algorithm. *Application Research of Computers*, No.11, p.p.3225-3228.

13. Hwang A.B., Bacharach S.L., Yom S.S. et al. (2009) Can positron emission tomography (PET) or PET/Computed Tomography (CT) acquired in a no treatment position be accurately registered to a head-and-neck radiotherapy planning CT?. *International Journal of Radiation Oncology, Biology, Physics*, 73(2), p.p.578-584.
14. He Z.M., Zhang Y., Gao L. (2014) Cloud computing resource schedule strategy based on QPS-FLA algorithm. *Computer Knowledge and Technology*, No.2, p.p.311-314.

A Perturbation Bound of the Partitioned Linear Response Eigenvalue Problem

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Abstract

In this paper, we focus on the linear response eigenvalue problem for $H=\begin{bmatrix}0 & K\\ M & 0\end{bmatrix}$, where K and admit a 2×2 block partitioning. When K and M are perturbed to $\tilde{K}$ and $\tilde{M}$ by two symmetric matrices E and F, the bound on how the changes of its eigenvalues is obtained, which is related to the Frobenius norm of E and F. Numerical experiment is presented to support our analysis.

Key words: LINEAR RESPONSE EIGENVALUE PROBLEMS, RANDOM PHASE APPROXIMATION, PERTURBATION BOUND

1. Introduction

In this paper, we consider the linear response eigenvalue problem (LREP) of the form:

$$Hz=\begin{bmatrix}0 & K\\ M & 0\end{bmatrix}\begin{bmatrix}y\\ x\end{bmatrix}=\lambda\begin{bmatrix}y\\ x\end{bmatrix}=\lambda z, \tag{1}$$

where K and M are $n\times n$ real symmetric positive definite. Such a problem arises in the linear response perturbation analysis of the time-dependent density functional theory in computational quantum chemistry and physics which is commonly used to analyze the electronic excitation spectrum of a quantum many-fermion system [1, 2, 3, 4]. It is also known as the random phase approximation eigenvalue problem.

Despite that this is a nonsymmetric eigenvalue problem since H is not symmetric, this eigenvalue problem exhibits many properties that one usually finds in a symmetric eigenvalue problem [5, 6, 7]. In fact, H is a special Hamiltonian matrix whose eigenvalues are real and come in pairs $\{\lambda,-\lambda\}$. Denote by $\pm\lambda_i$ the eigenvalues of H and order them as

$$-\lambda_n\le\ldots\le-\lambda_1<\lambda_1\le\ldots\le\lambda_n. \tag{2}$$

In particular, $\lambda_1>0$ since both K and M are positive definite. In practice, the first k smallest positive eigenvalues $\lambda_1\le\ldots\le\lambda_k$ are of interest.

Recently, Bai and Li [8, 9] has successfully obtained Ky Fan type trace min principle and Cauchy type interlacing inequalities, among others. Zhang [10, 11] got the Rayleigh-Ritz approximation theory and the backward perturbation bounds for LREP. Teng [12] study the perturbation bounds of the partitioned linear response eigenvalue problems, and obtain the bound that is of linear order with respect to the diagonal block perturbations and of quadratic order with respect to the off-diagonal block perturbations. In this paper, based on the paper [12], we will continue the effort in studying the partitioned linear response eigenvalue problems. Suppose LREP (1) in which K and M are already block diagonal:

$$K=\begin{matrix} & n_1 & n_2\\ n_1 & K_{11} & \\ n_2 & & K_{22}\end{matrix},\quad M=\begin{matrix} & n_1 & n_2\\ n_1 & M_{11} & \\ n_2 & & M_{22}\end{matrix}, \tag{3}$$

where M_{ii} and K_{ii} for $i=1,2$ are all symmetric positive definite, then

$$H=\begin{bmatrix}0 & 0 & K_{11} & 0\\ 0 & 0 & 0 & K_{22}\\ M_{11} & 0 & 0 & 0\\ 0 & M_{22} & 0 & 0\end{bmatrix}. \tag{4}$$

When K and M are perturbed to

$$\tilde{K}=K+E=\begin{bmatrix}K_{11}+E_{11} & E_{12}\\ E_{21} & K_{22}+E_{22}\end{bmatrix},$$

$$\tilde{M}=M+F=\begin{bmatrix}M_{11}+F_{11} & F_{12}\\ F_{21} & M_{22}+F_{22}\end{bmatrix}, \tag{5}$$

by perturbations E and F which are assumed symmetric, and $\tilde{K}$, $\tilde{M}$ are kept to be positive definite, we are interested in bounding how much the eigenvalues of H change. Let

$$H_1=\begin{bmatrix}0 & K_{11}\\ M_{11} & 0\end{bmatrix},\qquad H_2=\begin{bmatrix}0 & K_{22}\\ M_{22} & 0\end{bmatrix}, \tag{6}$$

$$\tilde{H}=\begin{bmatrix}0 & 0 & K_{11}+E_{11} & E_{12}\\ 0 & 0 & E_{21} & K_{22}+E_{22}\\ M_{11}+F_{11} & F_{12} & 0 & 0\\ F_{21} & M_{22}+F_{22} & 0 & 0\end{bmatrix}, \tag{7}$$

and denote the eigenvalues of $\tilde{H}$ and H_1 by

$-\tilde{\lambda}_n\le\ldots\le-\tilde{\lambda}_1<\tilde{\lambda}_1\le\ldots\le\tilde{\lambda}_n$, {}

$-\theta_{n_1}\le\ldots\le-\theta_1<\theta_1\le\ldots\le\theta_{n_1}$.

We are interested to bound the difference between the eigenvalues of H_1 and some n_1 eigenvalues of $\tilde{H}$.

Such a problem arises in one using some subspace projection type methods for large scale LREP. Recently, there are several rather efficient algorithms for LREP, such as the gradient type method [9, 13], the generalized Lanczos method [14, 15], and the block Chebyshev-Davidson method [16]. Each of these algorithms hopefully generates an approximate deflating subspace pair $\{\widetilde{\mathcal{U}},\widetilde{\mathcal{V}}\}$. Projecting LREP by the approximate deflating subspacepair $\{\widetilde{\mathcal{U}},\widetilde{\mathcal{V}}\}$ leads to $\tilde{H}$ in (7) with $E_{ii}=F_{ii}=0$ ($i=1,2$) and usually unknown K_{22} and M_{22}. Some norm estimates of E_{ij} and F_{ij} for $i\ne j$ are related to the residuals of the subspace type method. In such a case, our main results will help us understand how well the eigenvalues of H_1 approximate some of those of $\tilde{H}$. In [12], Teng obtains the bound of $|\theta_i - \tilde{\lambda}_{t_i}|$ ($1 \le i \le n_1$) with respect to 2-norm of the perturbation matrices E and F. In this paper, we will do further research on this problem and try to get the bound of $\sum_{t_i=1}^{n_1} |\theta_i - \tilde{\lambda}_{t_i}|$ related to the Frobenius norm of E and F.

The rest of the paper is organized as follows. In section 2, we will first collect some known results for the standard symmetric eigenvalue problem and LREP. These results are essential to our later development. We get our main results in section 3. Some numerical example is presented in Section 4 to support our analysis. Finally concluding remarks are made in Section 5.

Notation. $R^{m\times n}$ is the set of all $m\times n$ real matrices, $R^n = R^{n\times 1}$, and $R = R^1$. I_n is the $n\times n$ identity matrix or simply I if its dimension is clear from the context. The superscript "$\cdot^T$" takes transpose only, and $\|\cdot\|_2$ denote the ℓ_2-norm of a vector or the spectral norm of a matrix. For symmetric matrix $X \in R^{n\times n}$, we will use integer triplet

$(i_-(X), i_0(X), i_+(X))$

for its inertia, where $i_-(X)$, $i_0(X)$, and $i_+(X)$ are the number of negative, zero, and positive eigenvalues of X, respectively. For matrices or scalars X_i, $\mathrm{diag}(X_1,\ldots,X_k)$ denote the block diagonal matrix

$$\begin{bmatrix} X_1 & & \\ & \ddots & \\ & & X_k \end{bmatrix}.$$

2. Preliminaries

Recall (1). LREP can be turned into the following generalized eigenvalue problem by permuting the first and second block rows to get

$$\begin{bmatrix} M & 0 \\ 0 & K \end{bmatrix}\begin{bmatrix} y \\ x \end{bmatrix} = \lambda \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix}\begin{bmatrix} y \\ x \end{bmatrix}, \tag{8}$$

where I is the identity matrix of apt size. Later in this paper, we need the following known results from LREP, standard symmetric eigenvalue problems and the symmetric definite pencil for our later development.

Lemma 2. 1. There exist nonsingular $\Phi, \Psi \in R^{n\times n}$ such that

$$\Psi^{\mathrm{T}} K \Psi = \Lambda, \qquad \Phi^{\mathrm{T}} M \Phi = \Lambda, \qquad \Psi = \Phi^{-\mathrm{T}} \tag{9}$$

where $\Lambda = diag(\lambda_1, \lambda_2, \ldots, \lambda_n)$ and $0 < \lambda_1 \le \ldots \le \lambda_n$. Moreover,

$$\|\Psi\|_2^2 \le \frac{\|M\|_2}{\lambda_1} \quad \text{and} \quad \|\Phi\|_2^2 \le \frac{\|K\|_2}{\lambda_1}. \tag{10}$$

Lemma 2.2. Let A and $\tilde{A}$ be two $n\times n$ symmetric matrices, and denote their eigenvalues by $0 < \lambda_1 \le \ldots \le \lambda_n$ and $0 < \tilde{\lambda}_1 \le \ldots \le \tilde{\lambda}_n$, respectively.

(See [7]) $\sqrt{\sum_{i=1}^{n} |\tilde{\lambda}_i - \lambda_i|^2} \le \|\tilde{A} - A\|_F$.

(See [17]) Suppose that

$$A = \begin{matrix} & \begin{matrix} n_1 & n_2 \end{matrix} \\ \begin{matrix} n_1 \\ n_2 \end{matrix} & \begin{bmatrix} A_{11} & \\ & A_{22} \end{bmatrix} \end{matrix}, \qquad \tilde{A} = \begin{bmatrix} A_{11} & E^T \\ E & A_{22} \end{bmatrix}.$$

Denote by θ_i for $1 \le i \le n_1$ the eigenvalues of A_{11} with ascending order. Then there exist n_1 eigenvalues $\tilde{\lambda}_{t_1} \le \ldots \le \tilde{\lambda}_{t_{n_1}}$ of $\tilde{A}$ such that

$$\sqrt{\sum_{i=1}^{n_1} |\theta_i - \tilde{\lambda}_{t_i}|^2} \le \|E\|_F$$

Definition 2.1. $A - \lambda B$ is a symmetric pencil of order n if both $A, B \in R^{n\times n}$ are symmetric. $A - \lambda B$ is a positive definite matrix pencil of order n if it is a symmetric pencil of order n and if there exists $\in$ such that $A - \lambda_0 B$ is positive definite.

Lemma 2.3. ([18, 19, 20]). Suppose $A - \lambda B$ is a positive definite matrix pencil of order n with nonsingular B and let $\lambda_0 \in R$ such that $A - \lambda_0 B$ is positive definite. Denote the eigenvalues of the pencil $A - \lambda B$ by

$$\lambda_{n_-}^- \le \ldots \le \lambda_1^- < \lambda_1^+ \le \ldots \le \lambda_{n_+}^+, \tag{11}$$

where $n_+ = i_+(B)$ and $n_- = i_-(B)$. Then $\lambda_1^- < \lambda_0 < \lambda_1^+$, and there exists a nonsingular $W \in R^{n\times n}$ such that

$$W^{\mathrm{T}} A W = \begin{bmatrix} -\Lambda_- & \\ & \Lambda_+ \end{bmatrix}, \quad W^{\mathrm{T}} B W = \begin{bmatrix} -I_{n_-} & \\ & I_{n_+} \end{bmatrix}, \tag{12}$$

where $\Lambda_\pm = \mathrm{diag}(\lambda_1^\pm, \ldots, \lambda_{n_\pm}^\pm)$.

Lemma 2.4. ([21, Theorem A.2]). Suppose $A - \lambda B$ is a positive definite matrix pencil with nonsingular B and with the eigen-decomposition (12). Suppose it is perturbed to another positive definite pencil $\tilde{A} - \lambda \tilde{B}$ with nonsingular $\tilde{B}$. Suppose $\tilde{B}$ and B have the same inertia. Adopt the same notations for this perturbed pencil as those for $A - \lambda B$ except with a tilde on each symbol. Then,

$$\sqrt{\sum_{i=1}^{n_-} |\lambda_i^- - \tilde{\lambda}_i^-|^2 + \sum_{i=1}^{n_+} |\lambda_i^+ - \tilde{\lambda}_i^+|^2} \le \|W\|_2 \|\tilde{W}\|_2 \left(\|\tilde{A} - A\|_F + \varepsilon \|\tilde{B} - B\|_F \right) \tag{13}$$

where

$$\varepsilon = \max_{\substack{1\le i\le n_- \\ 1\le j\le n_+}} \{-\lambda_i^-, \lambda_j^+, -\tilde{\lambda}_i^-, \tilde{\lambda}_j^+\}.$$

Lemma 2.5. ([21, Theorem A.3]). Suppose $A-\lambda B$ is a positive definite matrix pencil with the eigen-decomposition (12), and the eigenvalues are ordered as in (11). Then for any $\lambda_0 \in (\lambda_1^-, \lambda_1^+)$

$$\| W \|_2 \le \sqrt{\max\{\lambda_{n_+}^+ - \lambda_0, \lambda_0 - \lambda_{n_-}^-\} \, \|(A-\lambda_0 B)^{-1}\|_2}. \quad (14)$$

Lemma 2.6. ([12, Lemma 2.7]). Let

$$A = \begin{bmatrix} A_1 & E^T \\ E & A_2 \end{bmatrix}, \qquad B = \begin{bmatrix} I_{n_+} & \\ & -I_{n_-} \end{bmatrix},$$

where $A_1 \in R^{n_+\times n_+}$, $A_2 \in R^{n_-\times n_-}$ and $A \in R^{n\times n}$ are symmetric positive definite, and $n_+ + n_- = n$. Denote the eigenvalues of $A-\lambda B$ by

$$\lambda_{n_-}^- \le \ldots \le \lambda_1^- < \lambda_1^+ \le \ldots \le \lambda_{n_+}^+,$$

where $\lambda_1^+ > 0$ and $\lambda_1^- < 0$, and the eigenvalues of A_1 and A_2 by

$$\alpha_1 \le \ldots \le \alpha_{n_+}, \quad \beta_1 \le \ldots \le \beta_{n_-},$$

respectively. Then, for $1 \le i \le n_+$ and $1 \le j \le n_-$,

$$-\beta_j \le \lambda_j^- < 0 < \lambda_i^+ \le \alpha_i. \quad (15)$$

3. Main result

Recall Theorem 2.1. For K_{ii} and M_{ii} in (3), there exist Ψ_i and Φ_i such that

$$\Psi_1^T K_{11}\Psi_1 = \Lambda_1, \quad \Phi_1^T M_{11}\Phi_1 = \Lambda_1, \quad \Psi_1 = \Phi_1^{-T},$$
$$\Psi_2^T K_{22}\Psi_2 = \Lambda_2, \quad \Phi_2^T M_{22}\Phi_2 = \Lambda_2, \quad \Psi_2 = \Phi_2^{-T},$$

where Λ_1 and Λ_2 are diagonal matrices with the diagonal entries consisting of the positive eigenvalues of H. In fact, $\lambda(\Lambda_1)\cup\lambda(\Lambda_2) = \lambda(\Lambda)$, where Λ is defined in (9).

Let

$$P = \begin{bmatrix} \Psi_1 & 0 & 0 & 0 \\ 0 & \Psi_2 & 0 & 0 \\ 0 & 0 & \Phi_1 & 0 \\ 0 & 0 & 0 & \Phi_2 \end{bmatrix}, \qquad Q = \begin{bmatrix} \Phi_1 & 0 & 0 & 0 \\ 0 & \Phi_2 & 0 & 0 \\ 0 & 0 & \Psi_1 & 0 \\ 0 & 0 & 0 & \Psi_2 \end{bmatrix}.$$

We have $P^T Q = I_{2n}$ and

$$P^T HQ = \begin{bmatrix} 0 & 0 & \Lambda_1 & 0 \\ 0 & 0 & 0 & \Lambda_2 \\ \Lambda_1 & 0 & 0 & 0 \\ 0 & \Lambda_2 & 0 & 0 \end{bmatrix}, \quad (16)$$

$$P^T \tilde{H} Q = \begin{bmatrix} 0 & 0 & \Lambda_1 + \tilde{E}_{11} & \tilde{E}_{12} \\ 0 & 0 & \tilde{E}_{21} & \Lambda_2 + \tilde{E}_{22} \\ \Lambda_1 + \tilde{F}_{11} & \tilde{F}_{12} & 0 & 0 \\ \tilde{F}_{21} & \Lambda_2 + \tilde{F}_{22} & 0 & 0 \end{bmatrix} = P^T HQ + \begin{bmatrix} 0 & \tilde{E} \\ \tilde{F} & 0 \end{bmatrix}. \quad (17)$$

where

$$\tilde{E} = \begin{bmatrix} \tilde{E}_{11} & \tilde{E}_{12} \\ \tilde{E}_{21} & \tilde{E}_{22} \end{bmatrix} = \begin{bmatrix} \Psi_1^T & 0 \\ 0 & \Psi_2^T \end{bmatrix} \begin{bmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{bmatrix} \begin{bmatrix} \Psi_1 & 0 \\ 0 & \Psi_2 \end{bmatrix},$$

$$\tilde{F} = \begin{bmatrix} \tilde{F}_{11} & \tilde{F}_{12} \\ \tilde{F}_{21} & \tilde{F}_{22} \end{bmatrix} = \begin{bmatrix} \Phi_1^T & 0 \\ 0 & \Phi_2^T \end{bmatrix} \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix} \begin{bmatrix} \Phi_1 & 0 \\ 0 & \Phi_2 \end{bmatrix}.$$

Making use of (10), we can bound $\tilde{E}_{ij}$ and $\tilde{F}_{ij}$ $(i,j=1,2)$ as follows

$$\|\tilde{E}_{ij}\|_2 = \|\Psi_i^T E_{ij}\Psi_j\|_2 \le \frac{\|M\|_2 \|E_{ij}\|_2}{\lambda_1},$$

$$\|\tilde{F}_{ij}\|_2 = \|\Phi_i^T F_{ij}\Phi_j\|_2 \le \frac{\|K\|_2 \|F_{ij}\|_2}{\lambda_1},$$

and similarly,

$$\|\tilde{E}\|_2 \le \frac{\|M\|_2 \|E\|_2}{\lambda_1} \qquad \|\tilde{F}\|_2 \le \frac{\|K\|_2 \|F\|_2}{\lambda_1}$$

Theorem 2.3. Suppose H in (4) is perturbed to $\tilde{H}$ in (7), where K, M and their perturbed ones are all symmetric positive definite. Adopt the notations introduced so far in this section. If $\max\{\|E\|_2 \|K^{-1}\|_2, \|F\|_2 \|M^{-1}\|_2\} < 1$, there are n_1 positive eigenvalues $\tilde{\lambda}_{t_1} \le \ldots \le \tilde{\lambda}_{t_{n_1}}$ of $\tilde{H}$ such that

$$\sqrt{\sum_{i=1}^{n_1} |\theta_i - \tilde{\lambda}_{t_i}|^2} \le \frac{1}{2}\left(\|\tilde{E}_{11} + \tilde{F}_{11}\|_F + \|\tilde{E}_{21} + \tilde{F}_{21}\|_F + \sqrt{\frac{\tilde{\lambda}_n(\lambda_n+\tau)}{2\tilde{\lambda}_1(\lambda_1-\tau)}} \left\|\tilde{E} - \tilde{F}\right\|_F \right)$$

where $\tau = \max\{\|\tilde{E}\|_2, \|\tilde{F}\|_2\}$.

Proof. Using (8), (16) and (17), we can transform LREP for H in (4) and LREP for $\tilde{H}$ in (7) equivalently to the generalized eigenvalue problems for $A-\lambda B$ and $\tilde{A}-\lambda B$, respectively, where

$$A = \begin{bmatrix} \Lambda_1 & 0 & 0 & 0 \\ 0 & \Lambda_2 & 0 & 0 \\ 0 & 0 & \Lambda_1 & 0 \\ 0 & 0 & 0 & \Lambda_2 \end{bmatrix}, \qquad B = \begin{bmatrix} 0 & 0 & I_{n_1} & 0 \\ 0 & 0 & 0 & I_{n_2} \\ I_{n_1} & 0 & 0 & 0 \\ 0 & I_{n_2} & 0 & 0 \end{bmatrix}$$

$$\tilde{A} = \begin{bmatrix} \Lambda_1 + \tilde{E}_{11} & \tilde{E}_{12} & 0 & 0 \\ \tilde{E}_{21} & \Lambda_2 + \tilde{E}_{22} & 0 & 0 \\ 0 & 0 & \Lambda_1 + \tilde{F}_{11} & \tilde{F}_{12} \\ 0 & 0 & \tilde{F}_{21} & \Lambda_2 + \tilde{F}_{22} \end{bmatrix}.$$

Both

$$\begin{bmatrix} \Lambda_1 + \tilde{E}_{11} & \tilde{E}_{12} \\ \tilde{E}_{21} & \Lambda_2 + \tilde{E}_{22} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} \Lambda_1 + \tilde{F}_{11} & \tilde{F}_{12} \\ \tilde{F}_{21} & \Lambda_2 + \tilde{F}_{22} \end{bmatrix}$$

are positive definite because $\tilde{K}$ and $\tilde{M}$ in (5) are assumed positive definite. Let $Z=\frac{1}{\sqrt{2}}\begin{bmatrix} I_n & I_n \\ I_n & -I_n \end{bmatrix}$.

We have

$$\hat{A}=Z^T\tilde{A}Z$$
$$=\begin{bmatrix} \Lambda_1+\frac{1}{2}\tilde{E}_{11}+\frac{1}{2}\tilde{F}_{11} & \frac{1}{2}\tilde{E}_{12}+\frac{1}{2}\tilde{F}_{12} & \frac{1}{2}\tilde{E}_{11}-\frac{1}{2}\tilde{F}_{11} & \frac{1}{2}\tilde{E}_{12}-\frac{1}{2}\tilde{F}_{12} \\ \frac{1}{2}\tilde{E}_{21}+\frac{1}{2}\tilde{F}_{21} & \Lambda_2+\frac{1}{2}\tilde{E}_{22}+\frac{1}{2}\tilde{F}_{22} & \frac{1}{2}\tilde{E}_{21}-\frac{1}{2}\tilde{F}_{21} & \frac{1}{2}\tilde{E}_{22}-\frac{1}{2}\tilde{F}_{22} \\ \frac{1}{2}\tilde{E}_{11}-\frac{1}{2}\tilde{F}_{11} & \frac{1}{2}\tilde{E}_{21}-\frac{1}{2}\tilde{F}_{21} & \Lambda_1+\frac{1}{2}\tilde{E}_{11}+\frac{1}{2}\tilde{F}_{11} & \frac{1}{2}\tilde{E}_{12}+\frac{1}{2}\tilde{F}_{12} \\ \frac{1}{2}\tilde{E}_{21}-\frac{1}{2}\tilde{F}_{21} & \frac{1}{2}\tilde{E}_{22}-\frac{1}{2}\tilde{F}_{22} & \frac{1}{2}\tilde{E}_{21}+\frac{1}{2}\tilde{F}_{21} & \Lambda_2+\frac{1}{2}\tilde{E}_{22}+\frac{1}{2}\tilde{F}_{22} \end{bmatrix}$$

$$\hat{B}=Z^{\mathrm{T}}BZ=\begin{bmatrix} I_{n_1} & 0 & 0 & 0 \\ 0 & I_{n_2} & 0 & 0 \\ 0 & 0 & -I_{n_1} & 0 \\ 0 & 0 & 0 & -I_{n_2} \end{bmatrix}.$$

In such a case, the generalized egienvalue problem $\hat{A}-\lambda\hat{B}$, $\tilde{A}-\lambda B$ and $\tilde{H}$ have the same eigenvalues. The matrix $\tilde{A}$ is positive definite; so are $\hat{A}$ and its leading $n\times n$ principle submatrix

$$\hat{A}^{(a)}=\begin{bmatrix} \Lambda_1+\frac{1}{2}\tilde{E}_{11}+\frac{1}{2}\tilde{F}_{11} & \frac{1}{2}\tilde{E}_{12}+\frac{1}{2}\tilde{F}_{12} \\ \frac{1}{2}\tilde{E}_{21}+\frac{1}{2}\tilde{F}_{21} & \Lambda_2+\frac{1}{2}\tilde{E}_{22}+\frac{1}{2}\tilde{F}_{22} \end{bmatrix}.$$

Denote the eigenvalues of $\hat{A}^{(a)}$ by

$\lambda_1^{(a)}\le\lambda_2^{(a)}\le\ldots\le\lambda_n^{(a)}$.

We first consider to estimate the difference between the eigenvalues of H_1 and some n_1 eigenvalues of $\hat{A}^{(a)}$. This can be done by two steps. First, bound the difference between the eigenvalues of $\Lambda_1+\frac{1}{2}\tilde{E}_{11}+\frac{1}{2}\tilde{F}_{11}$ and some n_1 eigenvalues of $\hat{A}^{(a)}$. Then, bound the difference between the eigenvalues of $\Lambda_1+\frac{1}{2}\tilde{E}_{11}+\frac{1}{2}\tilde{F}_{11}$ and those of H_1. By Lemma 2.2 (a) and Lemma 2.2 (b), there are n_1 eigenvalues $\lambda_{t_1}^{(a)}\le\ldots\le\lambda_{t_{n_1}}^{(a)}$ of $\hat{A}^{(a)}$ such that

$$\sqrt{\sum_{i=1}^{n_1}|\theta_i-\lambda_{t_i}^{(a)}|^2}\le\frac{1}{2}\left(\|\tilde{E}_{11}+\tilde{F}_{11}\|_F+\|\tilde{E}_{21}+\tilde{F}_{21}\|_F\right). \qquad (18)$$

Let

$$\bar{A}=\begin{bmatrix} \Lambda_1+\frac{1}{2}\tilde{E}_{11}+\frac{1}{2}\tilde{F}_{11} & \frac{1}{2}\tilde{E}_{12}+\frac{1}{2}\tilde{F}_{12} & & \\ \frac{1}{2}\tilde{E}_{21}+\frac{1}{2}\tilde{F}_{21} & \Lambda_2+\frac{1}{2}\tilde{E}_{22}+\frac{1}{2}\tilde{F}_{22} & & \\ & & \Lambda_1+\frac{1}{2}\tilde{E}_{11}+\frac{1}{2}\tilde{F}_{11} & \frac{1}{2}\tilde{E}_{12}+\frac{1}{2}\tilde{F}_{12} \\ & & \frac{1}{2}\tilde{E}_{21}+\frac{1}{2}\tilde{F}_{21} & \Lambda_2+\frac{1}{2}\tilde{E}_{22}+\frac{1}{2}\tilde{F}_{22} \end{bmatrix}.$$

By Lemma 2.3, $\hat{A}-\lambda\hat{B}$ and $\bar{A}-\lambda\hat{B}$ admit the follow eigen-decomposition

$$W^T\hat{A}W=\begin{bmatrix} \tilde{\Lambda} & \\ & \tilde{\Lambda} \end{bmatrix},\quad W^T\hat{B}W=\begin{bmatrix} -I_n & \\ & I_n \end{bmatrix},$$

$$\tilde{W}^T\bar{A}\tilde{W}=\begin{bmatrix} \bar{\Lambda} & \\ & \bar{\Lambda} \end{bmatrix},\quad \tilde{W}^T\hat{B}\tilde{W}=\begin{bmatrix} -I_n & \\ & I_n \end{bmatrix}.$$

where $\tilde{\Lambda}=\mathrm{diag}(\tilde{\lambda}_1,\ldots,\tilde{\lambda}_n)$ and $\bar{\Lambda}=\mathrm{diag}(\tilde{\lambda}_1^a,\ldots,\tilde{\lambda}_n^{(a)})$

Since $\tilde{A}$ and $\bar{A}$ are all positive definite, it is followed by Lemma 2.5 that

$$\|W\|_2\le\sqrt{\tilde{\lambda}_n\|\hat{A}^{-1}\|_2}=\sqrt{\tilde{\lambda}_n\|\tilde{A}^{-1}\|_2}.$$

Notice that

$$\|\tilde{A}^{-1}\|_2=\max\{\|(\Lambda+\tilde{E})^{-1}\|_2,\|(\Lambda+\tilde{F})^{-1}\|_2\}.$$

Since $\|\Lambda^{-1/2}\tilde{E}\Lambda^{-1/2}\|_2=\|\Lambda^{-1/2}\Psi^TE\Psi\Lambda^{-1/2}\|_2\le\|E\|_2\|\Psi\Lambda^{-1}\Psi^T\|_2=\|E\|_2\|K^{-1}\|_2<1$, we have

$$\|(\Lambda+\tilde{E})^{-1}\|_2=\left\|\left[\Lambda^{1/2}(I+\Lambda^{-1/2}\tilde{E}\Lambda^{-1/2})\Lambda^{1/2}\right]^{-1}\right\|_2$$
$$=\left\|\Lambda^{-1/2}(I+\Lambda^{-1/2}\tilde{E}\Lambda^{-1/2})^{-1}\Lambda^{-1/2}\right\|_2$$
$$\le\frac{1}{\lambda_1}\times\|(I+\Lambda^{-1/2}\tilde{E}\Lambda^{-1/2})^{-1}\|_2$$
$$\le\frac{1}{\lambda_1}\times\frac{1}{1-\|\Lambda^{-1/2}\tilde{E}\Lambda^{-1/2}\|_2}$$

$$\le \frac{1}{\lambda_1} \times \frac{1}{1 - \|\Lambda^{-1/2}\tilde{E}\Lambda^{-1/2}\|_2}$$

$$\le \frac{1}{\lambda_1 - \|\tilde{E}\|_2}.$$

and $\|(\Lambda + \tilde{F})^{-1}\|_2 \le \frac{1}{\lambda_1 - \|\tilde{F}\|_2}$.

Let $\tau = \max\{\|\tilde{E}\|_2, \|\tilde{F}\|_2\}$, it is followed that

$$\|W\|_2 \le \sqrt{\tilde{\lambda}_n \|\tilde{A}^{-1}\|_2} \le \sqrt{\frac{\tilde{\lambda}_n}{\lambda_1 - \tau}}.$$

Similarly,

$$\|\tilde{W}\|_2 \le \sqrt{\lambda_n^{(a)} \|\bar{A}^{-1}\|_2} = \sqrt{\frac{\lambda_n^{(a)}}{\lambda_1^{(a)}}} \le \sqrt{\frac{\lambda_n + \tau}{\lambda_1^{(a)}}} \le \sqrt{\frac{\lambda_n + \tau}{\tilde{\lambda}_1}}.$$

The last inequality holds because of (15). By using Lemma 2.4, we have

$$\sqrt{\sum_{i=1}^{n_1} |\lambda_{t_i}^{(a)} - \tilde{\lambda}_{t_i}|^2} \le \sqrt{\sum_{i=1}^{n} |\lambda_i^{(a)} - \tilde{\lambda}_i|^2}$$

$$\le \frac{1}{\sqrt{2}} \|W\|_2 \|\tilde{W}\|_2 \|\tilde{A} - \bar{A}\|_F$$

$$\le \frac{1}{2\sqrt{2}} \sqrt{\frac{\tilde{\lambda}_n(\lambda_n + \tau)}{\tilde{\lambda}_1(\lambda_1 - \tau)}} \left\|\tilde{E} - \tilde{F}\right\|_F. \quad (19)$$

Together (18) and (19), we have

$$\sqrt{\sum_{i=1}^{n_1} |\theta_i - \tilde{\lambda}_{t_i}|^2} \le \sqrt{\sum_{i=1}^{n_1} |\theta_i - \lambda_{t_i}^{(a)}|^2} + \sqrt{\sum_{i=1}^{n_1} |\lambda_{t_i}^{(a)} - \tilde{\lambda}_{t_i}|^2}$$

$$\le \frac{1}{2}\left(\|\tilde{E}_{11} + \tilde{F}_{11}\|_F + \|\tilde{E}_{21} + \tilde{F}_{21}\|_F + \sqrt{\frac{\tilde{\lambda}_n(\lambda_n + \tau)}{2\tilde{\lambda}_1(\lambda_1 - \tau)}} \left\|\tilde{E} - \tilde{F}\right\|_F \right),$$

as expected.

4. Numerical example

We test our results in Theorems 3.1 on the following parameterized LREP

$$\tilde{H}(\alpha)z = \begin{bmatrix} 0 & K + \alpha E \\ M + \alpha F & 0 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} = \lambda \begin{bmatrix} y \\ x \end{bmatrix} = \lambda z,$$

where the parameter α varies from 0 to 1 while $K + \alpha E$ and $M + \alpha F$ remain positive definite. Denote the eigenvalues of $\tilde{H}(\alpha)$ by

$$-\tilde{\lambda}_n(\alpha) \le \ldots \le -\tilde{\lambda}_1(\alpha) < \tilde{\lambda}_1(\alpha) \le \ldots \le \tilde{\lambda}_n(\alpha).$$

In particular, $\tilde{\lambda}_i(\alpha) = \lambda_i$ for $\alpha = 0$.

We construct a linear response eigenvalue problem using the eigenvalues $-\lambda_n \le \ldots \le -\lambda_1 < \lambda_1 \le \ldots \le \lambda_n$ from the LREP for the sodium dimer Na_2 [9] with $n = 1862$. Let

$$\Lambda_1 = \operatorname{diag}(\lambda_1, \ldots, \lambda_k), \qquad \Lambda_2 = \operatorname{diag}(\lambda_{k+1}, \ldots, \lambda_n),$$

and Q_1, Q_2 be the orthogonal matrices obtained by $\operatorname{qr}(\operatorname{randn}(k))$ and $\operatorname{qr}(\operatorname{randn}(n-k))$ within MATLAB, respectively. Finally, we make up an LREP with

$$K = \begin{bmatrix} K_{11} & \\ & K_{22} \end{bmatrix}, \quad M = \begin{bmatrix} M_{11} & \\ & M_{22} \end{bmatrix},$$

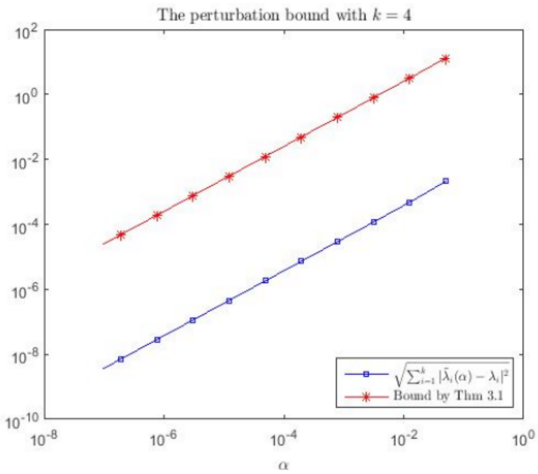
where

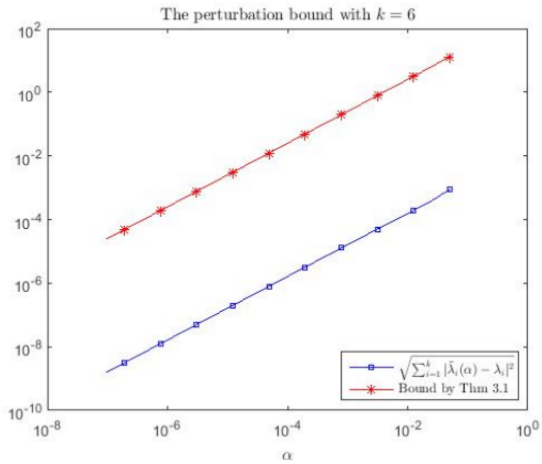
$$K_{11} = M_{11} = Q_1^T \Lambda_1 Q_1 \text{ and } K_{22} = M_{22} = Q_2^T \Lambda_2 Q_2.$$

The symmetric perturbation matrices

$$E = \begin{matrix} & k & n-k \\ k & E_{11} & E_{12} \\ n-k & E_{21} & E_{22} \end{matrix}, \qquad F = \begin{matrix} & k & n-k \\ k & F_{11} & F_{12} \\ n-k & F_{21} & F_{22} \end{matrix},$$

are also generated by the MATLAB function randn. We compute $\sqrt{\sum_{i=1}^{k} |\tilde{\lambda}(\alpha) - \lambda_i|^2}$ for k=4, 6, 8, 10 and their associated upper bounds from Theorem 3.1, and show the log-log plots in Figure 1. By Figure 1, it is clear that the bound by Theorem 3.1 is sharp in this example.





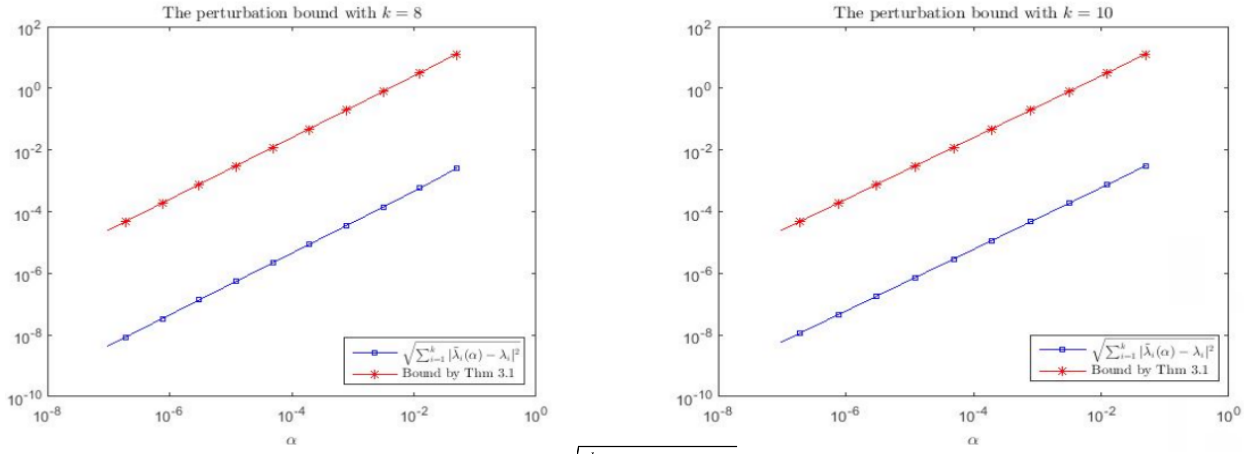


Figure 1. The perturbation bounds of $\sqrt{\sum_{i=1}^{k}(\tilde{\lambda}(\alpha)-\lambda_i)^2}$ from Theorem 3.1 with k =4, 6, 8, 10

5. Conclusions

In this paper, we focused on perturbation bounds for the partitioned LREP for H as in (1) perturbed to $\tilde{H}$ as in (7). The bound for the differences between the eigenvalues of H_1 as in (6) and some of those of $\tilde{H}$ are obtained. The main results are summarized in Theorems 3.1. The bound in Theorem 3.1 is referred to the Frobenius norm of the perturbation matrices E and F. It looks very sharp in the presented numerical examples. While we focused on real symmetric K and M so far, the development can be made to work for Hermitian K and M by simple modifications: replacing all R by C (the set of complex numbers) and each matrix/vector transpose by complex conjugate and transpose.

Acknowledgements

Research by Zhongming Teng was supported in part by Natural Science Foundation of Fujian province No. 2015J01580. Jinfu Liu research was supported in part by Natural Science Foundation of Fujian province No. 2015Y0042.

References

1. P. Ring, Z.-Y. Ma, N. Van Giai, D. Vretenar, A. Wandelt, and L.-G. Gao (2001) The time-dependent relativistic mean-field theory and the random phase approximation. *Nuclear Physics A*, p.p.249-268.
2. D. Rocca (2007) Time-Dependent Density Functional Perturbation Theory: New algorithms with Applications to Molecular Spectra. *PhD thesis, The International School for Advanced Studies*, Trieste, Italy.
3. R. E. Stratmann, G. E. Scuseria, and M. J. Frisch (1998) An efficient implementation of time-dependent density-functional theory for the calculation of excitation of large molecules. *The Journal of chemical physics,* 109, p.p.8218-8824.
4. E. V. Tsiper (2001) A classical mechanics technique for quantum linear response. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 34(12), p.p.401-407.
5. R. Bhatia (1996) *Matrix Analysis.* Graduate Texts in Mathematics. Springer, New York.
6. B. N. Parlett (1998) *The Symmetric Eigenvalue Problem.* SIAM, Philadelphia.
7. G. W. Stewart and J.-G. Sun (1990) *Matrix Perturbation Theory*. Academic Press, Boston.
8. Z. Bai and R.-C. Li (2012) Minimization principle for linear response eigenvalue problem I: Theory. *SIAM Journal on Matrix Analysis and Applications*, 33(4), p.p.1075-1100.
9. Z. Bai and R.-C. Li (2013) Minimization principle for linear response eigenvalue problem, {II}: Computation. *SIAM Journal on Matrix Analysis and Applications*, 34(2), p.p.392-416.
10. L.-H. Zhang, W.-W. Lin, and R.-C. Li (2014) Backward perturbation analysis and residual-based error bounds for the linear response eigenvalue problem. *BIT Numerical Mathematics*, p.p.1-28.
11. L.-H. Zhang, J. Xue, and R.-C. Li (2014) Rayleigh-Ritz approximation for the linear response eigenvalue problem. *SIAM Journal on Matrix Analysis and Applications*, 35(2), p.p.765-782.
12. Z. Teng, L. Z. Lu, and R.-C. Li (2015) Perturbation of partitioned linear response eigenvalue problems. *Electronic Transactions on Numerical Analysis*. Accept.
13. D. Rocca, Z. Bai, R.-C. Li, and G. Galli (2012) A block variational procedure for the iterative diagonalization of non-Hermitian random-phase approximation matrices. *The Journal of chemical physics*, 136, 034111.
14. Z. Teng and R.-C. Li (2013) Convergence ana-

lysis of Lanczos-type methods for the linear response eigenvalue problem. *Journal of Computational and Applied Mathematics*, 247, p.p.17-33.
15. E. V. Tsiper (1999) Variational procedure and generalized Lanczos recursion for small-amplitude classical oscillations. *JETP Letter*, 70(11), p.p.751-755.
16. Z. Teng, Y. Zhou, and R.-C. Li (2013) A block Chebyshev-Davidson method for linear response eigenvalue problems. *Technical Report 2013-11, Department of Mathematics, University of Texas at Arlington*. Available at http://www.uta.edu/math/preprint/, submitted.
17. W. Kahan (1967) Inclusion theorems for clusters of eigenvalues of Hermitian matrices. *Technical report, Computer Science Department, University of Toronto*.
18. D. C. Dzeng and W. W. Lin (1991) Homotopy continuation method for the numerical solutions of generalised symmetric eigenvalue problems. *The Journal of the Australian Mathematical Society. Series B.* Applied Mathematics, 32(4), p.p.437-456.
19. J. Kovač-Striko , K. Veselić (1995) Trace minimization and definiteness of symmetric pencils. *Linear Algebra and its Applications*, 216, p.p.139-158.
20. X. Liang, R.-C. Li, and Z. Bai (2013) Trace minimization principles for positive semi-definite pencils. *Linear Algebra and its Applications*, 438, p.p.3085-3106,.
21. X. Liang and R.-C. Li. (2015) The hyperbolic quadratic eigenvalue problem. *Forum of Mathematics, Sigma*, p.p.93-93.

Semantic Related Feature Analysis and Dynamic Evolution Based on Topic Temporal Chains under the Social Network

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