a scalar product on  $\mathbb{C}^n$   $\langle \cdot, \cdot \rangle_M$ , which is a bilinear or sesquilinear form, given by

$$\langle x, y \rangle_M = \begin{cases} x^T M y & \text{for bilinear forms,} \\ x^H M y & \text{for sesquilinear forms,} \end{cases} \quad (4)$$

for  $x, y \in \mathbb{C}^n$ . For a matrix  $A \in \mathbb{C}^{n \times n}$ ,  $A^*M \in \mathbb{C}^{n \times n}$  denotes the adjoint with respect to the scalar product defined by  $M$ . This is a uniquely defined matrix satisfying the identity

$$\langle Ax, y \rangle_M = \langle x, A^*M y \rangle_M$$

for all  $x, y \in \mathbb{C}^n$ . We call  $A^*M$  the  $M$ -adjoint of  $A$  and it holds

$$A^*M = M^{-1}A^*M,$$

where  $*$  can refer to the transpose  $^T$  or Hermitian transpose  $^H$ , depending on whether a bilinear or a sesquilinear form is considered. We call the matrix  $M$ -orthogonal if  $A^*M = A^{-1}$  (given the inverse exists),  $M$ -self-adjoint if  $A = A^*M$  and  $M$ -skew-adjoint if  $A = -A^*M$ .

The remaining paper is structured as follows. In Section 2 we compile theoretical results regarding the structured matrix forms. Here we see how both forms are connected and yield a similar spectral structure. A fundamental difference is given by the fact that a BSE matrix of form I can be mapped to a product eigenvalue problem of half the size, which is not possible for form II. This new framework is used in Section 3 to characterize three solution approaches. It becomes apparent that a variant involving the matrix square root is the least useful approach. This notion is confirmed by numerical experiments in Section 4. In Section 5 we apply our framework to devise new results concerning the non-definite case corresponding to excitations of finite lifetime. Here, not only real but also imaginary and complex eigenvalues appear. Most methods available in the literature are not applicable in this case. Our framework can again be used to map the eigenvalue problem to a smaller product eigenvalue problem and derive solution strategies.

## 2. Results on the spectral structure of BSE matrices

Non-definite scalar products introduced in (4) provide a language to describe the structure of the BSE matrices in a more concise way, not relying on the matrix block structure. The following two matrices, and the scalar products induced by them, play a central role:

$$J_n = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}, \quad K_n = \begin{bmatrix} I_n & 0 \\ 0 & -I_n \end{bmatrix}.$$

We drop the index when the dimension is clear from its context. The identities  $J^{-1} = -J$  and  $K^{-1} = K$  are regularly used in the following. The results compiled in this section are partly known and can be proven easily using the notion of generalized scalar products.

**Theorem 1.** A matrix  $H \in \mathbb{C}^{2n \times 2n}$  is a BSE matrix of form I as given in (2) if and only if both of the following conditions hold.

1.  $H$  is skew-adjoint with respect to the complex sesquilinear form induced by  $J$ , i.e.  $H = -H^*J = JH^HJ$ .
2.  $H$  is self-adjoint with respect to the complex sesquilinear form induced by  $K$ , i.e.  $H = H^*K = KH^HK$ .

**Theorem 2.** A matrix  $H$  is a BSE matrix of form II as given in (3) if and only if both of the following conditions hold.

1.  $H$  is skew-adjoint with respect to the complex bilinear form induced by  $J$ , i.e.  $H = -H^*J = JH^TJ$ .
2.  $H$  is self-adjoint with respect to the complex sesquilinear form induced by  $K$ , i.e.  $H = H^*K = KH^HK$ .

This new characterization is used to show that eigenvalues and eigenvectors also exhibit special structures. Matrices, that are skew-adjoint with respect to the sesquilinear form induced by  $J$  are called *Hamiltonian*, and play an important role in control theory and model order reduction (see e.g. [17]). The same property with respect to the bilinear form is called *J-symmetric* in [16] and explored further in [18].

The first two propositions of the following theorem are well known facts about Hamiltonian [17] and J-symmetric matrices [18]. Here,  $\bar{\lambda}$  denotes the complex conjugate of  $\lambda$ .

**Theorem 3.** Let  $H \in \mathbb{C}^{2n \times 2n}$ .

1. If  $H$  is skew-adjoint with respect to the sesquilinear form induced by  $J$ , i.e.  $JH = -H^HJ$ , then its eigenvalues come in pairs  $(\lambda, -\bar{\lambda})$ . If  $x$  is a right eigenvector of  $H$  corresponding to  $\lambda$ , then  $x^HJ$  is the left eigenvector of  $H$  corresponding to  $-\bar{\lambda}$ .
2. If  $H$  is skew-adjoint with respect to the bilinear form induced by  $J$ , i.e.  $JH = -H^TJ$ , then its eigenvalues come in pairs  $(\lambda, -\lambda)$ . If  $x$  is a right eigenvector of  $H$  corresponding to  $\lambda$ , then  $x^TJ$  is the left eigenvector of  $H$  corresponding to  $-\lambda$ .

3. If  $H$  is self-adjoint with respect to the sesquilinear form induced by  $K$ , i.e.  $KH = H^H K$ , then eigenvalues come in pairs  $(\lambda, \bar{\lambda})$ . If  $x$  is a right eigenvector of  $H$  corresponding to  $\lambda$ , then  $x^H K$  is the left eigenvector of  $H$  corresponding to  $\bar{\lambda}$ .

**Theorem 3** reveals that symmetries defined by the matrices  $J$  or  $K$  are reflected in connections between left and right eigenvectors of the considered matrix. The BSE matrices show a symmetry with respect to two scalar products ([Theorems 1](#) and [2](#)). This double-structure leads to eigenvalues that show up not only in pairs but also in quadruples if they have a real and an imaginary component. Additionally, it yields a connection between right eigenvectors, clarified in the following theorem.

**Theorem 4.** Let  $H \in \mathbb{C}^{2n \times 2n}$  be self-adjoint with respect to the sesquilinear scalar product induced by  $K$  and skew-adjoint with respect to (a) the sesquilinear scalar product or (b) the bilinear scalar product induced by  $J$ . Then

1. The eigenvalues of  $H$  come in pairs  $(\lambda, -\lambda)$  if  $\lambda \in \mathbb{R}$  or  $\lambda \in i\mathbb{R}$ , or in quadruples  $(\lambda, \bar{\lambda}, -\lambda, -\bar{\lambda})$ .
2. (a) If  $v$  is an eigenvector of  $H$  with respect to  $\lambda$ , then  $JKv$  is an eigenvector of  $H$  with respect to  $-\lambda$ .  
(b) If  $v$  is an eigenvector of  $H$  with respect to  $\lambda$ , then  $JK\bar{v}$  is an eigenvector of  $H$  with respect to  $-\bar{\lambda}$ .

In the practice of computing excitation properties of materials, often there is even more structure available. It can be exploited for devising efficient algorithms. The Hermitian matrices

$$\mathcal{H}_1 := KH_1 = \begin{bmatrix} A & B \\ B & A \end{bmatrix} > 0, \quad \mathcal{H}_2 := KH_2 = \begin{bmatrix} A & B \\ B^H & A^T \end{bmatrix} > 0, \quad (5)$$

introduced in [\(1\)](#), are typically positive definite [\[1,19\]](#) (indicated by the notation  $> 0$ ).

The definiteness property has consequences for the structure of the eigenvalue spectrum. To study these, we consider the more general class of  $\Sigma$ -Hermitian matrices. By this we mean matrices that are self-adjoint with respect to the scalar product induced by a signature matrix  $\Sigma$ .  $K$  is a particular example of a signature matrix.

**Theorem 5.** Let  $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_n)$ ,  $\sigma_i \in \{+1, -1\}$  be a signature matrix with  $p$  positive and  $n - p$  negative diagonal entries. Let  $H \in \mathbb{C}^{n \times n}$  be given such that  $\Sigma H$  is Hermitian positive definite. Then  $H$  is diagonalizable and its eigenvalues are real, of which  $p$  are positive and  $n - p$  are negative.

In the remaining part of this section we focus on BSE matrices of form [I](#), paving the way for a new unified framework relating different solution strategies. The following theorem plays the central role in this paper. Note that the definiteness property [\(5\)](#) is not required here. We use it as a new tool to derive the solution approach currently used in [\[1,2\]](#). Within this new framework other solution approaches become apparent yielding significant benefits.

**Theorem 6.** Let  $H$  be a BSE matrix of form [I](#) (see [\(2\)](#)) and  $M_1 := A + B$ ,  $M_2 = A - B$  be nonsingular. Let

$$M_1 M_2 v_1 = \mu v_1, \quad v_2^H M_1 M_2 = \mu v_2^H, \quad v_1^H v_2 = 1, \quad (6)$$

define a pair of right and left eigenvectors of the matrix product  $M_1 M_2$ , corresponding to an eigenvalue  $\mu \in \mathbb{R}$ . With  $Q := \frac{1}{2} \begin{bmatrix} I & I \\ -I & I \end{bmatrix}$  and scaling factors  $\lambda_1 := v_2^H M_1 v_2 \in \mathbb{R}$ ,  $\lambda_2 := v_1^H M_2 v_1 \in \mathbb{R}$ , an eigenpair of  $H$  is given by

$$\lambda = \begin{cases} \mu^{\frac{1}{2}} & \text{if } (\lambda_1 > 0 \text{ and } \lambda_2 > 0) \text{ or } \text{sign}(\lambda_1) \text{sign}(\lambda_2) = -1, \\ -\mu^{\frac{1}{2}} & \text{if } \lambda_1 < 0 \text{ and } \lambda_2 < 0 \end{cases}, \quad v_\lambda = Q \begin{bmatrix} v_1 \lambda_1^{\frac{1}{4}} \lambda_2^{-\frac{1}{4}} \\ v_2 \lambda_1^{-\frac{1}{4}} \lambda_2^{\frac{1}{4}} \end{bmatrix}, \quad (7)$$

i.e.  $H v_\lambda = \lambda v_\lambda$ . If  $\gamma$  is an eigenvalue of  $M_1 M_2$  and  $v_\gamma$  is the corresponding constructed vector, it holds

$$v_\lambda^H K v_\gamma = \begin{cases} 1 & \text{if } \lambda = \gamma \in \mathbb{R}, \\ 0 & \text{if } \lambda = \gamma \in i\mathbb{R}, \\ 0 & \text{if } \lambda \neq \gamma, \end{cases} \quad v_\lambda^H J v_\gamma = \begin{cases} 0 & \text{if } \lambda = \gamma \in \mathbb{R} \text{ or if } \lambda \neq \gamma, \\ i & \text{if } \lambda = \gamma \in i\mathbb{R} \text{ and } \lambda_1 > 0, \lambda_2 < 0, \\ -i & \text{if } \lambda = \gamma \in i\mathbb{R} \text{ and } \lambda_1 < 0, \lambda_2 > 0. \end{cases} \quad (8)$$

**Proof.** It follows from [\(6\)](#) that

$$M_1 M_2 M_1 v_2 = \mu M_1 v_2,$$

i.e.  $M_1 v_2$  lies in the eigenspace of  $M_1 M_2$  corresponding to  $\mu$ . If  $M_1 v_2$  is not a multiple of  $v_1$  it must hold  $(M_1 v_2)^H v_2 = 0$ , which contradicts the fact, that  $M_1$  is nonsingular. So there is  $\lambda_1 \in \mathbb{C}$ , s.t.

$$M_1 v_2 = \lambda_1 v_1. \quad (9)$$

Similarly it follows from [\(6\)](#) that there is  $\lambda_2 \in \mathbb{C}$ , s.t.

$$M_2 v_1 = \lambda_2 v_2. \quad (10)$$

Following from (9) and (10) and using  $v_1^H v_2 = 1$ ,  $\lambda_1$  and  $\lambda_2$  can be computed as

$$\lambda_1 = v_2^H M_1 v_2, \quad \lambda_2 = v_1^H M_2 v_1.$$

It follows that  $\lambda_1, \lambda_2 \in \mathbb{R}$  because  $M_1$  and  $M_2$  are Hermitian. Inserting (10) in (9) we get

$$M_1 M_2 v_1 = \lambda_1 \lambda_2 v_1. \quad (11)$$

With (6) it follows  $\lambda_1 \lambda_2 = \mu$ . For  $\lambda \in \mathbb{C}$ ,

$$\begin{bmatrix} 0 & M_1 \\ M_2 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} x \\ y \end{bmatrix}$$

holds if and only if

$$M_1 y = \lambda x \quad \text{and} \quad M_2 x = \lambda y. \quad (12)$$

This is achieved by  $x := v_1 \lambda_1^{\frac{1}{4}} \lambda_2^{-\frac{1}{4}}$ ,  $y := v_2 \lambda_1^{-\frac{1}{4}} \lambda_2^{\frac{1}{4}}$  and  $\lambda = \lambda_1^{\frac{1}{2}} \lambda_2^{\frac{1}{2}}$ . If  $\lambda_1$  and  $\lambda_2$  are both positive, or if they have opposing signs, it holds  $(\lambda_1 \lambda_2)^{\frac{1}{2}} = \lambda_1^{\frac{1}{2}} \lambda_2^{\frac{1}{2}}$ , so that we have  $\lambda = \lambda_1^{\frac{1}{2}} \lambda_2^{\frac{1}{2}} = \mu^{\frac{1}{2}}$ . If  $\lambda_1$  and  $\lambda_2$  are both negative, it holds  $(\lambda_1 \lambda_2)^{\frac{1}{2}} = -\lambda_1^{\frac{1}{2}} \lambda_2^{\frac{1}{2}}$ , so that  $\lambda = \lambda_1^{\frac{1}{2}} \lambda_2^{\frac{1}{2}} = -\mu^{\frac{1}{2}}$ . We observe that

$$Q^{-1} H Q = \begin{bmatrix} 0 & M_1 \\ M_2 & 0 \end{bmatrix}$$

and conclude

$$H v_\lambda = H Q \begin{bmatrix} x \\ y \end{bmatrix} = Q \begin{bmatrix} 0 & M_1 \\ M_2 & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \lambda Q \begin{bmatrix} x \\ y \end{bmatrix} = \lambda v_\lambda.$$

The orthogonality conditions (8) remain to be shown. We see with scaling factors  $s_\lambda = \lambda_1^{\frac{1}{4}} \lambda_2^{-\frac{1}{4}}$ ,  $s_\gamma = \gamma_1^{\frac{1}{4}} \gamma_2^{-\frac{1}{4}}$  and

$$v_\lambda = Q \begin{bmatrix} x_\lambda \\ y_\lambda \end{bmatrix}, \quad x_\lambda = v_{1,\lambda} s_\lambda, \quad y_\lambda = v_{2,\lambda} s_\lambda^{-1}, \quad v_\gamma = Q \begin{bmatrix} x_\gamma \\ y_\gamma \end{bmatrix}, \quad x_\gamma = v_{1,\gamma} s_\gamma, \quad y_\gamma = v_{2,\gamma} s_\gamma^{-1},$$

that

$$v_\lambda^H K v_\gamma = \frac{1}{2} (\overline{s_\lambda} s_\gamma^{-1} v_{1,\lambda}^H v_{2,\gamma} + \overline{s_\lambda^{-1}} s_\gamma v_{2,\lambda}^H v_{1,\gamma}), \quad v_\lambda^H J v_\gamma = \frac{1}{2} (\overline{s_\lambda} s_\gamma^{-1} v_{1,\lambda}^H v_{2,\gamma} - \overline{s_\lambda^{-1}} s_\gamma v_{2,\lambda}^H v_{1,\gamma}).$$

For  $\lambda \neq \gamma$  both expressions are zero because  $v_{1,\lambda}^H v_{2,\gamma} = 0$ . For  $\gamma = \lambda$  we have

$$v_\lambda^H K v_\lambda = \frac{1}{2} (\overline{s_\lambda} s_\lambda^{-1} + \overline{s_\lambda^{-1}} s_\lambda), \quad v_\lambda^H J v_\lambda = \frac{1}{2} (\overline{s_\lambda} s_\lambda^{-1} - \overline{s_\lambda^{-1}} s_\lambda).$$

If  $\lambda$  is real then  $\mu$  is positive and  $\lambda_1$  and  $\lambda_2$  have the same sign. Then it holds  $s_\lambda = (\lambda_1 \lambda_2^{-1})^{\frac{1}{4}}$ .  $s_\lambda$  is real and so it holds  $\overline{s_\lambda} s_\lambda^{-1} = 1 = \overline{s_\lambda^{-1}} s_\lambda$ , which shows  $v_\lambda^H J v_\lambda = 0$  and  $v_\lambda^H K v_\lambda = 1$ . If  $\lambda$  is imaginary, then  $\mu$  is negative and  $\lambda_1$  and  $\lambda_2$  have opposing signs. Here we have

$$\overline{s_\lambda} s_\lambda^{-1} = \begin{cases} i & \text{if } \lambda_1 > 0, \lambda_2 < 0, \\ -i & \text{if } \lambda_1 < 0, \lambda_2 > 0, \end{cases}$$

leading to the final results  $v_\lambda^H J v_\lambda = \pm i$  and  $v_\lambda^H K v_\lambda = 0$ .  $\square$

We have seen that the sign of the eigenvalue of the computed eigenpair of  $H$  via Theorem 6 does not necessarily match the sign of the principal square root of the eigenvalue of the matrix product  $M_1 M_2$ . In the definite case (5), i.e. where  $KH$  is positive definite we have positive definite  $M_1$  and  $M_2$ .  $\lambda_1$  and  $\lambda_2$  are positive and the sign switch does not take place. If a sign switch happened and the eigenvectors corresponding to the principal square root are of interest, they can easily be computed via Theorem 4, 2. (a).

The product eigenvalue problem resulting from Theorem 6 can also be interpreted as a generalized eigenvalue problem of the matrix pencil  $(M_2, M_1^{-1})$ . However, computing a matrix inverse is not necessary and the product eigenvalue problem can be tackled directly as we see in the following section.

### 3. Algorithms for crystalline systems (form I)

#### 3.1. Ways to solve the definite product eigenvalue problem

We have seen in Theorem 6 that the BSE problem of form I with size  $2n \times 2n$  can be interpreted as a product eigenvalue problem with two Hermitian factors of size  $n \times n$ . In this section we assume that the definiteness property (5) holds. Then the factors of the product eigenvalue problem are Hermitian positive definite.

In practice, the complete set of eigenvectors provides additional insight into excitonic effects. To compute them, left and right eigenvectors of the smaller product eigenvalue problem are needed. Product eigenvalue problems are well studied (see e.g. [20]). A general way to solve these problems, taking the product structure into account to improve numerical properties, is the periodic QR algorithm. This tool can be used for solving general Hamiltonian eigenvalue problems [21]. In this work we focus on non-iterative methods that work for Hermitian factors and transform the problem such that it can be treated using available HPC libraries.

The algorithms presented in this section compute the positive part of the spectrum of a BSE matrix and the corresponding eigenvectors. If the eigenvectors corresponding to the negative mirror eigenvalues are of interest, they can easily be computed by employing [Theorem 4](#), 2. (a).

A widely used approach for solving the BSE problem of form I [1,2,12] relies on the computation of the matrix square root of  $M_2 = A - B$ . We present it in the following, relating it to the framework given by [Theorem 6](#).

Starting with (6), we see

$$M_1 M_2 V_1 = V_1 \Lambda^2 \Leftrightarrow M_2^{\frac{1}{2}} M_1 M_2^{\frac{1}{2}} \hat{V} = \hat{V} \Lambda^2, \quad (13)$$

$$V_2^H M_1 M_2 = \Lambda^2 V_2^H \Leftrightarrow \hat{V}^H M_2^{\frac{1}{2}} M_1 M_2^{\frac{1}{2}} = \Lambda^2 \hat{V}^H, \quad (14)$$

where  $\hat{V} = M_2^{\frac{1}{2}} V_1 = M_2^{-\frac{1}{2}} V_2$  contains the eigenvectors of the Hermitian matrix  $M_2^{\frac{1}{2}} M_1 M_2^{\frac{1}{2}}$ . The following theorem clarifies how this approach leads to a simple algorithm.

**Theorem 7.** Let  $H$ ,  $M_1$ ,  $M_2$  and  $Q$  be given as in [Theorem 6](#), with  $KH$  positive definite,  $S = M_2^{\frac{1}{2}}$  and  $SM_1 S \hat{V} = \hat{V} \Lambda^2$  be an eigenvalue decomposition with  $\hat{V}^H \hat{V} = I$ ,  $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n) \in \mathbb{R}_+^{n \times n}$ . Then

$$V = Q \begin{bmatrix} S^{-1} \hat{V} \Lambda^{\frac{1}{2}} \\ S \hat{V} \Lambda^{-\frac{1}{2}} \end{bmatrix}$$

contains eigenvectors of  $H$  corresponding to  $\Lambda$ , i.e.  $HV = V\Lambda$ .

**Proof.** We see from (13) and (14) that right and left eigenvectors of  $M_1 M_2$  are given by  $V_1 = S^{-1} \hat{V}$  and  $V_2 = S \hat{V}$ . It holds  $V_1^H V_2 = I$  so that we are in a position to apply [Theorem 6](#). The scaling factors  $\lambda_1$  and  $\lambda_2$  for each eigenvector follow from observing  $M_2 V_1 = V_2$  and  $M_1 V_2 = V_1 \Lambda^2$ . So we have  $\lambda_1 = \lambda^2$ ,  $\lambda_2 = 1$  for each eigenvalue  $\lambda$ .  $V_1$  needs to be scaled by  $\Lambda_1^{\frac{1}{4}} \Lambda_2^{-\frac{1}{4}} = \Lambda^{\frac{1}{2}}$ ,  $V_2$  needs to be scaled by  $\Lambda^{-\frac{1}{2}}$ .  $\square$

The essential work of this approach is the computation of the matrix square root and the solution of a Hermitian eigenvalue problem. Computing the (principal) square root of a matrix is a nontrivial task (see e.g. [22], Chapter 6) with a (perhaps surprisingly) high computational demand. Its efficient computation has been an active area of research. Given a Hermitian positive definite matrix  $C$ , its principal square root  $S$ , s.t.  $S^2 = C$ , can be computed by diagonalizing  $M = V_C D_C V_C^H$ , and taking the square roots of the diagonal entries of  $D_C$ . Then  $S := V_C D_C^{\frac{1}{2}} V_C^H$ . The main computational effort is therefore the subsequent solution of two Hermitian eigenvalue problems.

We now lay out how the product eigenvalue problem given in (6) can be solved by using Cholesky factorizations. Let the Cholesky factorization  $M_2 = L L^H$  be given. This approach is also followed in [23]. Starting with (6) we see

$$M_1 M_2 V_1 = V_1 \Lambda^2 \Leftrightarrow L^H M_1 L \hat{V} = \hat{V} \Lambda^2,$$

$$V_2^H M_1 M_2 = \Lambda^2 V_2^H \Leftrightarrow \hat{V}^H L^H M_1 L = \Lambda^2 \hat{V}^H,$$

where  $\hat{V} = L^H V_1 = L^{-1} V_2$  contains the eigenvectors of the Hermitian matrix  $L^H M_1 L$ .

The analogy to [Theorem 7](#) is given in the following, which is proven in a similar way.

**Theorem 8.** Let  $H$ ,  $M_1$ ,  $M_2$  and  $Q$  be given as in [Theorem 6](#), with  $KH$  positive definite,  $L L^H = M_2$  be a Cholesky decomposition and  $L^H M_1 L \hat{V} = \hat{V} \Lambda^2$  be an eigenvalue decomposition with  $\hat{V}^H \hat{V} = I$ ,  $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n) \in \mathbb{R}_+^{n \times n}$ . Then

$$V = Q \begin{bmatrix} L^{-H} \hat{V} \Lambda^{\frac{1}{2}} \\ L \hat{V} \Lambda^{-\frac{1}{2}} \end{bmatrix}$$

contains eigenvectors of  $H$  corresponding to  $\Lambda$ , i.e.  $HV = V\Lambda$ .

Comparing algorithms resulting from [Theorems 7](#) and [8](#) we see that the essential work in both algorithms is solving Hermitian positive definite  $n \times n$  eigenvalue problems. The Cholesky variant solves one explicitly, the square root variant solves one for computing the matrix square root, which is then used to set up the matrix for the second eigenvalue problem. Then both left and right eigenvectors of the product eigenvalue problem can be inferred from the computed eigenvectors.

Both approaches compute the squared eigenvalues of the original problem. In the numerical linear algebra community this procedure is well known to limit the attainable accuracy [24]. The methods essentially work on the (transformed) matrix product  $M_1 M_2$ . It corresponds to the squared matrix  $H^2$  as

$$Q^{-1} H^2 Q = \begin{bmatrix} M_1 M_2 & 0 \\ 0 & M_2 M_1 \end{bmatrix}.$$

$H$  belongs to the class of Hamiltonian matrices (see Section 2). When the eigenvalues are computed from the squared matrix  $H^2$ , employing a backward-stable method, the computational error can be approximated using first-order perturbation theory [24–26]. It is given as

$$|\lambda - \hat{\lambda}| \approx \epsilon \frac{\|H\|_2}{s(\lambda)} \min \left\{ \frac{\|H\|_2}{\lambda}, \frac{1}{\sqrt{\epsilon}} \right\}, \quad (15)$$

where  $\lambda$  denotes an exact eigenvalue of  $H$ ,  $\hat{\lambda}$  the corresponding computed value,  $s(\lambda)$  the condition number of the eigenvalue, and  $\epsilon$  the machine precision. Unless  $\lambda$  is very large, the expression is dominated by  $\frac{\sqrt{\epsilon}\|H\|_2}{s(\lambda)}$ . Essentially, the number of significant digits of the eigenvalues is halved, compared to direct backward-stable methods. For example, applying the QR algorithm on the original matrix  $H$  would yield an approximate error of  $\frac{\epsilon\|H\|_2}{s(\lambda)}$ . It fails however, to preserve and exploit the structure of the problem and is undesirable from a numerical as well as from a performance point of view. A remedy is given by making use of the singular value decomposition (SVD).

Given the Cholesky factorizations  $L_1 L_1^H = M_1$ ,  $L_2 L_2^H = M_2$ , the product eigenvalue problem can be rewritten in the following form:

$$M_1 M_2 V_1 = V_1 \Lambda^2 \Leftrightarrow L_1^H L_2 (L_1^H L_2)^H \hat{V}_1 = \hat{V}_1 \Lambda^2, \quad (16)$$

$$V_2^H M_1 M_2 = \Lambda^2 V_2^H \Leftrightarrow \hat{V}_2^H (L_1^H L_2)^H L_1^H L_2 = \Lambda^2 \hat{V}_2^H, \quad (17)$$

where  $\hat{V}_1 = L_1^{-1} V_1$ ,  $\hat{V}_2 = L_2^{-1} V_2$ .  $\Lambda$  contains the positive eigenvalues of the BSE matrix, i.e. the square roots of the eigenvalues of the matrix product  $M_1 M_2$ . (16) and (17) can be further simplified using the SVD  $U_{SVD} \Lambda_{SVD} V_{SVD}^H = L_1^H L_2$ . Then  $L_1^H L_2 (L_1^H L_2)^H = U_{SVD} \Lambda_{SVD}^2 U_{SVD}^H$  and  $(L_1^H L_2)^H L_1^H L_2 = V_{SVD} \Lambda_{SVD}^2 V_{SVD}^H$ . It becomes apparent that  $\hat{V} = U_{SVD}$ ,  $\hat{V}_2 = V_{SVD}$  and  $\Lambda = \Lambda_{SVD}$  solve (16) and (17). The following theorem gives the details of the eigenvector computation from the SVD including scaling factors.

**Theorem 9.** Let  $H$ ,  $M_1$ ,  $M_2$  and  $Q$  be given as in Theorem 6, with  $KH$  positive definite,  $L_1 L_1^H = M_1$ ,  $L_2 L_2^H = M_2$  be Cholesky decompositions and  $U_{SVD} \Lambda V_{SVD}^H = L_1^H L_2$  be a singular value decomposition,  $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n) \in \mathbb{R}_+^{n \times n}$ . Then

$$V = Q \begin{bmatrix} L_1 U_{SVD} \Lambda^{-\frac{1}{2}} \\ L_2 V_{SVD} \Lambda^{-\frac{1}{2}} \end{bmatrix}$$

contains eigenvectors of  $H$  corresponding to  $\Lambda$ , i.e.  $HV = V\Lambda$ .

**Proof.** We see from (16) and (17) that  $V_1 = L_1 U_{SVD} \Lambda^{-\frac{1}{2}}$  and  $V_2 = L_2 V_{SVD} \Lambda^{-\frac{1}{2}}$  are right and left eigenvectors of the matrix product  $M_1 M_2$ . The diagonal scaling matrix  $\Lambda^{-\frac{1}{2}}$  was chosen s.t. it holds  $V_1^H V_2 = I$  and we can apply Theorem 6. We observe  $M_2 V_1 = V_2 \Lambda$  and  $M_1 V_2 = V_1 \Lambda$ . So scaling factors are given as  $\lambda_1 = \lambda_2 = \lambda$  for each  $\lambda$ . Then  $V_1$  needs to be scaled by  $\Lambda_1^{\frac{1}{4}} \Lambda_2^{-\frac{1}{4}} = I$  according to (7), i.e. not at all, just as  $V_2$ .  $\square$

The main difference between the SVD-based algorithm and the other ones, from a numerical point of view, is that the eigenvalue matrix  $\Lambda$  is computed directly by the SVD and not as a square root of another diagonal matrix. The way real BSE matrices of form II (3) are treated in [27] is based on the same idea.

We can expect to see a higher accuracy in the eigenvalues than in the square root and the Cholesky approach, because the eigenvalues are computed directly, using a backward-stable method for the singular value decomposition. Perturbation theory [28] yields an approximate error of

$$|\lambda - \hat{\lambda}| \approx \epsilon \frac{\|H\|_2}{s(\lambda)}.$$

In the other approaches, a similar approximation only holds for the error of the squared eigenvalues  $\lambda^2$ , and translates in form of (15) to the non-squared ones.

### 3.2. Comparison

In recent years, various packages have been developed to facilitate the computation of the electronic structure of materials. See e.g. [29–31] or <https://www.nomad-coe.eu/externals/codes> for an overview. In particular, computing excited states via methods based on many-body perturbation theory has come into focus, as powerful computational



**Table 1**

Algorithmic steps of the different methods. The number in brackets estimates the number of flops, where lower-order terms are neglected.

	SQRT (Theorem 7)	CHOL (Theorem 8)	CHOL+SVD (Theorem 9)
1. Preprocessing	$S = (A - B)^{\frac{1}{2}},$ $M = S(A + B)S$ ( $11n^3$ ) ( $4n^3$ )	$LL^H = A - B,$ $M = L(A + B)L^H$ ( $\frac{1}{3}n^3$ ) ( $2n^3$ )	$L_1L_1^H = A + B, \quad L_2L_2^H = A - B,$ $M = L_1^H L_2$ ( $\frac{2}{3}n^3$ ) ( $n^3$ )
2. Decomposition	$M = \hat{V}A^2\hat{V}^H$ ( $9n^3$ )	$M = \hat{V}A^2\hat{V}^H$ ( $9n^3$ )	$M = U_{SVD}AV_{SVD}^H$ ( $21n^3$ )
3. Postprocessing	$V_1 := S^{-1}\hat{V}A^{\frac{1}{2}},$ $V_2 = S\hat{V}A^{-\frac{1}{2}}$ ( $\frac{8}{3}n^3$ ) ( $2n^3$ )	$V_1 = L^{-H}\hat{V}A^{\frac{1}{2}},$ $V_2 = L\hat{V}A^{-\frac{1}{2}}$ ( $n^3$ ) ( $n^3$ )	$V_1 = L_1U_{SVD}A^{-\frac{1}{2}},$ $V_2 = L_2V_{SVD}A^{-\frac{1}{2}}$ ( $n^3$ ) ( $n^3$ )
4. Final setup	$V = \begin{bmatrix} \frac{1}{2}(V_1 + V_2) \\ \frac{1}{2}(V_2 - V_1) \end{bmatrix}.$		

resources become more widely available. Here, the Bethe–Salpeter approach constitutes a state-of-the art method for computing optical properties such as the optical absorption spectrum. To this end, an algorithm based on Theorem 7 is typically used to solve the resulting eigenvalue problem after the matrices  $A$  and  $B$  have been set up [1].

The main contribution of the previous section was to provide a unified frame of reference, which can be used to derive the currently used approach (Theorem 7) as well as two alternative ones (Theorems 8 and 9). Here, the similarities between the realizations of the different approaches become apparent. In all resulting algorithms we clearly see four steps.

1. Preprocessing: Setup a matrix  $M$ .
2. Decomposition: Compute spectral, respectively, singular value decomposition of  $M$ .
3. Postprocessing: Transform resulting vectors to (left and right) eigenvectors of matrix  $(A + B)(A - B)$ .
4. Final setup: Form eigenvectors of original BSE matrix.

A detailed compilation is given in Table 1.

Seeing the algorithms side by side enables a direct comparison. The amount of flops is based on estimates for sequential, non-blocked implementations [32], and lower order terms i.e.  $\mathcal{O}(n^2)$  and  $\mathcal{O}(n)$ , are neglected. The preprocessing step is most expensive in the square root approach. Computing the square root of a Hermitian matrix involves the solution of a Hermitian eigenvalue problem. Additionally, the matrices  $S$  and  $M$  need to be set up, using 3 matrix–matrix products. This makes the preprocessing step even more expensive than the following “main” eigenvalue computation. The CHOL and the CHOL+SVD approach, on the other hand, only rely on one or two Cholesky factorizations and matrix multiplications, which are comparatively cheap to realize. The computational effort in the decomposition step is the highest in the CHOL+SVD step. The post-processing step again is most expensive in the SQRT approach, because the matrix  $S$  is a general square matrix, while the  $L$  matrices in CHOL and CHOL+SVD are triangular. In total, SQRT takes an estimated amount of  $28\frac{2}{3}n^3$  flops, CHOL takes  $13\frac{1}{3}n^3$  flops and CHOL+SVD takes  $24\frac{2}{3}n^3$  flops. The classical QR algorithm applied to the full, non-Hermitian matrix takes about  $25(2n)^3 = 200n^3$  flops (not including the computation of eigenvectors from the Schur vectors). Solving the Hermitian-definite eigenvalue problem (1) can exploit symmetry, but still acts on the large problem and can be expected to perform  $14(2n)^3 = 112n^3$  flops.

According to this metric, we expect the Cholesky and the SVD approach to perform faster than the square root approach. The actual performance of algorithms on modern architectures is not simply determined by the number of operations performed, but by their parallelizability and communication costs. All presented approaches have a high computational intensity of  $\mathcal{O}(n^3)$ , such that the memory bandwidth is not likely to be a bottleneck. All methods rely on the same standard building blocks from numerical linear algebra, for which optimized versions (e.g. blocked variants for cache-efficiency) are available. This setting makes a fair comparison possible where the arithmetic complexity has a high explanatory power.

To summarize, we expect CHOL to be about twice as fast as SQRT, while keeping the same accuracy. CHOL+SVD performs more computations than CHOL, and will take more time, but could improve the accuracy of the computations. It might be faster than SQRT, depending on how efficient the diagonalizations in SQRT and the SVD in CHOL+SVD are implemented.

The comparison in Table 1 is helpful when implementing the new approaches in codes that already use the square root approach. For the Cholesky approach we need to substitute the computation of the matrix square root with the computation of a Cholesky factorization (LAPACK routine `zpotrf`), compute the matrix  $M$  using triangular matrix multiplications (`ztrmm`), and use a triangular solve (`ztrs`) and a triangular matrix multiplication (`ztrmm`) in the post-processing step. For the CHOL+SVD approach, an additional Cholesky factorization is necessary and the Hermitian eigenvalue decomposition is substituted by a singular value decomposition (`zgesvd`). The post-processing involves two triangular matrix products instead of a matrix inversion and two general matrix products.

#### 4. Numerical experiments

We implemented and compared serial versions of algorithms presented in Table 1 in MATLAB. They compute positive eigenvalues and associated eigenvectors of a BSE matrix  $H \in \mathbb{C}^{2n \times 2n}$  of form I (2), which fulfills the definiteness property



**Table 2**Comparison of different methods for eigenvalue computation for Bethe–Salpeter matrix of form I of size  $400 \times 400$ .

Method	Relative Error				Runtime
	$\kappa = 10$	$\kappa = 10^3$	$\kappa = 10^6$	$\kappa = 10^9$	
eig	1.28e−14	5.08e−14	3.82e−11	1.26e−08	62.7 ms
generalized eig	7.89e−15	6.67e−15	1.89e−11	1.97e−09	10.7 ms
haeig	4.73e−15	7.82e−15	4.32e−11	2.23e−08	50.9 ms
SQRT	5.45e−15	3.11e−12	4.64e−06	1.39e+00	5.87 ms
CHOL	4.23e−15	2.17e−12	1.32e−06	1.19e−05	3.09 ms
CHOL + SVD	1.23e−15	2.20e−14	2.53e−11	2.38e−09	4.28 ms

$KH > 0$ . The eigenvalues are given as a diagonal matrix  $D \in \mathbb{R}^{n \times n}$ . The eigenvectors  $V \in \mathbb{C}^{2n \times n}$  are scaled s.t.  $K$ -orthogonality holds, i.e.  $V^H K V = I_n$ . The  $K$ -orthogonality is an important property in the application. It is exploited in order to construct the polarizability operator ultimately used for the computation of the absorption spectrum.

We also include the MATLAB eigensolver `eig` for comparison. `eig` can either work on the BSE matrix  $H$  or solve the generalized eigenvalue problem for the matrix pencil  $(KH, K)$ . In this formulation, both matrices are Hermitian and one is positive definite, which allows for a faster computation.

The experiments were performed on a laptop with an Intel(R) Core(TM) i7-8550U processor using MATLAB R2018a.

The first experiments aim to assess the accuracy of the computed eigenvalues. The matrices  $A$  and  $B$  are of size  $n = 200$  and are created in the following way for a given value  $\kappa \in \mathbb{R}$ . Let  $d = [1, \dots, \frac{1}{3}\kappa] \in \mathbb{R}^n$  be a vector with elements equally spaced between 1 and  $\frac{1}{3}\kappa$ . The BSE matrix is constructed as

$$H = \begin{bmatrix} A & B \\ -B & -A \end{bmatrix} := \begin{bmatrix} Q & 0 \\ 0 & Q \end{bmatrix}^H \begin{bmatrix} \text{diag}(d) & \frac{1}{2} \text{diag}(d) \\ -\frac{1}{2} \text{diag}(d) & -\text{diag}(d) \end{bmatrix} \begin{bmatrix} Q & 0 \\ 0 & Q \end{bmatrix},$$

where  $Q \in \mathbb{C}^{n \times n}$  is a randomly generated, unitary matrix. It can be shown, that  $\text{cond } H = \kappa$  and the eigenvalues are given as  $\frac{\sqrt{3}}{2}d$ .

Table 2 shows the relative error in the smallest eigenvalue  $\lambda = \frac{\sqrt{3}}{2}$ , using the methods discussed in Section 3. We also include the routine `haeig` from the SLICOT package [33,34]. Because `haeig` can only compute eigenvalues, not eigenvectors, we also only compute eigenvalues in the other methods in order to make the runtimes comparable.

The MATLAB `eig` function has the largest runtime. `haeig` is slightly faster, because it exploits the available Hamiltonian structure. However, the routine is not optimized for cache-reuse, which is why this effect cannot be observed more clearly and vanishes for larger matrices. The generalized eigenvalue problem can be solved much faster, because it can be transformed to a Hermitian eigenvalue problem of size  $2n \times 2n$ . The other methods ultimately act on Hermitian matrices of size  $n \times n$ , which explains the much lower runtimes.

The observed eigenvalue errors also comply with the error analysis given in Section 3.1. The currently used square root approach performs even worse than expected, yielding a completely wrong eigenvalue for matrices with a condition number  $\kappa = 10^9$ . In the application context, the small eigenvalues are of special interest. They correspond to bound exciton states, representing a strong electron–hole interaction. They are the reason why the Bethe–Salpeter approach is used instead of simpler schemes based on time-dependent density functional theory [3]. The smallest eigenvalues suffer the most from this numerical inaccuracy.

The second experiment aims to assess the runtime of the sequential implementations, including the eigenvector computation in the measurement. The matrices  $A$  and  $B$  are setup as random matrices, where the diagonal of  $A$  has been scaled up in order to guarantee the definiteness property  $KH > 0$ . The measured runtimes are found in Fig. 1 and serve as a rough indicator of computational effort.

As expected, the Cholesky approach yields the fastest runtime of all approaches. The SVD approach also performs better than the square root approach. However, this picture could easily look different in another computational setup.

An approach based on the `eig` command becomes prohibitively slow, when larger matrices are considered. Matrices in real applications become extremely large, up to dimensions of order 100 000, in order to get reasonable results. The effect would be even more drastic in a parallel setting, as the solution of a non-symmetric dense eigenvalue problem is notoriously difficult to parallelize.

Fig. 2 shows the achieved  $K$ -orthogonality of the eigenvector matrices for matrices with certain condition numbers. To this end, we manipulate the diagonal of the randomly generated matrix  $A$  such that badly conditioned BSE matrices  $H$  are generated. For the square root and the Cholesky approach, the  $K$ -orthogonality breaks down completely for badly conditioned matrices. This can have dramatic consequences and can lead to completely wrong results, when further computations rely on this property.

To show the applicability to real life examples, we extracted a Bethe–Salpeter matrix corresponding to the excitation of Lithium-Fluoride from the `exciting` software package [29]. Computational details on how the matrix is generated

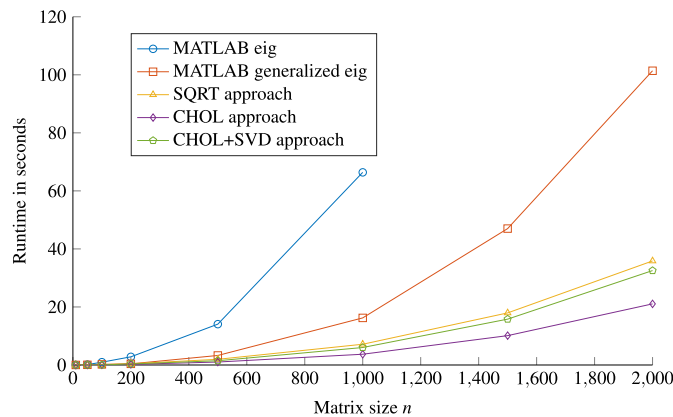


Fig. 1. Runtimes for different methods,  $A, B \in \mathbb{C}^{n \times n}$  with varying matrix sizes.

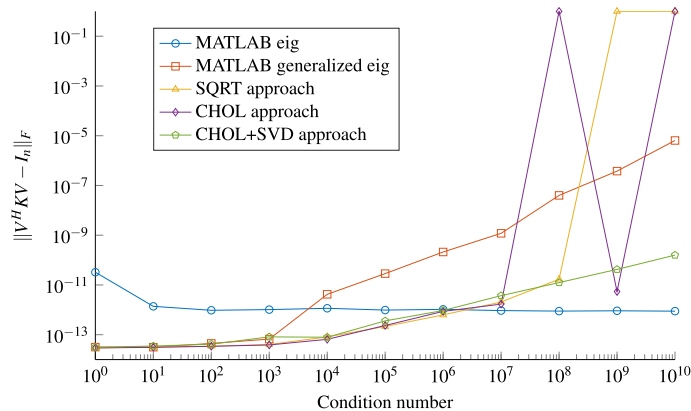


Fig. 2. Deviation from  $K$ -orthogonality for different methods,  $A, B \in \mathbb{C}^{200 \times 200}$  with a certain condition number.

Table 3

Computed eigenvalues for Lithium Fluoride example.

	$\lambda_1$	$\lambda_2$	$\lambda_3$	Runtime
eig	4.6423352497493209e-01	4.6524229149750918e-01	4.6872644706731720e-01	32.49 s
generalized eig	4.6423352497493126e-01	4.6524229149750407e-01	4.6872644706732447e-01	10.62 s
haeig	4.6423352497493725e-01	4.6524229149750940e-01	4.6872644706732514e-01	71.43 s
SQR	4.6423352497493120e-01	4.6524229149750490e-01	4.6872644706732541e-01	3.44 s
CHOL	4.6423352497493031e-01	4.6524229149750573e-01	4.6872644706732414e-01	2.06 s
CHOL + SVD	4.6423352497493092e-01	4.6524229149750473e-01	4.6872644706732453e-01	3.41 s
TDA	4.6427305979874345e-01	4.6528180480128906e-01	4.6877150201685513e-01	0.88 s

can be found in the documentation<sup>1</sup>. Here, it is pointed out that a Tamm–Dancoff approximation, i.e. setting the off-diagonal block  $B$  to zero, already yields satisfactory results. The resulting  $2560 \times 2560$  BSE matrix has a condition number (computed using `cond` in MATLAB) of 5.33. We do not expect the algorithms to suffer from the numerical difficulties observed in the first example.

The three smallest eigenvalues computed by different methods are found in Table 3. Indeed, all approaches coincide in the first 14 significant digits. The Tamm–Dancoff approximation (TDA) applies MATLAB `eig` on the diagonal Block  $A$  and provides eigenvalues, that are correct up to 4 significant digits which is sufficient for practical applications. The measured runtimes reflect the results of the other experiments. Now the lack of low-level optimization in the `haeig` routine becomes apparent and leads to the lowest performance of all approaches.

<sup>1</sup> <http://exciting-code.org/carbon-excited-states-from-bse>

**Table 4**

Algorithmic steps of the different methods applicable in the non-definite setting, i.e. (5) does not necessarily hold.

	$LDL^T$	$LDL^T + \text{GSVD}$
1. Preprocessing	$LT L^H = A - B,$ $M = L(A + B)L^H T$	$L_1 T_1 L_1^H = A + B, \quad L_2 T_2 L_2^H = A - B,$ $M = L_1^H L_2$
2. Decomposition	$M = \hat{V} D \hat{V}^{-1},$ where $\hat{V}^H T \hat{V} = S,$ $\Lambda = D^{\frac{1}{2}}$	$M = U_{\text{GSVD}}^{-H} \Lambda V_{\text{GSVD}}^{-1},$ where $U_{\text{GSVD}}^H T_1 U_{\text{GSVD}} = \hat{T}_1,$ $V_{\text{GSVD}}^H T_2 V_{\text{GSVD}} = \hat{T}_2$
3. Postprocessing	$V_1 = L^{-H} \hat{V} \Lambda^{\frac{1}{2}},$ $V_2 = L T \hat{V} \hat{T} \Lambda^{-\frac{1}{2}}$	$V_1 = L_1 U_{\text{GSVD}} (\Lambda^{-\frac{1}{2}})^H,$ $V_2 = L_2 V_{\text{GSVD}} \Lambda^{-\frac{1}{2}} P,$ where $P = I_k \oplus i I_l \oplus S_{2m}$
4. Sign switches	$\hat{T}$ is the diagonal matrix containing the signature of $S$ .	$\hat{T}$ is the diagonal matrix containing the signature of $\hat{T}_1$ .
4. Final setup	$V = \begin{bmatrix} \frac{1}{2}(V_1 + V_2) \\ \frac{1}{2}(V_2 - V_1) \end{bmatrix}, \quad \hat{\Lambda} = \Lambda \hat{T}$	

## 5. Towards structure preserving methods for non-definite problems

The presented algorithms assume (5) to hold, i.e.  $KH$  is assumed to be positive definite. However, as pointed out in [8,13], complex eigenvalues can occur in certain contexts and are related to finite lifetimes of particles. In this section, we point out how our framework can be used to gain insight into this case. In contrast to the definite case, the stable computation of required quantities can be more challenging and routines are not as readily available. This section serves as a motivation for future algorithm development. This is why the numerical experiments in the previous section focus on the definite case.

Similarly to Theorem 6, complex eigenvalues can be related to a smaller product eigenvalue problem.

**Theorem 10.** Let  $H$  be a BSE matrix of form  $I$ , with  $M_1 := A + B$  and  $M_2 := A - B$  nonsingular. Let  $V_1 = \begin{bmatrix} v_{11} & v_{12} \end{bmatrix} \in \mathbb{C}^{n \times 2}$  contain two right eigenvectors of the matrix  $M_1 M_2$ , and let  $V_2 = \begin{bmatrix} v_{21} & v_{22} \end{bmatrix} \in \mathbb{C}^{n \times 2}$  contain the corresponding right eigenvector pair, s.t.

$$M_1 M_2 V_1 = V_1 M \quad V_2^H M_1 M_2 = M V_2^H, \quad V_1^H V_2 = I_2, \quad (18)$$

where  $M = \begin{bmatrix} \mu & \\ & \bar{\mu} \end{bmatrix}$  contains the eigenvalue pair.

Define the scaling factors

$$\lambda_1 := v_{21}^H M_1 v_{22}, \quad \lambda_2 := v_{12}^H M_2 v_{11}, \quad \hat{\lambda} := \lambda_1^{1/4} \lambda_2^{-1/4}, \quad (19)$$

$$\hat{\Lambda}_1 := \begin{bmatrix} \hat{\lambda} & 0 \\ 0 & \bar{\hat{\lambda}} \end{bmatrix}, \quad \hat{\Lambda}_2 := \begin{bmatrix} 0 & \hat{\lambda}^{-1} \\ \hat{\lambda}^{-1} & 0 \end{bmatrix}.$$

Then, with  $Q = \frac{1}{2} \begin{bmatrix} I & I \\ -I & I \end{bmatrix}$ , two eigenvectors of  $H$  are given as columns of the matrix  $V_\lambda = Q \begin{bmatrix} V_1 \hat{\Lambda}_1 \\ V_2 \hat{\Lambda}_2 \end{bmatrix}$  and it holds

$$H V_\lambda = V_\lambda S \begin{bmatrix} \mu^{\frac{1}{2}} & \\ & \frac{1}{\mu^{\frac{1}{2}}} \end{bmatrix}, \quad S = \begin{cases} -1 & \text{if } \arg \lambda_1 + \arg \lambda_2 < -\pi \text{ or } \arg \lambda_1 + \arg \lambda_2 > \pi, \\ 1 & \text{else.} \end{cases} \quad (20)$$

Furthermore, it holds

$$V_\lambda^H K V_\gamma = \begin{cases} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} & \text{if } \{\lambda, \bar{\lambda}\} = \{\gamma, \bar{\gamma}\}, \\ \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix} & \text{if } \{\lambda, \bar{\lambda}\} \neq \{\gamma, \bar{\gamma}\}, \end{cases} \quad V_\lambda^H J V_\gamma = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}, \quad (21)$$

$$V_\lambda^H K v_\gamma = \begin{bmatrix} 0 & 0 \end{bmatrix}^T, \quad V_\lambda^H J v_\gamma = \begin{bmatrix} 0 & 0 \end{bmatrix}^T, \quad (22)$$

where  $V_\gamma$  contains two eigenvectors corresponding to a complex eigenvalue pair  $\{\gamma, \bar{\gamma}\}$ , constructed according to this theorem.  $v_\gamma$  is an eigenvector corresponding to a real or an imaginary eigenvalue  $\gamma$ , constructed according to Theorem 6.

**Proof.** Starting with  $M_1 M_2 v_{11} = \mu v_{11}$ , we get

$$M_2 M_1 M_2 v_{11} = \mu M_2 v_{11} \Leftrightarrow (M_2 v_{11})^H M_1 M_2 = \bar{\mu} (M_2 v_{11})^H.$$

$M_2 v_{11}$  must be a multiple of  $v_{22}$ . Otherwise it would hold  $(M_2 v_{11})^H v_{12} = 0$ , which contradicts  $M_2$  being nonsingular. So there is  $\lambda_2 \in \mathbb{C}$ , s.t.

$$M_2 v_{11} = \lambda_2 v_{22}.$$

Similarly it can be concluded, that  $\lambda_1 \in \mathbb{C}$  exists, and

$$M_1 v_{22} = \lambda_1 v_{11}, \quad M_1 v_{21} = \bar{\lambda}_1 v_{12}, \quad M_2 v_{12} = \bar{\lambda}_2 v_{21}.$$

With the normalization condition (18) we get

$$V_1^H M_2 V_1 = \begin{bmatrix} 0 & \bar{\lambda}_2 \\ \lambda_2 & 0 \end{bmatrix} =: \Lambda_2, \quad V_2^H M_1 V_2 = \begin{bmatrix} 0 & \lambda_1 \\ \bar{\lambda}_1 & 0 \end{bmatrix} =: \Lambda_1$$

and

$$M_1 M_2 V_1 = V_1 \Lambda_1 \Lambda_2.$$

With (18) it follows that  $\Lambda_1 \Lambda_2 = M$ . Note that  $Q^{-1} H Q = \begin{bmatrix} 0 & M_1 \\ M_2 & 0 \end{bmatrix}$  and

$$\begin{bmatrix} 0 & M_1 \\ M_2 & 0 \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} = \begin{bmatrix} X \\ Y \end{bmatrix} \Lambda$$

holds for  $X, Y \in \mathbb{C}^{n \times 2}$  if and only if

$$M_1 Y = X \Lambda \quad \text{and} \quad M_2 X = Y \Lambda. \quad (23)$$

Simple algebra shows that

$$\Lambda_1 \hat{\Lambda}_2 = s \hat{\Lambda}_1 M^{\frac{1}{2}} \quad \text{and} \quad \Lambda_2 \hat{\Lambda}_1 = s \hat{\Lambda}_2 M^{\frac{1}{2}} \quad \text{for } s = \begin{cases} -1 & \text{if } \arg \lambda_1 + \arg \lambda_2 < -\pi \text{ or } \arg \lambda_1 + \arg \lambda_2 > \pi, \\ 1 & \text{else.} \end{cases} \quad (24)$$

Using (24), we see that (23) holds for  $X := V_1 \hat{\Lambda}_1$ ,  $Y := V_2 \hat{\Lambda}_2$  and  $\Lambda := s M^{\frac{1}{2}} = s \operatorname{diag}(\mu^{\frac{1}{2}}, \bar{\mu}^{\frac{1}{2}})$ . In conclusion we have

$$H V_\lambda = H Q \begin{bmatrix} X \\ Y \end{bmatrix} = Q \begin{bmatrix} 0 & M_1 \\ M_2 & 0 \end{bmatrix} \begin{bmatrix} X \\ Y \end{bmatrix} = Q \begin{bmatrix} X \\ Y \end{bmatrix} \Lambda = V_\lambda \Lambda.$$

The orthogonality conditions (21) remain to be shown. We observe  $Q^H K Q = \frac{1}{2} \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix}$  and with

$$\begin{aligned} V_\lambda &= Q \begin{bmatrix} X_\lambda \\ Y_\lambda \end{bmatrix}, \quad X_\lambda = V_{1,\lambda} \hat{\Lambda}_1, \quad Y_\lambda = V_{2,\lambda} \hat{\Lambda}_2, \\ V_\gamma &= Q \begin{bmatrix} X_\gamma \\ Y_\gamma \end{bmatrix}, \quad X_\gamma = V_{1,\gamma} \hat{\Lambda}_1, \quad Y_\gamma = V_{2,\gamma} \hat{\Lambda}_2, \end{aligned}$$

we see

$$V_\lambda^H K V_\gamma = \frac{1}{2} (\hat{\Lambda}_1^H V_{1,\lambda}^H V_{2,\gamma} \hat{\Lambda}_2 + \hat{\Lambda}_2^H V_{2,\lambda}^H V_{1,\gamma} \hat{\Lambda}_1), \quad V_\lambda^H J V_\gamma = \frac{1}{2} (\hat{\Lambda}_1^H V_{1,\lambda}^H V_{2,\gamma} \hat{\Lambda}_2 - \hat{\Lambda}_2^H V_{2,\lambda}^H V_{1,\gamma} \hat{\Lambda}_1). \quad (25)$$

These expressions are equal to 0 if  $V_{2,\lambda}$  and  $V_{1,\gamma}$  contain left and right eigenvectors corresponding to different eigenvalue pairs  $\{\lambda, \bar{\lambda}\} \neq \{\gamma, \bar{\gamma}\}$  of  $M_1 M_2$ . If  $\lambda = \gamma$  and if  $V_\lambda$  and  $V_\gamma$  were constructed in the same way, we have  $\hat{\Lambda}_1 = \hat{\Lambda}_1$  and  $\hat{\Lambda}_2 = \hat{\Lambda}_2$ . (25) simplifies to  $V_\lambda^H K V_\lambda = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$  and  $V_\lambda^H J V_\lambda = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$ . We used the normalization of the vectors given in (18) and that  $\hat{\Lambda}_1^H \hat{\Lambda}_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$  following from the definition (19). (22) is shown in a similar way.  $\square$

In the definite case in Section 3, a Cholesky factorization was used to transform the eigenvalue problem. This role is now played by a generalized Cholesky factorization. We use a scaled  $LDL^T$  decomposition to arrive at an eigenvalue problem of half the size. The resulting matrix is pseudo-Hermitian, i.e. Hermitian up to sign changes of certain rows or columns. The same idea is explored in [13]. Let  $M_2 = L T L^H$  be a decomposition, where  $T$  is a signature matrix, i.e.  $T = \operatorname{diag}(t_1, \dots, t_n)$ ,  $t_j \in \{1, -1\}$  for  $j = 1, \dots, n$ . Then we see

$$M_1 M_2 V_1 = V_1 D \quad \Leftrightarrow \quad L^H M_1 L T \hat{V}_1 = \hat{V}_1 D, \quad (26)$$

where  $\hat{V}_1 = L^H V_1$  contains the right eigenvectors of the pseudo-Hermitian matrix  $L^H M_1 L T$ . Similarly, the left eigenvectors of  $M_1 M_2$  show the relation

$$V_2^H M_1 M_2 = D V_2^H \quad \Leftrightarrow \quad \hat{V}_2^H L^H M_1 L T = D \hat{V}_2^H,$$

where  $\hat{V}_2 = L^{-1} V_2$  contains the left eigenvectors of the pseudo-Hermitian matrix  $L^H M_1 L T$ .

For Hermitian matrices occurring in the definite case, left and right eigenvectors are the same. For pseudo-Hermitian matrices this does not hold, but they are nevertheless related. This is pointed out in the following theorem stating a normal form for pseudo-Hermitian matrices (see [35]).

**Theorem 11.** Let  $M \in \mathbb{C}$  be diagonalizable and selfadjoint with respect to a signature matrix  $\Sigma$ , i.e.  $M\Sigma = (M\Sigma)^H$ , and let  $S_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ . Then there exists an eigenvalue decomposition

$$V^{-1}MV = D := D_+ \oplus D_- \oplus D_{\text{complex}},$$

$$V^H \Sigma V = S := \text{diag}(\sigma_1, \dots, \sigma_{k+l}, S_2, \dots, S_2).$$

$D_+ = \text{diag}(\lambda_1, \dots, \lambda_k)$  contains the positive real eigenvalues of  $M$ ,  $D_- = \text{diag}(\lambda_{k+1}, \dots, \lambda_{k+l})$  contains the negative real eigenvalues of  $M$  and  $D_{\text{complex}} = \text{diag}(\lambda_{k+l+1}, \bar{\lambda}_{k+l+1}, \dots, \lambda_{k+l+m}, \bar{\lambda}_{k+l+m})$  contains the  $2m$  complex eigenvalues of  $M$ .  $(\sigma_1, \dots, \sigma_{k+l})$  is an ordered list of signs  $\pm 1$ .

Given the decomposition from Theorem 11, the left eigenvectors of  $M$  are given as the columns of

$$V_2 = V^{-H} = \Sigma V S.$$

Structure preserving algorithms such as the HR algorithm [36–39] can be employed to compute a structured eigenvalue decomposition. This idea is described for product eigenvalues in [40]. A well-known downside of this approach is that it is not guaranteed to be stable. Further investigation is needed in order to devise satisfactory algorithms. Given a structured decomposition, the following theorem explains how to use it to construct eigenvalues of  $H$ .

**Theorem 12.** Let  $H$  be a BSE matrix of form  $I$ , with  $M_1 := A + B$  and  $M_2 = A - B$  nonsingular. Moreover, let  $M_2 = LTL^H$  be a decomposition, where  $T$  is a signature matrix, and assume

$$\hat{V}^{-1}M\hat{V} = D$$

be the structured eigenvalue decomposition of  $M = L^H M_1 L T$  given in Theorem 11, i.e.

$$\hat{V}^{-1} = S \hat{V}^H T, \quad S = \text{diag}(\sigma_1, \dots, \sigma_{k+l}, S_2, \dots, S_2).$$

Then with  $\hat{T} = \text{diag}(\sigma_1, \dots, \sigma_{k+l}, I_2, \dots, I_2)$  and  $Q := \frac{1}{2} \begin{bmatrix} I & I \\ -I & I \end{bmatrix}$ , the columns of the matrix

$$V = Q \begin{bmatrix} L^{-H} \hat{V} D^{1/4} \\ L T \hat{V} \hat{T} D^{-1/4} \end{bmatrix},$$

provide eigenvectors of  $H$  fulfilling  $HV = V\hat{\Lambda}$ , where  $\hat{\Lambda} = D^{\frac{1}{2}} \hat{T}$ . The complete set of eigenvectors is given by

$$V_{\text{full}} = \begin{bmatrix} V & -iKV \end{bmatrix}, \quad (27)$$

for which it holds that

$$V_{\text{full}}^H K V_{\text{full}} = \begin{bmatrix} I_k & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & I_l & 0 \\ 0 & 0 & S_{2m} & 0 & 0 & 0 \\ 0 & 0 & 0 & -I_k & 0 & 0 \\ 0 & I_l & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -S_{2m} \end{bmatrix}, \quad S_{2m} = \text{diag}(\dots, S_2) \in \mathbb{R}^{2m \times 2m}. \quad (28)$$

**Proof.** We see in (26) that  $L^{-H} \hat{V} =: V_1$  contains right eigenvectors of the matrix product  $M_1 M_2$ . Similarly, it can be seen that  $L \hat{V}^{-H} = L T \hat{V} S =: V_2$  contains left eigenvectors of  $M_1 M_2$ . We aim to apply Theorems 6 and 10 to compute the needed scaling factors for  $V_1$  and  $V_2$ . We observe that

$$M_1 V_2 = V_1 D S, \quad M_2 V_1 = V_2 S. \quad (29)$$

$V_{1,\text{ri}} := V_1(:, 1:k+l)$  and  $V_{2,\text{ri}} := V_2(:, 1:k+l)$  correspond to the real eigenvalues of  $M$ , and will turn out to correspond to real and imaginary eigenvalues of  $H$  (explaining the subscript choice). For the leading parts of  $S$  and  $T$  it holds

$$S_{\text{ri}} := S(1:k+l, 1:k+l) = \text{diag}(\sigma_1, \dots, \sigma_{k+l}) = \hat{T}_{\text{ri}} := \hat{T}(1:k+l, 1:k+l).$$

It follows with  $D_{\text{ri}} = D(1:k+l, 1:k+l)$  that

$$M_1 V_{2,\text{ri}} = V_{1,\text{ri}} D_{\text{ri}} \hat{T}_{\text{ri}}, \quad M_2 V_{1,\text{ri}} = V_{2,\text{ri}} \hat{T}_{\text{ri}}.$$

According to Theorem 6, the scaling factors  $\lambda_1$  and  $\lambda_2$  are given by the diagonal elements of  $D_{\text{ri}} \hat{T}_{\text{ri}}$  and  $\hat{T}_{\text{ri}}$ . Let  $\mu$  be an eigenvalue of  $M_1 M_2$  given as a diagonal element of  $D_{\text{ri}}$ . We consider the four possible cases

1.  $\mu > 0$

- (a)  $\lambda_1 > 0$  and  $\lambda_2 > 0 \Leftrightarrow$  Corresponding diagonal value in  $\hat{T}_{ri}$  is  $+1$ ,  
 (b)  $\lambda_1 < 0$  and  $\lambda_2 < 0 \Leftrightarrow$  Corresponding diagonal value in  $\hat{T}_{ri}$  is  $-1$ ,

2.  $\mu < 0$

- (a)  $\lambda_1 < 0$  and  $\lambda_2 > 0 \Leftrightarrow$  Corresponding diagonal value in  $\hat{T}_{ri}$  is  $+1$ .  
 (b)  $\lambda_1 > 0$  and  $\lambda_2 < 0 \Leftrightarrow$  Corresponding diagonal value in  $\hat{T}_{ri}$  is  $-1$ ,

In cases 1 (a) and 2 (a), the constructed vector corresponds to  $\lambda = \mu^{\frac{1}{2}}$  with no sign switch occurring according to [Theorem 6](#). In case 1 (b), a sign switch occurs according to [Theorem 6](#). In these three cases the corresponding scaling factor is given as  $\lambda_1^{\frac{1}{4}} \lambda_2^{-\frac{1}{4}} = \mu^{\frac{1}{4}}$ . In case 2 (b), no sign switch occurs according to [Theorem 6](#), but the proper scaling factor is given as  $\lambda_1^{\frac{1}{4}} \lambda_2^{-\frac{1}{4}} = \mu^{\frac{1}{4}} = -i\mu^{\frac{1}{4}}$ . If instead a scaling factor of  $\mu^{\frac{1}{4}}$  is chosen, this yields the eigenvector corresponding to  $-\mu^{\frac{1}{2}}$  as we see in the following. Let  $v = Q \begin{bmatrix} v_1 s_1 \\ v_2 s_1^{-1} \end{bmatrix}$  be the properly constructed eigenvector  $H$  corresponding to  $\mu$  with the scaling factor  $s_1 = -i\mu^{\frac{1}{4}}$ . According to [Theorem 4](#), 2. (a) the eigenvector corresponding to  $-\mu^{\frac{1}{2}}$  is given by

$$JKv = Q \begin{bmatrix} v_1 s_1 \\ -v_2 s_1^{-1} \end{bmatrix} = -iQ \begin{bmatrix} v_1 \mu^{\frac{1}{4}} \\ v_2 \mu^{-\frac{1}{4}} \end{bmatrix}, \quad (30)$$

where we used  $JKQ = QK$ . Scaling this eigenvector with  $i$  gives the vector, that is constructed using  $\mu^{\frac{1}{4}}$  as a scaling factor, as is proposed here. In summary, the proposed construction leads to a sign change whenever  $\hat{T}$  has negative values and it holds

$$HV_{ir} = V_{ir} D_{ir}^{\frac{1}{2}} \hat{T}_{ir}, \quad V_{ir} = Q \begin{bmatrix} L^{-H} \hat{V}_{ir} D_{ir}^{\frac{1}{4}} \\ LT \hat{V}_{ir} \hat{T}_{ir} D_{ir}^{-\frac{1}{4}} \end{bmatrix}. \quad (31)$$

The scaling matrices for the remaining vectors  $V_c = V(:, k+l+1 : n)$  associated with complex eigenvalues are constructed via [Theorem 10](#). From (29) we see that the scaling factors for a given  $\mu$  are given as  $\lambda_1 = \mu$  and  $\lambda_2 = 1$ , resulting in  $\hat{\lambda} = \mu^{\frac{1}{4}}$  and the scaling matrices

$$\hat{\lambda}_1 = \begin{bmatrix} \mu^{\frac{1}{4}} & 0 \\ 0 & \mu^{-\frac{1}{4}} \end{bmatrix}, \quad \hat{\lambda}_2 = \begin{bmatrix} 0 & \mu^{-\frac{1}{4}} \\ \mu^{-\frac{1}{4}} & 0 \end{bmatrix} = S_2 \hat{\lambda}_1^{-1}.$$

$D_c$ ,  $\hat{V}_c$ ,  $V_{1,c}$  and  $V_{2,c}$  denote the trailing diagonal matrix or the trailing columns of the respective matrix, corresponding to the  $2m$  complex eigenvalues of  $H$  with non-vanishing real and imaginary part. The scaling matrices for  $V_{1,c}$  and  $V_{2,c}$  are given as  $\hat{\lambda}_{1,c} = D_c^{\frac{1}{4}}$ ,  $\hat{\lambda}_{2,c} = S_{2m} \hat{\lambda}_{1,c}^{-1}$ . According to (20), no sign switch occurs with the given  $\lambda_1$  and  $\lambda_2$  and it holds

$$HV_c = V_c D_c^{\frac{1}{2}}, \quad V_c = Q \begin{bmatrix} V_{1,c} \hat{\lambda}_{1,c} \\ V_{2,c} \hat{\lambda}_{2,c} \end{bmatrix} = Q \begin{bmatrix} L^{-H} \hat{V}_c D_c^{\frac{1}{4}} \\ LT \hat{V}_c D_c^{-\frac{1}{4}} \end{bmatrix}. \quad (32)$$

(31) and (32) together give the first part of the proposed theorem.

$V_{full}$  provides a full set of eigenvectors according to [Theorem 4](#), 2. (a). It remains to show (28). The upper left quadrant of  $V_{full}^H K V_{full}$  is given as proposed according to [Theorems 6](#) and [10](#). The lower right quadrant is evaluated as  $(-iJKV)^H K (-iJKV) = -V^H K V$ . The remaining quadrants are determined by the entries  $v_\lambda^H K (-iJKv_\gamma) = i v_\lambda^H J v_\gamma$ , where  $v_\lambda$  and  $v_\gamma$  refer to vectors given as columns of  $V$ . This term evaluates as 0 when  $\lambda \neq \gamma$  or when the corresponding eigenvalue is not purely imaginary. For imaginary eigenvalues, we distinguish cases 2 (a) and 2 (b) defined above. In case 2 (a) ( $\lambda_1 < 0$ ,  $\lambda_2 > 0$ ), we have  $i v_\lambda^H J v_\gamma = i(-i) = 1$  according to (8). In case 2 (b) ( $\lambda_1 > 0$ ,  $\lambda_2 < 0$ ), we used the scaling factor  $\mu^{\frac{1}{4}}$  instead of  $-i\mu^{\frac{1}{4}}$  proposed by [Theorem 6](#). (30) states that the original vector, for which [Theorem 6](#) holds, is given by  $-iKJv_\lambda$ . So the  $J$ -orthogonality condition from [6](#) holds for  $-iKJv_\lambda$ , i.e. in this case we have  $(-iKJv_\lambda)^H J (-iKJv_\lambda) = -v_\lambda^H J v_\lambda = i$ . The quadrant entry then evaluates as  $i v_\lambda^H J v_\gamma = 1$ .  $\square$

The right tool for generalizing the SVD-based approach in [Theorem 9](#) is a generalized SVD given in form of [Theorem 4.1](#) in [41]. The following version concerns the special case of diagonalizable matrices and gives a generalized SVD with respect to two signature matrices  $T_1$  and  $T_2$ .

**Theorem 13.** Let  $A \in \mathbb{C}^{n \times n}$  be nonsingular and diagonalizable and let  $T_1, T_2 \in \mathbb{R}^{n \times n}$  be two signature matrices. Then there exist nonsingular matrices  $U, V \in \mathbb{C}^{n \times n}$ , s.t.

$$U^H A V = A_r \oplus A_i \oplus A_c, \quad U^H T_1 U = \hat{T}_1 = \text{diag}(s_1, \dots, s_{k+l}, S_2, \dots, S_2), \quad V^H T_2 V = \hat{T}_2 = \text{diag}(\hat{s}_1, \dots, \hat{s}_{k+l}, S_2, \dots, S_2),$$



where  $\Lambda_r = \text{diag}(\lambda_1, \dots, \lambda_k)$ ,  $\Lambda_i = \text{diag}(\lambda_{k+1}, \dots, \lambda_{k+l})$  are diagonal matrices containing positive real values,

$$\Lambda_c = \text{diag}(\lambda_{k+l+1}, \bar{\lambda}_{k+l+1}, \dots, \lambda_{k+l+m}, \bar{\lambda}_{k+l+m})$$

is a diagonal matrix containing complex conjugate pairs of complex values,  $\arg \lambda_j \in (0, \pi/2)$  for  $j = k+l+1, \dots, k+l+m$ .  $s$  and  $\hat{s}$  are signs,  $s_j, \hat{s}_j \in \{1, -1\}$ . It holds  $s_j \hat{s}_j = 1$  for  $j = 1, \dots, k$  and  $s_j \hat{s}_j = -1$  for  $j = k+1, \dots, k+l$ . For the matrices  $M = T_1 A T_2 A^H$ ,  $\hat{M} = T_2 A^H T_1 A$  the decomposition presented in Theorem 11 is given as

$$U^{-1} M U = \Lambda_r^2 \oplus -\Lambda_i^2 \oplus (\Lambda_c^2)^H, \quad V^{-1} \hat{M} V = \Lambda_r^2 \oplus -\Lambda_i^2 \oplus \Lambda_c^2.$$

Using scaled  $LDL^T$  decompositions  $M_1 = L_1 T_1 L_1^H$ ,  $M_2 = L_2 T_2 L_2^H$ , where  $T_1$  and  $T_2$  are signature matrices, the product eigenvalue problem considered in Theorem 6 and Theorem 10 is rewritten as

$$M_1 M_2 V_1 = V_1 D \Leftrightarrow T_1 L_1^H L_2 T_2 (L_1^H L_2)^H \hat{V}_1 = \hat{V}_1 D, \quad (33)$$

$$V_2^H M_1 M_2 = D V_2^H \Leftrightarrow \hat{V}_2^H (L_1^H L_2)^H T_1 (L_1^H L_2) T_2 = D \hat{V}_2^H, \quad (34)$$

where  $\hat{V}_1 = L_1^{-1} V_1$ ,  $\hat{V}_2 = L_2^{-1} V_2$ .

Here, the connection to the GSVD in Theorem 13 becomes apparent by setting  $A = L_1^H L_2$ . The following theorem explores this idea and gives guidance for computing eigenpairs of the BSE matrix via the GSVD.

**Theorem 14.** Let  $M_1 = L_1 T_1 L_1^H$ ,  $M_2 = L_2 T_2 L_2^H$  be decompositions, where  $T_1$ ,  $T_2$  are signature matrices and

$$\hat{U}^H M \hat{V} = \Lambda = \Lambda_r \oplus \Lambda_i \oplus \Lambda_c$$

be the GSVD of  $M = L_1^H L_2$  with respect to  $T_1$  and  $T_2$  given in Theorem 13, i.e.

$$\hat{U}^{-1} = \hat{T}_1 \hat{U}^H T_1, \quad \hat{T}_1 = \text{diag}(s_1, \dots, s_{k+l}, S_2, \dots, S_2),$$

$$\hat{V}^{-1} = \hat{T}_2 \hat{V}^H T_2, \quad \hat{T}_2 = \text{diag}(\hat{s}_1, \dots, \hat{s}_{k+l}, S_2, \dots, S_2).$$

Then

$$V = Q \begin{bmatrix} L_1 \hat{U} (\Lambda^{-1/2})^H \\ L_2 \hat{V} \Lambda^{-1/2} P \end{bmatrix}, \quad P = I_k \oplus i I_l \oplus S_2 \oplus \dots \oplus S_2$$

yields eigenvectors of  $H$  fulfilling  $HV = V \hat{\Lambda}$ , where  $\hat{\Lambda} = \Lambda \hat{T}$ ,  $\hat{T} = \text{diag}(s_1, \dots, s_{k+l}, I_{2m})$ . The complete set of eigenvectors is given by

$$V_{\text{full}} = [V \quad i j K V],$$

for which it holds that

$$V_{\text{full}}^H K V_{\text{full}} = \begin{bmatrix} I_k & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & I_l & 0 \\ 0 & 0 & S_{2m} & 0 & 0 & 0 \\ 0 & 0 & 0 & -I_k & 0 & 0 \\ 0 & I_l & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -S_{2m} \end{bmatrix}, \quad S_{2m} = \text{diag}(S_2, \dots, S_2) \in \mathbb{R}^{2m \times 2m}. \quad (35)$$

**Proof.** We use the GSVD of  $M = L_1^H L_2$  from Theorem 13,  $\hat{U}^H M \hat{V} = \Lambda$ . Then it holds

$$T_1 M T_2 M^H = \hat{U} (\Lambda^2)^H \hat{U}^{-1}, \quad S = I_k \oplus -I_l \oplus I_{2m},$$

and (33) is equivalent to

$$\hat{U} (\Lambda^2)^H \hat{U}^{-1} \hat{V}_1 = \hat{V}_1 D, \quad \hat{V}_1 = L_1^{-1} V_1.$$

This equation holds for  $D = (\Lambda^2)^H S$  and  $V_1 = L_1 \hat{U} (\Lambda^{-\frac{1}{2}})^H$ . Similarly it can be seen that (34) is solved by  $V_2 = L_2 \hat{V} \Lambda^{-\frac{1}{2}}$  and  $D = (\Lambda^2)^H S$ .  $(\Lambda^{-\frac{1}{2}})^H$  and  $\Lambda^{\frac{1}{2}}$  are diagonal matrices scaling the eigenvectors and have been chosen s.t. it holds  $V_1^H V_2 = I_n$ . Now we are in a position to apply Theorems 6 and 10. With some simple algebra we see that the scaling factors are given as (block-) diagonal elements of

$$\Lambda_1 = V_2^H M_1 V_2 = \hat{T}_1 \Lambda, \quad \Lambda_2 = V_1^H M_2 V_1 = \Lambda \hat{T}_2.$$

The scaling factor corresponding to a real diagonal value  $\lambda_j$ ,  $j = 1, \dots, k+l$ , of  $\Lambda$  can be evaluated as

$$\lambda_{1,j} \lambda_{2,j}^{-\frac{1}{4}} = (\lambda_j s_j)^{\frac{1}{4}} (\lambda_j \hat{s}_j)^{-\frac{1}{4}} = \begin{cases} 1 & \text{if } s_j \hat{s}_j = 1, \\ i^{-\frac{1}{2}} = \sqrt{2}^{-1} - \sqrt{2}^{-1} i & \text{if } s_j = 1 \text{ and } \hat{s}_j = -1, \\ i^{\frac{1}{2}} = \sqrt{2}^{-1} + \sqrt{2}^{-1} i & \text{if } s_j = -1 \text{ and } \hat{s}_j = 1. \end{cases} \quad (36)$$

The  $2 \times 2$  scaling blocks for complex eigenvalues evaluate as the identity matrix. Therefore, a non-trivial scaling is only needed for eigenvectors corresponding to imaginary eigenvalues ( $s_j \hat{s}_j = -1$ ).

(36) suggests for the case where  $s_j = 1$  and  $\hat{s}_j = -1$  to use the scaling factors  $i^{-\frac{1}{2}}$  for the corresponding vectors in  $V_1$  and  $i^{\frac{1}{2}}$  in  $V_2$ . We further multiply all vectors with  $i^{\frac{1}{2}}$ , s.t. only  $V_2$  is scaled by  $i$ . This does not change the fact that they are normalized eigenvectors, but simplifies notation.

In the case  $s_j = -1$ ,  $\hat{s}_j = 1$  the wrong scaling factor has been chosen. This is the same situation as in the proof of Theorem 12. Similarly, it can be shown that using the “wrong” scaling factor leads to the computation of an eigenvector corresponding to an eigenvalue of switched sign. In the case  $s_j = -1$ ,  $\hat{s}_j = -1$ , a sign switch occurs according to Theorem 6. No sign switch occurs for the complex eigenvalues according to (20), because we have  $\lambda_1 = \lambda_2$  and  $\arg \lambda_1 \in [0, \pi/2]$  according to the definition of the GSVD (Theorem 13). So in total, a sign switch occurs whenever  $s_j = -1$ . This is encoded in  $\hat{\Lambda} = \Lambda \hat{T}$ , where  $\hat{T} = \text{diag}(s_1, \dots, s_{k+l}, I_{2m})$ . The normalization condition (35) is shown similarly to the proof of Theorem 12.  $\square$

Table 4 summarizes and compares the two algorithmic approaches following from Theorems 12 and 14. Unfortunately, stable algorithms computing the necessary structured decompositions (Theorem 11 and Theorem 13) are hard to find. Filling these gaps is a topic of future research.

## 6. Conclusions and discussion

We presented a unifying framework for solving the Bethe–Salpeter eigenvalue problem as it appears in the computation of optical properties of crystalline systems. Two presented methods are superior to the one often used in current implementations, which is based on the computation of a matrix square root. Computing the matrix square root constitutes a high computational effort for non-diagonal matrices. Our first proposed method substitutes the matrix square root with a Cholesky factorization which can be computed much easier. The total runtime is reduced by about 40% in preliminary experiments, while the same accuracy is achieved. In order to achieve a higher accuracy we proposed a second method, which also relies on Cholesky factorizations and uses a singular value decomposition instead of an eigenvalue decomposition.

We gave new theoretical results on structured matrices, which served as a foundation of the proposed algorithms. These results were further extended to be applicable in a setting where non-definite matrices and complex eigenvalues occur. The previously presented methods found direct analogies in this setting. Most methods available in the literature on the other hand rely on the definiteness property (5).

In the definite setting many available methods, such as the iterative ones presented in [8,14], are implicitly connected to the presented product eigenvalue structure given in Theorems 6 and 10. The contribution of this manuscript in this regard is to clarify the common basis of methods that seem unconnected at first glimpse. The treatment of the non-definite case in Theorem 10 is completely new and can serve as a basis for further algorithm development. In this manuscript, we only presented direct methods based on structured decompositions. Future research can explore the possibility of an iterative approach solving the indefinite product eigenvalue problem in Theorem 10. A candidate might be based on an indefinite Lanczos method [42–44].

Iterative methods have benefits when only a fraction of the eigenpairs are sought. Typically, the eigenpairs corresponding to a few smallest eigenvalues already provide a lot of information about the considered system. It is also possible to reduce the computational costs of direct methods when only few eigenpairs are sought. For example, the needed decompositions can partially be computed in a divide-and-conquer fashion [45]. On an implementational level it is also possible to save some operations in the computation of symmetric eigenvalue decompositions in particular in the context of high performance computing [46].

## References

- [1] T. Sander, E. Maggio, G. Kresse, Beyond the Tamm–Dancoff approximation for extended systems using exact diagonalization, *Phys. Rev. B* 92 (2015) 045209, <http://dx.doi.org/10.1103/PhysRevB.92.045209>.
- [2] C. Vorwerk, B. Aurich, C. Cocchi, C. Draxl, Bethe–Salpeter equation for absorption and scattering spectroscopy: implementation in the exciting code, *Electron. Struct.* 1 (3) (2019) 037001, <http://dx.doi.org/10.1088/2516-1075/ab3123>.
- [3] S. Sagmeister, C. Ambrosch-Draxl, Time-dependent density functional theory versus Bethe–Salpeter equation: an all-electron study, *Phys. Chem. Chem. Phys.* 11 (2009) 4451–4457, <http://dx.doi.org/10.1039/B903676H>.
- [4] C. Penke, A. Marek, C. Vorwerk, C. Draxl, P. Benner, High performance solution of skew-symmetric eigenvalue problems with applications in solving the Bethe–Salpeter eigenvalue problem, *Parallel Comput.* 96 (2020) 102639, <http://dx.doi.org/10.1016/j.parco.2020.102639>.
- [5] The Top500 list, Available at <http://www.top500.org>.
- [6] L. Hedin, S. Lundqvist, Effects of electron–electron and electron–phonon interactions on the one-electron states of solids, in: F. Seitz, D. Turnbull, H. Ehrenreich (Eds.), *Solid State Physics*, Vol. 23, Academic Press, 1970, pp. 1–181, [http://dx.doi.org/10.1016/S0081-1947\(08\)60615-3](http://dx.doi.org/10.1016/S0081-1947(08)60615-3).
- [7] Z. Bai, R.-C. Li, Minimization principles for the linear response eigenvalue problem I: Theory, *SIAM J. Matrix Anal. Appl.* 33 (4) (2012) 1075–1100, <http://dx.doi.org/10.1137/110838960>.
- [8] Z. Bai, R.-C. Li, Minimization principles for the linear response eigenvalue problem II: Computation, *SIAM J. Matrix Anal. Appl.* 34 (2) (2013) 392–416, <http://dx.doi.org/10.1137/110838972>.
- [9] Z. Bai, R.-C. Li, Minimization principles and computation for the generalized linear response eigenvalue problem, *BIT* 54 (1) (2014) 31–54, <http://dx.doi.org/10.1007/s10543-014-0472-6>.

- [10] Z. Bai, R.-C. Li, W.-W. Lin, Linear response eigenvalue problem solved by extended locally optimal preconditioned conjugate gradient methods, *Sci. China Math.* 59 (8) (2016) 1443–1460, <http://dx.doi.org/10.1007/s11425-016-0297-1>.
- [11] Z. Bai, R.-C. Li, Recent progress in linear response eigenvalue problems, in: *Eigenvalue Problems: Algorithms, Software and Applications in Petascale Computing*, in: *Lect. Notes Comput. Sci. Eng.*, vol. 117, Springer, Cham, 2017, pp. 287–304, [http://dx.doi.org/10.1007/978-3-319-62426-6\\_18](http://dx.doi.org/10.1007/978-3-319-62426-6_18).
- [12] M. Casida, Time-dependent density functional response theory for molecules, in: *Recent Advances in Density Functional Methods*, World Scientific, 1995, pp. 155–192, [http://dx.doi.org/10.1142/9789812830586\\_0005](http://dx.doi.org/10.1142/9789812830586_0005).
- [13] P. Papakonstantinou, Reduction of the RPA eigenvalue problem and a generalized Cholesky decomposition for real-symmetric matrices, *Europhys. Lett.* 78 (1) (2007) 12001, <http://dx.doi.org/10.1209/0295-5075/78/12001>.
- [14] M. Shao, F.H. da Jornada, L. Lin, C. Yang, J. Deslippe, S.G. Louie, A structure preserving Lanczos algorithm for computing the optical absorption spectrum, *SIAM J. Matrix Anal. Appl.* 39 (2) (2018) 683–711, <http://dx.doi.org/10.1137/16M1102641>.
- [15] F. Henneke, L. Lin, C. Vorwerk, C. Draxl, R. Klein, C. Yang, Fast optical absorption spectra calculations for periodic solid state systems, *Commun. Appl. Math. Comput. Sci.* 15 (1) (2020) 89–113, <http://dx.doi.org/10.2140/camcos.2020.15.89>.
- [16] D.S. Mackey, N. Mackey, F. Tisseur, Structured factorizations in scalar product spaces, *SIAM J. Matrix Anal. Appl.* 27 (3) (2005) 821–850, <http://dx.doi.org/10.1137/040619363>.
- [17] P. Benner, D. Kressner, V. Mehrmann, Skew-Hamiltonian and Hamiltonian eigenvalue problems: Theory, algorithms and applications, in: *Proc. Conf. Appl. Math. Scientific Comp.*, Springer-Verlag, 2005, pp. 3–39, [http://dx.doi.org/10.1007/1-4020-3197-1\\_1](http://dx.doi.org/10.1007/1-4020-3197-1_1).
- [18] P. Benner, H. Faßbender, C. Yang, Some remarks on the complex J-symmetric eigenproblem, *Linear Algebra Appl.* 544 (2018) 407–442, <http://dx.doi.org/10.1016/j.laa.2018.01.014>.
- [19] G. Onida, L. Reining, A. Rubio, Electronic excitations: density-functional versus many-body Green's-function approaches, *Rev. Modern Phys.* 74 (2002) 601–659, <http://dx.doi.org/10.1103/RevModPhys.74.601>.
- [20] D. Kressner, *Numerical Methods for General and Structured Eigenvalue Problems*, in: *Lecture Notes in Computational Science and Engineering*, vol. 46, Springer-Verlag, Berlin Heidelberg, 2005, p. xiv+258.
- [21] P. Benner, V. Mehrmann, H. Xu, A numerically stable, structure preserving method for computing the eigenvalues of real Hamiltonian or symplectic pencils, *Numer. Math.* 78 (3) (1998) 329–358, <http://dx.doi.org/10.1007/s002110050315>.
- [22] N.J. Higham, *Functions of Matrices: Theory and Computation*, in: *Applied Mathematics, Society for Industrial and Applied Mathematics*, Philadelphia, PA, 2008, p. xx+425, <http://dx.doi.org/10.1137/1.9780898717778>.
- [23] B.E. Chi, The eigenvalue problem for collective motion in the random phase approximation, *Nuclear Phys. A* 146 (2) (1970) 449–456, [http://dx.doi.org/10.1016/0375-9474\(70\)90738-4](http://dx.doi.org/10.1016/0375-9474(70)90738-4).
- [24] C.F. Van Loan, A symplectic method for approximating all the eigenvalues of a Hamiltonian matrix, *Linear Algebra Appl.* 61 (1984) 233–251, [http://dx.doi.org/10.1016/0024-3795\(84\)90034-X](http://dx.doi.org/10.1016/0024-3795(84)90034-X).
- [25] J.H. Wilkinson, *The Algebraic Eigenvalue Problem*, Oxford University Press, Oxford, 1965.
- [26] P. Benner, R. Byers, E. Barth, Algorithm 800. Fortran 77 subroutines for computing the eigenvalues of Hamiltonian matrices I: The square-reduced method, *ACM Trans. Math. Softw.* 26 (1) (2000) 49–77, <http://dx.doi.org/10.1145/347837.347852>.
- [27] M. Shao, F.H. da Jornada, C. Yang, J. Deslippe, S.G. Louie, Structure preserving parallel algorithms for solving the Bethe-Salpeter eigenvalue problem, *Linear Algebra Appl.* 488 (2016) 148–167, <http://dx.doi.org/10.1016/j.laa.2015.09.036>.
- [28] G.W. Stewart, J.-G. Sun, *Matrix Perturbation Theory*, Academic Press, New York, 1990.
- [29] A. Gulans, S. Kontur, C. Meisenbichler, D. Nabok, P. Pavone, S. Rigamonti, S. Sagmeister, U. Werner, C. Draxl, Exciting: a full-potential all-electron package implementing density-functional theory and many-body perturbation theory, *J. Phys.: Condens. Matter* 26 (36) (2014) 363202, <http://dx.doi.org/10.1088/0953-8984/26/36/363202>.
- [30] J. Deslippe, G. Samsonidze, D.A. Strubbe, M. Jain, M.L. Cohen, S.G. Louie, BerkeleyGW: A massively parallel computer package for the calculation of the quasiparticle and optical properties of materials and nanostructures, *Comput. Phys. Comm.* 183 (6) (2012) 1269–1289, <http://dx.doi.org/10.1016/j.cpc.2011.12.006>.
- [31] D. Sangalli, A. Ferretti, H. Miranda, C. Attaccalite, I. Marri, E. Cannuccia, P. Melo, M. Marsili, F. Paleari, A. Marrazzo, G. Prandini, P. Bonfà, M.O. Atambo, F. Affinito, M. Palumbo, A. Molina-Sánchez, C. Hogan, M. Grüning, D. Varsano, A. Marini, Many-body perturbation theory calculations using the yambo code, *J. Phys.: Condens. Matter* 31 (32) (2019) 325902, <http://dx.doi.org/10.1088/1361-648x/ab15d0>.
- [32] G.H. Golub, C.F. Van Loan, *Matrix Computations*, fourth ed., in: *Johns Hopkins Studies in the Mathematical Sciences*, Johns Hopkins University Press, Baltimore, 2013.
- [33] P. Benner, V. Mehrmann, H. Xu, A note on the numerical solution of complex Hamiltonian and skew-Hamiltonian eigenvalue problems, *Electron. Trans. Numer. Anal.* 8 (1999) 115–126.
- [34] P. Benner, D. Kressner, V. Sima, A. Varga, Die SLICOT-toolboxen für MATLAB, at–Automatisierungstechnik 58 (1) (2010) 15–25, <http://dx.doi.org/10.1524/auto.2010.0814>.
- [35] C. Mehl, Finite-dimensional indefinite inner product spaces and applications in numerical analysis, in: *Operator Theory*, Springer Basel, Basel, 2015, pp. 1–17, [http://dx.doi.org/10.1007/978-3-0348-0692-3\\_34-1](http://dx.doi.org/10.1007/978-3-0348-0692-3_34-1).
- [36] P. Benner, H. Faßbender, D.S. Watkins, Two connections between the SR and HR eigenvalue algorithms, *Linear Algebra Appl.* 272 (1997) 17–32.
- [37] D. Watkins, *The Matrix Eigenvalue Problem*, Society for Industrial and Applied Mathematics, 2007, <http://dx.doi.org/10.1137/1.9780898717808>.
- [38] A. Bunse-Gerstner, An analysis of the HR algorithm for computing the eigenvalues of a matrix, *Linear Algebra Appl.* 35 (1981) 155–173, [http://dx.doi.org/10.1016/0024-3795\(81\)90271-8](http://dx.doi.org/10.1016/0024-3795(81)90271-8).
- [39] A. Bunse-Gerstner, An algorithm for the symmetric generalized eigenvalue problem, *Linear Algebra Appl.* 58 (1984) 43–68.
- [40] M. Brebner, J. Grad, Eigenvalues of  $Ax = \lambda Bx$  for real symmetric matrices  $A$  and  $B$  computed by reduction to a pseudosymmetric form and the HR process, *Linear Algebra Appl.* 43 (1982) 99–118, [http://dx.doi.org/10.1016/0024-3795\(82\)90246-4](http://dx.doi.org/10.1016/0024-3795(82)90246-4).
- [41] C. Mehl, V. Mehrmann, H. Xu, Structured decompositions for matrix triples: SVD-like concepts for structured matrices, *Oper. Matrices* 3 (3) (2009) 303–356, <http://dx.doi.org/10.7153/oam-03-19>.
- [42] B.N. Parlett, H.C. Chen, Use of indefinite pencils for computing damped natural modes, *Linear Algebra Appl.* 140 (1990) 53–88, [http://dx.doi.org/10.1016/0024-3795\(90\)90222-X](http://dx.doi.org/10.1016/0024-3795(90)90222-X).
- [43] D. Day, An efficient implementation of the nonsymmetric Lanczos algorithm, *SIAM J. Matrix Anal. Appl.* 18 (3) (1997) 566–589, <http://dx.doi.org/10.1137/S0895479895292503>.
- [44] C. Campos, J.E. Roman, Restarted Q-Arnoldi-type methods exploiting symmetry in quadratic eigenvalue problems, *BIT* 56 (4) (2016) 1213–1236, <http://dx.doi.org/10.1007/s10543-016-0601-5>.
- [45] Y. Nakatsukasa, N.J. Higham, Stable and efficient spectral divide and conquer algorithms for the symmetric eigenvalue decomposition and the SVD, *SIAM J. Sci. Comput.* 35 (3) (2013) A1325–A1349, <http://dx.doi.org/10.1137/120876605>.
- [46] T. Auckenthaler, V. Blum, H.-J. Bungartz, T. Huckle, R. Johanni, L. Krämer, B. Lang, H. Lederer, P. Willems, Parallel solution of partial symmetric eigenvalue problems from electronic structure calculations, *Parallel Comput.* 37 (12) (2011) 783–794, <http://dx.doi.org/10.1016/j.parco.2011.05.002>.