Electronic Transactions on Numerical Analysis.
Volume 44, pp. 624–638, 2015.
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ISSN 1068–9613.

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PERTURBATION OF PARTITIONED LINEAR RESPONSE EIGENVALUE PROBLEMS*

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Abstract. This paper is concerned with bounds for the linear response eigenvalue problem for $H = \begin{bmatrix} 0 & K \\ M & 0 \end{bmatrix}$, where K and M admit a 2×2 block partitioning. Bounds on how the changes of its eigenvalues are obtained when K and M are perturbed. They are of linear order with respect to the diagonal block perturbations and of quadratic order with respect to the off-diagonal block perturbations in K and M. The result is helpful in understanding how the Ritz values move towards eigenvalues in some efficient numerical algorithms for the linear response eigenvalue problem. Numerical experiments are presented to support the analysis.

Key words. linear response eigenvalue problem, random phase approximation, perturbation, quadratic perturbation bound

AMS subject classifications. 15A42, 65F15

1. Introduction.

Linear response perturbation analysis of time-dependent density functional theory in computational quantum chemistry and physics is commonly used to analyze the electronic excitation spectrum of a quantum many-fermion system [12, 13, 16, 20]. From the analysis arises the following eigenvalue problem, known as the linear response eigenvalue problem (LREP) (also known as the random phase approximation eigenvalue problem),

$$Hz = \begin{bmatrix} 0 & K \\ M & 0 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} = \lambda \begin{bmatrix} y \\ x \end{bmatrix} = \lambda z, \tag{1.1}$$

where K and M are $n \times n$ real symmetric positive definite matrices.

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 [3, 11, 15]. In fact, H is a special Hamiltonian matrix whose eigenvalues are real and in pairs $\{\lambda, -\lambda\}$. Denote by $\pm\lambda_i$ the eigenvalues of H and order them as

$$-\lambda_n \le \cdots \le -\lambda_1 < \lambda_1 \le \cdots \le \lambda_n. \tag{1.2}$$

In particular, $\lambda_1 > 0$ since both K and M are positive definite. In practice, the first k smallest positive eigenvalues $\lambda_1 \le \cdots \le \lambda_k$ are of interest. Recently, Bai and Li [1, 2] have successfully obtained Ky Fan-type trace min principle and Cauchy-type interlacing inequalities, among others. In this paper, we will continue the effort by extending the quadratic residual bounds, such as the ones in [7, 10] for the symmetric eigenvalue problem, to LREP.

In this paper, we are concerned with perturbations of an LREP (1.1) in which K and M

*Received July 13, 2015. Accepted September 17, 2015. Published online on December 3, 2015. Recommended by Wen-Wei Lin. The work of the first author is supported in part by Natural Science Foundation of Fujian province No. 2015J01580 and No. 2013J05005. The work of the second author is supported in part by National Natural Science Foundation of China grant 11261012 and 11428104. The work of the third author is supported in part by NSF grants DMS-1115834, DMS-1317330, CCF-1527091, and NSFC grant 11428104.

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are already block diagonal:

$$K = \begin{array}{cc} & \begin{array}{cc} n_1 & n_2 \end{array} \\ \begin{array}{c} n_1 \\ n_2 \end{array} & \begin{bmatrix} K_{11} & \\ & K_{22} \end{bmatrix} \end{array}, \qquad M = \begin{array}{cc} & \begin{array}{cc} n_1 & n_2 \end{array} \\ \begin{array}{c} n_1 \\ n_2 \end{array} & \begin{bmatrix} M_{11} & \\ & M_{22} \end{bmatrix} \end{array}, \tag{1.3}$$

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

$$H = \begin{bmatrix} 0 & 0 & K_{11} & 0 \\ 0 & 0 & 0 & K_{22} \\ M_{11} & 0 & 0 & 0 \\ 0 & M_{22} & 0 & 0 \end{bmatrix}. \tag{1.4}$$

When K and M are perturbed to

$$\widetilde{K} = K + E = \begin{bmatrix} K_{11} + E_{11} & E_{12} \\ E_{21} & K_{22} + E_{22} \end{bmatrix}, \widetilde{M} = M + F = \begin{bmatrix} M_{11} + F_{11} & F_{12} \\ F_{21} & M_{22} + F_{22} \end{bmatrix}, \tag{1.5}$$

by perturbations E and F which are assumed symmetric, we are interested in bounding how much the eigenvalues of H change. Let

$$H_1 = \begin{bmatrix} 0 & K_{11} \\ M_{11} & 0 \end{bmatrix}, \quad H_2 = \begin{bmatrix} 0 & K_{22} \\ M_{22} & 0 \end{bmatrix}. \tag{1.6}$$

Two kinds of bounds will be established in this paper:

- Bounds on the difference between the eigenvalues of H and those of

$$\widetilde{H} = \begin{bmatrix} 0 & 0 & K_{11} + E_{11} & E_{12} \\ 0 & 0 & E_{21} & K_{22} + E_{22} \\ M_{11} + F_{11} & F_{12} & 0 & 0 \\ F_{21} & M_{22} + F_{22} & 0 & 0 \end{bmatrix}. \tag{1.7}$$

  Assume that $\widetilde{H}$ is also an LREP, i.e, $\widetilde{K}$ and $\widetilde{M}$ are also symmetric positive definite. This assumption holds if E and F are sufficiently tiny in norm.
- Bounds on the difference between the eigenvalues of H_1 and some n_1 eigenvalues of $\widetilde{H}$.

There are two immediate applicable situations. The first one arises from using algorithms that try to reduce both K and M to the diagonal form. In running such algorithms, K and M are gradually turned into block diagonal, i.e., for some $i \neq j$, $E_{ii} = F_{ii} = 0$ $(i = 1, 2)$ and E_{ij} and F_{ij} have tiny magnitude. When E_{ij} and F_{ij} are deemed sufficiently tiny, it is natural to regard them simply as 0. Our results can be used to show what the effect of doing so is.

The other situation is when one uses some subspace projection type methods for large scale LREP. Recently, there are several rather efficient algorithms for LREP, such as the locally optimal block preconditioned 4-D conjugate gradient method (LOBP4DCG) [2, 14], the generalized Lanczos method [17, 19], and the block Chebyshev-Davidson method [18]. These algorithms are all based on the pair of deflating subspaces which is a generalization of the concept of the invariant subspace in the standard eigenvalue problem. A pair of subspaces $\{\mathcal{U}, \mathcal{V}\}$ are called a *pair of deflating subspaces* if they satisfy

$$K\mathcal{U} \subset \mathcal{V} \quad \text{and} \quad M\mathcal{V} \subset \mathcal{U}.$$

Each of these algorithms hopefully generates an approximate deflating subspace pair $\{\widetilde{\mathcal{U}}, \widetilde{\mathcal{V}}\}$. Projecting LREP by the approximate deflating subspace pair $\{\widetilde{\mathcal{U}}, \widetilde{\mathcal{V}}\}$ leads to $\widetilde{H}$ in (1.7) with

$E_{ii} = F_{ii} = 0$ ($i = 1, 2$) and usually unknown K_{22} and M_{22}. In such a case, our main results will help us to understand how well the eigenvalues of H_1 approximate some of those of $\widetilde{H}$.

The rest of this paper is organized as follows. In Section 2, we first collect some known results for the standard symmetric eigenvalue problem and LREP. These results are essential to the later analysis in this paper. Analogous to the estimate results of perturbed Hermitian eigenvalue problems [7] and Hermitian definite generalized eigenvalue problems [8], we obtain our main results in Section 3. Some numerical examples are presented in Section 4 to support our analysis. Concluding remarks are given in Section 5.

The following is a list of notation used in this paper: $\mathbb{R}^{m\times n}$ is the set of all $m \times n$ real matrices, $\mathbb{R}^n = \mathbb{R}^{n\times 1}$, $\mathbb{R} = \mathbb{R}^1$, and I_n is the $n \times n$ identity matrix or simply I if its dimension is clear from the context. The superscript "${}^{\mathrm{T}}$" represents the transpose. $\|\cdot\|_2$ denotes the ℓ_2-norm of a vector or the spectral norm of a matrix. For any Hermitian matrix $X \in \mathbb{R}^{n\times n}$, we will use the integer triplet

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

to represent 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, both $\operatorname{diag}(X_1, \ldots, X_k)$ and $X_1 \oplus \cdots \oplus X_k$ denote the same block diagonal matrix.

2. Preliminaries. In the rest of this paper, unless otherwise explicitly stated, we always assume that K and M are symmetric positive definite. The LREP (1.1) can be turned into the following generalized eigenvalue problem by permuting the first and second block rows to get

$$\begin{bmatrix} M & 0 \\ 0 & K \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} = \lambda \begin{bmatrix} 0 & I_n \\ I_n & 0 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix}. \tag{2.1}$$

We collect several properties of LREP in Theorems 2.1–2.2; see [1] for more detail.

THEOREM 2.1. *There exist nonsingular X, $Y \in \mathbb{R}^{n\times n}$, such that*

$$K = Y\varLambda^2 Y^{\mathrm{T}}, \quad M = XX^{\mathrm{T}}, \quad X^{\mathrm{T}}Y = I_n, \tag{2.2}$$

where $\varLambda = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ and $0 < \lambda_1 \le \cdots \le \lambda_n$. As a consequence,

$$KX = Y\varLambda^2, \quad MY = X, \tag{2.3}$$

or equivalently

$$H \begin{bmatrix} Y & \\ & X \end{bmatrix} = \begin{bmatrix} Y & \\ & X \end{bmatrix} \begin{bmatrix} & \varLambda^2 \\ I_n & \end{bmatrix}. \tag{2.4}$$

THEOREM 2.2. *There exist nonsingular $\varPhi$, $\varPsi \in \mathbb{R}^{n\times n}$, such that*

$$\varPsi^{\mathrm{T}} K \varPsi = \varLambda, \qquad \varPhi^{\mathrm{T}} M \varPhi = \varLambda, \qquad \varPsi = \varPhi^{-\mathrm{T}}, \tag{2.5}$$

where $\varLambda$ is the same as in Theorem 2.1. Moreover,

$$\|\varPsi\|_2^2 \le \frac{\|M\|_2}{\lambda_1} \quad \text{and} \quad \|\varPhi\|_2^2 \le \frac{\|K\|_2}{\lambda_1}. \tag{2.6}$$

Proof. From Theorem 2.1, taking $\varPsi = X\varLambda^{-1/2}$ and $\varPhi = Y\varLambda^{1/2}$, we have (2.5). We also have (2.6) from

$$\|K\|_2 = \|\varPhi^{\mathrm{T}}\varLambda\varPhi\|_2 \ge \lambda_1\|\varPhi\|_2^2,$$
$$\|M\|_2 = \|\varPsi^{\mathrm{T}}\varLambda\varPsi\|_2 \ge \lambda_1\|\varPsi\|_2^2. \qquad \square$$

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Later in this paper, we also need the following known results from the standard symmetric eigenvalue problem.

LEMMA 2.3. *Let A and $\tilde{A}$ be two $n \times n$ symmetric matrices. Denote their eigenvalues in the ascending order by λ_i and $\tilde{\lambda}_i$, for $1 \le i \le n$, respectively. Then*

(a) (See [15]) $|\tilde{\lambda}_i - \lambda_i| \le \|\tilde{A} - A\|_2$, *for* $1 \le i \le n$.

(b) (See [7]) *Suppose that*

$$A = \begin{array}{c c} & \begin{array}{cc} n_1 & n_2 \end{array} \\ \begin{array}{c} n_1 \\ n_2 \end{array} & \begin{bmatrix} A_{11} & \\ & A_{22} \end{bmatrix} \end{array}, \qquad \widetilde{A} = \begin{bmatrix} A_{11} & E^{\mathrm{T}} \\ E & A_{22} \end{bmatrix}. \tag{2.7}$$

Then for $1 \le i \le n$,

$$|\tilde{\lambda}_i - \lambda_i| \le \frac{2\|E\|_2^2}{\eta_i + \sqrt{\eta_i^2 + 4\|E\|_2^2}} \le \frac{2\|E\|_2^2}{\eta + \sqrt{\eta^2 + 4\|E\|_2^2}},$$

where

$$\eta_i = \begin{cases} \min\limits_{\mu_2 \in \lambda(A_{22})} |\lambda_i - \mu_2|, & \text{if } \lambda_i \in \lambda(A_{11}), \\ \min\limits_{\mu_1 \in \lambda(A_{11})} |\lambda_i - \mu_1|, & \text{if } \lambda_i \in \lambda(A_{22}), \end{cases}$$

$$\eta = \min_{1 \le i \le n} \eta_i = \min_{\mu_1 \in \lambda(A_{11}),\, \mu_2 \in \lambda(A_{22})} |\mu_1 - \mu_2|.$$

(c) (See [5]) *Denote by θ_i, for $1 \le i \le n_1$, the eigenvalues of A_{11} in (2.7) in the ascending order. Then there exist n_1 eigenvalues $\widetilde{\lambda}_{t_1} \le \cdots \le \widetilde{\lambda}_{t_{n_1}}$ of $\widetilde{A}$, such that*

$$|\theta_i - \widetilde{\lambda}_{t_i}| \le \|E\|_2, \quad \text{for } 1 \le i \le n_1.$$

We also need the following definition of positive (semi-)definite matrix pencil.

DEFINITION 2.4. (See [9]) *$A - \lambda B$ is a* symmetric matrix pencil *of order n if both A, $B \in \mathbb{R}^{n\times n}$ are symmetric. $A - \lambda B$ is a* positive (semi-)definite matrix pencil *of order n if it is a symmetric matrix pencil of order n and if there exists $\lambda_0 \in \mathbb{R}$ such that $A - \lambda_0 B$ is positive (semi-)definite.*

It can be proved that any positive semidefinite matrix pencil $A - \lambda B$ with nonsingular B has only real eigenvalues and $i_-(B)$ of them are no larger than λ_0 and the rest $i_+(B)$ of them are no less than λ_0 [4, 6, 9]. We implicitly use this fact in the following lemmas in ordering the eigenvalues of involved positive (semi-)definite matrix pencils.

LEMMA 2.5 ([6, Theorem 2.1]). *Let A and $J = \mathrm{diag}(\pm 1) \in \mathbb{R}^{n\times n}$ be a positive semidefinite pencil partitioned as*

$$A = \begin{array}{c c} & \begin{array}{cc} k & \ell \end{array} \\ \begin{array}{c} k \\ \ell \end{array} & \begin{bmatrix} A_1 & E^{\mathrm{T}} \\ E & A_2 \end{bmatrix} \end{array}, \quad J = \begin{array}{c c} & \begin{array}{cc} k & \ell \end{array} \\ \begin{array}{c} k \\ \ell \end{array} & \begin{bmatrix} J_1 & \\ & J_2 \end{bmatrix} \end{array},$$

and let

$$\begin{aligned} n_+ &= i_+(J), & n_- &= i_-(J), & n_+ + n_- &= n, \\ k_+ &= i_+(J_1), & k_- &= i_-(J_1), & k_+ + k_- &= k, \\ \ell_+ &= i_+(J_2), & \ell_- &= i_-(J_2), & \ell_+ + \ell_- &= \ell. \end{aligned}$$

Denote by

$$\lambda_{n_-}^- \le \cdots \le \lambda_1^- \le \lambda_1^+ \cdots \le \lambda_{n_+}^+ ,$$
$$\alpha_{k_-}^- \le \cdots \le \alpha_1^- \le \alpha_1^+ \cdots \le \alpha_{k_+}^+ ,$$
$$\beta_{\ell_-}^- \le \cdots \le \beta_1^- \le \beta_1^+ \cdots \le \beta_{\ell_+}^+ ,$$

the eigenvalues of the pencils $A - \lambda J$, $A_1 - \lambda J_1$ and $A_2 - \lambda J_2$, respectively. Then

$$\lambda_i^+ \le \alpha_i^+ \le \lambda_{i+n-k}^+ , \quad i = 1, 2, \dots, k_+ ,$$
$$\lambda_{j+n-k}^- \le \alpha_j^- \le \lambda_j^- , \quad j = 1, 2, \dots, k_- ,$$

and

$$\lambda_i^+ \le \beta_i^+ \le \lambda_{i+n-\ell}^+ , \quad i = 1, 2, \dots, \ell_+ ,$$
$$\lambda_{j+n-\ell}^- \le \beta_j^- \le \lambda_j^- , \quad j = 1, 2, \dots, \ell_- ,$$

where $\lambda_t^+ = +\infty$ if $t > n_+$ and $\lambda_t^- = -\infty$ if $t > n_-$.

LEMMA 2.6. *Suppose $A - \lambda B$ is a positive definite matrix pencil of order n with nonsingular B and let $\lambda_0 \in \mathbb{R}$ such that $A - \lambda_0 B$ is positive definite. Denote the eigenvalues of $A - \lambda B$ by*

$$\lambda_{n_-}^- \le \cdots \le \lambda_1^- < \lambda_1^+ \le \cdots \le \lambda_{n_+}^+, \tag{2.8}$$

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

$$W^{\mathrm{T}} A W = \begin{bmatrix} -\Lambda_- & \\ & \Lambda_+ \end{bmatrix}, \quad W^{\mathrm{T}} B W = \begin{bmatrix} -I_{n_-} & \\ & I_{n_+} \end{bmatrix}, \tag{2.9}$$

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

Proof. The key is to prove the eigen-decomposition (2.9). This is a corollary of more general results [4, 6, 9]. In fact, the current case is much simpler; the matrices A and $A - \lambda_0 B$ are simultaneously congruent to diagonal matrices since $A - \lambda_0 B$ is positive definite, and then the eigen-decomposition can be constructed. We omit the detail here. ◻

LEMMA 2.7. *Let*

$$A = \begin{bmatrix} A_1 & E^{\mathrm{T}} \\ E & A_2 \end{bmatrix}, \quad B = \begin{bmatrix} I_{n_+} & \\ & -I_{n_-} \end{bmatrix}, \tag{2.10}$$

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

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

where[1] *$\lambda_1^+ > 0$ and $\lambda_1^- < 0$, and the eigenvalues of A_1 and A_2 by*

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

[1] $A - \lambda B$ is a positive definite pencil with $\lambda_0 = 0$ in Definition 2.4. Thus we know it has n_- negative and n_+ positive eigenvalues.

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

$$-\beta_j \le \lambda_j^- < 0 < \lambda_i^+ \le \alpha_i, \tag{2.11}$$

and

$$|\alpha_i - \lambda_i^+| \le \frac{\|E\|_2^2}{\beta_1 + \lambda_i^+} \le \frac{\|E\|_2^2}{\lambda_i^+ - \lambda_1^-}, \tag{2.12a}$$

$$|(-\beta_j) - \lambda_j^-| \le \frac{\|E\|_2^2}{\alpha_1 - \lambda_j^-} \le \frac{\|E\|_2^2}{\lambda_1^+ - \lambda_j^-}. \tag{2.12b}$$

In particular, if $\lambda_i^+ - \lambda_1^- \ge 2\|E\|_2$ *and* $\lambda_1^+ - \lambda_j^- \ge 2\|E\|_2$*, then*[2]

$$|\alpha_i - \lambda_i^+| \le \frac{2\|E\|_2^2}{(\beta_1 + \alpha_i) + \sqrt{(\beta_1 + \alpha_i)^2 - 4\|E\|_2^2}} \tag{2.13a}$$

$$\le \frac{2\|E\|_2^2}{(\lambda_i^+ - \lambda_1^-) + \sqrt{(\lambda_i^+ - \lambda_1^-)^2 - 4\|E\|_2^2}}, \tag{2.13b}$$

$$|(-\beta_j) - \lambda_j^-| \le \frac{2\|E\|_2^2}{(\alpha_1 + \beta_j) + \sqrt{(\alpha_1 + \beta_j)^2 - 4\|E\|_2^2}} \tag{2.13c}$$

$$\le \frac{2\|E\|_2^2}{(\lambda_1^+ - \lambda_j^-) + \sqrt{(\lambda_1^+ - \lambda_j^-)^2 - 4\|E\|_2^2}}. \tag{2.13d}$$

Proof. We may suppose that $A_1 = \mathrm{diag}(\alpha_1, \ldots, \alpha_{n_+})$ and $A_2 = \mathrm{diag}(\beta_1, \ldots, \beta_{n_-})$. Otherwise, replace A by

$$(U_+ \oplus U_-)^{\mathrm{T}} A (U_+ \oplus U_-),$$

where $U_+^{\mathrm{T}} A_1 U_+$ and $U_-^{\mathrm{T}} A_2 U_-$ are in diagonal form with their diagonal entries arranged in ascending order and $U_\pm^{\mathrm{T}} U_\pm = I_{n_\pm}$. Doing so will keep the eigenvalues of $A - \lambda B$ unchanged since $B = (U_+ \oplus U_-)^{\mathrm{T}} B (U_+ \oplus U_-)$.

The inequalities in (2.11) are consequences of Lemma 2.5.

Let k be the multiplicity of λ_i^+ and assume that

$$\lambda_{i-k_1}^+ < \lambda_{i-k_1+1}^+ = \cdots = \lambda_i^+ = \cdots = \lambda_{i+k_2}^+ < \lambda_{i+k_2+1}^+,$$

where $k_1 + k_2 = k$. Let $X = \begin{bmatrix} I_{n_+} & 0 \\ -(A_2 + \lambda_i^+ I_{n_-})^{-1} E & I_{n_-} \end{bmatrix}$. It can be verified that

$$X^{\mathrm{T}}(A - \lambda_i^+ B) X = X^{\mathrm{T}} \begin{bmatrix} A_1 - \lambda_i^+ I_{n_+} & E^{\mathrm{T}} \\ E & A_2 + \lambda_i^+ I_{n_-} \end{bmatrix} X = \begin{bmatrix} M(\lambda_i^+) & 0 \\ 0 & A_2 + \lambda_i^+ I_{n_-} \end{bmatrix},$$

where $M(\lambda_i^+) = A_1 - \lambda_i^+ I_{n_+} - E^{\mathrm{T}} (A_2 + \lambda_i^+ I_{n_-})^{-1} E$. Since $X^{\mathrm{T}}(A - \lambda_i^+ B) X$ and $A - \lambda_i^+ B$ have the same inertia, by using Lemma 2.6 we conclude

$$\begin{aligned} i_+(X^{\mathrm{T}}(A - \lambda_i^+ B) X) &= 2n - i - k_2, \\ i_-(X^{\mathrm{T}}(A - \lambda_i^+ B) X) &= i - k_1, \\ i_0(X^{\mathrm{T}}(A - \lambda_i^+ B) X) &= k. \end{aligned}$$

[2] By (2.11), $\lambda_i^+ - \lambda_1^- \ge 2\|E\|_2$ and $\lambda_1^+ - \lambda_j^- \ge 2\|E\|_2$ imply that $\beta_1 + \alpha_i \ge 2\|E\|_2$ and $\alpha_1 + \beta_j \ge 2\|E\|_2$, respectively.

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Notice that the eigenvalues of $A_2 + \lambda_i^+ I_{n_-}$ are all positive. Thus, the inertia of $M(\lambda_i^+)$ is given by

$$i_0(M(\lambda_i^+)) = k, \quad i_-(M(\lambda_i^+)) = i - k_1, \quad i_+(M(\lambda_i^+)) = n_+ - i - k_2. \tag{2.14}$$

Denote by $\omega_1 \le \omega_2 \le \cdots \le \omega_{n_+}$ the eigenvalues of $M(\lambda_i^+)$. By (2.14), it is clear that

$$\omega_{i-k_1+1} = \cdots = \omega_i = \cdots = \omega_{i+k_2} = 0. \tag{2.15}$$

Notice that the eigenvalues of $A_1 - \lambda_i^+ I_{n_+}$ are

$$\alpha_1 - \lambda_i^+ \le \alpha_2 - \lambda_i^+ \le \cdots \le \alpha_i - \lambda_i^+ \le \alpha_{i+1} - \lambda_i^+ \le \cdots \le \alpha_{n_+} - \lambda_i^+.$$

Therefore, we have by (2.15) and Lemma 2.3 (a),

$$\begin{aligned} |\omega_i - (\alpha_i - \lambda_i^+)| = |\alpha_i - \lambda_i^+| &\le \|E(A_2 + \lambda_i^+ I_{n_-})^{-1} E^{\mathrm{T}}\|_2 \\ &\le \|E\|_2^2 \, \|(A_2 + \lambda_i^+ I_{n_-})^{-1}\|_2 \\ &\le \frac{\|E\|_2^2}{\beta_1 + \lambda_i^+} \, . \end{aligned}$$

This together with (2.11) yields

$$|\alpha_i - \lambda_i^+| \le \frac{\|E\|_2^2}{\lambda_i^+ - \lambda_1^-},$$

which gives (2.12a), and

$$|\alpha_i - \lambda_i^+| \le \frac{\|E\|_2^2}{\beta_1 + \alpha_i - |\alpha_i - \lambda_i^+|}.$$

Consequently, if $\lambda_i^+ - \lambda_1^- \ge 2\|E\|_2$, which implies $\beta_1 + \alpha_i \ge 2\|E\|_2$, then

$$\begin{aligned} |\alpha_i - \lambda_i^+| &\le \frac{2\|E\|_2^2}{(\beta_1 + \alpha_i) + \sqrt{(\beta_1 + \alpha_i)^2 - 4\|E\|_2^2}} \\ &\le \frac{2\|E\|_2^2}{(\lambda_i^+ - \lambda_1^-) + \sqrt{(\lambda_i^+ - \lambda_1^-)^2 - 4\|E\|_2^2}} \, , \end{aligned}$$

which are (2.13a) and (2.13b). Similarly, we can prove (2.12b), (2.13c), and (2.13d). ∎

3. Main Results.

Consider LREP (1.1) with (1.3). Denote by $\pm\widetilde{\lambda}_i$ the eigenvalues of $\widetilde{H}$ and order them, similarly to (1.2), as

$$-\widetilde{\lambda}_n \le \cdots \le -\widetilde{\lambda}_1 < \widetilde{\lambda}_1 \le \cdots \le \widetilde{\lambda}_n. \tag{3.1}$$

First we bound the difference between the eigenvalues of H and $\widetilde{H}$.

From Theorem 2.2, we know that for K_{ii} and M_{ii} in (1.3), there exist Ψ_i and Φ_i, such that

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

where Λ_1 and Λ_2 are diagonal matrices with the diagonal entries consisting of the positive eigenvalues of H. Also $\lambda(\Lambda_1) \cup \lambda(\Lambda_2) = \lambda(\Lambda)$, where Λ is defined in (2.2).

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Define, for $1 \le i \le n$,

$$\eta_i = \begin{cases} \min_{\mu_2 \in \lambda(\varLambda_2)} |\lambda_i - \mu_2|, & \text{if } \lambda_i \in \lambda(\varLambda_1), \\ \min_{\mu_1 \in \lambda(\varLambda_1)} |\lambda_i - \mu_1|, & \text{if } \lambda_i \in \lambda(\varLambda_2), \end{cases} \tag{3.2}$$

$$\eta = \min_{1 \le i \le n} \eta_i = \min_{\mu_i \in \lambda(\varLambda_1),\, \mu_j \in \lambda(\varLambda_2)} |\mu_i - \mu_j|. \tag{3.3}$$

The quantity η is the spectral gap between $\lambda(H_1)$ and $\lambda(H_2)$, where H_1 and H_2 are as given in (1.6). Set

$$P = \begin{bmatrix} \varPsi_1 & 0 & 0 & 0 \\ 0 & \varPsi_2 & 0 & 0 \\ 0 & 0 & \varPhi_1 & 0 \\ 0 & 0 & 0 & \varPhi_2 \end{bmatrix}, \qquad Q = \begin{bmatrix} \varPhi_1 & 0 & 0 & 0 \\ 0 & \varPhi_2 & 0 & 0 \\ 0 & 0 & \varPsi_1 & 0 \\ 0 & 0 & 0 & \varPsi_2 \end{bmatrix}.$$

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

$$P^{\mathrm{T}}HQ = \begin{bmatrix} 0 & 0 & \varLambda_1 & 0 \\ 0 & 0 & 0 & \varLambda_2 \\ \varLambda_1 & 0 & 0 & 0 \\ 0 & \varLambda_2 & 0 & 0 \end{bmatrix}, \tag{3.4}$$

$$\begin{aligned} P^{\mathrm{T}}\widetilde{H}Q &= \begin{bmatrix} 0 & 0 & \varLambda_1 + \widetilde{E}_{11} & \widetilde{E}_{12} \\ 0 & 0 & \widetilde{E}_{21} & \varLambda_2 + \widetilde{E}_{22} \\ \varLambda_1 + \widetilde{F}_{11} & \widetilde{F}_{12} & 0 & 0 \\ \widetilde{F}_{21} & \varLambda_2 + \widetilde{F}_{22} & 0 & 0 \end{bmatrix} \\ &= P^{\mathrm{T}}HQ + \begin{bmatrix} 0 & \widetilde{E} \\ \widetilde{F} & 0 \end{bmatrix}, \end{aligned} \tag{3.5}$$

where

$$\widetilde{E} \equiv \begin{bmatrix} \widetilde{E}_{11} & \widetilde{E}_{12} \\ \widetilde{E}_{21} & \widetilde{E}_{22} \end{bmatrix} = \begin{bmatrix} \varPsi_1^{\mathrm{T}} & 0 \\ 0 & \varPsi_2^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{bmatrix} \begin{bmatrix} \varPsi_1 & 0 \\ 0 & \varPsi_2 \end{bmatrix}, \tag{3.6a}$$

$$\widetilde{F} \equiv \begin{bmatrix} \widetilde{F}_{11} & \widetilde{F}_{12} \\ \widetilde{F}_{21} & \widetilde{F}_{22} \end{bmatrix} = \begin{bmatrix} \varPhi_1^{\mathrm{T}} & 0 \\ 0 & \varPhi_2^{\mathrm{T}} \end{bmatrix} \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix} \begin{bmatrix} \varPhi_1 & 0 \\ 0 & \varPhi_2 \end{bmatrix}. \tag{3.6b}$$

Using (2.6), we can bound $\widetilde{E}_{ij}$ and $\widetilde{F}_{ij}$ $(i, j = 1, 2)$ as follows

$$\|\widetilde{E}_{ij}\|_2 = \|\varPsi_i^{\mathrm{T}} E_{ij} \varPsi_j\|_2 \le \frac{\|M\|_2 \|E_{ij}\|_2}{\lambda_1}, \tag{3.7a}$$

$$\|\widetilde{F}_{ij}\|_2 = \|\varPhi_i^{\mathrm{T}} F_{ij} \varPhi_j\|_2 \le \frac{\|K\|_2 \|F_{ij}\|_2}{\lambda_1}, \tag{3.7b}$$

and similarly,

$$\|\widetilde{E}\|_2 \le \frac{\|M\|_2 \|E\|_2}{\lambda_1}, \quad \|\widetilde{F}\|_2 \le \frac{\|K\|_2 \|F\|_2}{\lambda_1}. \tag{3.8}$$

In the following theorem, we use the notation introduced so far in this section.

THEOREM 3.1. *Suppose that H in (1.4) is perturbed to $\widetilde{H}$ in (1.7), where K, M, and the corresponding perturbed matrices are all symmetric positive definite. Then, for all $1 \le i \le n$,*

$$|\widetilde{\lambda}_i - \lambda_i| \le \epsilon_1 + \epsilon_2 + \epsilon_3, \tag{3.9}$$

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where

$$\epsilon_1 = \frac{\|\widetilde{E}-\widetilde{F}\|_2^2}{4\,(\widetilde{\lambda}_1+\widetilde{\lambda}_i)}, \quad \epsilon_2 = \max_{j=1,2}\frac{1}{2}\|\widetilde{E}_{jj}+\widetilde{F}_{jj}\|_2,$$
$$\epsilon_3 = \frac{\|\widetilde{E}_{21}+\widetilde{F}_{21}\|_2^2}{2\,\eta_i + 2\sqrt{\eta_i^2+\|\widetilde{E}_{21}+\widetilde{F}_{21}\|_2^2}} \le \frac{\|\widetilde{E}_{21}+\widetilde{F}_{21}\|_2^2}{2\,\eta + 2\sqrt{\eta^2+\|\widetilde{E}_{21}+\widetilde{F}_{21}\|_2^2}}.$$

Proof. Using (2.1), (3.4) and (3.5), we can transform LREP for H in (1.4) and LREP for $\widetilde{H}$ in (1.7) equivalently to the generalized eigenvalue problems for $A-\lambda B$ and $\widetilde{A}-\lambda B$, respectively, where

$$A = \begin{bmatrix} \Lambda_1 & 0 & 0 & 0 \\ 0 & \Lambda_2 & 0 & 0 \\ 0 & 0 & \Lambda_1 & 0 \\ 0 & 0 & 0 & \Lambda_2 \end{bmatrix}, \quad B = \begin{bmatrix} 0 & 0 & I_{n_1} & 0 \\ 0 & 0 & 0 & I_{n_2} \\ I_{n_1} & 0 & 0 & 0 \\ 0 & I_{n_2} & 0 & 0 \end{bmatrix},$$
$$\widetilde{A} = \begin{bmatrix} \Lambda_1+\widetilde{E}_{11} & \widetilde{E}_{12} & 0 & 0 \\ \widetilde{E}_{21} & \Lambda_2+\widetilde{E}_{22} & 0 & 0 \\ 0 & 0 & \Lambda_1+\widetilde{F}_{11} & \widetilde{F}_{12} \\ 0 & 0 & \widetilde{F}_{21} & \Lambda_2+\widetilde{F}_{22} \end{bmatrix}.$$

Both

$$\begin{bmatrix} \Lambda_1+\widetilde{E}_{11} & \widetilde{E}_{12} \\ \widetilde{E}_{21} & \Lambda_2+\widetilde{E}_{22} \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} \Lambda_1+\widetilde{F}_{11} & \widetilde{F}_{12} \\ \widetilde{F}_{21} & \Lambda_2+\widetilde{F}_{22} \end{bmatrix}. \tag{3.10}$$

are positive definite because $\widetilde{K}$ and $\widetilde{M}$ in (1.5) are assumed positive definite. Let $Z = \frac{1}{\sqrt{2}}\begin{bmatrix} I_n & I_n \\ I_n & -I_n \end{bmatrix}$. We have

$$\widehat{A} = Z^{\mathrm{T}}\widetilde{A}Z$$
$$= \begin{bmatrix} \Lambda_1+\frac{1}{2}\widetilde{E}_{11}+\frac{1}{2}\widetilde{F}_{11} & \frac{1}{2}\widetilde{E}_{12}+\frac{1}{2}\widetilde{F}_{12} & \frac{1}{2}\widetilde{E}_{11}-\frac{1}{2}\widetilde{F}_{11} & \frac{1}{2}\widetilde{E}_{12}-\frac{1}{2}\widetilde{F}_{12} \\ \frac{1}{2}\widetilde{E}_{21}+\frac{1}{2}\widetilde{F}_{21} & \Lambda_2+\frac{1}{2}\widetilde{E}_{22}+\frac{1}{2}\widetilde{F}_{22} & \frac{1}{2}\widetilde{E}_{21}-\frac{1}{2}\widetilde{F}_{21} & \frac{1}{2}\widetilde{E}_{22}-\frac{1}{2}\widetilde{F}_{22} \\ \frac{1}{2}\widetilde{E}_{11}-\frac{1}{2}\widetilde{F}_{11} & \frac{1}{2}\widetilde{E}_{12}-\frac{1}{2}\widetilde{F}_{12} & \Lambda_1+\frac{1}{2}\widetilde{E}_{11}+\frac{1}{2}\widetilde{F}_{11} & \frac{1}{2}\widetilde{E}_{12}+\frac{1}{2}\widetilde{F}_{12} \\ \frac{1}{2}\widetilde{E}_{21}-\frac{1}{2}\widetilde{F}_{21} & \frac{1}{2}\widetilde{E}_{22}-\frac{1}{2}\widetilde{F}_{22} & \frac{1}{2}\widetilde{E}_{21}+\frac{1}{2}\widetilde{F}_{21} & \Lambda_2+\frac{1}{2}\widetilde{E}_{22}+\frac{1}{2}\widetilde{F}_{22} \end{bmatrix},$$
$$\widehat{B} = Z^{\mathrm{T}}BZ = \begin{bmatrix} I_{n_1} & 0 & 0 & 0 \\ 0 & I_{n_2} & 0 & 0 \\ 0 & 0 & -I_{n_1} & 0 \\ 0 & 0 & 0 & -I_{n_2} \end{bmatrix}.$$

The matrix $\widetilde{A}$ is positive definite; so are $\widehat{A}$ and its leading $n\times n$ principal submatrix

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

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Next, we consider the following four eigenvalue problems:

1. EIG(a): $\widehat{A} - \lambda\widehat{B}$ (which has the same eigenvalues as $\widetilde{A} - \lambda B$);
2. EIG(b): $\begin{bmatrix} \Lambda_1 + \frac{1}{2}\widetilde{E}_{11} + \frac{1}{2}\widetilde{F}_{11} & \frac{1}{2}\widetilde{E}_{12} + \frac{1}{2}\widetilde{F}_{12} \\ \frac{1}{2}\widetilde{E}_{21} + \frac{1}{2}\widetilde{F}_{21} & \Lambda_2 + \frac{1}{2}\widetilde{E}_{22} + \frac{1}{2}\widetilde{F}_{22} \end{bmatrix} - \lambda I_n$;
3. EIG(c): $\begin{bmatrix} \Lambda_1 & \frac{1}{2}\widetilde{E}_{12} + \frac{1}{2}\widetilde{F}_{12} \\ \frac{1}{2}\widetilde{E}_{21} + \frac{1}{2}\widetilde{F}_{21} & \Lambda_2 \end{bmatrix} - \lambda I_n$;
4. EIG(d): $\begin{bmatrix} \Lambda_1 & \\ & \Lambda_2 \end{bmatrix} - \lambda I_n$.

For x=b, c, and d, denote the eigenvalues of EIG(x) by $\lambda_i^{(\mathrm{x})}$ in the ascending order, i.e.,

$$\lambda_1^{(\mathrm{x})} \le \lambda_2^{(\mathrm{x})} \le \cdots \le \lambda_n^{(\mathrm{x})}.$$

For $\mathrm{EIG}(\mathrm{a})$, the eigenvalues are given by (3.1). Now, we can bound the eigenvalue differences between any two adjacent eigenvalue problems in the above list as follows:

$\mathrm{EIG}(\mathrm{a})$ and $\mathrm{EIG}(\mathrm{b})$: By Lemma 2.7,

$$|\widetilde{\lambda}_i - \lambda_i^{(\mathrm{b})}| \le \epsilon_1 = \frac{\|\widetilde{E} - \widetilde{F}\|_2^2}{4(\widetilde{\lambda}_1 + \widetilde{\lambda}_i)}.$$

$\mathrm{EIG}(\mathrm{b})$ and $\mathrm{EIG}(\mathrm{c})$: By Lemma 2.3 (a),

$$\begin{aligned} |\lambda_i^{(\mathrm{b})} - \lambda_i^{(\mathrm{c})}| \le \epsilon_2 &= \left\| \begin{bmatrix} \frac{1}{2}\widetilde{E}_{11} + \frac{1}{2}\widetilde{F}_{11} & 0 \\ 0 & \frac{1}{2}\widetilde{E}_{22} + \frac{1}{2}\widetilde{F}_{22} \end{bmatrix} \right\|_2 \\ &= \frac{1}{2} \max\left\{ \|\widetilde{E}_{11} + \widetilde{F}_{11}\|_2, \|\widetilde{E}_{22} + \widetilde{F}_{22}\|_2 \right\}. \end{aligned}$$

$\mathrm{EIG}(\mathrm{c})$ and $\mathrm{EIG}(\mathrm{d})$: By Lemma 2.3 (b),

$$|\lambda_i^{(\mathrm{c})} - \lambda_i^{(\mathrm{d})}| \le \epsilon_3 = \frac{2\left\|\frac{1}{2}\widetilde{E}_{21} + \frac{1}{2}\widetilde{F}_{21}\right\|_2^2}{\eta_i + \sqrt{\eta_i^2 + 4\left\|\frac{1}{2}\widetilde{E}_{21} + \frac{1}{2}\widetilde{F}_{21}\right\|_2^2}},$$

where η_i and η are given in (3.2) and (3.3), respectively.

Combining the above three inequalities, we have

$$\begin{aligned} |\widetilde{\lambda}_i - \lambda_i| &= |\widetilde{\lambda}_i - \lambda_i^{(\mathrm{d})}| \\ &\le |\widetilde{\lambda}_i - \lambda_i^{(\mathrm{b})}| + |\lambda_i^{(\mathrm{b})} - \lambda_i^{(\mathrm{c})}| + |\lambda_i^{(\mathrm{c})} - \lambda_i^{(\mathrm{d})}| \\ &\le \epsilon_1 + \epsilon_2 + \epsilon_3. \qquad \square \end{aligned}$$

Next, we bound the difference between the eigenvalues of H_1 and some n_1 eigenvalues of $\widetilde{H}$.

THEOREM 3.2. *Assume that the conditions of Theorem 3.1. Denote the eigenvalues of H_1 by*

$$-\mu_{n_1} \le \cdots \le -\mu_1 < \mu_1 \le \cdots \le \mu_{n_1}.$$

There are n_1 positive eigenvalues $\widetilde{\lambda}_{t_1} \le \cdots \le \widetilde{\lambda}_{t_{n_1}}$ of $\widetilde{H}$, such that for $1 \le i \le n_1$,

$$|\mu_i - \widetilde{\lambda}_{t_i}| \le \tilde{\epsilon}_1 + \tilde{\epsilon}_2 + \tilde{\epsilon}_3, \tag{3.11}$$

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where

$$\tilde{\epsilon}_1 = \frac{\|\widetilde{E} - \widetilde{F}\|_2^2}{4(\widetilde{\lambda}_1 + \widetilde{\lambda}_{t_i})}, \quad \tilde{\epsilon}_2 = \frac{1}{2}\|\widetilde{E}_{11} + \widetilde{F}_{11}\|_2, \quad \tilde{\epsilon}_3 = \frac{1}{2}\|\widetilde{E}_{21} + \widetilde{F}_{21}\|_2.$$

Proof. We follow the notation used in the proof of Theorem 3.1. We first consider estimating the difference between the eigenvalues of H_1 and some n_1 eigenvalues of EIG(b). This can be done in two steps. First, we bound the difference between the eigenvalues of $\Lambda_1 + \frac{1}{2}\widetilde{E}_{11} + \frac{1}{2}\widetilde{F}_{11}$ and some n_1 eigenvalues of EIG(b), and then bound the difference between the eigenvalues of $\Lambda_1 + \frac{1}{2}\widetilde{E}_{11} + \frac{1}{2}\widetilde{F}_{11}$ and those of H_1.

By Lemma 2.3 (a) and (c), there are n_1 eigenvalues $\lambda_{t_1}^{(\mathrm{b})} \le \cdots \le \lambda_{t_{n_1}}^{(\mathrm{b})}$ of EIG(b), such that

$$|\mu_i - \lambda_{t_i}^{(\mathrm{b})}| \le \frac{1}{2}\Big(\|\widetilde{E}_{11} + \widetilde{F}_{11}\|_2 + \|\widetilde{E}_{21} + \widetilde{F}_{21}\|_2\Big). \tag{3.12}$$

For $1 \le i \le n_1$, we have by Lemma 2.7,

$$|\widetilde{\lambda}_{t_i} - \lambda_{t_i}^{(\mathrm{b})}| \le \frac{\|\widetilde{E} - \widetilde{F}\|_2^2}{4(\widetilde{\lambda}_1 + \widetilde{\lambda}_{t_i})}. \tag{3.13}$$

Therefore, it follows from (3.12) and (3.13) that

$$\begin{aligned} |\mu_i - \widetilde{\lambda}_{t_i}| &\le |\mu_i - \lambda_{t_i}^{(\mathrm{b})}| + |\lambda_{t_i}^{(\mathrm{b})} - \widetilde{\lambda}_{t_i}| \\ &\le \frac{1}{2}\Big(\|\widetilde{E}_{11} + \widetilde{F}_{11}\|_2 + \|\widetilde{E}_{21} + \widetilde{F}_{21}\|_2\Big) + \frac{\|\widetilde{E} - \widetilde{F}\|_2^2}{4(\widetilde{\lambda}_1 + \widetilde{\lambda}_{t_i})}, \end{aligned}$$

which is (3.11). □

REMARK 3.3. Listed below are some comparisons between Theorems 3.1 and 3.2.

(a) The bound in Theorem 3.1 is quadratic with respect to the off-diagonal blocks of $\widetilde{E}$ and $\widetilde{F}$, but is only linear with respect to the diagonal blocks of $\widetilde{E}$ and $\widetilde{F}$, whereas in Theorem 3.2, the bound is linear with respect to both diagonal and off-diagonal blocks of $\widetilde{E}$ and $\widetilde{F}$. Thus, the bound in Theorem 3.1 is much tighter in the case of no perturbations in the diagonal blocks, i.e., $E_{ii} = F_{ii} = 0$ for $i = 1, 2$. Theorem 3.1 achieves this supremacy over Theorem 3.2 in the case when $E_{ii} = F_{ii} = 0$ for $i = 1, 2$ through the availability of the gaps as defined in (3.2), which Theorem 3.2 does not require, i.e., Theorem 3.2 uses less information.

(b) Theorem 3.1 provides bounds for the changes of all of eigenvalues of H, while Theorem 3.2 provides only for those of H_1.

4. Numerical examples.

We test our results in Theorems 3.1 and 3.2 on the following parameterized LREP,

$$\widetilde{H}(\alpha)z = \begin{bmatrix} 0 & K + \alpha E \\ M + \alpha F & 0 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} = \lambda \begin{bmatrix} y \\ x \end{bmatrix} = \lambda z, \tag{4.1}$$

where the parameter α varies from 0 to 1 while $K + \alpha E$ and $M + \alpha F$ remain positive definite. Two types of perturbations E and F are considered: Perturbations in all blocks

$$E = \begin{bmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{bmatrix}, \quad F = \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix}, \tag{4.2}$$

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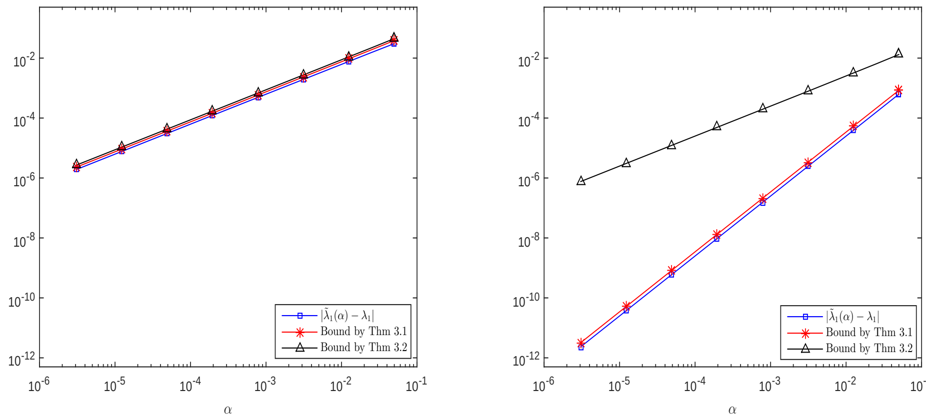

FIG. 4.1. $|\widetilde{\lambda}_1(\alpha)-\lambda_1|$ *and its bounds in Theorems 3.1 and 3.2. The* left *plot is for the perturbations in* (4.4) *and all three lines have the same slope. The* right *plot is for the perturbations in* (4.5) *and the line corresponding to Theorem 3.2 has flatter slope than the other two lines. This is due to the fact that under* (4.5), $\widetilde{\lambda}_1(\alpha)-\lambda_1$ *varies quadratically in* α *and such dependency is correctly reflected by the bound in Theorem 3.1 but incorrectly by the bound in Theorem 3.2.*

and perturbations in off-diagonal blocks only

$$E=\begin{bmatrix} & E_{12}\\ E_{21} & \end{bmatrix},\quad F=\begin{bmatrix} & F_{12}\\ F_{21} & \end{bmatrix}. \tag{4.3}$$

Denote the eigenvalues of $\widetilde{H}(\alpha)$ by

$$-\widetilde{\lambda}_n(\alpha)\le\cdots\le-\widetilde{\lambda}_1(\alpha)<\widetilde{\lambda}_1(\alpha)\le\cdots\le\widetilde{\lambda}_n(\alpha).$$

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

EXAMPLE 4.1. For simplicity, we first take $K=M=\operatorname{diag}(1,2)$. In such case, Φ_i and Ψ_i $(i=1,2)$ in (3.6) are $I_1=1$. Therefore, in (3.6), we have

$$\widetilde{E}_{ij}=E_{ij},\qquad \widetilde{F}_{ij}=F_{ij}\qquad \text{for } i,j=1,2.$$

Furthermore, the eigenvalues of H are $\pm\lambda_1=\pm1$, $\pm\lambda_2=\pm2$, and the gap $\eta=1$. We consider two perturbation pairs (E,F):

$$\text{Perturbing all blocks,}\qquad E=\begin{bmatrix}1 & 1\\ 1 & 1/2\end{bmatrix},\quad F=\begin{bmatrix}1/4 & -1/2\\ -1/2 & 1\end{bmatrix}, \tag{4.4}$$

and

$$\text{perturbing only off-diagonal blocks,}\qquad E=\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix},\quad F=\begin{bmatrix}0 & -1/2\\ -1/2 & 0\end{bmatrix}. \tag{4.5}$$

Since $n=2$, we can directly compute $|\widetilde{\lambda}_1(\alpha)-\lambda_1|$ to get, under (4.5),

$$\left|\widetilde{\lambda}_1(\alpha)-\lambda_1\right|=\left|\sqrt{1-\frac{\alpha^2}{2}}-1\right|=\frac{1}{2}\alpha^2+O(\alpha^3), \tag{4.6}$$

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and under (4.4),

$$\left|\widetilde{\lambda}_1(\alpha) - \lambda_1\right| = \left|\sqrt{1 + \frac{5\alpha - \alpha^2}{4}} - 1\right| = \frac{5}{8}\alpha + O(\alpha^2). \tag{4.7}$$

Figure 4.1 shows log-log plots for $|\widetilde{\lambda}_1(\alpha) - \lambda_1|$ and the bounds in Theorems 3.1 and 3.2 under perturbations in (4.4) (left) and perturbations in (4.5) (right), respectively. The vertical axes in both plots are purposefully made to have the same range, in an attempt to highlight the linear and quadratic behaviors of eigenvalue changes with respect to different perturbation patterns in (4.4) and (4.5). It is noted that the bound in Theorem 3.1 is sharp in this example. In fact, the exact value $|\widetilde{\lambda}_1(\alpha) - \lambda_1|$ and its bounds all approach 0 linearly in α in the left-hand side plot, correctly reflecting the true behavior. In the right-hand side part, the exact value $|\widetilde{\lambda}_1(\alpha) - \lambda_1|$ and its bound of Theorem 3.1 approaches 0 quadratically in α while the bound in Theorem 3.2 still approaches 0 linearly, as commented on in Remark 3.3(a).

EXAMPLE 4.2. In this example, we construct a linear response eigenvalue problem using the eigenvalues $-\lambda_n \le \cdots \le -\lambda_1 < \lambda_1 \le \cdots \le \lambda_n$ from the LREP for the sodium dimer Na_2 [2] with $n = 1862$. Let

$$\Lambda_1 = \operatorname{diag}(\lambda_1, \dots, \lambda_4), \qquad \Lambda_2 = \operatorname{diag}(\lambda_5, \dots, \lambda_n),$$

and Q_1, Q_2 be random orthogonal matrices obtained by

$$\texttt{qr(randn(4))} \text{ and } \texttt{qr(randn(}n-4\texttt{))},$$

in MATLAB, respectively. Finally, we define an LREP with

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

where $K_{11} = M_{11} = Q_1^{\mathrm{T}} \Lambda_1 Q_1$ and $K_{22} = M_{22} = Q_2^{\mathrm{T}} \Lambda_2 Q_2$. The symmetric perturbation matrices

$$E = \begin{array}{c c} & \begin{array}{cc} 4 & n-4 \end{array} \\ \begin{array}{c} 4 \\ n-4 \end{array} & \begin{bmatrix} E_{11} & E_{12} \\ E_{21} & E_{22} \end{bmatrix} \end{array}, \quad F = \begin{array}{c c} & \begin{array}{cc} 4 & n-4 \end{array} \\ \begin{array}{c} 4 \\ n-4 \end{array} & \begin{bmatrix} F_{11} & F_{12} \\ F_{21} & F_{22} \end{bmatrix} \end{array}$$

are also generated by the MATLAB function `randn`. $|\widetilde{\lambda}_i(\alpha) - \lambda_i|$ for $i = 1, 2, 3, 4$ and their associated upper bounds under the two different types of perturbations in (4.2) and (4.3) are shown in Figure 4.2. Again it can be seen that off-diagonal-block-only perturbations change λ_i, for $i = 1, 2, 3, 4$, much less than all-block perturbations do and the bounds in Theorem 3.1 reflect that well. In addition, in this example, $\widetilde{E}_{22} + \widetilde{F}_{22}$ has much larger norm than $\widetilde{E}_{11} + \widetilde{F}_{11}$ since the norms of E_{22} and F_{22} are larger than those of E_{11} and F_{11}. Consequently, the bounds in Theorem 3.2 under perturbations in (4.5) appear sharper than those in Theorem 3.1.

5. Conclusion.

In this paper, we have obtained perturbation bounds for the partitioned LREP for H as in (1.4) perturbed to $\widetilde{H}$ as in (1.7), as well as bounds for the differences between the eigenvalues of H_1 as in (1.6) and some of those of $\widetilde{H}$. The main results are summarized in Theorems 3.1 and 3.2. The bound in Theorem 3.1 depends linearly on the norms of diagonal perturbation blocks E_{ii}, F_{ii} but quadratically on those of off-diagonal perturbation blocks E_{ij} and F_{ij} ($i \neq j$). These bounds are shown to be very sharp in the presented numerical examples.

While the analysis in this paper is for real symmetric K and M, it also holds for the case of Hermitian K and M, simply by replacing all $\mathbb{R}$ by $\mathbb{C}$ (the set of complex numbers) and each matrix/vector transpose by complex conjugate and transpose.

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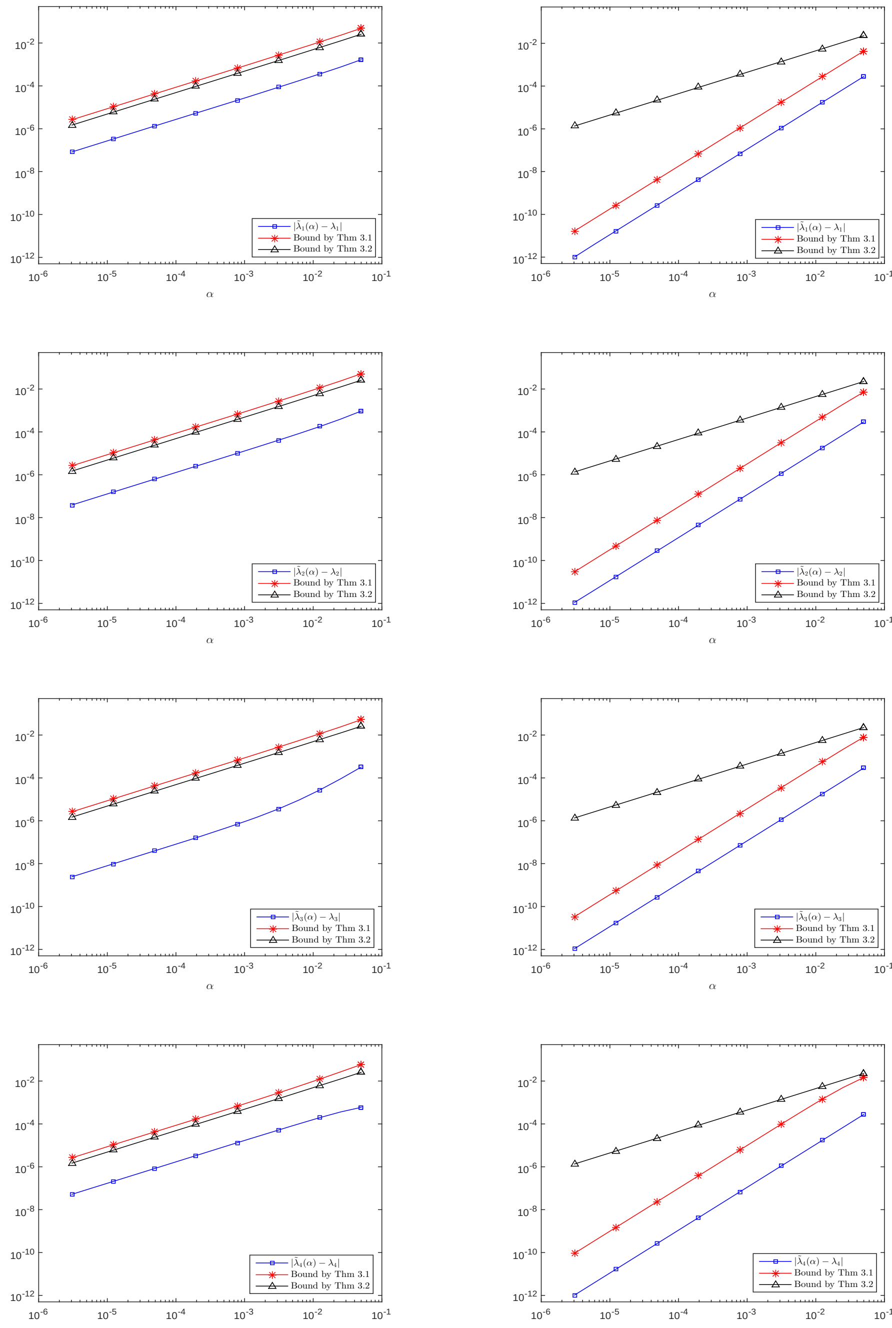

FIG. 4.2. $|\widetilde{\lambda}_i(\alpha) - \lambda_i|$ *for* $i = 1, 2, 3, 4$ *and their bounds in Theorems 3.1 and 3.2 under all-block perturbations (left plots) and off-diagonal perturbations (right plots), respectively. In particular, in the left plots, the bounds in Theorem 3.2 under all-block perturbations are sharper than those in Theorem 3.1 due to* $\|\widetilde{E}_{22} + \widetilde{F}_{22}\|_2 \geq \|\widetilde{E}_{11} + \widetilde{F}_{11}\|_2$.

REFERENCES

[1] Z. BAI AND R.-C. LI, *Minimization principles for linear response eigenvalue problem I: Theory*, SIAM J. Matrix Anal. Appl., 33 (2012), pp. 1075–1100.

[2] ———, *Minimization principle for linear response eigenvalue problem, II: Computation*, SIAM J. Matrix Anal. Appl., 34 (2013), pp. 392–416.

[3] R. BHATIA, *Matrix Analysis*, Springer, New York, 1997.

[4] D. C. DZENG AND W. W. LIN, *Homotopy continuation method for the numerical solutions of generalised symmetric eigenvalue problems*, J. Austral. Math. Soc. Ser. B, 32 (1991), pp. 437–456.

[5] W. KAHAN, *Inclusion theorems for clusters of eigenvalues of hermitian matrices*, Technical Report, Computer Science Department, University of Toronto, Toronto, 1967.

[6] J. KOVAČ-STRIKO AND K. VESELIĆ, *Trace minimization and definiteness of symmetric pencils*, Linear Algebra Appl., 216 (1995), pp. 139–158.

[7] C.-K. LI AND R.-C. LI, *A note on eigenvalues of perturbed Hermitian matrices*, Linear Algebra Appl., 395 (2005), pp. 183–190.

[8] R.-C. LI, Y. NAKATSUKASA, N. TRUHAR, AND S. XU, *Perturbation of partitioned Hermitian definite generalized eigenvalue problems*, SIAM J. Matrix Anal. Appl., 32 (2011), pp. 642–663.

[9] X. LIANG, R.-C. LI, AND Z. BAI, *Trace minimization principles for positive semi-definite pencils*, Linear Algebra Appl., 438 (2013), pp. 3085–3106.

[10] R. MATHIAS, *Quadratic residual bounds for the Hermitian eigenvalue problem*, SIAM J. Matrix Anal. Appl., 19 (1998), pp. 541–550.

[11] B. N. PARLETT, *The Symmetric Eigenvalue Problem*, SIAM, Philadelphia, 1998.

[12] P. RING, Z.-Y. MA, N. V. GIAI, D. VRETENAR, A. WANDELT, AND L.-G. GAO, *The time-dependent relativistic mean-field theory and the random phase approximation*, Nuclear Phys. A, 694 (2001), pp. 249–268.

[13] D. ROCCA, *Time-Dependent Density Functional Perturbation Theory: New Algorithms with Applications to Molecular Spectra*, Ph.D. Thesis, The International School for Advanced Studies, Trieste, Italy, 2007.

[14] D. ROCCA, Z. BAI, R.-C. LI, AND G. GALLI, *A block variational procedure for the iterative diagonalization of non-Hermitian random-phase approximation matrices*, J. Chem. Phys., 136 (2012), 034111 (8 pages).

[15] G. W. STEWART AND J. G. SUN, *Matrix Perturbation Theory* , Academic Press, Boston, 1990.

[16] R. E. STRATMANN, G. E. SCUSERIA, AND M. J. FRISCH, *An efficient implementation of time-dependent density-functional theory for the calculation of excitation of large molecules*, J. Chem. Phys., 109 (1998), pp. 8218–8824.

[17] Z. TENG AND R.-C. LI, *Convergence analysis of Lanczos-type methods for the linear response eigenvalue problem*, J. Comput. Appl. Math., 247 (2013), pp. 17–33.

[18] Z. TENG, Y. ZHOU, AND R.-C. LI, *A block Chebyshev-Davidson method for linear response eigenvalue problems*, Technical Report 2013-11, Department of Mathematics, University of Texas at Arlington, Arlington, September 2013.

[19] E. V. TSIPER, *Variational procedure and generalized Lanczos recursion for small-amplitude classical oscillations*, JETP Lett., 70 (1999), pp. 751–755.

[20] ———, *A classical mechanics technique for quantum linear response*, J. Phys. B: At. Mol. Opt. Phys., 34 (2001), pp. L401–L407.