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RAYLEIGH–RITZ APPROXIMATION FOR THE LINEAR RESPONSE EIGENVALUE PROBLEM*

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Abstract. Large scale eigenvalue computation is about approximating certain invariant subspaces associated with the interesting part of the spectrum, and the interesting eigenvalues are then extracted through projecting the problem through approximate invariant subspaces into a much smaller eigenvalue problem. In the case of the linear response eigenvalue problem (aka the random phase eigenvalue problem), it is the pair of deflating subspaces associated with the first few smallest positive eigenvalues that needs to be computed. This paper is concerned with approximation accuracy relationships between a pair of approximate deflating subspaces and approximate eigenvalues extracted by the pair. Lower and upper bounds on eigenvalue approximation errors are obtained in terms of canonical angles between an exact and computed pair of deflating subspaces. These bounds can also be interpreted as lower/upper bounds on the canonical angles in terms of eigenvalue approximation errors. They are useful in analyzing numerical solutions to linear response eigenvalue problems.

Key words. linear response eigenvalue problem, eigenvalue approximation, Rayleigh–Ritz approximation, canonical angles, deflating subspace, error bounds

AMS subject classifications. Primary, 65L15, 65F15; Secondary, 15A18, 15A42, 81Q15

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1. Introduction.

In computational quantum chemistry and physics, the so-called random phase approximation (RPA) describes the excitation states (energies) of physical systems in the study of collective motion of many-particle systems [1, 21, 22], which has applications in silicon nanoparticles and nanoscale materials and analysis of interstellar clouds [1, 2]. One important question in RPA is to compute a few eigenpairs associated with the smallest *positive* eigenvalues of the following eigenvalue problem:

$$\mathscr{H}\boldsymbol{w} := \begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{v} \end{bmatrix} = \lambda \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{v} \end{bmatrix}, \tag{1.1}$$

where $A, B \in \mathbb{R}^{n\times n}$ are both symmetric matrices and

$$\begin{bmatrix} A & B \\ B & A \end{bmatrix} \quad \text{is positive definite.} \tag{1.2}$$

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The matrix $\mathscr{H}$ is a special Hamiltonian matrix: all of its eigenvalues are real and appear in pairs $\{\lambda, -\lambda\}$. The eigenvalue problem (1.1) is referred to as the *linear response eigenvalue problem* (LREP) in the literature of computational quantum chemistry and physics, and several minimization principles were recently established and, as a result, CG type optimization algorithms were proposed to solve (1.1) [1, 2, 17].

Using the symmetric orthogonal matrix

$$J = \frac{1}{\sqrt{2}} \begin{bmatrix} I_n & I_n \\ I_n & -I_n \end{bmatrix}, \tag{1.3}$$

which satisfies $J^{\mathrm{T}}J = J^2 = I_{2n}$, we can transform the matrix $\mathscr{H}$ similarly to [1, 2]

$$J^{\mathrm{T}}\mathscr{H}J = \begin{bmatrix} 0 & A-B \\ A+B & 0 \end{bmatrix} =: \begin{bmatrix} 0 & K \\ M & 0 \end{bmatrix} =: H \tag{1.4}$$

and thus, by the relation:

$$\boldsymbol{z} := \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{x} \end{bmatrix} = J^{\mathrm{T}} \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{v} \end{bmatrix}, \quad \begin{bmatrix} \boldsymbol{u} \\ \boldsymbol{v} \end{bmatrix} = J \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{x} \end{bmatrix}, \tag{1.5}$$

the eigenvalue problem (1.1) is equivalent to

$$H\boldsymbol{z} := \begin{bmatrix} 0 & K \\ M & 0 \end{bmatrix} \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{x} \end{bmatrix} = \lambda \begin{bmatrix} \boldsymbol{y} \\ \boldsymbol{x} \end{bmatrix}, \tag{1.6}$$

which was still referred to as the LREP [1, 16, 24] and will be in this paper, too. The condition (1.2) implies that both K and M are symmetric and positive definite [1].

In the rest of this paper, unless otherwise explicitly stated, we relax the positive definiteness of both K and M to that *both are positive semidefinite and one of them is definite*. Denote the ordered eigenvalues of H (and they are of $\mathscr{H}$ as well) by

$$-\lambda_n \le \cdots \le -\lambda_1 \le \lambda_1 \le \cdots \le \lambda_n. \tag{1.7}$$

In the case when both K and M are positive definite, $\lambda_1 > 0$; $\lambda_1 = 0$ if one of K and M is singular [1]. In practice, the first k smallest eigenvalues with the positive sign[1] $\lambda_1 \le \cdots \le \lambda_k$ are of interest.

The classical Thouless's minimization principle stated in terms of (1.6) is

$$\lambda_1 = \min_{\boldsymbol{x},\boldsymbol{y}} \frac{\boldsymbol{x}^{\mathrm{T}}K\boldsymbol{x} + \boldsymbol{y}^{\mathrm{T}}M\boldsymbol{y}}{2|\boldsymbol{x}^{\mathrm{T}}\boldsymbol{y}|},$$

assuming both K and M are positive definite. In [1], a subspace version of this for characterizing the first k smallest eigenvalues with the positive sign $\lambda_1 \le \cdots \le \lambda_k$ was obtained[2]

$$\sum_{i=1}^{k} \lambda_i = \frac{1}{2} \inf_{U^{\mathrm{T}}V = I_k} \operatorname{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV), \tag{1.8}$$

where $U, V \in \mathbb{R}^{n\times k}$.

[1] We adopt the notion in [1, footnote 2 on p. 1077] of calling λ_i's the eigenvalues with the positive sign to encompass the case when some first few $\lambda_i = 0$.

[2] The "inf" in (1.8) is used to allow the case when one of K or M may be singular. But when both are positive definite, as in the case of original LREP, the minimum is attainable and then "inf" can be replaced by "min."

An important notion for LREP [1] is the so-called pair of deflating subspaces $\{\mathcal{U}, \mathcal{V}\}$ by which we mean that both $\mathcal{U}$ and $\mathcal{V}$ are subspaces of $\mathbb{R}^n$ and satisfy

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

More discussions on this are in section 2.2. It is a generalization of the concept of the invariant subspace (or eigenspace) in the standard eigenvalue problem upon considering the special structure in the LREP (1.6). This notion is not only vital in analyzing the theoretical properties such as the subspace version of Thouless's minimization principle (1.8) and the Cauchy-like interlacing inequalities [2], but also fundamental for several rather efficient algorithms, e.g., the locally optimal block preconditioned four-dimensional conjugate gradient method (LOBP4DCG) [2], the block Chebyshev–Davidson method [20], and the generalized Lanczos method [19, 23, 24]. Each of these algorithms generates a sequence of approximate deflating subspace pairs $\{\mathcal{U}_j, \mathcal{V}_j\}$ that hopefully converge to or contain subspaces near the pair of deflating subspaces $\{\mathcal{U}, \mathcal{V}\}$ of interest. Therefore, it is important to establish relationships between the accuracy in eigenvalue approximations and the distances from the exact deflating subspaces to their approximate ones.

Analogously to error estimate results for Rayleigh–Ritz approximations in the standard symmetric eigenvalue problem [8, 10, 11, 15, 25], in this paper we will establish results on error bounds for approximating eigenvalues computed by a pair of approximate deflating subspaces and conversely the error bounds on approximate deflating subspaces in terms of eigenvalue approximation errors. These estimates are useful in analyzing certain iterative methods.

The rest of the paper is organized as follows. In section 2, we will first provide some basic concepts about the angles between subspaces as well as some basic properties of LREP and the notion of the pair of deflating subspaces. Section 3 contains our main results: (i) lower and upper bounds on eigenvalue approximation errors in terms of canonical angles between exact and approximate pair of deflating subspaces and (ii) lower and upper bounds on the canonical angles in terms of eigenvalue approximation errors. In section 4, we discuss possible extensions of our main results in section 3 to deal with the more general LREP. Finally, conclusions are drawn in section 5.

Notation. $\mathbb{R}^{n\times k}$ is the set of all $n\times k$ real matrices, $\mathbb{R}^n = \mathbb{R}^{n\times 1}$, and $\mathbb{R} = \mathbb{R}^1$. I_n (or simply I if its dimension is clear from the context) is the $n\times n$ identity matrix, and $\boldsymbol{e}_j$ is its jth column. All vectors are column vectors and are in boldface. For a matrix Z, Z^{T} denotes its transpose; $\mathcal{R}(Z)$ is its column space, spanned by its column vectors; $\|Z\|_2$, $\|Z\|_{\mathrm{F}}$, and $\|Z\|_{\mathrm{ui}}$ are the spectral norm, the Frobenius norm, and a general unitarily invariant norm, respectively; and Z's submatrices $Z_{(k:\ell,i:j)}$, $Z_{(k:\ell,:)}$, and $Z_{(:,i:j)}$ consist of intersections of row k to row ℓ and column i to column j, row k to row ℓ, and column i to column j, respectively. The trace of a square matrix Z is $\operatorname{trace}(Z)$ and its eigenvalue set is $\operatorname{eig}(Z)$. For real symmetric matrices Z and W, $Z \succeq W$ (resp., $Z \succ W$) means that $Z - W$ is positive semidefinite (resp., positive definite).

2. Preliminary results. A matrix norm $\|\cdot\|$ is called a unitarily invariant norm on $\mathbb{C}^{m\times n}$ (the set of all $m \times n$ complex matrices) if it is a matrix norm and has the following two properties:

1. $\|XZY\| = \|Z\|$ for all unitary matrices X and Y of apt sizes and $Z \in \mathbb{C}^{m\times n}$.
2. $\|Z\| = \|Z\|_2$, the spectral norm of Z, if $\operatorname{rank}(Z) = 1$.

Two commonly used unitarily invariant norms are the spectral norm $\|Z\|_2$ and the Frobenius norm $\|Z\|_{\mathrm{F}}$. In what follows, we use $\|\cdot\|_{\mathrm{ui}}$ for a general unitarily invariant norm.

2.1. Canonical angles. For two subspaces $\mathcal{X}$ and $\mathcal{Y}$ of $\mathbb{R}^n$, suppose

$$k := \dim(\mathcal{X}) \le \dim(\mathcal{Y}) =: \ell, \tag{2.1}$$

and the canonical angles $\theta_i(\mathcal{X},\mathcal{Y})$ can be defined recursively [9] for $i = 1, 2, \dots, k$, by

$$\cos\theta_i(\mathcal{X},\mathcal{Y}) = \max_{\boldsymbol{x}\in\mathcal{X}} \max_{\boldsymbol{y}\in\mathcal{Y}} \langle \boldsymbol{x}, \boldsymbol{y}\rangle =: \langle \boldsymbol{x}_i, \boldsymbol{y}_i\rangle \tag{2.2}$$

subject to

$$\|\boldsymbol{x}\|_2 = \|\boldsymbol{y}\|_2 = 1, \quad \langle \boldsymbol{x}, \boldsymbol{x}_j\rangle = \langle \boldsymbol{y}, \boldsymbol{y}_j\rangle = 0 \quad \text{for } j = 1, 2, \dots, i-1, \tag{2.3}$$

where the *standard inner-product* $\langle \boldsymbol{x}, \boldsymbol{y}\rangle$ is defined by

$$\langle \boldsymbol{x}, \boldsymbol{y}\rangle := \boldsymbol{x}^{\mathrm{T}}\boldsymbol{y} \quad \text{for } \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n.$$

If $X \in \mathbb{R}^{n\times k}$ and $Y \in \mathbb{R}^{n\times \ell}$ are orthonormal basis matrices of $\mathcal{X}$ and $\mathcal{Y}$, respectively, i.e.,

$$X^{\mathrm{T}}X = I_k,\ \mathcal{X} = \mathcal{R}(X), \quad \text{and} \quad Y^{\mathrm{T}}Y = I_\ell,\ \mathcal{Y} = \mathcal{R}(Y),$$

and σ_j for $1 \le j \le k$ in ascending order, i.e., $\sigma_1 \le \cdots \le \sigma_k$, are the singular values of $Y^{\mathrm{T}}X$, then the k canonical angles $\theta_j(\mathcal{X},\mathcal{Y})$ from[3] $\mathcal{X}$ to $\mathcal{Y}$ are given by

$$0 \le \theta_j(\mathcal{X},\mathcal{Y}) := \arccos\sigma_j \le \frac{\pi}{2} \quad \text{for } 1 \le j \le k. \tag{2.4}$$

They are in descending order, i.e., $\theta_1(\mathcal{X},\mathcal{Y}) \ge \cdots \ge \theta_k(\mathcal{X},\mathcal{Y})$. Set

$$\Theta(\mathcal{X},\mathcal{Y}) = \operatorname{diag}(\theta_1(\mathcal{X},\mathcal{Y}), \dots, \theta_k(\mathcal{X},\mathcal{Y})). \tag{2.5}$$

It can be seen that angles so defined are independent of the orthonormal basis matrices X and Y which are not unique. The *angle* $\theta(\mathcal{X},\mathcal{Y})$ between $\mathcal{X}$ and $\mathcal{Y}$ is defined to be

$$\theta(\mathcal{X},\mathcal{Y}) := \max_i \arccos(\sigma_i) = \arccos(\min_i \sigma_i) = \theta_1(\mathcal{X},\mathcal{Y}). \tag{2.6}$$

When $k = 1$, i.e., X is a vector, there is only one canonical angle from $\mathcal{X}$ to $\mathcal{Y}$ and so $\theta(\mathcal{X},\mathcal{Y}) = \Theta(\mathcal{X},\mathcal{Y})$.

In what follows, we sometimes place a vector or matrix in one of or both arguments of $\theta_j(\,\cdot\,,\,\cdot\,)$, $\theta(\,\cdot\,,\,\cdot\,)$, and $\Theta(\,\cdot\,,\,\cdot\,)$, e.g., $\theta(X,Y)$, with the understanding that it is about the subspace spanned by the vector or the columns of the matrix argument.

Denote by $\mathbb{G}_k^n$ the set of all subspaces of dimension k in $\mathbb{R}^n$. It is famously known as the *Grassmannian manifold*. For any unitarily invariant norm $\|\cdot\|_{\mathrm{ui}}$, $\|\sin\Theta(\cdot,\cdot)\|_{\mathrm{ui}}$ defines a *distance metric* on $\mathbb{G}_k^n$ [18, p. 94].

Let $Y_\perp$ be an orthonormal basis matrix of the orthogonal complement of $\mathcal{Y}$ in $\mathbb{R}^n$. It can be proved that the k singular values of $X^{\mathrm{T}}Y_\perp$ are $\sin\theta_i(\mathcal{X},\mathcal{Y})$, and thus[4]

$$\|\sin\Theta(\mathcal{X},\mathcal{Y})\|_{\mathrm{ui}} = \left\|X^{\mathrm{T}}Y_\perp\right\|_{\mathrm{ui}}.$$

[3] If $k = \ell$, we may say that these angles are *between* $\mathcal{X}$ and $\mathcal{Y}$.

[4] We assume that any $\|\cdot\|_{\mathrm{ui}}$ we use is generic to matrix sizes in the sense that it applies to matrices of all sizes. Examples include the matrix spectral norm $\|\cdot\|_2$ and the Frobenius norm $\|\cdot\|_{\mathrm{F}}$.

In particular, we have

$$\|\sin\Theta(\mathcal{X},\mathcal{Y})\|_2 = \sin\theta(\mathcal{X},\mathcal{Y}) = \sin\theta_1(\mathcal{X},\mathcal{Y}).$$

Given a symmetric and positive definite matrix $W \in \mathbb{R}^{n\times n}$, the *$W$-inner product* is defined by

$$\langle \boldsymbol{x},\boldsymbol{y}\rangle_W = \boldsymbol{x}^{\mathrm{T}} W \boldsymbol{y} \quad \text{for } \boldsymbol{x},\boldsymbol{y} \in \mathbb{R}^n.$$

Replacing the standard inner-product $\langle \boldsymbol{x},\boldsymbol{y}\rangle$ in (2.2) and (2.3) by the W-inner-product $\langle \boldsymbol{x},\boldsymbol{y}\rangle_W$ leads to the W-canonical angles between $\mathcal{X}$ and $\mathcal{Y}$, which will be denoted by $\theta_{W;i}(\mathcal{X},\mathcal{Y})$ and also

$$\Theta_W(\mathcal{X},\mathcal{Y}) = \operatorname{diag}\left(\theta_{W;1}(\mathcal{X},\mathcal{Y}),\dots,\theta_{W;k}(\mathcal{X},\mathcal{Y})\right).$$

The W-canonical angles can also be stated in terms of the standard canonical angles (i.e., the ones under $W = I_n$) through a linear transformation of the involved subspaces. In fact, let $W = CC^{\mathrm{T}}$, where $C \in \mathbb{R}^{n\times n}$ is nonsingular. Such a decomposition is not unique, but for our purpose, any one of them suffices. Then [9, Theorem 4.2]

$$\theta_{W;i}(\mathcal{X},\mathcal{Y}) = \theta_i(C^{\mathrm{T}}\mathcal{X}, C^{\mathrm{T}}\mathcal{Y}),\ \Theta_W(\mathcal{X},\mathcal{Y}) = \Theta(C^{\mathrm{T}}\mathcal{X}, C^{\mathrm{T}}\mathcal{Y}),\ \theta_W(\mathcal{X},\mathcal{Y}) = \theta(C^{\mathrm{T}}\mathcal{X}, C^{\mathrm{T}}\mathcal{Y}). \tag{2.7}$$

There are important implications of (2.7):

$$\|\sin\Theta_W(\mathcal{X},\mathcal{Y})\|_{\mathrm{ui}} = \left\|\sin\Theta(C^{\mathrm{T}}\mathcal{X}, C^{\mathrm{T}}\mathcal{Y})\right\|_{\mathrm{ui}}, \tag{2.8}$$

and $\|\sin\Theta_W(\cdot,\cdot)\|_{\mathrm{ui}}$ is a distance metric on $\mathbb{G}_k^n$.

2.2. Basic properties of LREP and pair of deflating subspaces. Throughout the rest of this paper, $K, M \in \mathbb{R}^{n\times n}$ are symmetric and at least positive semidefinite. To facilitate our discussions, we next collect several necessary properties of the LREP in Theorem 2.1, and the reader is referred to [1, section 2] for proofs and more.

THEOREM 2.1. *Suppose that M is definite. Then the following statements are true:*

(i) *There exists a nonsingular $\Phi \in \mathbb{R}^{n\times n}$ such that*

$$K = \Psi\Lambda^2\Psi^{\mathrm{T}} \quad \text{and} \quad M = \Phi\Phi^{\mathrm{T}}, \tag{2.9}$$

where $\Lambda = \operatorname{diag}(\lambda_1,\lambda_2,\dots,\lambda_n)$ and $\Psi = \Phi^{-\mathrm{T}}$.

(ii) *If K is also definite, then all $\lambda_i > 0$ and H is diagonalizable:*

$$H\begin{bmatrix}\Psi\Lambda & \Psi\Lambda \\ \Phi & -\Phi\end{bmatrix} = \begin{bmatrix}\Psi\Lambda & \Psi\Lambda \\ \Phi & -\Phi\end{bmatrix}\begin{bmatrix}\Lambda & \\ & -\Lambda\end{bmatrix}. \tag{2.10}$$

(iii) *The eigen-decompostions of KM and MK are*

$$(KM)\Psi = \Psi\Lambda^2 \quad \text{and} \quad (MK)\Phi = \Phi\Lambda^2, \tag{2.11}$$

respectively.

The property (2.11) follows directly from (2.9) which implies that we can alternatively solve the LREP via solving any product eigenvalue problem in (2.11) for the k smallest positive eigenvalues and their associated eigenvectors.

Given two k-dimensional subspaces $\mathcal{U} \subseteq \mathbb{R}^n$ and $\mathcal{V} \subseteq \mathbb{R}^n$, the pair $\{\mathcal{U}, \mathcal{V}\}$ is called *a pair of deflating subspaces* of $\{K, M\}$ if

$$K\mathcal{U} \subseteq \mathcal{V} \quad \text{and} \quad M\mathcal{V} \subseteq \mathcal{U}. \tag{2.12}$$

This definition is essentially the same as the existing ones for the product eigenvalue problem [5, 7, 12]. Let $U \in \mathbb{R}^{n\times k}$ and $V \in \mathbb{R}^{n\times k}$ be the basis matrices for $\mathcal{U}$ and $\mathcal{V}$, respectively. Alternatively, (2.12) implies that there exist $K_{\mathrm{R}} \in \mathbb{R}^{k\times k}$ and $M_{\mathrm{R}} \in \mathbb{R}^{k\times k}$ such that

$$KU = VK_{\mathrm{R}} \quad \text{and} \quad MV = UM_{\mathrm{R}}$$

and vice versa. Equivalently,

$$H \begin{bmatrix} V & \\ & U \end{bmatrix} = \begin{bmatrix} V & \\ & U \end{bmatrix} \begin{bmatrix} & K_{\mathrm{R}} \\ M_{\mathrm{R}} & \end{bmatrix}.$$

This implies that $\mathcal{V} \oplus \mathcal{U}$ is an invariant subspace of H [1, Theorem 2.4], and conversely, if $\mathcal{R}([\begin{smallmatrix} V \\ U \end{smallmatrix}])$ is an invariant subspace of H, i.e.,

$$\begin{bmatrix} KU \\ MV \end{bmatrix} = H \begin{bmatrix} V \\ U \end{bmatrix} = \begin{bmatrix} V \\ U \end{bmatrix} D = \begin{bmatrix} VD \\ UD \end{bmatrix} \quad \text{for some } D \in \mathbb{R}^{k\times k},$$

then $\{\mathcal{R}(U), \mathcal{R}(V)\}$ is a pair of deflating subspace of $\{K, M\}$. The eigenvalues of D are part of those of H, i.e., $\mathrm{eig}(D) \subseteq \mathrm{eig}(H)$, and we are interested in the pair of deflating subspaces so that $\mathrm{eig}(D) = \{\lambda_1, \ldots, \lambda_k\}$.

Given a pair of deflating subspaces $\{\mathcal{R}(U), \mathcal{R}(V)\}$, partial eigenpairs of H can be obtained via solving the smaller eigenvalue problem [1, Theorem 2.5]: if

$$H_{\mathrm{R}}\hat{\boldsymbol{z}} := \begin{bmatrix} & K_{\mathrm{R}} \\ M_{\mathrm{R}} & \end{bmatrix} \begin{bmatrix} \hat{\boldsymbol{y}} \\ \hat{\boldsymbol{x}} \end{bmatrix} = \lambda \begin{bmatrix} \hat{\boldsymbol{y}} \\ \hat{\boldsymbol{x}} \end{bmatrix} =: \lambda\hat{\boldsymbol{z}}, \tag{2.13}$$

then $(\lambda, [\begin{smallmatrix} V\hat{\boldsymbol{y}} \\ U\hat{\boldsymbol{x}} \end{smallmatrix}])$ is an eigenpair of H. The matrix H_{R} is the restriction of H onto $\mathcal{V} \oplus \mathcal{U}$ with respect to the basis matrices $V \oplus U$.

It is shown that if one of K and M is definite, then $U^{\mathrm{T}}V$ is nonsingular [1, Lemma 2.7]. In that case, decompose $U^{\mathrm{T}}V$ as $U^{\mathrm{T}}V = W_1^{\mathrm{T}}W_2$, where $W_1 \in \mathbb{R}^{k\times k}$ and $W_2 \in \mathbb{R}^{k\times k}$ are nonsingular. We choose new basis matrices for $\mathcal{R}(U)$ and $\mathcal{R}(V)$ as UW_1^{-1} and VW_2^{-1}, respectively, upon which the restriction of H onto $\mathcal{V} \oplus \mathcal{U}$ becomes

$$H_{\mathrm{SR}} = \begin{bmatrix} & W_1^{-\mathrm{T}}U^{\mathrm{T}}KUW_1^{-1} \\ W_2^{-\mathrm{T}}V^{\mathrm{T}}MVW_2^{-1} & \end{bmatrix}, \tag{2.14}$$

whose off-diagonal blocks are both symmetric and positive (semi)definite.

Roughly speaking, calculating the k smallest positive eigenvalues of LREP (1.6) is about finding the pair of deflating subspaces $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$, where

$$\Phi_1 = \Phi_{(:,1:k)} \quad \text{and} \quad \Psi_1 = \Psi_{(:,1:k)}. \tag{2.15}$$

To this end, usually a sequence of approximate deflating subspace pairs $\{\mathcal{U}_j, \mathcal{V}_j\}$ (the dimensions of $\mathcal{U}_j$ and $\mathcal{V}_j$ can be larger than k) are generated to converge or contain $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$. For example,

- for the first Lanczos type algorithm in [19], $\mathcal{U}_j$ and $\mathcal{V}_j$ are the Krylov subspaces generated by initial vectors $\boldsymbol{u}_0 \in \mathbb{R}^n$ and $\boldsymbol{v}_0 \in \mathbb{R}^n$ [19, Lemma 3.1]:

$$\mathcal{U}_j = \mathcal{K}_j(MK, \boldsymbol{u}_0) \quad \text{and} \quad \mathcal{V}_j = \mathcal{K}_j(KM, \boldsymbol{v}_0), \tag{2.16}$$

  and the basis matrices U_j and V_j for $\mathcal{U}_j$ and $\mathcal{V}_j$, respectively, obey the relation [19, Theorem 3.1]:

$$U_j^{\mathrm{T}} V_j = I_j, \quad KU_j = V_j T_j + \beta_j \boldsymbol{v}_{j+1} \boldsymbol{e}_j^{\mathrm{T}}, \quad MV_j = U_j D_j, \tag{2.17}$$

  where $\boldsymbol{v}_i$ is the ith column of V_j, $\beta_j \in \mathbb{R}$ and $T_j, D_j \in \mathbb{R}^{j\times j}$;
- in [2], $\mathcal{U}_j$ and $\mathcal{V}_j$ are constructed based on the LOBP4DCG based on the minimization principle (1.8);
- in [20], $\mathcal{U}_j$ and $\mathcal{V}_j$ are generated by a block Chebyshev–Davidson type method, where the block Chebyshev filter procedure is used to refine and to expand the subspaces.

Suppose $\{\mathcal{R}(U), \mathcal{R}(V)\}$ is a pair of approximate deflating subspace and $U^{\mathrm{T}}V$ is nonsingular; then it is proved [1, Theorem 2.9] that the eigenvalues of H_{SR} defined by (2.14) are invariant with respect to the different choice of basis matrices U and V. In particular, if $U^{\mathrm{T}}V = I_k$, then H_{SR} becomes

$$H_{\mathrm{SR}} = \begin{bmatrix} & U^{\mathrm{T}}KU \\ V^{\mathrm{T}}MV & \end{bmatrix}. \tag{2.18}$$

The eigenpairs of H_{SR} are shown to give the *best possible* approximate eigenpairs, the so-called Ritz pairs, for H. (See [2] for more details.)

Given an approximation $\{\mathcal{R}(U), \mathcal{R}(V)\}$ to the pair of deflating subspaces $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$, we will investigate how good the Ritz pairs are in approximating the exact eigenpairs of H. In measuring the difference between $\{\mathcal{R}(U), \mathcal{R}(V)\}$ and $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$, we have three choices

$$\sin\Theta_{M^{-1}}(U, \Phi_1) \text{ and } \sin\Theta_{K^{-1}}(V, \Psi_1), \tag{2.19a}$$

$$\sin\Theta_{M^{-1}}(U, \Phi_1) \text{ and } \sin\Theta_{M^{-1}}(U, MV), \text{ or} \tag{2.19b}$$

$$\sin\Theta_{K^{-1}}(V, \Psi_1) \text{ and } \sin\Theta_{K^{-1}}(V, KU). \tag{2.19c}$$

While it seems that (2.19a) is most natural, (2.19b) and (2.19c) are more convenient to use for our purpose. In the case of $K \succ 0$ and $M \succ 0$, they are equivalent, as the following theorem shows.

THEOREM 2.2. *Suppose $K \succ 0$ and $M \succ 0$. If both sines in any one of* (2.19) *are zeros, $\{\mathcal{R}(U), \mathcal{R}(V)\}$ is the pair of deflating subspaces with the corresponding H_{SR} having eigenvalues $\pm\lambda_i$ for $1 \le i \le k$.*

Proof. We will use (2.19a) as an example. Let $\Lambda_1 = \Lambda_{(1:k,1:k)}$. Suppose

$$\text{both } \sin\Theta_{M^{-1}}(U, \Phi_1) = 0 \text{ and } \sin\Theta_{K^{-1}}(V, \Psi_1) = 0.$$

Thus there exist nonsingular $Q_1, Q_2 \in \mathbb{R}^{k\times k}$ such that

$$U = \Phi_1 Q_1, \quad V = \Psi_1 Q_2. \tag{2.20}$$

Then

$$KU = \Psi \Lambda^2 \Psi^{\mathrm{T}} \Phi_1 Q_1 = \Psi_1 \Lambda_1^2 Q_1 = V(Q_2^{-1} \Lambda_1^2 Q_1),$$
$$MV = \Phi \Phi^{\mathrm{T}} \Psi_1 Q_2 = \Phi_1 Q_2 = U(Q_1^{-1} Q_2).$$

They imply that $\{\mathcal{R}(U), \mathcal{R}(V)\}$ is a pair of deflating subspaces.

It remains to show that the corresponding H_{SR} has eigenvalues $\pm\lambda_i$ for $1 \le i \le k$. As different choices of basis matrices for $\mathcal{R}(U)$ and $\mathcal{R}(V)$ do not change the eigenvalues of H_{SR} [1, Theorem 2.9], we can assume, without loss of generality, $Q_1 = Q_2 = I_k$ in (2.20) for which

$$H_{\text{SR}} = \begin{bmatrix} 0 & \Lambda_1^2 \\ I_k & 0 \end{bmatrix}$$

whose eigenvalues are $\pm\lambda_i$ for $1 \le i \le k$. ∎

3. Main results. Suppose one of K and M is definite. Let $\{\mathcal{R}(U), \mathcal{R}(V)\}$ be a pair of approximate deflating subspaces intended to approximate $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$, where Φ_1 and Ψ_1 are given by (2.15), $U, V \in \mathbb{R}^{n\times k}$, and $U^{\mathrm{T}}V = I_k$. With the pair, a restriction H_{SR} given in (2.18) is constructed. Since H_{SR} is of the same structure as H in (1.6), it has eigenvalues

$$-\mu_k \le \cdots \le -\mu_1 \le \mu_1 \le \cdots \le \mu_k. \tag{3.1}$$

We are interested in bounding

1. the errors in μ_i as approximations to λ_i in terms of the error in $\{\mathcal{R}(U), \mathcal{R}(V)\}$ as an approximation to $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$, and conversely
2. the error in $\{\mathcal{R}(U), \mathcal{R}(V)\}$ as an approximation to $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$ in terms of the errors in μ_i as approximations to λ_i.

Define

$$\delta_k := \sum_{i=1}^{k} (\mu_i^2 - \lambda_i^2). \tag{3.2}$$

We know $0 \le \lambda_i \le \mu_i$ (see [1, Theorem 4.1]); so δ_k defines an error measurement in all μ_i as approximations to λ_i for $1 \le i \le k$. This is what we will be using for measuring the total eigenvalue approximation error in all μ_i. We have already discussed how to measure approximation accuracy in deflating subspaces by one of (2.19a)–(2.19c).

THEOREM 3.1. *Assume that M is definite. Let $\{\mathcal{R}(U), \mathcal{R}(V)\}$ be an approximate pair to $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$, where $U, V \in \mathbb{R}^{n\times k}$ and $\operatorname{rank}(U^{\mathrm{T}}V) = k$, and let the eigenvalues of H_{SR} be given by* (3.1). *Then for δ_k defined by* (3.2)*, it holds that*

$$(\lambda_{k+1}^2 - \lambda_k^2)\|\sin\Theta_{M^{-1}}(U, \Phi_1)\|_{\mathrm{F}}^2 \le \delta_k \le \sum_{i=1}^{k} \lambda_i^2 \cdot \tan^2\theta_{M^{-1}}(U, MV) + \frac{\lambda_n^2 - \lambda_1^2}{\cos^2\theta_{M^{-1}}(U, MV)}\|\sin\Theta_{M^{-1}}(U, \Phi_1)\|_{\mathrm{F}}^2. \tag{3.3}$$

As a result,

$$\|\sin\Theta_{M^{-1}}(U, \Phi_1)\|_{\mathrm{F}} \le \sqrt{\frac{\delta_k}{\lambda_{k+1}^2 - \lambda_k^2}}. \tag{3.4}$$

Proof. As different choices of basis matrices for $\mathcal{R}(U)$ and $\mathcal{R}(V)$ do not change the eigenvalues of H_{SR} [1, Theorem 2.9], we can assume, without loss of generality, that $U^{\mathrm{T}}V = I_k$. Define

$$\widetilde{U} := \Psi^{\mathrm{T}}U = \Phi^{-1}U \quad \text{and} \quad \widetilde{V} := \Phi^{\mathrm{T}}V = \Psi^{-1}V \tag{3.5}$$

which satisfy $\widetilde{U}^{\mathrm{T}}\widetilde{V} = U^{\mathrm{T}}\Psi\Phi^{\mathrm{T}}V = U^{\mathrm{T}}V = I_k$. It can be verified that

$$\Theta_{M^{-1}}(U, \Phi_1) = \Theta(\Psi^{\mathrm{T}}U, \Psi^{\mathrm{T}}\Phi_1) = \Theta(\widetilde{U}, I_{(:,1:k)}), \tag{3.6}$$

using (2.7). Partition $\widetilde{U}$ and Λ as

$$\widetilde{U} = \begin{matrix} \scriptstyle k \\ \scriptstyle n-k \end{matrix} \overset{\scriptstyle k}{\begin{bmatrix} \widetilde{U}_1 \\ \widetilde{U}_2 \end{bmatrix}}, \quad \Lambda = \begin{matrix} \scriptstyle k \\ \scriptstyle n-k \end{matrix} \overset{\begin{matrix}\scriptstyle k & \scriptstyle n-k\end{matrix}}{\begin{bmatrix} \Lambda_1 & \\ & \Lambda_2 \end{bmatrix}}. \tag{3.7}$$

According to Theorem 2.1, μ_i^2 for $i = 1, \ldots, k$ are the eigenvalues of the product matrix $(U^{\mathrm{T}}KU)(V^{\mathrm{T}}MV)$. Therefore,

$$\begin{aligned} \sum_{i=1}^{k} \mu_i^2 &= \operatorname{trace}((U^{\mathrm{T}}KU)(V^{\mathrm{T}}MV)) \\ &= \operatorname{trace}((U^{\mathrm{T}}\Psi\Lambda^2\Psi^{\mathrm{T}}U)(V^{\mathrm{T}}\Phi\Phi^{\mathrm{T}}V)) \\ &= \operatorname{trace}((\widetilde{U}^{\mathrm{T}}\Lambda^2\widetilde{U})(\widetilde{V}^{\mathrm{T}}\widetilde{V})) \\ &= \operatorname{trace}(\Lambda_1^2\widetilde{U}_1\widetilde{V}^{\mathrm{T}}\widetilde{V}\widetilde{U}_1^{\mathrm{T}}) + \operatorname{trace}(\Lambda_2^2\widetilde{U}_2\widetilde{V}^{\mathrm{T}}\widetilde{V}\widetilde{U}_2^{\mathrm{T}}). \end{aligned} \tag{3.8}$$

We have pointed out that the eigenvalues of H_{SR} are unchanged with different choices of the basis matrices for $\mathcal{R}(U)$ and $\mathcal{R}(V)$; we next choose specific basis matrices U and V to simplify (3.8). Specifically, let the QR decompositions of $\widetilde{U}$ and $\widetilde{V}$ be

$$\widetilde{U} = Q_1R_1 \quad \text{and} \quad \widetilde{V} = Q_2R_2,$$

respectively, where Q_1 and Q_2 are n-by-k with orthonormal columns. By [18, p. 40], there exist orthogonal matrices $P \in \mathbb{R}^{n\times n}$ and $S_i \in \mathbb{R}^{k\times k}$ such that

- for $2k \le n$,

$$PQ_1S_1 = \begin{matrix} \scriptstyle k \\ \scriptstyle k \\ \scriptstyle n-2k \end{matrix} \overset{\scriptstyle k}{\begin{bmatrix} I_k \\ 0 \\ 0 \end{bmatrix}}, \quad PQ_2S_2 = \begin{matrix} \scriptstyle k \\ \scriptstyle k \\ \scriptstyle n-2k \end{matrix} \overset{\scriptstyle k}{\begin{bmatrix} \Gamma \\ \Sigma \\ 0 \end{bmatrix}},$$

$$\begin{aligned} &\Gamma = \operatorname{diag}(\gamma_1, \ldots, \gamma_k), \quad 0 \le \gamma_1 \le \cdots \le \gamma_k, \\ &\Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_k), \quad \sigma_1 \ge \cdots \ge \sigma_k \ge 0, \\ &\gamma_i = \cos\theta_i(\widetilde{U}, \widetilde{V}),\ \sigma_i = \sin\theta_i(\widetilde{U}, \widetilde{V}) \text{ for } 1 \le i \le k; \end{aligned}$$

- for $2k > n$,

$$PQ_1S_1 = \begin{matrix} \scriptstyle n-k \\ \scriptstyle 2k-n \\ \scriptstyle n-k \end{matrix} \overset{\begin{matrix}\scriptstyle n-k & \scriptstyle 2k-n\end{matrix}}{\begin{bmatrix} I_{n-k} & 0 \\ 0 & I_{2k-n} \\ 0 & 0 \end{bmatrix}}, \quad PQ_2S_2 = \begin{matrix} \scriptstyle n-k \\ \scriptstyle 2k-n \\ \scriptstyle n-k \end{matrix} \overset{\begin{matrix}\scriptstyle n-k & \scriptstyle 2k-n\end{matrix}}{\begin{bmatrix} \Gamma & 0 \\ 0 & I_{2k-n} \\ \Sigma & 0 \end{bmatrix}},$$

$$\begin{aligned} &\Gamma = \operatorname{diag}(\gamma_1, \ldots, \gamma_{n-k}), \quad 0 \le \gamma_1 \le \cdots \le \gamma_{n-k}, \\ &\Sigma = \operatorname{diag}(\sigma_1, \ldots, \sigma_{n-k}), \quad \sigma_1 \ge \cdots \ge \sigma_{n-k} \ge 0, \\ &\gamma_i = \cos\theta_i(\widetilde{U}, \widetilde{V}),\ \sigma_i = \sin\theta_i(\widetilde{U}, \widetilde{V}) \text{ for } 1 \le i \le n-k, \\ &\theta_i(\widetilde{U}, \widetilde{V}) = 0 \text{ for } n-k+1 \le i \le k. \end{aligned}$$

Now, we reset

$$\widetilde{U} = P^{\mathrm{T}} \begin{bmatrix} \Gamma^{-1} \\ 0 \\ 0 \end{bmatrix}, \qquad \widetilde{V} = P^{\mathrm{T}} \begin{bmatrix} \Gamma \\ \Sigma \\ 0 \end{bmatrix} \qquad \text{if } 2k \le n, \tag{3.9a}$$

$$\widetilde{U} = P^{\mathrm{T}} \begin{bmatrix} \Gamma^{-1} & 0 \\ 0 & I_{2n-k} \\ 0 & 0 \end{bmatrix}, \quad \widetilde{V} = P^{\mathrm{T}} \begin{bmatrix} \Gamma & 0 \\ 0 & I_{2n-k} \\ \Sigma & 0 \end{bmatrix} \quad \text{if } 2k > n, \tag{3.9b}$$

which essentially change the basis matrices for $\mathcal{R}(U)$ and $\mathcal{R}(V)$ from U and V to $UR_1^{-1}S_1$ and $VR_2^{-1}S_2$, respectively. Moreover, the new $\widetilde{U}$ and $\widetilde{V}$ in (3.9) satisfy

$$\widetilde{U}^{\mathrm{T}}\widetilde{V} = I_k, \quad \widetilde{V}^{\mathrm{T}}\widetilde{V} = I_k,$$
$$\|\widetilde{U}\|_2 = \|\Gamma^{-1}\|_2 = \frac{1}{\cos\theta(\widetilde{U},\widetilde{V})} = \frac{1}{\cos\theta(\Psi^{\mathrm{T}}U, \Phi^{\mathrm{T}}V)} = \frac{1}{\cos\theta_{M^{-1}}(U, MV)}. \tag{3.10}$$

Thus, from (3.8), we have

$$\sum_{i=1}^{k} \mu_i^2 = \operatorname{trace}(\Lambda_1^2 \widetilde{U}_1 \widetilde{U}_1^{\mathrm{T}}) + \operatorname{trace}(\Lambda_2^2 \widetilde{U}_2 \widetilde{U}_2^{\mathrm{T}}). \tag{3.11}$$

Partition

$$P = \begin{matrix} & \scriptstyle k & \scriptstyle n-k \\ \scriptstyle k & P_{11} & P_{12} \\ \scriptstyle n-k & P_{21} & P_{22} \end{matrix}.$$

By (3.9), $\mathcal{R}(\widetilde{U}) = \mathcal{R}((P^{\mathrm{T}})_{(:,1:k)})$, and therefore

$$\Theta_{M^{-1}}(U, \Phi_1) = \Theta(\widetilde{U}, I_{(:,1:k)}) = \Theta\left(\begin{bmatrix} P_{11}^{\mathrm{T}} \\ P_{12}^{\mathrm{T}} \end{bmatrix}, \begin{bmatrix} I_k \\ 0 \end{bmatrix} \right). \tag{3.12}$$

On the other hand, from (3.9) and with $\widetilde{U}$ partitioned as in (3.7), we have

$$\begin{aligned} \widetilde{U}_1 &= \begin{cases} P_{11}^{\mathrm{T}} \Gamma^{-1} & \text{if } 2k \le n, \\ P_{11}^{\mathrm{T}} \begin{bmatrix} \Gamma^{-1} & \\ & I_{2k-n} \end{bmatrix} & \text{if } 2k > n, \end{cases} \\ \widetilde{U}_2 &= \begin{cases} P_{12}^{\mathrm{T}} \Gamma^{-1} & \text{if } 2k \le n, \\ P_{12}^{\mathrm{T}} \begin{bmatrix} \Gamma^{-1} & \\ & I_{2k-n} \end{bmatrix} & \text{if } 2k > n, \end{cases} \end{aligned} \tag{3.13}$$

from which we can verify that for $i = 1, 2$

$$P_{1i}^{\mathrm{T}} P_{1i} \le \widetilde{U}_i \widetilde{U}_i^{\mathrm{T}} \le \frac{1}{\gamma_1^2} P_{1i}^{\mathrm{T}} P_{1i}, \quad \text{where } \gamma_1 := \cos\theta_{M^{-1}}(U, MV).$$

Therefore

$$\begin{aligned} &\operatorname{trace}(\Lambda_1^2 P_{11}^{\mathrm{T}} P_{11}) + \operatorname{trace}(\Lambda_2^2 P_{12}^{\mathrm{T}} P_{12}) \\ &\qquad \le \sum_{i=1}^{k} \mu_i^2 \le \frac{1}{\gamma_1^2} \Big[\operatorname{trace}(\Lambda_1^2 P_{11}^{\mathrm{T}} P_{11}) + \operatorname{trace}(\Lambda_2^2 P_{12}^{\mathrm{T}} P_{12}) \Big]. \end{aligned} \tag{3.14}$$

We claim that

$$(\lambda_{k+1}^2-\lambda_k^2)\|\sin\Theta_{M^{-1}}(U,\Phi_1)\|_{\mathrm{F}}^2 \le \operatorname{trace}(\Lambda_1^2P_{11}^{\mathrm{T}}P_{11})+\operatorname{trace}(\Lambda_2^2P_{12}^{\mathrm{T}}P_{12})-\sum_{i=1}^k\lambda_i^2 \tag{3.15a}$$

$$\le(\lambda_n^2-\lambda_1^2)\|\sin\Theta_{M^{-1}}(U,\Phi_1)\|_{\mathrm{F}}^2. \tag{3.15b}$$

To prove (3.15), we note

$$\begin{aligned} I_k-P_{11}^{\mathrm{T}}P_{11}\succeq 0,\qquad\qquad & P_{12}^{\mathrm{T}}P_{12}\succeq 0,\\ \lambda_1^2\cdot I_k\preceq\Lambda_1^2\preceq\lambda_k^2\cdot I_k,\quad & \lambda_{k+1}^2\cdot I_{n-k}\preceq\Lambda_2^2\preceq\lambda_n^2\cdot I_{n-k},\end{aligned}$$

and therefore

$$\begin{aligned}\lambda_1^2\cdot(I_k-P_{11}^{\mathrm{T}}P_{11})\preceq(I_k-P_{11}^{\mathrm{T}}P_{11})^{1/2}\Lambda_1^2(I_k-P_{11}^{\mathrm{T}}P_{11})^{1/2}&\preceq\lambda_k^2\cdot(I_k-P_{11}^{\mathrm{T}}P_{11}),\\ \lambda_{k+1}^2\cdot P_{12}^{\mathrm{T}}P_{12}\preceq\qquad(P_{12}^{\mathrm{T}}P_{12})^{1/2}\Lambda_2^2(P_{12}^{\mathrm{T}}P_{12})^{1/2}\qquad&\preceq\lambda_n^2\cdot P_{12}^{\mathrm{T}}P_{12}.\end{aligned}$$

So for the right-hand side of (3.15a),

$$\begin{aligned}&\operatorname{trace}(\Lambda_1^2P_{11}^{\mathrm{T}}P_{11})+\operatorname{trace}(\Lambda_2^2P_{12}^{\mathrm{T}}P_{12})-\sum_{i=1}^k\lambda_i^2\\ &\quad=-\operatorname{trace}((I_k-P_{11}^{\mathrm{T}}P_{11})\Lambda_1^2)+\operatorname{trace}(P_{12}\Lambda_2^2P_{12}^{\mathrm{T}})\\ &\quad\ge\lambda_{k+1}^2\cdot\operatorname{trace}(P_{12}^{\mathrm{T}}P_{12})-\lambda_k^2\cdot\operatorname{trace}(I_k-P_{11}^{\mathrm{T}}P_{11})\\ &\quad=\lambda_{k+1}^2\cdot\operatorname{trace}(P_{12}^{\mathrm{T}}P_{12})-\lambda_k^2\cdot[k-\operatorname{trace}(P_{11}P_{11}^{\mathrm{T}})]\\ &\quad=\lambda_{k+1}^2\cdot\operatorname{trace}(P_{12}^{\mathrm{T}}P_{12})-\lambda_k^2\cdot[k-\operatorname{trace}(I_k-P_{12}P_{12}^{\mathrm{T}})]\\ &\quad=(\lambda_{k+1}^2-\lambda_k^2)\cdot\|P_{12}\|_{\mathrm{F}}^2\\ &\quad=(\lambda_{k+1}^2-\lambda_k^2)\|\sin\Theta_{M^{-1}}(U,\Phi_1)\|_{\mathrm{F}}^2.\end{aligned}$$

This proves (3.15a) and thus the first inequality in (3.3). Similarly,

$$-\operatorname{trace}((I_k-P_{11}^{\mathrm{T}}P_{11})\Lambda_1^2)+\operatorname{trace}(P_{12}\Lambda_2^2P_{12}^{\mathrm{T}})\le(\lambda_n^2-\lambda_1^2)\|\sin\Theta_{M^{-1}}(U,\Phi_1)\|_{\mathrm{F}}^2,$$

which proves (3.15b). Noticing $\gamma_1=\cos\theta_{M^{-1}}(U,MV)$, we have

$$\begin{aligned}\sum_{i=1}^k\mu_i^2-\sum_{i=1}^k\lambda_i^2&\le\frac{\sum_{i=1}^k\lambda_i^2+(\lambda_n^2-\lambda_1^2)\|\sin\Theta_{M^{-1}}(U,\Phi_1)\|_{\mathrm{F}}^2}{\gamma_1^2}-\sum_{i=1}^k\lambda_i^2\\ &\le\frac{(\lambda_n^2-\lambda_1^2)\|\sin\Theta_{M^{-1}}(U,\Phi_1)\|_{\mathrm{F}}^2}{\gamma_1^2}+\frac{1-\gamma_1^2}{\gamma_1^2}\sum_{i=1}^k\lambda_i^2\\ &=\frac{(\lambda_n^2-\lambda_1^2)\|\sin\Theta_{M^{-1}}(U,\Phi_1)\|_{\mathrm{F}}^2}{\cos^2\theta_{M^{-1}}(U,MV)}+\tan^2\theta_{M^{-1}}(U,MV)\cdot\sum_{i=1}^k\lambda_i^2,\end{aligned}$$

which proves the second inequality in (3.3). ∎

Remark 3.1. We make several remarks for Theorem 3.1:

(1) We first consider the special case $k = 1$ for which the lower and upper bounds in Theorem 3.1 reduce to

$$(\lambda_2^2 - \lambda_1^2) \cdot \sin^2 \theta_{M^{-1}}(\boldsymbol{u}, \Phi_1) \le \delta_1 \le \lambda_1^2 \cdot \tan^2 \theta_{M^{-1}}(\boldsymbol{u}, M\boldsymbol{v}) + \frac{\lambda_n^2 - \lambda_1^2}{\cos^2 \theta_{M^{-1}}(\boldsymbol{u}, M\boldsymbol{v})} \sin^2 \theta_{M^{-1}}(\boldsymbol{u}, \Phi_1), \tag{3.16}$$

where we have written $\boldsymbol{u}$ for U and $\boldsymbol{v}$ for V since $k = 1$. It is interesting to note that in this case, the upper bound (3.16) is sharp in the sense that when

$$\lambda_1 \le \lambda_2 = \cdots = \lambda_n, \tag{3.17}$$

it becomes an equality. This can be seen as follows. Suppose (3.17) holds. Then (3.11) becomes

$$\mu_1^2 = \lambda_1^2 (\tilde{\boldsymbol{v}}^{\mathrm{T}} \tilde{\boldsymbol{v}})(\tilde{\boldsymbol{u}}_1^{\mathrm{T}} \tilde{\boldsymbol{u}}_1) + \lambda_n^2 (\tilde{\boldsymbol{v}}^{\mathrm{T}} \tilde{\boldsymbol{v}})(\tilde{\boldsymbol{u}}_2^{\mathrm{T}} \tilde{\boldsymbol{u}}_2), \tag{3.18}$$

where $\tilde{\boldsymbol{u}} = [\tilde{\boldsymbol{u}}_1^{\mathrm{T}}, \tilde{\boldsymbol{u}}_2^{\mathrm{T}}]^{\mathrm{T}}$ and $\tilde{\boldsymbol{v}}$ are defined as in (3.5) and (3.7). Therefore, by noting $\tilde{\boldsymbol{u}}^{\mathrm{T}} \tilde{\boldsymbol{u}} = \tilde{\boldsymbol{u}}_1^{\mathrm{T}} \tilde{\boldsymbol{u}}_1 + \tilde{\boldsymbol{u}}_2^{\mathrm{T}} \tilde{\boldsymbol{u}}_2$, we have from (3.18) that

$$\mu_1^2 = \lambda_1^2 (\tilde{\boldsymbol{v}}^{\mathrm{T}} \tilde{\boldsymbol{v}})(\tilde{\boldsymbol{u}}^{\mathrm{T}} \tilde{\boldsymbol{u}}) + (\lambda_n^2 - \lambda_1^2)(\tilde{\boldsymbol{v}}^{\mathrm{T}} \tilde{\boldsymbol{v}})(\tilde{\boldsymbol{u}}_2^{\mathrm{T}} \tilde{\boldsymbol{u}}_2). \tag{3.19}$$

Moreover, for $k = 1$,

$$(\tilde{\boldsymbol{v}}^{\mathrm{T}} \tilde{\boldsymbol{v}})(\tilde{\boldsymbol{u}}^{\mathrm{T}} \tilde{\boldsymbol{u}}) = \frac{1}{\cos^2 \theta_{M^{-1}}(\boldsymbol{u}, M\boldsymbol{v})}, \quad (\tilde{\boldsymbol{v}}^{\mathrm{T}} \tilde{\boldsymbol{v}})(\tilde{\boldsymbol{u}}_2^{\mathrm{T}} \tilde{\boldsymbol{u}}_2) = \left[\frac{\sin \theta_{M^{-1}}(\boldsymbol{u}, \Phi_1)}{\cos \theta_{M^{-1}}(\boldsymbol{u}, M\boldsymbol{v})} \right]^2,$$

which, together with (3.19), imply that the second inequality in (3.16) is an equality.

(2) When $M = I_n$, the LREP reduces to the symmetric eigenvalue problem and $\Phi = \Psi$ is orthogonal. Therefore, only one of $\mathcal{R}(U)$ and $\mathcal{R}(V)$ is needed, i.e., $U = V$, which then leads to

$$\tan \theta_{M^{-1}}(U, MV) = 0 \quad \text{and} \quad \cos \theta_{M^{-1}}(U, MV) = 1,$$

and (3.16) becomes the well-known one

$$(\lambda_{k+1}^2 - \lambda_k^2) \| \sin \Theta(U, \Phi_1) \|_{\mathrm{F}}^2 \le \sum_{i=1}^{k} (\mu_i^2 - \lambda_i^2) \le (\lambda_n^2 - \lambda_1^2) \| \sin \Theta(U, \Phi_1) \|_{\mathrm{F}}^2 \tag{3.20}$$

for the symmetric eigenvalue problem [8, 10, 11, 15, 25].

By comparing the lower and upper bounds for δ_k in Theorem 3.1, one may argue that an unsatisfactory part in the lower bound for δ_k is that a term in the order of

$$\| \sin \Theta_{M^{-1}}(U, MV) \|_{\mathrm{F}}^2$$

is absent because it would be reasonable to expect that $\Theta_{M^{-1}}(U, MV) = 0$ if $\delta_k = 0$. However, this is false, as demonstrated by Example 3.1 below.

Example 3.1. Let $K = \mathrm{diag}(0, 0, 1)$ and $M = I_3$. The eigenvalues of H are ± 0, ± 0, and ± 1, i.e., $\lambda_1 = \lambda_2 = 0$ and $\lambda_3 = 1$, and $\Phi = \Psi = I_n$ in (2.9). Consider $k = 2$

and

$$U = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad V = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 1 \end{bmatrix}. \tag{3.21}$$

It can be verified that

$$U^{\mathrm{T}}V = I_2,\ U^{\mathrm{T}}KU = 0 \quad \text{and} \quad V^{\mathrm{T}}MV = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix},$$

which implies that $\mu_1 = \mu_2 = 0$ and thus $\delta_k = 0$. However,

$$\Theta_{M^{-1}}(U, \Phi_1) = 0, \qquad \Theta_{M^{-1}}(U, MV) = \operatorname{diag}\left(\frac{\pi}{4}, 0\right),$$
$$(\lambda_3^2 - \lambda_2^2)\|\sin\Theta_{M^{-1}}(U, MV)\|_{\mathrm{F}}^2 = (\lambda_3^2 - \lambda_2^2)\|\sin\Theta_{M^{-1}}(U, MV)\|_2^2 = \frac{1}{2}.$$

This phenomenon that $\delta_k = 0$ but $\|\sin\Theta_{M^{-1}}(U, MV)\|_F \neq 0$ is caused by the indefiniteness of K, and in Theorem 3.4, we will establish a lower bound (see (3.36)) of δ_k using $\|\sin\Theta_{M^{-1}}(U, MV)\|_{\mathrm{F}}^2$ under the assumption that both K and M are definite.

So far, we have considered $K \succeq 0$ and $M \succ 0$. It is not difficult to state a version for $K \succ 0$ and $M \succeq 0$ by swapping the roles of K and M. In fact, when $K \succ 0$ and $M \succeq 0$, we have, instead of (2.9),

$$M = \widehat{\Phi}\Lambda^2\widehat{\Phi}^{\mathrm{T}}, \quad K = \widehat{\Psi}\widehat{\Psi}^{\mathrm{T}}, \tag{3.22}$$

where $\widehat{\Psi} \in \mathbb{R}^{n\times n}$ is nonsingular, $\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$, and $\widehat{\Phi} = \widehat{\Psi}^{-\mathrm{T}}$. Let (cf. (2.15))

$$\widehat{\Phi}_1 = \widehat{\Phi}_{(:,1:k)} \quad \text{and} \quad \widehat{\Psi}_1 = \widehat{\Psi}_{(:,1:k)}. \tag{3.23}$$

Remark 3.2. In the case when $K \succ 0$ and $M \succ 0$, if $\lambda_k < \lambda_{k+1}$, then

$$\mathcal{R}(\Phi_1) = \mathcal{R}(\widehat{\Phi}_1) \quad \text{and} \quad \mathcal{R}(\Psi_1) = \mathcal{R}(\widehat{\Psi}_1).$$

In fact, for the case H is diagonalizable (see Theorem 2.1) and

$$\begin{bmatrix} \Psi_1\Lambda_1 \\ \Phi_1 \end{bmatrix}, \qquad \begin{bmatrix} \widehat{\Psi}_1 \\ \widehat{\Phi}_1\Lambda_1 \end{bmatrix}$$

are two different basis matrices for the eigenspace of H associated with the eigenvalues λ_i for $1 \le i \le k$, which are different from the rest of the eigenvalues of H, where $\Lambda_1 = \Lambda_{(1:k,1:k)}$. So the eigenspace is unique and thus there exists a nonsingular $Q \in \mathbb{R}^{k\times k}$ such that

$$\begin{bmatrix} \Psi_1\Lambda_1 \\ \Phi_1 \end{bmatrix} = \begin{bmatrix} \widehat{\Psi}_1 \\ \widehat{\Phi}_1\Lambda_1 \end{bmatrix} Q,$$

which implies $\mathcal{R}(\Phi_1) = \mathcal{R}(\widehat{\Phi}_1)$ and $\mathcal{R}(\Psi_1) = \mathcal{R}(\widehat{\Psi}_1)$. An implication of this remark is that there is no need to distinguish Φ_1 from $\widehat{\Phi}_1$ and Ψ_1 from $\widehat{\Psi}_1$.

THEOREM 3.2. *Suppose that $K \succ 0$ and $M \succeq 0$. Let $\{\mathcal{R}(U), \mathcal{R}(V)\}$ be an approximate pair to $\{\mathcal{R}(\widehat{\Phi}_1), \mathcal{R}(\widehat{\Psi}_1)\}$, where $U, V \in \mathbb{R}^{n\times k}$ satisfying* $\operatorname{rank}(U^{\mathrm{T}}V) = k$*,* *and let the nonnegative eigenvalues of* $H_{\rm SR}$ *given by* (2.14)*. Then for the* δ_k *given by* (3.2)*, it holds that*

$$(\lambda_{k+1}^2-\lambda_k^2)\|\sin\Theta_{K^{-1}}(V,\widehat{\Psi}_1)\|_{\rm F}^2 \le \delta_k \le \sum_{i=1}^{k}\lambda_i^2\cdot\tan^2\theta_{K^{-1}}(V,KU) + \frac{\lambda_n^2-\lambda_1^2}{\cos^2\theta_{K^{-1}}(V,KU)}\|\sin\Theta_{K^{-1}}(V,\widehat{\Psi}_1)\|_{\rm F}^2. \tag{3.24}$$

As a result,

$$\|\sin\Theta_{K^{-1}}(V,\widehat{\Psi}_1)\|_{\rm F} \le \sqrt{\frac{\delta_k}{\lambda_{k+1}^2-\lambda_k^2}}. \tag{3.25}$$

Suppose $K\succ 0$ and $M\succ 0$. The inequalities (3.4) and (3.25) imply that if $\delta_k=0$ and if the gap

$$\eta_k := \lambda_{k+1}^2-\lambda_k^2 > 0, \tag{3.26}$$

then the two sines in (2.19a) are zeros. By Theorem 2.2, all sines in (2.19) are zeros in this case, but it does not lead to quantitative upper bounds on some of the angles, most notably on $\sin\Theta_{M^{-1}}(U,MV)$ and $\sin\Theta_{K^{-1}}(V,KU)$.

LEMMA 3.3. *Suppose* $K\succ 0$ *and* $M\succ 0$*, and let* $U,V\in\mathbb{R}^{n\times k}$ *satisfying* $\operatorname{rank}(U^{\rm T}V)=k$*. Then for any unitarily invariant norm* $\|\cdot\|_{\rm ui}$

$$\left\|\sin\Theta_{M^{-1}}(U,MV)\right\|_{\rm ui} \le \left\|\sin\Theta_{M^{-1}}(U,\Phi_1)\right\|_{\rm ui} + \kappa\left\|\sin\Theta_{K^{-1}}(V,\Psi_1)\right\|_{\rm ui}, \tag{3.27}$$

$$\left\|\sin\Theta_{K^{-1}}(V,KU)\right\|_{\rm ui} \le \left\|\sin\Theta_{K^{-1}}(V,\Psi_1)\right\|_{\rm ui} + \kappa\left\|\sin\Theta_{M^{-1}}(U,\Phi_1)\right\|_{\rm ui}, \tag{3.28}$$

where $\kappa=\lambda_n/\lambda_1$*.*

Proof. Recall (2.7), (3.5), and (3.6). Noting $\Phi^{\rm T}\Psi=I$, $K^{-1}=\Phi\Lambda^{-2}\Phi^{\rm T}$, and $M^{-1}=\Psi\Psi^{\rm T}$, we have

$$\Theta_{K^{-1}}(V,\Psi_1)=\Theta(\Lambda^{-1}\Phi^{\rm T}V,\Lambda^{-1}\Phi^{\rm T}\Psi_1)=\Theta(\Lambda^{-1}\widetilde{V},I_{(:,1:k)}), \tag{3.29a}$$

$$\Theta_{M^{-1}}(U,MV)=\Theta(\Psi^{\rm T}U,\Psi^{\rm T}MV)=\Theta(\widetilde{U},\Phi^{\rm T}V)=\Theta(\widetilde{U},\widetilde{V}), \tag{3.29b}$$

$$\Theta_{K^{-1}}(V,KU)=\Theta(\Lambda^{-1}\Phi^{\rm T}V,\Lambda^{-1}\Phi^{\rm T}KU)=\Theta(\Lambda^{-1}\widetilde{V},\Lambda\widetilde{U}). \tag{3.29c}$$

In obtaining the last equality in (3.29a), we have used $\Lambda^{-1}\Phi^{\rm T}\Psi_1=\Lambda^{-1}I_{(:,1:k)}$ whose columns span the same subspace as $I_{(:,1:k)}$. Partition $\widetilde{U}$ and Λ as in (3.7) and $\widetilde{V}$ accordingly as

$$\widetilde{V}=\begin{matrix} \\ k \\ n-k\end{matrix}\begin{bmatrix} k \\ \widetilde{V}_1 \\ \widetilde{V}_2\end{bmatrix}. \tag{3.30}$$

For any unitarily invariant norm $\|\cdot\|_{\rm ui}$, we have

$$\left\|\sin\Theta(\widetilde{U},\widetilde{V})\right\|_{\rm ui} \le \left\|\sin\Theta(\widetilde{U},I_{(:,1:k)})\right\|_{\rm ui} + \left\|\sin\Theta(I_{(:,1:k)},\widetilde{V})\right\|_{\rm ui}, \tag{3.31a}$$

$$\left\|\sin\Theta(\Lambda^{-1}\widetilde{V},\Lambda\widetilde{U})\right\|_{\rm ui} \le \left\|\sin\Theta(\Lambda^{-1}\widetilde{V},I_{(:,1:k)})\right\|_{\rm ui} + \left\|\sin\Theta(I_{(:,1:k)},\Lambda\widetilde{U})\right\|_{\rm ui}. \tag{3.31b}$$

We need to relate $\Theta(\Lambda^{-1}\widetilde{V}, I_{(:,1:k)})$ to $\Theta(\widetilde{V}, I_{(:,1:k)})$. Without loss of generality, we may normalize V from the right so that $\widetilde{V}^{\mathrm{T}}\widetilde{V} = I_k$. We know that $\sin\Theta(I_{(:,1:k)}, \widetilde{V})$ and $\sin\Theta(\Lambda^{-1}\widetilde{V}, I_{(:,1:k)})$ consist of the singular values of

$$\widetilde{V}_2, \quad \Lambda_2^{-1}\widetilde{V}_2(\widetilde{V}^{\mathrm{T}}\Lambda^{-2}\widetilde{V})^{-1/2},$$

respectively. Denote their singular values by $\alpha_1 \geq \cdots \geq \alpha_k$ and $\beta_1 \geq \cdots \geq \beta_k$, respectively. It can be verified that

$$\lambda_1^2 I_k \preceq (\widetilde{V}^{\mathrm{T}}\Lambda^{-2}\widetilde{V})^{-1} \preceq \lambda_n^2 I_k,$$

$$\lambda_1^2\Lambda_2^{-1}\widetilde{V}_2\widetilde{V}_2^{\mathrm{T}}\Lambda_2^{-1} \preceq \Lambda_2^{-1}\widetilde{V}_2(\widetilde{V}^{\mathrm{T}}\Lambda^{-2}\widetilde{V})^{-1}\widetilde{V}_2^{\mathrm{T}}\Lambda_2^{-1} \preceq \lambda_n^2\Lambda_2^{-1}\widetilde{V}_2\widetilde{V}_2^{\mathrm{T}}\Lambda_2^{-1},$$

$$(1/\lambda_n^2)\widetilde{V}_2^{\mathrm{T}}\widetilde{V}_2 \preceq \widetilde{V}_2^{\mathrm{T}}\Lambda_2^{-2}\widetilde{V}_2 \preceq (1/\lambda_{k+1}^2)\widetilde{V}_2^{\mathrm{T}}\widetilde{V}_2.$$

These matrix inequalities imply

$$\frac{\lambda_1}{\lambda_n}\,\alpha_i \leq \beta_i \leq \frac{\lambda_n}{\lambda_{k+1}}\,\alpha_i,$$

which yields

(3.32)
$$\frac{\lambda_1}{\lambda_n}\left\|\sin\Theta(\widetilde{V}, I_{(:,1:k)})\right\|_{\mathrm{ui}} \leq \left\|\sin\Theta(\Lambda^{-1}\widetilde{V}, I_{(:,1:k)})\right\|_{\mathrm{ui}} \leq \frac{\lambda_n}{\lambda_{k+1}}\left\|\sin\Theta(\widetilde{V}, I_{(:,1:k)})\right\|_{\mathrm{ui}}.$$

Combine (3.6), (3.29b), (3.31a), and (3.32) to get (3.27).

We now relate $\Theta(I_{(:,1:k)}, \Lambda\widetilde{U})$ to $\Theta(I_{(:,1:k)}, \widetilde{U})$. Without loss of generality, we may normalize U from the right so that $\widetilde{U}^{\mathrm{T}}\widetilde{U} = I_k$. We know $\sin\Theta(I_{(:,1:k)}, \widetilde{U})$ and $\sin\Theta(I_{(:,1:k)}, \Lambda\widetilde{U})$ consist of the singular values of

$$\widetilde{U}_2, \quad \Lambda_2\widetilde{U}_2(\widetilde{U}^{\mathrm{T}}\Lambda^2\widetilde{U})^{-1/2},$$

respectively. Denote their singular values by $\hat{\alpha}_1 \geq \cdots \geq \hat{\alpha}_k$ and $\hat{\beta}_1 \geq \cdots \geq \hat{\beta}_k$, respectively. It can be verified that

$$(1/\lambda_n^2)I_k \preceq (\widetilde{U}^{\mathrm{T}}\Lambda^2\widetilde{U})^{-1} \preceq (1/\lambda_1^2)I_k,$$

$$(1/\lambda_n^2)\Lambda_2\widetilde{U}_2\widetilde{U}_2^{\mathrm{T}}\Lambda_2 \preceq \Lambda_2\widetilde{U}_2(\widetilde{U}^{\mathrm{T}}\Lambda^2\widetilde{U})^{-1}\widetilde{U}_2^{\mathrm{T}}\Lambda_2 \preceq (1/\lambda_1^2)\Lambda_2\widetilde{U}_2\widetilde{U}_2^{\mathrm{T}}\Lambda_2,$$

$$\lambda_{k+1}^2\widetilde{U}_2^{\mathrm{T}}\widetilde{U}_2 \preceq \widetilde{U}_2^{\mathrm{T}}\Lambda_2^2\widetilde{U}_2 \preceq \lambda_n^2\widetilde{U}_2^{\mathrm{T}}\widetilde{U}_2.$$

These matrix inequalities imply

$$\frac{\lambda_{k+1}}{\lambda_n}\,\hat{\alpha}_i \leq \hat{\beta}_i \leq \frac{\lambda_n}{\lambda_1}\,\hat{\alpha}_i,$$

which yields

(3.33)
$$\frac{\lambda_{k+1}}{\lambda_n}\left\|\sin\Theta(I_{(:,1:k)}, \widetilde{U})\right\|_{\mathrm{ui}} \leq \left\|\sin\Theta(I_{(:,1:k)}, \Lambda\widetilde{U})\right\|_{\mathrm{ui}} \leq \frac{\lambda_n}{\lambda_1}\left\|\sin\Theta(I_{(:,1:k)}, \widetilde{U})\right\|_{\mathrm{ui}}.$$

Combine (3.29a), (3.29c), (3.31b), and (3.33) to get (3.28). ∎

THEOREM 3.4. *Add to the conditions of Theorem* 3.1 *and Theorem* 3.2 *that* $K \succ 0$ *and* $M \succ 0$*. If* $\eta_k = \lambda_{k+1}^2 - \lambda_k^2 > 0$*, then*

$$\|\sin\Theta_{M^{-1}}(U, MV)\|_{\rm F} \le (\kappa+1)\sqrt{\frac{\delta_k}{\eta_k}}, \tag{3.34}$$

$$\|\sin\Theta_{K^{-1}}(V, KU)\|_{\rm F} \le (\kappa+1)\sqrt{\frac{\delta_k}{\eta_k}}, \tag{3.35}$$

where $\kappa = \lambda_n/\lambda_1$*.*

Remark 3.3. While (3.4), (3.25), (3.34), and (3.35) are naturally interpreted as providing upper bounds on various canonical angles between interested subspaces, each of them can also be understood to yield a lower bound on δ_k, e.g., by (3.34), we have

$$\delta_k \ge \frac{\eta_k}{(1+\kappa)^2}\,\|\sin\Theta_{M^{-1}}(U, MV)\|_{\rm F}^2. \tag{3.36}$$

We omit the rest. Upper bounds on δ_k come from the second inequalities in (3.3) and (3.24).

4. Extension to the more general case. In this section, we discuss how to extend our results in section 3 to the following more general LREP:

$$H\boldsymbol{z} := \begin{bmatrix} & K \\ M & \end{bmatrix}\begin{bmatrix}\boldsymbol{y}\\ \boldsymbol{x}\end{bmatrix} = \lambda\begin{bmatrix} E_+ & \\ & E_-\end{bmatrix}\begin{bmatrix}\boldsymbol{y}\\ \boldsymbol{x}\end{bmatrix} =: \lambda E\begin{bmatrix}\boldsymbol{y}\\ \boldsymbol{x}\end{bmatrix}, \tag{4.1}$$

where $E_+^{\rm T} = E_- \in \mathbb{R}^{n\times n}$ are nonsingular and K and M have the same property as before, i.e., $K, M \in \mathbb{R}^{n\times n}$ are symmetric and at least positive semidefinite. It is a generalized eigenvalue problem for the matrix pencil $H - \lambda E$ and has been discussed in [3, 4, 6, 13, 14].

Decompose $E_-^{\rm T} = E_+$ as $E_-^{\rm T} = E_+ = CD^{\rm T}$, where $C, D \in \mathbb{R}^{n\times n}$ are nonsingular. The eigenvalue problem (4.1) can be equivalenly transformed to [3]

$$\widetilde{H}\tilde{\boldsymbol{z}} := \begin{bmatrix} & \widetilde{K} \\ \widetilde{M} & \end{bmatrix}\begin{bmatrix}\tilde{\boldsymbol{y}}\\ \tilde{\boldsymbol{x}}\end{bmatrix} = \lambda\begin{bmatrix}\tilde{\boldsymbol{y}}\\ \tilde{\boldsymbol{x}}\end{bmatrix}, \tag{4.2}$$

returning in form to the standard LREP (1.6), where

(4.3)
$$\widetilde{K} = C^{-1}KC^{-\rm T}, \quad \widetilde{M} = D^{-1}MD^{-\rm T}, \quad \begin{bmatrix}\tilde{\boldsymbol{y}}\\ \tilde{\boldsymbol{x}}\end{bmatrix} = \Gamma^{\rm T}\begin{bmatrix}\boldsymbol{y}\\ \boldsymbol{x}\end{bmatrix}, \quad \text{and} \quad \Gamma = \begin{bmatrix} D & \\ & C\end{bmatrix}.$$

Although this transformation (4.3) equivalently transforms the general case to the original form in (1.6), it is of significance only in theory because in practice K, M, and $E_\pm$ may not be available and their very existences are through matrix-vector multiplications.

By Theorem 2.1, there exist nonsingular $\widetilde{\Phi}$, $\widetilde{\Psi} \in \mathbb{R}^{n\times n}$ such that

$$\widetilde{K} = \widetilde{\Psi}\Lambda^2\widetilde{\Psi}^{\rm T}, \quad \widetilde{M} = \widetilde{\Phi}\widetilde{\Phi}^{\rm T}, \quad \widetilde{\Phi}^{\rm T}\widetilde{\Psi} = I_n, \tag{4.4}$$

where $\Lambda = {\rm diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ and $\pm\lambda_i$ ordered as in (1.7) are the eigenvalues of (4.1) (cf. (4.2) and (4.3)). Let

$$\Phi = C^{-\rm T}\widetilde{\Phi}, \quad \Psi = D^{-\rm T}\widetilde{\Psi}.$$

The decompositions in (4.4) become

$$K\Phi = E_+\Psi\Lambda^2, \quad M\Psi = E_-\Phi, \quad \Phi^{\mathrm{T}}E_+\Psi = I_n. \tag{4.5}$$

The notion of the pair of deflating subspaces for $H - \lambda E$ was also introduced in [3, 4]: For two k-dimensional subspaces $\mathcal{R}(U)$ and $\mathcal{R}(V)$ of $\mathbb{R}^n$, we call $\{\mathcal{R}(U), \mathcal{R}(V)\}$ a *pair of deflating subspaces* of $H - \lambda E$ if

$$K\mathcal{R}(U) \subseteq E_+\mathcal{R}(V) \quad \text{and} \quad M\mathcal{R}(V) \subseteq E_-\mathcal{R}(U).$$

Let $\Phi_1 = \Phi_{(:,1:k)}$, $\Psi_1 = \Psi_{(:,1:k)}$, and $\Lambda_1 = \Lambda_{(1:k,1:k)}$. Then $K\Phi_1 = E_+\Psi_1\Lambda_1^2$ and $M\Psi_1 = E_-\Phi_1$. So $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$ is a pair of deflating subspaces of $H - \lambda E$.

Now, let $\{\mathcal{R}(U), \mathcal{R}(V)\}$ be an approximate pair to $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$ and decompose $U^{\mathrm{T}}E_+V$ as $U^{\mathrm{T}}E_+V = W_1^{\mathrm{T}}W_2$, where W_1, $W_2 \in \mathbb{R}^{k\times k}$ are nonsingular. It is shown that the first k smallest eigenvalues with the positive sign of H_{SR} defined also as in (2.14) are the best approximations to $\lambda_1 \le \cdots \le \lambda_k$ by the pair $\{\mathcal{R}(U), \mathcal{R}(V)\}$ in the sense specified there [4, Theorem 4.1].

Upon exploiting the equivalent relationship between (4.1) and (4.2), we can generalize Theorems 3.1, 3.2, and 3.4 to the more general LREP (4.1). As an example, here we only consider generalizing Theorem 3.1. This gives Theorem 4.1, below, whose detailed proof can be found in [26].

THEOREM 4.1. *Assume that M is definite. Let $\{\mathcal{R}(U), \mathcal{R}(V)\}$ be an approximate pair to the pair of deflating subspaces $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$ of $H - \lambda E$, where U, $V \in \mathbb{R}^{n\times k}$ and* $\operatorname{rank}(U^{\mathrm{T}}E_+V) = k$. *Denote the eigenvalues of H_{SR} as in* (2.14) *again by $\pm\mu_i$ ordered as in* (3.1)*. Then for δ_k defined by* (3.2)*, it holds that*

$$\begin{aligned}(\lambda_{k+1}^2 - \lambda_k^2)\|\sin\Theta_{M^{-1}}(E_-U, E_-\Phi_1)\|_{\mathrm{F}}^2 \\ \le \delta_k \le \sum_{i=1}^{k} \lambda_i^2 \cdot \tan^2\theta_{M^{-1}}(E_-U, MV) \\ + \frac{\lambda_n^2 - \lambda_1^2}{\cos^2\theta_{M^{-1}}(E_-U, MV)}\|\sin\Theta_{M^{-1}}(E_-U, E_-\Phi_1)\|_{\mathrm{F}}^2.\end{aligned} \tag{4.6}$$

As a result,

$$\|\sin\Theta_{M^{-1}}(E_-U, E_-\Phi_1)\|_{\mathrm{F}} \le \sqrt{\frac{\delta_k}{\lambda_{k+1}^2 - \lambda_k^2}}. \tag{4.7}$$

5. Conclusions. As an important notion in the LREP, the pair of deflating subspaces for $\{K, M\}$ is not only a vital object in analyzing the theoretical properties such as the subspace version of Thouless minimization principle and the Cauchy-like interlacing inequalities, but also leads to very efficient algorithms (e.g., the LOBP4DCG [2], a block Chebyshev–Davidson method [20], and the generalized Lanczos method [19]). Related, the estimation for the approximation of the pair of deflating pair $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$ also becomes important. In this paper, following the approximation for the Ritz values and Ritz vectors for the symmetric eigenvalue problem, we have established similar Ritz approximation results for the eigenvalues $\lambda_1 \le \cdots \le \lambda_k$ as well as for the pair of deflating subspaces $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$. These estimations cannot only reveal some properties of the LREP, but are also useful in analyzing certain iterative methods.

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