Minimization Principle for Linear Response Eigenvalue Problem I: Theory

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Abstract

We present two theoretical results for the linear response eigenvalue problem. The first result is a minimization principle for the sum of the smallest eigenvalues with the positive sign. The second result is Cauchy-like interlacing inequalities. Although the linear response eigenvalue problem is a nonsymmetric eigenvalue problem, these results mirror the well-known trace minimization principle and Cauchy interlacing inequalities for the symmetric eigenvalue problem.

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1 Introduction

In this paper, we consider the eigenvalue problem of the form:

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

where K and M are $n \times n$ symmetric positive semi-definite matrices and one of them is definite. We refer to it as a *linear response (LR) eigenvalue problem* for the reason to be explained later.

The LR eigenvalue problem (1.1) arises from computing excitation states (energies) of physical systems in the study of collective motion of many particle systems, ranging from silicon nanoparticles and nanoscale materials to analysis of interstellar clouds (see for example [8, 20, 24]). In computational quantum chemistry and physics, the excitation states are described by the *random phase approximation* (RPA), a linear response perturbation analysis in the time-dependent Hatree-Fock and time-dependent density function theories. There are a great deal of recent work and interests in developing efficient numerical algorithms and simulation techniques for excitation response calculations of molecules for materials design in energy science [10, 21, 28, 29].

The heart of (nonrelativistic) RPA calculation is to compute a few smallest positive eigenvalues and corresponding eigenvectors of the following eigenvalue problem

$$\boldsymbol{H} \begin{pmatrix} u \\ v \end{pmatrix} \equiv \begin{pmatrix} A & B \\ -B & -A \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = \lambda \begin{pmatrix} u \\ v \end{pmatrix}, \tag{1.2}$$

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where A and B are $n \times n$ real symmetric matrices such that the symmetric matrix $\begin{pmatrix} A & B \\ B & A \end{pmatrix}$ is positive definite[1] [27, 32]. In physics literature, it is this eigenvalue problem that is referred to as *the LR eigenvalue problem* (see, e.g., [23]), or *the RPA eigenvalue problem* (see e.g., [11]). We point out that this eigenvalue problem is also a special case of the so-called *Hamiltonian eigenvalue problem* because $\boldsymbol{H}$ in (1.2) is a Hamiltonian matrix. Therefore existing developments in, e.g., [4, 5, 18, 35], on the Hamiltonian eigenvalue problem apply. In general, the eigenvalues of a Hamiltonian matrix come in pairs $\{\mu, -\bar{\mu}\}$ for the real case and in quadruples $\{\pm\mu, \mp\bar{\mu}\}$ for the complex case [18, Table 1]. But (1.2) is a special one: its eigenvalues are real and come in pairs $\{\mu, -\mu\}$.

Define the symmetric orthogonal matrix

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

where I_n is the $n \times n$ identity matrix. It can be verified that $J^{\mathrm{T}} J = J^2 = I_{2n}$ and

$$J^{\mathrm{T}} \boldsymbol{H} J = \begin{pmatrix} 0 & A - B \\ A + B & 0 \end{pmatrix} \tag{1.4}$$

which is H in (1.1) with

$$K = A - B, \quad M = A + B. \tag{1.5}$$

Hence the Hamiltonian matrix $\boldsymbol{H}$ in (1.2) and the matrix H in (1.1) with (1.5) are similar through J, making it equivalent to solve the eigenvalue problem for one by the one for the other. In fact, both have the same eigenvalues with corresponding eigenvectors related by

$$\begin{pmatrix} y \\ x \end{pmatrix} = J^{\mathrm{T}} \begin{pmatrix} u \\ v \end{pmatrix}, \quad \begin{pmatrix} u \\ v \end{pmatrix} = J \begin{pmatrix} y \\ x \end{pmatrix}. \tag{1.6}$$

Furthermore, the positive definiteness of the matrix $\begin{pmatrix} A & B \\ B & A \end{pmatrix}$ is equivalent to that both K and M are positive definite since

$$J^{\mathrm{T}} \begin{pmatrix} A & B \\ B & A \end{pmatrix} J = \begin{pmatrix} A + B & 0 \\ 0 & A - B \end{pmatrix}. \tag{1.7}$$

By the equivalence of the eigenvalue problems (1.2) and (1.1), in this paper, we also refer to the eigenvalue problem (1.1) as the *linear response eigenvalue problem*.

When both K and M are symmetric positive definite, as in the case for RPA [26, 31, 34], it can be shown that the Hamiltonian matrix $\boldsymbol{H}$ in (1.2) and thus the matrix H in (1.1) have only nonzero real eigenvalues and their nonzero eigenvalues come in pairs $\{\pm\mu\}$ (see section 2). In this case, Thouless [31] showed that the smallest positive eigenvalue $\lambda_{\min}$ admits the following minimization principle:

$$\lambda_{\min} = \min_{u,v} \varrho(u, v), \tag{1.8}$$

where $\varrho(u, v)$ is defined by

$$\varrho(u, v) = \frac{\begin{pmatrix} u \\ v \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} A & B \\ B & A \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}}{|u^{\mathrm{T}} u - v^{\mathrm{T}} v|}, \tag{1.9}$$

[1] In this article we will focus on very much this case, except that the eigenvalue 0 is allowed, i.e., (1.2) has only real eigenvalues and some of them may be 0.

and the minimization is taken among all vectors u, v such that $u^{\mathrm{T}}u - v^{\mathrm{T}}v \neq 0$. By the similarity transformation (1.4) and using the relationships in (1.6), we have

$$\varrho(u, v) \equiv \rho(x, y) \stackrel{\text{def}}{=} \frac{x^{\mathrm{T}}Kx + y^{\mathrm{T}}My}{2|x^{\mathrm{T}}y|}, \tag{1.10}$$

and thus equivalently [34]

$$\lambda_{\min} = \min_{x,y} \rho(x, y), \tag{1.11}$$

where the minimization is taken among all x and y such that either $x^{\mathrm{T}}y \neq 0$ or $x^{\mathrm{T}}y = 0$ but $x^{\mathrm{T}}Kx + y^{\mathrm{T}}My > 0$. This removes those x and y that annihilate both the numerator and the denominator from the domain. In particular $x = y = 0$ is excluded.

We will refer to both $\varrho(u, v)$ and $\rho(x, y)$ as the *Thouless functional* but in different forms. Although $\varrho(u, v) \equiv \rho(x, y)$ under (1.6), in this paper we primarily work with $\rho(x, y)$ to develop extensions of (1.11) and efficient numerical methods.

The theoretical part of our contributions in this paper are three-folds:

1. We extend the minimization principle (1.11) to include the case when one of K and M is singular and thus $\lambda_{\min} = 0$ for which "min" needs to be replaced by "inf".

2. We prove a subspace version of the minimization principle (1.8):

$$\sum_{i=1}^{k} \lambda_i = \frac{1}{2} \inf_{U^{\mathrm{T}}V = I_k} \operatorname{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV), \tag{1.12}$$

   where λ_i $(1 \leq i \leq k)$ are the k smallest eigenvalues with the positive sign[2] of H, and $U, V \in \mathbb{R}^{n\times k}$. Moreover, "inf" can be replaced by "min" if both K and M are definite.

   Equation (1.12) suggests that

$$\frac{1}{2} \operatorname{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV) \quad \text{subject to } U^{\mathrm{T}}V = I_n \tag{1.13}$$

   is a *proper subspace version* of the Thouless functional in the form of $\rho(\cdot, \cdot)$. By exploiting the close relation through (1.6) between ρ and ϱ, we also obtain a subspace version of the minimization principle (1.8) in Theorem 3.3 for the original LR eigenvalue problem (1.2) and, at the same time, a *proper subspace version* of the Thouless functional in the form of $\varrho(\cdot, \cdot)$.

3. We prove that the ith eigenvalue with the positive sign of a structure-preserving projection matrix H_{SR} of H onto a pair of subspaces is no smaller than the corresponding λ_i of H. In many ways, H_{SR} plays the same role for the LR eigenvalue problem (1.1) as the Rayleigh quotient matrix for the symmetric eigenvalue problem [25].

[2] H has an even number of eigenvalue 0, if any. It happens when one of K and M is semi-definite, i.e., singular. Perturbing the singular one by ϵI and then letting $\epsilon \to 0^+$, we see that half of the 0s comes from some of the positive eigenvalues of perturbed H going to 0 from the right and the other half from the opposites of these positive eigenvalues going to 0 from the left. In recognizing this, we will associate the plus sign to half of the 0s and the negative sign to the other half, and speak of H having n eigenvalues with the positive sign and n eigenvalues with the negative sign without causing any ambiguity. Our distinguishing $+0$ and -0 here is not unprecedent. In fact, it is rather beneficial sometimes in computations [13] and it is built into the IEEE floating point standard 754-1985 [1].

These three theoretical contributions mirror the three well-known results for the symmetric eigenvalue problem, namely the minimization principle of the Rayleigh quotient, the trace minimization principle (a corollary of Wielandt's theorem [30, p.199]), and Cauchy's interlacing inequalities. They will be reviewed at the beginning of section 3 (see for example [16, 25, 30]).

The eigenvalue problem (1.1) is equivalent to the generalize eigenvalue problem for the matrix pencil

$$\boldsymbol{A} - \lambda \boldsymbol{B} \equiv \begin{pmatrix} M & 0 \\ 0 & K \end{pmatrix} - \lambda \begin{pmatrix} 0 & I_n \\ I_n & 0 \end{pmatrix}. \tag{1.14}$$

It is not hard to show that $\boldsymbol{A} - \lambda \boldsymbol{B}$ is diagonalizable (using Theorem 2.3, for example) if K and M are symmetric positive definite. So the results in [15, 22] apply. Also when K and M are symmetric positive definite, $\boldsymbol{A}$ is definite and thus $\boldsymbol{A} - \lambda \boldsymbol{B}$ is a symmetric definite pencil. Fischer's min-max principle [30, p.201] (naturally extended to the generalized eigenvalue problem [17, Appendix A]) is applicable. Later we will comment on what possible results may come out of such applications and compare them to ours.

This is the first paper of ours in a sequel of two. Here we focus on treating the theoretical aspect of the eigenvalue problem for H, and its numerical aspect will be the subject of study in the second paper [2]. The rest of this paper is organized as follows. In section 2, we review basic theoretical results about the eigenvalue problem (1.1) and then introduce the concept of a pair of deflating subspaces and its approximation properties. In section 3, we extend the minimization principle (1.11) by Thouless and Tsiper to include several eigenvalues and present our Cauchy-like interlacing inequalities and more. We will also discuss the metric about the best approximation from a pair of approximate deflating subspaces. For simplicity of exposition, most proofs are deferred to appendix A Concluding remarks are in section 4.

Throughout this paper, $\mathbb{R}^{n\times m}$ is the set of all $n \times m$ 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 e_j is its jth column. The superscript "$\cdot^{\mathrm{T}}$" takes transpose only. We shall also adopt MATLAB-like convention to access the entries of vectors and matrices. $i : j$ is the set of integers from i to j inclusive. For a vector u and an matrix X, $u_{(j)}$ is u's jth entry, $X_{(i,j)}$ is X's (i, j)th entry; X's submatrices $X_{(k:\ell,i:j)}$, $X_{(k:\ell,:)}$, and $X_{(:,i:j)}$ 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. If X is nonsingular, $\kappa(X) \stackrel{\text{def}}{=} \|X\|_2\|X^{-1}\|_2$ is its spectral condition number, where $\|\cdot\|_2$ denotes the ℓ_2-norm of a vector or the spectral norm of a matrix. For matrices or scalars X_i, both $\mathrm{diag}(X_1, \ldots, X_k)$ and $X_1 \oplus \cdots \oplus X_k$ denote the same matrix

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

The assignments in (1.1) will be assumed, namely H is always defined that way for given K, $M \in \mathbb{R}^{n\times n}$ which are assumed by default to be symmetric positive semi-definite and one of which is definite, unless explicitly stated differently. This assumption is essential to our main contributions in this paper and its following one [2], although a few results do not require this. We will point them out along the way.

2 Basic theory and pair of deflating subspaces

2.1 Basic theory

In this subsection, we discuss some basic theoretical results on the eigenvalue problem (1.1). Most results are likely known, but cannot be found in one place. They are collected here for

the convenience of our later developments. Proofs of these results which can be found in the technical report [3] are not hard and thus will be omitted.

Theorem 2.1.

1. *Each nonzero $\mu = \lambda^2$ as an eigenvalue of KM (and MK) leads to two distinct eigenvalues of H and two corresponding eigenvectors z.*

2. *The number of eigenvalues 0 of H is twice as many as the number of eigenvalues 0 of KM (or MK).*

REMARK **2.1.** Theorem 2.1 is valid for all square matrices K and M. $\diamond$

Suppose that K and M are symmetric positive semi-definite. Since $KM = K^{1/2}K^{1/2}M$ has the same eigenvalues as $K^{1/2}MK^{1/2}$ which is also symmetric positive semi-definite, all eigenvalues of KM are real and nonnegative. Denote these eigenvalues by λ_i^2 $(1 \le i \le n)$ in ascending order, i.e.,

$$0 \le \lambda_1^2 \le \lambda_2^2 \le \cdots \le \lambda_n^2, \tag{2.1}$$

where all $\lambda_i \ge 0$ and thus $0 \le \lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$. The eigenvalues of MK are λ_i^2 $(1 \le i \le n)$, too. Theorem 2.1 implies the eigenvalues of H are

$$\pm\lambda_i \quad \text{for } i = 1, 2, \ldots, n. \tag{2.2}$$

An immediate consequence of this is that the eigenvalues of H come in $\pm\lambda$ pairs. In particular, it has an even number of eigenvalues 0. As we mentioned in the footnote 2, for convenience, we shall associate half of eigenvalues 0 with the positive sign and the other half with the negative sign. Doing so legitimizes the use of the phrase "the first k smallest eigenvalues with the positive sign of H" to refer to λ_i for $1 \le i \le k$ without ambiguity. Throughout this paper, we will stick to using λ_i^2 $(1 \le i \le n)$ in ascending order as in (2.1) to denote the eigenvalues of KM (when K and M are symmetric positive semi-definite).

Set

$$\mathscr{I} = \begin{pmatrix} 0 & I_n \\ I_n & 0 \end{pmatrix} \tag{2.3}$$

which is symmetric but indefinite. The matrix $\mathscr{I}$ induces an *indefinite inner product* on $\mathbb{R}^{2n}$:

$$\langle z_1, z_2 \rangle_{\mathscr{I}} \stackrel{\text{def}}{=} z_1^{\mathrm{T}} \mathscr{I} z_2.$$

The following theorem tells us some orthogonality properties among the eigenvectors of H. It does not require that one of K and M are definite.

Theorem 2.2. *Suppose K, $M \in \mathbb{R}^{n\times n}$ are symmetric and positive semi-definite.*

1. *Let (α, z) be an eigenpair of H, i.e., $Hz = \alpha z$ and $z = \begin{pmatrix} y \\ x \end{pmatrix} \ne 0$, where x, $y \in \mathbb{R}^n$. Then $\alpha\langle z, z\rangle_{\mathscr{I}} = 2\alpha\, x^{\mathrm{T}} y > 0$ if $\alpha \ne 0$. In particular, this implies $\langle z, z\rangle_{\mathscr{I}} = 2x^{\mathrm{T}} y \ne 0$ if $\alpha \ne 0$.*

2. *Let (α_i, z_i) $(i = 1, 2)$ be two eigenpairs of H. Partition $z_i = \begin{pmatrix} y_i \\ x_i \end{pmatrix} \ne 0$, where x_i, $y_i \in \mathbb{R}^n$.*

   (a) If $\alpha_1 \ne \alpha_2$, then $\langle z_1, z_2\rangle_{\mathscr{I}} = y_1^{\mathrm{T}} x_2 + x_1^{\mathrm{T}} y_2 = 0$.
   (b) If $\alpha_1 \ne \pm\alpha_2 \ne 0$, then $y_1^{\mathrm{T}} x_2 = x_1^{\mathrm{T}} y_2 = 0$.

More can be said when one of K and M are definite. For the sake of presentation, we shall always either assume that M is definite or only provide proofs for definite M whenever one of K and M is required to be definite. Doing so loses no generality because the interchangeable roles played by K and M makes it rather straightforward to create a version for the case when K is definite by simply swapping K and M in each of their appearances. The following theorem is critical to our theoretical developments.

Theorem 2.3. *Suppose that M is definite. Then the following statements are true:*

1. *There exists a nonsingular $Y \in \mathbb{R}^{n\times n}$ such that*

$$K = Y\Lambda^2 Y^{\mathrm{T}}, \quad M = XX^{\mathrm{T}}, \tag{2.4}$$

   where $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n)$ and $X = Y^{-\mathrm{T}}$.

2. *If K is also definite, then all $\lambda_i > 0$ and H is diagonalizable:*

$$H \begin{pmatrix} Y\Lambda & Y\Lambda \\ X & -X \end{pmatrix} = \begin{pmatrix} Y\Lambda & Y\Lambda \\ X & -X \end{pmatrix} \begin{pmatrix} \Lambda & \\ & -\Lambda \end{pmatrix}. \tag{2.5}$$

3. *H is not diagonalizable if and only if $\lambda_1 = 0$ which happens when and only when K is singular.*

4. *The ith column of $Z = \begin{pmatrix} Y\Lambda \\ X \end{pmatrix}$ is the eigenvector corresponding to λ_i and it is unique if*

   (a) λ_i is a simple eigenvalue of H, or

   (b) $i = 1$, $\lambda_1 = +0 < \lambda_2$. In this case, 0 is a double eigenvalue of H but there is only one eigenvector associated with it.

5. *If $0 = \lambda_1 = \cdots = \lambda_\ell < \lambda_{\ell+1}$, then H's Jordan canonical form is*

$$\underbrace{\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \oplus \cdots \oplus \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}}_{\ell} \oplus \mathrm{diag}(\lambda_{\ell+1}, -\lambda_{\ell+1}, \ldots, \lambda_n, -\lambda_n). \tag{2.6}$$

   Thus H has 0 as an eigenvalue of algebraic multiplicity 2ℓ with only ℓ linear independent eigenvectors which are the columns of $\begin{pmatrix} 0 \\ X_{(:,1:\ell)} \end{pmatrix}$.

2.2 Pair of deflating subspaces

Let $\mathcal{U}, \mathcal{V} \subseteq \mathbb{R}^n$ be subspaces. We call $\{\mathcal{U}, \mathcal{V}\}$ a *pair of deflating subspaces* of $\{K, M\}$ if

$$K\mathcal{U} \subseteq \mathcal{V} \quad \text{and} \quad M\mathcal{V} \subseteq \mathcal{U}. \tag{2.7}$$

This definition is essentially the same as the existing ones for the product eigenvalue problem [6, 9, 19]. Let $U \in \mathbb{R}^{n\times k}$ and $V \in \mathbb{R}^{n\times \ell}$ be the basis matrices for the subspaces $\mathcal{U}$ and $\mathcal{V}$, respectively, where $\dim(\mathcal{U}) = k$ and $\dim(\mathcal{V}) = \ell$. Then (2.7) implies that there exist $K_{\mathrm{R}} \in \mathbb{R}^{\ell\times k}$ and $M_{\mathrm{R}} \in \mathbb{R}^{k\times \ell}$ such that

$$KU = VK_{\mathrm{R}}, \quad MV = UM_{\mathrm{R}}. \tag{2.8}$$

Given U and V, both $K_{\rm R}$ and $M_{\rm R}$ are uniquely determined by respective equations in (2.8), but there are numerous way to express them. In fact for any left generalized inverses $U^{\dashv}$ and $V^{\dashv}$ of U and V, respectively, i.e., $U^{\dashv}U = I_k$ and $V^{\dashv}V = I_\ell$,

$$K_{\rm R} = V^{\dashv}KU, \quad M_{\rm R} = U^{\dashv}MV. \tag{2.9}$$

There are infinitely many left generalized inverses $U^{\dashv}$ and $V^{\dashv}$. For example, two of them for U are

$$U^{\dashv} = (U^{\rm T}U)^{-1}U^{\rm T}$$

or

$$U^{\dashv} = (V^{\rm T}U)^{-1}V^{\rm T} \quad \text{if } (V^{\rm T}U)^{-1} \text{ exists.} \tag{2.10}$$

But still $K_{\rm R}$ and $M_{\rm R}$ are unique. The second left generalized inverse (2.10) will become important later in preserving symmetry in K and M.

Define

$$H_{\rm R} = \begin{pmatrix} 0 & K_{\rm R} \\ M_{\rm R} & 0 \end{pmatrix}. \tag{2.11}$$

Then $H_{\rm R}$ is the restriction of H onto $\mathcal{V} \oplus \mathcal{U}$ with respect to the basis matrix $V \oplus U$:

$$\begin{pmatrix} 0 & K \\ M & 0 \end{pmatrix} \begin{pmatrix} V & \\ & U \end{pmatrix} = \begin{pmatrix} V & \\ & U \end{pmatrix} \begin{pmatrix} 0 & K_{\rm R} \\ M_{\rm R} & 0 \end{pmatrix}. \tag{2.12}$$

This also says that $\mathcal{V} \oplus \mathcal{U}$ is an invariant subspace of H. On the other hand, every invariant subspace of H yields a pair of deflating subspaces of $\{K, M\}$ as well.

Theorem 2.4. *1. If $\{\mathcal{U}, \mathcal{V}\}$ is a pair of deflating subspaces of $\{K, M\}$, then $\mathcal{V} \oplus \mathcal{U}$ is an invariant subspace of H.*

2. Let $\mathcal{Z}$ be invariant subspace of H and let $Z = \begin{pmatrix} V \\ U \end{pmatrix}$ be a basis matrix of $\mathcal{Z}$, where $V \in \mathbb{R}^{n\times\ell}$. Then $\{\mathrm{span}(U), \mathrm{span}(V)\}$ is a pair of deflating subspaces of $\{K, M\}$.

Proof. 1. That $\mathcal{V} \oplus \mathcal{U}$ is an invariant subspace of H is a consequence of (2.12).

2. There is a matrix D such that $HZ = ZD$ which leads to $KU = VD$ and $MV = UD$. Thus (2.7) holds for $\mathcal{U} = \mathrm{span}(U)$ and $\mathcal{V} = \mathrm{span}(V)$. □

The following theorem says a subset of eigenvalues and eigenvectors of H can be recovered from those of $H_{\rm R}$.

Theorem 2.5. *Let $\{\mathcal{U}, \mathcal{V}\}$ be a pair of deflating subspaces of $\{K, M\}$ and $U \in \mathbb{R}^{n\times k}$ and $V \in \mathbb{R}^{n\times\ell}$ be the basis matrices for the subspaces $\mathcal{U}$ and $\mathcal{V}$, respectively. Define $K_{\rm R}$, $M_{\rm R}$, and $H_{\rm R}$ by the equations in* (2.8) *and* (2.11)*. Then*

$$H_{\rm R}\hat{z} \equiv \begin{pmatrix} 0 & K_{\rm R} \\ M_{\rm R} & 0 \end{pmatrix} \begin{pmatrix} \hat{y} \\ \hat{x} \end{pmatrix} = \lambda \begin{pmatrix} \hat{y} \\ \hat{x} \end{pmatrix} \equiv \lambda\hat{z}$$

implies (1.1) *with $x = U\hat{x}$ and $y = V\hat{y}$, where $\hat{z} = \begin{pmatrix} \hat{y} \\ \hat{x} \end{pmatrix}$ conformably partitioned.*

Proof. $H_{\rm R}\hat{z} = \lambda\hat{z}$ yields $K_{\rm R}\hat{x} = \lambda\hat{y}$ and $M_{\rm R}\hat{y} = \lambda\hat{x}$. Therefore

$$\begin{aligned} KU\hat{x} &= VK_{\rm R}\hat{x} = \lambda V\hat{y}, \\ MV\hat{y} &= UM_{\rm R}\hat{y} = \lambda U\hat{x}, \end{aligned}$$

as was to be shown. □

$H_{\rm R}$ in (2.11) inherits the block structure in H in (1.1): zero blocks remain zero blocks. But when K and M are symmetric, as in the RPA case, in general $H_{\rm R}$ may lose the symmetry property in its off-diagonal blocks $K_{\rm R}$ and $M_{\rm R}$, not to mention preserving the positive semi-definiteness of K and M. We propose a modification to $H_{\rm R}$ to overcome this potential loss, when $W \stackrel{\rm def}{=} U^{\rm T}V$ is nonsingular. Factorize $W = W_1^{\rm T}W_2$, where W_1 and W_2 are nonsingular, and define

$$H_{\rm SR} = \begin{pmatrix} 0 & W_1^{-\,\rm T}U^{\rm T}KUW_1^{-1} \\ W_2^{-\,\rm T}V^{\rm T}MVW_2^{-1} & 0 \end{pmatrix}. \tag{2.13}$$

Note $H_{\rm SR}$ shares not only the block structure in H but also the symmetry and semi-definiteness in its off-diagonal blocks. In defining $H_{\rm SR}$ here, it is assumed that $U^{\rm T}V$ is nonsingular. For this, we have the following lemma.

Lemma 2.1. *Suppose that one of K and M is definite. Let $\{\mathcal{U},\mathcal{V}\}$ be a pair of deflating subspaces of $\{K,M\}$ with $\dim(\mathcal{U}) = \dim(\mathcal{V}) = k$, and let $U \in \mathbb{R}^{n\times k}$ and $V \in \mathbb{R}^{n\times k}$ be the basis matrices of the subspaces $\mathcal{U}$ and $\mathcal{V}$, respectively. Then $U^{\rm T}V$ is nonsingular.*

Proof. Equations in (2.8) hold for some $K_{\rm R}$ and $M_{\rm R}$. Thus

$$U^{\rm T}KU = U^{\rm T}V\,K_{\rm R}, \quad V^{\rm T}MV = V^{\rm T}U\,M_{\rm R}.$$

Suppose that M is definite. Then $V^{\rm T}MV$ is definite and thus nonsingular; so $V^{\rm T}U$ is nonsingular from the second equation. □

Theorem 2.6. *Let $\{\mathcal{U},\mathcal{V}\}$ be a pair of deflating subspaces of $\{K,M\}$ and $U \in \mathbb{R}^{n\times k}$ and $V \in \mathbb{R}^{n\times \ell}$ be the basis matrices for the subspaces $\mathcal{U}$ and $\mathcal{V}$, respectively. Suppose that $W \stackrel{\rm def}{=} U^{\rm T}V$ is nonsingular and is factorized as $W = W_1^{\rm T}W_2$ with both W_1 and W_2 being nonsingular, and define $H_{\rm SR}$ by (2.13). Then $H_{\rm SR}$ is the restriction of H onto $\mathcal{V}\oplus\mathcal{U}$ with respect to the basis matrix $VW_2^{-1}\oplus UW_1^{-1}$:*

$$H\begin{pmatrix} VW_2^{-1} & \\ & UW_1^{-1}\end{pmatrix} = \begin{pmatrix} VW_2^{-1} & \\ & UW_1^{-1}\end{pmatrix} H_{\rm SR}. \tag{2.14}$$

Consequently, $H_{\rm SR}\hat{z} = \lambda\hat{z}$ implies (1.1) with $x = UW_1^{-1}\hat{x}$ and $y = VW_2^{-1}\hat{y}$, where $\hat{z} = \begin{pmatrix}\hat{y}\\ \hat{x}\end{pmatrix}$ conformably partitioned.

Proof. Equations in (2.8) hold for some $K_{\rm R}$ and $M_{\rm R}$. Thus

$$\begin{aligned} U^{\rm T}KU &= (U^{\rm T}V)K_{\rm R} = W_1^{\rm T}W_2K_{\rm R}, \\ V^{\rm T}MV &= (V^{\rm T}U)M_{\rm R} = W_2^{\rm T}W_1M_{\rm R}, \end{aligned}$$

which gives

$$W_1^{-\,\rm T}U^{\rm T}KUW_1^{-1} = W_2K_{\rm R}W_1^{-1}, \quad W_2^{-\,\rm T}V^{\rm T}MVW_2^{-1} = W_1M_{\rm R}W_2^{-1}. \tag{2.15}$$

Now use (2.8) and (2.15) to get

$$\begin{aligned} K(UW_1^{-1}) &= VK_{\rm R}W_1^{-1} \\ &= (VW_2^{-1})(W_2K_{\rm R}W_1^{-1}) \\ &= (VW_2^{-1})(W_1^{-\,\rm T}U^{\rm T}KUW_1^{-1}), \\ M(VW_2^{-1}) &= (UW_1^{-1})(W_2^{-\,\rm T}V^{\rm T}MVW_2^{-1}). \end{aligned}$$

They yield (2.14). Apply Theorem 2.5 to conclude the proof. □

Equations in (2.15) imply that *under the conditions of* Theorem 2.6, H_{R} *and* H_{SR} *are similar:*

$$H_{\mathrm{SR}} = \begin{pmatrix} 0 & W_2 K_{\mathrm{R}} W_1^{-1} \\ W_1 M_{\mathrm{R}} W_2^{-1} & 0 \end{pmatrix} = \begin{pmatrix} W_2 & 0 \\ 0 & W_1 \end{pmatrix} H_{\mathrm{R}} \begin{pmatrix} W_2 & 0 \\ 0 & W_1 \end{pmatrix}^{-1}, \tag{2.16}$$

which is not at all obvious from (2.11) and (2.13).

A trivial pair of deflating subspaces $\{\mathcal{U}, \mathcal{V}\}$ is when $\mathcal{U} = \mathcal{V} = \mathbb{R}^n$. In particular, for U, $V \in \mathbb{R}^{n\times n}$ satisfying $U^{\mathrm{T}}V = I_n$, matrices

$$H = \begin{pmatrix} 0 & K \\ M & 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & U^{\mathrm{T}}KU \\ V^{\mathrm{T}}MV & 0 \end{pmatrix} \tag{2.17}$$

have the same eigenvalues. In fact, the two matrices in (2.17) are similar because of (2.12) and for the current case

$$\begin{pmatrix} V & \\ & U \end{pmatrix}^{-1} = \begin{pmatrix} U^{\mathrm{T}} & \\ & V^{\mathrm{T}} \end{pmatrix}.$$

Remark **2.2.** For this subsection, our default assumption on $K, M \in \mathbb{R}^{n\times n}$ is not required, except for Lemma 2.1. ◇

2.3 Invariant properties of H_{SR}

In the previous subsection, H_{SR} was introduced as a structure-preserving projection of H onto a pair of deflating subspaces $\{\mathcal{U}, \mathcal{V}\}$. But its definition in (2.13) does not require $\{\mathcal{U}, \mathcal{V}\}$ being a pair of deflating subspaces. In fact, it is well-defined so long as $U^{\mathrm{T}}V$ is nonsingular, where $U, V \in \mathbb{R}^{n\times k}$ are the basis matrices of $\mathcal{U} \subset \mathbb{R}^n$ and $\mathcal{V} \subset \mathbb{R}^n$, respectively. This observation will become critically important in the second part of this paper [2] where H_{SR} is often defined for a pair of *approximate* deflating subspaces and will play the same role in the LR eigenvalue computation as the Rayleigh quotient matrix does for the symmetric eigenvalue computation.

As we just pointed out, we need the non-singularity assumption on $U^{\mathrm{T}}V$ to define H_{SR}. We note that this assumption is independent of the freedom in choosing basis matrices. Now we present a necessary and sufficient condition in terms of canonical angles between subspaces for this assumption. Recall that the *canonical angles* between $\mathcal{U}$ and $\mathcal{V}$ are defined to be [30, Definition 5.3 on p.43]

$$\arccos \sigma_i, \quad i = 1, 2, \ldots, k,$$

where σ_i $(1 \le i \le k)$ are the singular values of $(U^{\mathrm{T}}U)^{-1/2}U^{\mathrm{T}}V(V^{\mathrm{T}}V)^{-1/2}$. Furthermore, we define the angle $\angle(\mathcal{U}, \mathcal{V})$ between $\mathcal{U}$ and $\mathcal{V}$ to be

$$\angle(\mathcal{U}, \mathcal{V}) = \max_i \arccos(\sigma_i) = \arccos(\min_i \sigma_i).$$

Note the canonical angles $\arccos \sigma_i$ and the angle $\angle(\mathcal{U}, \mathcal{V})$ are independent of the choices of basis matrices.

Lemma 2.2. *Let* $U, V \in \mathbb{R}^{n\times k}$ *be basis matrices of* $\mathcal{U} \subset \mathbb{R}^n$ *and* $\mathcal{V} \subset \mathbb{R}^n$*, respectively.*

1. $U^{\mathrm{T}}V$ *is nonsingular if and only if* $\angle(\mathcal{U}, \mathcal{V}) < \pi/2$.
2. *If* $\angle(\mathcal{U}, \mathcal{V}) < \pi/2$*, then* $\mathbb{R}^n = \mathcal{U} \oplus \mathcal{V}^{\perp} = \mathcal{V} \oplus \mathcal{U}^{\perp}$*, where* $\mathcal{U}^{\perp}$ *and* $\mathcal{V}^{\perp}$ *are the orthogonal complements of* $\mathcal{U}$ *and* $\mathcal{V}$*, respectively.*

Proof. Use the notations in the definition of $\angle(\mathcal{U},\mathcal{V})$ above. $U^{\mathrm{T}}V$ is nonsingular if and only if all $1 \geq \sigma_i > 0$ which is equivalent to all $\arccos(\sigma_i) < \pi/2$. This proves item *1*.

Suppose $\angle(\mathcal{U},\mathcal{V}) < \pi/2$ and thus $U^{\mathrm{T}}V$ is nonsingular. Any $x \in \mathbb{R}^n$ can be written as $x = Px + (I-P)x$, where

$$P = U(V^{\mathrm{T}}U)^{-1}V^{\mathrm{T}}. \tag{2.18}$$

Evidently $Px \in \mathcal{U}$. It can be verified that $V^{\mathrm{T}}(I-P) = 0$ which implies $(I-P)x \in \mathcal{V}^{\perp}$. Hence $\mathbb{R}^n = \mathcal{U} + \mathcal{V}^{\perp}$. Furthermore, if $x \in \mathcal{U}$ and $x \in \mathcal{V}^{\perp}$, then

$$x = U\hat{x}, \quad 0 = V^{\mathrm{T}}x = V^{\mathrm{T}}U\hat{x}$$

which implies $\hat{x} = 0$ and so must $x = 0$ because $V^{\mathrm{T}}U$ is nonsingular. This proves $\mathbb{R}^n = \mathcal{U} \oplus \mathcal{V}^{\perp}$. Similarly $\mathbb{R}^n = \mathcal{V} \oplus \mathcal{U}^{\perp}$. □

Unique subspaces:

$$\mathcal{U} = \mathrm{span}(U), \quad \mathcal{V} = \mathrm{span}(V)$$

are implied by the way H_{SR} is defined, and they satisfy $\angle(\mathcal{U},\mathcal{V}) < \pi/2$. On the other hand, two subspaces $\mathcal{U}$ and $\mathcal{V}$ satisfying $\angle(\mathcal{U},\mathcal{V}) < \pi/2$ lead to (infinitely) many H_{SR}, due to the following two non-unique choices:

$$\begin{cases} 1.\ \text{Factorization } W = W_1^{\mathrm{T}}W_2 \text{ is not unique.} \\ 2.\ \text{Basis matrices } U \text{ and } V \text{ are not unique.} \end{cases} \tag{2.19}$$

In the next theorem, we present two invariant properties of H_{SR} with respect to these two non-unique choices. The properties are important in speaking about eigenvalue and eigenvector approximations from a pair of approximate deflating subspaces in [2].

Theorem 2.7. *Let $\mathcal{U},\mathcal{V} \subset \mathbb{R}^n$ be two subspaces of dimension k such that $\angle(\mathcal{U},\mathcal{V}) < \pi/2$. We have the following invariant properties of H_{SR}.*

1. *The eigenvalues of H_{SR} defined by* (2.13) *are invariant with respect to any of the non-uniqueness listed in* (2.19)*;*

2. *For any invariant subspace $\mathcal{E}$ of H_{SR},*

$$\left\{ \begin{pmatrix} VW_2^{-1} & \\ & UW_1^{-1} \end{pmatrix} \hat{z} \,:\, \hat{z} \in \mathcal{E} \right\} \tag{2.20}$$

is invariant with respect to any of the non-uniqueness listed in (2.19)*. By which we mean for any two realizations H_0 and H_1 of H_{SR} and the subspace* (2.20) *obtained from an invariant subspace $\mathcal{E}_0$ of H_0, there exists an invariant subspace $\mathcal{E}_1$ of H_1 which produces the same subspace* (2.20)*. In particular, if $\mathcal{E}$ has dimension* 1*, this gives an invariant property on the eigenvectors of H_{SR}.*

Proof. We first show the invariant properties with respect to different factorizations $W = W_1^{\mathrm{T}}W_2$. To this end, we note that $H_1 \stackrel{\mathrm{def}}{=} H_{\mathrm{SR}}$ with $W = W_1^{\mathrm{T}}W_2$ and $H_0 \stackrel{\mathrm{def}}{=} H_{\mathrm{SR}}$ with $W = I_k^{\mathrm{T}} \cdot W$ are similar:

$$\begin{pmatrix} W_1^{-\mathrm{T}} & \\ & W_1 \end{pmatrix}^{-1} H_1 \begin{pmatrix} W_1^{-\mathrm{T}} & \\ & W_1 \end{pmatrix} = \begin{pmatrix} W_1^{\mathrm{T}} & \\ & W_1^{-1} \end{pmatrix} H_1 \begin{pmatrix} W_1^{-\mathrm{T}} & \\ & W_1 \end{pmatrix} = H_0.$$

Next we verify the invariant properties with respect to different choices of basis matrices. To this end, it suffices to verify the invariant properties under the following substitutions:

$$UR \leftarrow U, \quad VS \leftarrow V, \quad W_1R \leftarrow W_1, \quad W_2S \leftarrow W_2, \tag{2.21}$$

where R, $S \in \mathbb{R}^{k\times k}$ are nonsingular because we have just proved the properties with respect to different decompositions of W. The verification is straightforward because H_{SR} and

$$\begin{pmatrix} VW_2^{-1} & \\ & UW_1^{-1} \end{pmatrix}$$

do not change under the substitutions (2.21). □

REMARK **2.3.** For this subsection, our default assumption on $K, M \in \mathbb{R}^{n\times n}$ is not required. ◇

3 Minimization principles

We recall three well-known results for a symmetric matrix $\boldsymbol{\Xi} \in \mathbb{R}^{m\times m}$. Denote by θ_i $(1 \le i \le m)$ $\boldsymbol{\Xi}$'s eigenvalues in ascending order. The first well-known result is the following minimization principle for $\boldsymbol{\Xi}$'s smallest eigenvalue θ_1:

$$\theta_1 = \min_x \frac{x^{\mathrm{T}}\boldsymbol{\Xi}x}{x^{\mathrm{T}}x}. \tag{3.1}$$

The trace (or subspace) version of (3.1), the second well-known result, is

$$\sum_{i=1}^{k} \theta_i = \min_{U\in\mathbb{R}^{m\times k}, U^{\mathrm{T}}U=I_k} \operatorname{trace}(U^{\mathrm{T}}\boldsymbol{\Xi}U) \tag{3.2}$$

which is a corollary of Wielandt's theorem [30, p.199]. Furthermore, given any $U \in \mathbb{R}^{n\times k}$ such that $U^{\mathrm{T}}U = I_k$, denote by μ_i $(1 \le i \le k)$ the eigenvalues of the projection matrix $U^{\mathrm{T}}\boldsymbol{\Xi}U$ in ascending order. We have Cauchy's interlacing inequalities – the third well-known result:

$$\theta_i \le \mu_i \le \theta_{i+m-k} \quad \text{for } 1 \le k. \tag{3.3}$$

The proofs of these well-known theoretical results can be found, for example, in [7, 25, 30]. They are crucial to the establishment of efficient numerical methods for the symmetric eigenvalue problem, and largely responsible for why the symmetric eigenvalue problems are regarded as *nice* eigenvalue problems in a wide range of applications.

In this section, we establish analogs of these results mainly for the LR eigenvalue problem (1.1).

3.1 Minimization principles

Theorem 3.1 is an analog of the minimization principle (3.1) for the symmetric matrix $\boldsymbol{\Xi}$. It is essentially (1.11) due to Tsiper [33, 34] who deduced it from (1.8) due to Thouless [31], except we allow one of K and M to be singular. We note that Theorem 3.2 presents a subspace version of Theorem 3.1. Although Theorem 3.1 is a corollary of Theorem 3.2, we decide to give a short proof because the proof of Theorem 3.2 is long and complicated, and is deferred to appendix A.

Theorem 3.1. *Suppose that one of K, $M \in \mathbb{R}^{n\times n}$ is definite. Then we have*

$$\lambda_1 = \inf_{x,y} \rho(x, y), \tag{3.4}$$

where the infimum is taken over all $x, y \in \mathbb{R}^n$ such that $x^{\mathrm{T}}y \neq 0$. Moreover, "inf" can be replaced by "min" if and only if both K and M are definite. When they are definite, the optimal argument pair (x, y) gives rise to an eigenvector $z = \begin{pmatrix} y \\ x \end{pmatrix}$ of H associated with λ_1.

Proof. Note $\rho(x,y) \geq 0$ for any x and y. If K is singular, then $\lambda_1 = +0$. Pick $x \neq 0$ such that $Kx = 0$. Then $x^{\mathrm{T}}Mx > 0$ since one of K and M is assumed definite. We have

$$\rho(x, \epsilon x) = |\epsilon|\, x^{\mathrm{T}}Mx/(2|x^{\mathrm{T}}x|) \to 0 \quad \text{as} \quad \epsilon \to 0.$$

This is (3.4) for the case. We now show that "inf" cannot be replaced by "min". Suppose there were x and y such that $x^{\mathrm{T}}y \neq 0$ and $\rho(x,y) = 0$. We note that $\rho(x,y) = 0$ and $x^{\mathrm{T}}y \neq 0$ imply $x^{\mathrm{T}}Kx = y^{\mathrm{T}}My = 0$ which in turn implies $Kx = My = 0$, contradicting that one of K and M is definite.

Suppose K and M are definite. Then $\lambda_1 > 0$ and equations in (2.4) hold for some nonsingular $Y \in \mathbb{R}^{n\times n}$ and $X = Y^{-\mathrm{T}}$. We have

$$\begin{aligned}
\min_{x,y} \frac{x^{\mathrm{T}}Kx + y^{\mathrm{T}}My}{2|x^{\mathrm{T}}y|} &= \min_{x,y} \frac{x^{\mathrm{T}}Y\Lambda^2Y^{\mathrm{T}}x + y^{\mathrm{T}}Y^{-\mathrm{T}}Y^{-1}y}{2|x^{\mathrm{T}}YY^{-1}y|} \\
&= \min_{\widetilde{x},\widetilde{y}} \frac{\widetilde{x}^{\mathrm{T}}\Lambda^2\widetilde{x} + \widetilde{y}^{\mathrm{T}}\widetilde{y}}{2|\widetilde{x}^{\mathrm{T}}\widetilde{y}|} \\
&\geq \min_{\widetilde{x},\widetilde{y}} \frac{2\sum_i \lambda_i |\widetilde{x}_{(i)}\widetilde{y}_{(i)}|}{2|\sum_i \widetilde{x}_{(i)}\widetilde{y}_{(i)}|} \qquad (3.5) \\
&\geq \lambda_1, \qquad (3.6)
\end{aligned}$$

where $\widetilde{x} = Y^{\mathrm{T}}x$ and $\widetilde{y} = Y^{-1}y$. Suppose $0 < \lambda_1 = \cdots = \lambda_\ell < \lambda_{\ell+1} \leq \cdots \leq \lambda_n$. Both equality signs in (3.5) and (3.6) hold if and only if

$$\begin{aligned}
\widetilde{x}_{(i)}\lambda_i &= \widetilde{y}_{(i)} \qquad \text{for } 1 \leq i \leq n, \\
\widetilde{x}_{(i)} &= \widetilde{y}_{(i)} = 0 \quad \text{for } \ell < i \leq n,
\end{aligned}$$

i.e., $\widetilde{y} = \Lambda\widetilde{x}$ and $\widetilde{x}_{(\ell+1:n)} = \widetilde{y}_{(\ell+1:n)} = 0$. So for their corresponding optimal argument pair (x,y),

$$Kx = KY^{-\mathrm{T}}\widetilde{x} = KX\widetilde{x} = Y\Lambda^2\widetilde{x} = Y\Lambda\widetilde{y} = \lambda_1 Y\widetilde{y} = \lambda_1 y,$$

and similarly $My = \lambda_1 x$. □

Remark **3.1.** Equation (3.4) is actually true even if both K and M are singular (but still positive semi-definite, of course). There are two cases.

1. Both K and M are singular and their kernels are not orthogonal to each other, i.e., there are nonzero vectors x and y such that $Kx = My = 0$ and $x^{\mathrm{T}}y \neq 0$. For such a case, we have
$$\lambda_1 = \min_{x,y} \rho(x,y). \qquad (3.7)$$

2. Both K and M are singular but their kernels are orthogonal to each other. For such a case, we have (3.4) but "inf" cannot be replaced by "min". Here is why. Since K is singular, we pick $x \neq 0$ such that $Kx = 0$. Then $Mx \neq 0$ because the kernels of K and M are orthogonal to each other. So $x^{\mathrm{T}}M = (Mx)^{\mathrm{T}} \neq 0$ which says at least one of the columns of M is not orthogonal to x, and take y to be one of such a column. Now we see
$$\rho(x, \epsilon y) = |\epsilon|\, y^{\mathrm{T}}My/(2|x^{\mathrm{T}}y|) \to 0 \quad \text{as} \quad \epsilon \to 0.$$
This gives (3.4) since $\rho(\cdot,\cdot) \geq 0$ always. To see "inf" cannot be replaced by "min", we assume there were x and y such that $x^{\mathrm{T}}y \neq 0$ and $\rho(x,y) = 0$. We note that $\rho(x,y) = 0$ and $x^{\mathrm{T}}y \neq 0$ imply $x^{\mathrm{T}}Kx = y^{\mathrm{T}}My = 0$ which in turn implies $Kx = My = 0$, contradicting the assumption that the kernels of K and M are orthogonal to each other. ◇

Remark **3.2.** The first part of Theorem 3.1 – equation (3.4) for positive definite K and M – can also be deduced from the equivalence between the eigenvalue problem (1.1) and the one for (1.14). Suppose that both K and M are definite; so is $\boldsymbol{A}$ in (1.14). Note that λ_1^{-1} is the largest and $-\lambda_1^{-1}$ the smallest eigenvalue of the definite pencil $\boldsymbol{B}-\lambda\boldsymbol{A}$, and thus for any $0 \neq z = \begin{pmatrix} y \\ x \end{pmatrix} \in \mathbb{R}^{2n}$

$$\left[-\lambda_1^{-1}, \lambda_1^{-1}\right] \ni \frac{z^{\mathrm{T}}\boldsymbol{B}z}{z^{\mathrm{T}}\boldsymbol{A}z} \Rightarrow \frac{z^{\mathrm{T}}\boldsymbol{A}z}{z^{\mathrm{T}}\boldsymbol{B}z} \in (-\infty, -\lambda_1] \cup [\lambda_1, \infty). \tag{3.8}$$

Since $\pm\lambda_1^{-1}$ are eigenvalues of $\boldsymbol{B}-\lambda\boldsymbol{A}$ and thus attainable by $z^{\mathrm{T}}\boldsymbol{B}z/z^{\mathrm{T}}\boldsymbol{A}z$ for some z; so are $\pm\lambda_1$ are by $z^{\mathrm{T}}\boldsymbol{A}z/z^{\mathrm{T}}\boldsymbol{B}z$ for some z. By (3.8) and that $z^{\mathrm{T}}\boldsymbol{A}z > 0$ for $z \neq 0$, we have

$$\lambda_1 = \min_{z\neq 0}\left|\frac{z^{\mathrm{T}}\boldsymbol{A}z}{z^{\mathrm{T}}\boldsymbol{B}z}\right| = \min_{z\neq 0}\frac{x^{\mathrm{T}}Kx + y^{\mathrm{T}}My}{2|x^{\mathrm{T}}y|}$$

which is equation (3.4) (with "inf" replaced by "min") for positive definite K and M. One may also use Fischer's min-max principle [30, p.201] on $\boldsymbol{B}-\lambda\boldsymbol{A}$ to deduce expressions for other λ_j^{-1}:

$$\lambda_j^{-1} = \max_{\mathcal{S}_j}\min_{0\neq z\in\mathcal{S}_j}\frac{z^{\mathrm{T}}\boldsymbol{B}z}{z^{\mathrm{T}}\boldsymbol{A}z} = \max_{\mathcal{S}_j}\min_{0\neq z\in\mathcal{S}_j}\frac{2x^{\mathrm{T}}y}{x^{\mathrm{T}}Kx + y^{\mathrm{T}}My}, \tag{3.9a}$$

$$\lambda_j^{-1} = \min_{\mathcal{S}_{2n-j+1}}\max_{0\neq z\in\mathcal{S}_{2n-j+1}}\frac{z^{\mathrm{T}}\boldsymbol{B}z}{z^{\mathrm{T}}\boldsymbol{A}z} = \min_{\mathcal{S}_{2n-j+1}}\max_{0\neq z\in\mathcal{S}_{2n-j+1}}\frac{2x^{\mathrm{T}}y}{x^{\mathrm{T}}Kx + y^{\mathrm{T}}My}. \tag{3.9b}$$

But it seems that they do not yield any min-max principle of λ_j in terms of $(x^{\mathrm{T}}Kx+y^{\mathrm{T}}My)/(2x^{\mathrm{T}}y)$ because it can be positive, 0, and negative. ◇

Our next theorem – Theorem 3.2 – presents a subspace version of Theorem 3.1. It is the reason we mentioned in section 1 that the expression in (1.13) can be regarded as a *proper subspace version* of the Thouless functional in the form of $\rho(\cdot,\cdot)$.

Theorem 3.2. *Suppose that one of K, $M \in \mathbb{R}^{n\times n}$ is definite. Then we have*

$$\sum_{i=1}^{k}\lambda_i = \frac{1}{2}\inf_{U^{\mathrm{T}}V=I_k}\operatorname{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV). \tag{3.10}$$

*Moreover, "*inf*" can be replaced by "*min*" if and only if both K and M are definite. When they are definite and if also $\lambda_k < \lambda_{k+1}$, then for any U and V that attain the minimum, $\{\operatorname{span}(U), \operatorname{span}(V)\}$ is a pair of deflating subspaces of $\{K, M\}$ and the corresponding H_{SR} (and H_{R}, too) has eigenvalues $\pm\lambda_i$ $(1 \le i \le k)$.*

Proof. The proof is long and deferred to appendix A. □

Corollary 3.1. *Suppose that one of K, $M \in \mathbb{R}^{n\times n}$ is definite. Then*

$$\sum_{i=1}^{n}\lambda_i = \frac{1}{2}\inf_{U^{\mathrm{T}}V=I_n}\operatorname{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV). \tag{3.11}$$

Remark **3.3.** In (3.2) which is for the symmetric eigenvalue problem of $\boldsymbol{\Xi} = \boldsymbol{\Xi}^{\mathrm{T}} \in \mathbb{R}^{m\times m}$, if $k = m$, then

$$\sum_{i=1}^{m}\theta_i = \operatorname{trace}(U^{\mathrm{T}}\boldsymbol{\Xi}U), \tag{3.12}$$

regardless of $U \in \mathbb{R}^{m\times m}$ so long as $U^{\mathrm{T}}U = I_m$. There is certainly a strong resemblance between (3.11) and (3.12), but a fundamental difference, too. That is that "inf" has to be there in (3.11). Without "inf", (3.11) becomes

$$\sum_{i=1}^{n} \lambda_i \le \frac{1}{2}\,\mathrm{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV) \tag{3.13}$$

for any two U, $V \in \mathbb{R}^{n\times n}$ satisfying $U^{\mathrm{T}}V = I_n$. For example, consider

$$K = \begin{pmatrix} \lambda_1^2 & 0 \\ 0 & \lambda_2^2 \end{pmatrix}, \quad M = I_2, \quad U = \begin{pmatrix} \xi_1 & 0 \\ 0 & \xi_2 \end{pmatrix}, \quad V = U^{-\,\mathrm{T}} = \begin{pmatrix} \xi^{-1} & 0 \\ 0 & \xi_2^{-1} \end{pmatrix},$$

where $0 < \lambda_1 \le \lambda_2$ and $0 \ne \xi_i \in \mathbb{R}$. Then we have

$$\frac{1}{2}\,\mathrm{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV) = \sum_{i=1}^{2} \frac{\xi_i^2\lambda_i^2 + \xi_i^{-2}}{2} \ge \sum_{i=1}^{2} \lambda_i,$$

where the equality sign holds if and only if $|\xi_i| = 1/\sqrt{\lambda_i}$ for $i = 1, 2$. ◇

Exploiting the close relation through (1.6) between the two different forms of the Thouless functionals $\varrho(\cdot,\cdot)$ and $\rho(\cdot,\cdot)$, we have by Theorem 3.2 the following theorem. It suggests that

$$\frac{1}{2}\,\mathrm{trace}\Big(\begin{pmatrix} U \\ V \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} A & B \\ B & A \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}\Big) \quad \text{subject to } U^{\mathrm{T}}U - V^{\mathrm{T}}V = 2I_k,\ U^{\mathrm{T}}V = V^{\mathrm{T}}U \tag{3.14}$$

is a *proper subspace version* of the Thouless functional in the form of $\varrho(\cdot,\cdot)$.

Theorem 3.3. *Suppose that A and B are $n \times n$ real symmetric matrices and that $A + B$ and $A - B$ are positive semi-definite and one of them is definite. Then we have*

$$\sum_{i=1}^{k} \lambda_i = \frac{1}{2} \inf_{\substack{U^{\mathrm{T}}U - V^{\mathrm{T}}V = 2I_k \\ U^{\mathrm{T}}V = V^{\mathrm{T}}U}} \mathrm{trace}\Big(\begin{pmatrix} U \\ V \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} A & B \\ B & A \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}\Big). \tag{3.15}$$

*Moreover, "*inf*" can be replaced by "*min*" if and only if both $A \pm B$ are definite.*

Proof. Assume the assignments in (1.5) for K and M. We have by (1.7)

$$\begin{pmatrix} U \\ V \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} A & B \\ B & A \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix} = \begin{pmatrix} \hat{V} \\ \hat{U} \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} M & \\ & K \end{pmatrix} \begin{pmatrix} \hat{V} \\ \hat{U} \end{pmatrix} = \hat{U}^{\mathrm{T}}K\hat{U} + \hat{V}^{\mathrm{T}}M\hat{V},$$

where

$$\begin{pmatrix} \hat{V} \\ \hat{U} \end{pmatrix} = J^{\mathrm{T}} \begin{pmatrix} U \\ V \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} U + V \\ U - V \end{pmatrix},$$

and J is given by (1.3). Therefore

$$\begin{aligned} &\inf_{\hat{U}^{\mathrm{T}}\hat{V} = I_k} \mathrm{trace}(\hat{U}^{\mathrm{T}}K\hat{U} + \hat{V}^{\mathrm{T}}M\hat{V}) \\ &\qquad = \inf_{(U-V)^{\mathrm{T}}(U+V) = 2I_k} \mathrm{trace}\Big(\begin{pmatrix} U \\ V \end{pmatrix}^{\mathrm{T}} \begin{pmatrix} A & B \\ B & A \end{pmatrix} \begin{pmatrix} U \\ V \end{pmatrix}\Big). \end{aligned} \tag{3.16}$$

We claim

$$(U - V)^{\mathrm{T}}(U + V) = 2I_k \quad \Leftrightarrow \quad U^{\mathrm{T}}U - V^{\mathrm{T}}V = 2I_k \text{ and } U^{\mathrm{T}}V = V^{\mathrm{T}}U. \tag{3.17}$$

This is because $(U-V)^{\mathrm{T}}(U+V)=2I_k$ and its transpose version give

$$U^{\mathrm{T}}U+U^{\mathrm{T}}V-V^{\mathrm{T}}U-V^{\mathrm{T}}V=2I_k, \tag{3.18a}$$

$$U^{\mathrm{T}}U+V^{\mathrm{T}}U-U^{\mathrm{T}}V-V^{\mathrm{T}}V=2I_k. \tag{3.18b}$$

Add both equations in (3.18) to get $U^{\mathrm{T}}U-V^{\mathrm{T}}V=2I_k$ and subtract one from the other to get $U^{\mathrm{T}}V=V^{\mathrm{T}}U$. That the right-hand side in (3.17) implies its left-hand side can be seen from any of the equations in (3.18). Equation (3.15) is now a consequence of Theorem 3.2, (3.16), and (3.17). □

3.2 Cauchy-like interlacing inequalities

In the following theorem, we obtain inequalities that can be regarded as an extension of Cauchy's interlacing inequalities (3.3).

Theorem 3.4. *Suppose that one of K, $M\in\mathbb{R}^{n\times n}$ is definite. Let $U,V\in\mathbb{R}^{n\times k}$ such that $U^{\mathrm{T}}V$ is nonsingular. Write $W=U^{\mathrm{T}}V=W_1^{\mathrm{T}}W_2$, where $W_i\in\mathbb{R}^{k\times k}$ are nonsingular, and define H_{SR} by* (2.13)*. Denote by $\pm\mu_i$ $(1\le i\le k)$ the eigenvalues of H_{SR}, where $0\le\mu_1\le\cdots\le\mu_k$. Then*

$$\lambda_i\le\mu_i\le\frac{\sqrt{\min\{\kappa(K),\kappa(M)\}}}{\cos\angle(\mathcal{U},\mathcal{V})}\,\lambda_{i+n-k}\quad \textit{for } 1\le i\le k, \tag{3.19}$$

where $\mathcal{U}=\operatorname{span}(U)$ and $\mathcal{V}=\operatorname{span}(V)$, and $\kappa(K)$ and $\kappa(M)$ are spectral condition numbers. Furthermore, if $\lambda_k<\lambda_{k+1}$ and $\lambda_i=\mu_i$ for $1\le i\le k$, then[3]

1. *$\mathcal{U}=\operatorname{span}(X_{(1:k,:)})$ when M is definite, where X is as in* Theorem 2.3*;*
2. *$\{\mathcal{U},\mathcal{V}\}$ is a pair of deflating subspaces of $\{K,M\}$ corresponding to the eigenvalues $\pm\lambda_i$ $(1\le i\le k)$ of H when both K and M are definite.*

Proof. The proof is long and deferred to appendix A. □

Remark **3.4.** Strengthen the conditions of Theorem 3.4 to: both K and M are definite. Recall the equivalence between the eigenvalue problem (1.1) and the one for (1.14). Let

$$Z=\begin{pmatrix} VW_2^{-1} & \\ & UW_1^{-1}\end{pmatrix}.$$

We have

$$Z^{\mathrm{T}}\boldsymbol{A}Z=\begin{pmatrix} W_2^{-\mathrm{T}}V^{\mathrm{T}}MVW_2^{-1} & 0\\ 0 & W_1^{-\mathrm{T}}U^{\mathrm{T}}KUW_1^{-1}\end{pmatrix},\quad Z^{\mathrm{T}}\boldsymbol{B}Z=\begin{pmatrix}0 & I_k\\ I_k & 0\end{pmatrix}. \tag{3.20}$$

The eigenvalues of H_{SR} are the same as those for the pencil $Z^{\mathrm{T}}\boldsymbol{A}Z-\lambda Z^{\mathrm{T}}\boldsymbol{B}Z$. Apply Cauchy's interlacing inequalities (extended for the generalized eigenvalue problem) to $\boldsymbol{B}-\lambda\boldsymbol{A}$ and $Z^{\mathrm{T}}\boldsymbol{B}Z-\lambda Z^{\mathrm{T}}\boldsymbol{A}Z$ to get

$$\lambda_i^{-1}\ge\mu_i^{-1}\ge\begin{cases}\lambda_{i+2n-2k}^{-1}, & \text{if } i+2n-2k\le n,\\ 0, & \text{otherwise.}\end{cases}$$

Equivalently

$$\lambda_i\le\mu_i\le\lambda_{i+2n-2k}\quad\text{for } 1\le i\le k, \tag{3.21}$$

where $\lambda_j=\infty$ for $j>n$. The second inequality in (3.21) looks more elegant than those in (3.19) but not without a price that some of them could be ∞. Later in Remark 3.5, we will present an example to show the factor $[\cos\angle(\mathcal{U},\mathcal{V})]^{-1}$ in (3.19) cannot be removed. ◇

[3] A similar statement for the case in which K is definite (but M is semi-definite) can be made, noting that the decompositions in (2.4) no longer hold but similar decompositions exist.

Corollary 3.2. *Suppose that one of K, $M \in \mathbb{R}^{n\times n}$ is definite. Let K_p and M_p be $k\times k$ principal submatrices of K and M, extracted with same row and column indices for both. Denote by $\pm\mu_i$ $(1 \le i \le k)$ the eigenvalues of $\begin{pmatrix} 0 & K_p \\ M_p & 0 \end{pmatrix}$, where $0 \le \mu_1 \le \cdots \le \mu_k$. Then*

$$\lambda_i \le \mu_i \le \sqrt{\min\{\kappa(K), \kappa(M)\}}\, \lambda_{i+n-k} \quad \text{for } 1 \le i \le k. \tag{3.22}$$

Proof. Let $i_1, i_2, \ldots, i_k$ be the row and column indices of K and M that give K_p and M_p, and let $U = (e_{i_1}, e_{i_2}, \ldots, e_{i_k}) \in \mathbb{R}^{n\times k}$. Then $K_p = U^{\mathrm{T}}KU$ and $M_p = U^{\mathrm{T}}MU$. Apply Theorem 3.4 with $V = U$ to conclude the proof. □

Remark **3.5.** Inequalities (3.19), (3.21), and (3.22) mirror Cauchy's interlacing inequalities (3.3). But the upper bounds on μ_i by (3.19) and (3.22) are more complicated. The following example shows that the factor $[\cos\angle(\mathcal{U},\mathcal{V})]^{-1}$ in general cannot be removed. Consider

$$K = \begin{pmatrix} \alpha^2 & 0 \\ 0 & \beta^2 \end{pmatrix}, \quad M = I_2, \quad U = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad V = \begin{pmatrix} t \\ 1 \end{pmatrix},$$

where $0 < \alpha < \beta$ and $t = \tan\angle(\mathcal{U},\mathcal{V})$. Then the positive eigenvalue of H_{SR} is

$$\mu_1 = \sqrt{U^{\mathrm{T}}KUV^{\mathrm{T}}MV} = \beta\sqrt{1+t^2} = \frac{\lambda_2}{\cos\angle(\mathcal{U},\mathcal{V})}.$$

An application of (3.21) leads to $\alpha = \lambda_1 \le \mu_1 \le \lambda_{1+4-2} = \infty$. *We suspect that* $\sqrt{\min\{\kappa(K), \kappa(M)\}}$ *in* (3.19) *and* (3.22) *could be removed or at least be replaceable by something that does not depend on the condition numbers*, but we have no proof, except for the special case as detailed in the following theorem. ◇

Theorem 3.5. *Under the assumptions of* Theorem 3.4*, if either $\mathcal{U} \subseteq M\mathcal{V}$ when M is definite or $\mathcal{V} \subseteq K\mathcal{U}$ when K is definite, then*

$$\lambda_i \le \mu_i \le \lambda_{i+n-k} \quad \text{for } 1 \le i \le k. \tag{3.23}$$

Proof. We will prove (3.23), assuming M is definite and $\mathcal{U} \subseteq M\mathcal{V}$. Since M is definite, $\dim(M\mathcal{V})^{\perp} = n-k$, where $(M\mathcal{V})^{\perp}$ is the orthogonal complement of $M\mathcal{V}$. Let $V_{\perp} \in \mathbb{R}^{n\times(n-k)}$ be a basis matrix of $(M\mathcal{V})^{\perp}$. Then $V_{\perp}^{\mathrm{T}}MV = 0$ and also $U^{\mathrm{T}}V_{\perp} = 0$ because $\mathcal{U} \subseteq M\mathcal{V}$. Let

$$\boldsymbol{U} = \left(UW_1^{-1}, MV_{\perp}(V_{\perp}^{\mathrm{T}}MV_{\perp})^{-1/2}\right), \quad \boldsymbol{V} = \left(VW_2^{-1}, V_{\perp}(V_{\perp}^{\mathrm{T}}MV_{\perp})^{-1/2}\right).$$

It can be verified that $\boldsymbol{U}^{\mathrm{T}}\boldsymbol{V} = I_n$ (which implies $\boldsymbol{V}^{\mathrm{T}}\boldsymbol{U} = I_n$ also) and

$$\widehat{M} \stackrel{\text{def}}{=} \boldsymbol{V}^{\mathrm{T}}M\boldsymbol{V} = \begin{pmatrix} W_2^{-\mathrm{T}}V^{\mathrm{T}}MVW_2^{-1} & \\ & I_{n-k} \end{pmatrix}.$$

Let $\widehat{K} = \boldsymbol{U}^{\mathrm{T}}K\boldsymbol{U}$. Notice that

$$\mathrm{eig}(\widehat{K}\widehat{M}) = \mathrm{eig}(\widehat{M}^{1/2}\widehat{K}\widehat{M}^{1/2}) = \{\lambda_i^2,\ i = 1, 2, \ldots, n\},$$

where $\mathrm{eig}(\cdot)$ is the set of eigenvalues of a matrix. The $k\times k$ leading principal matrix of $\widehat{M}^{1/2}\widehat{K}\widehat{M}^{1/2}$ is

$$(W_2^{-\mathrm{T}}V^{\mathrm{T}}MVW_2^{-1})^{1/2}(W_1^{-\mathrm{T}}U^{\mathrm{T}}KUW_1^{-1})(W_2^{-\mathrm{T}}V^{\mathrm{T}}MVW_2^{-1})^{1/2} \tag{3.24}$$

whose eigenvalues are μ_i^2, $i = 1, 2, \ldots, k$. Apply Cauchy's interlacing inequalities to $\widehat{M}^{1/2}\widehat{K}\widehat{M}^{1/2}$ and its $k\times k$ leading principal matrix (3.24) to get

$$\lambda_i^2 \le \mu_i^2 \le \lambda_{i+n-k}^2 \quad \text{for } 1 \le i \le k$$

which yield (3.23). □

3.3 Minimization principle and deflation

Deflation is a commonly used technique in solving eigenvalue problems. The basic idea is to avoid computing these eigenpairs that have been already computed to a prescribed accuracy, and it is accomplished by orthogonalizing current vectors against all already converged eigenvectors. Return to the symmetric eigenvalue problem for $\boldsymbol{\Xi}$ we discussed at the beginning of this section. Denote by x_i $(1 \le i \le m)$ the eigenvectors of $\boldsymbol{\Xi}$ corresponding to θ_i. We may assume $x_i^{\mathrm{T}} x_j = 0$ for $i \ne j$. In (3.1), if "min" is restricted to all x that is orthogonal to x_i $(1 \le i \le \ell)$, then the minimum becomes $\theta_{\ell+1}$. Similarly, if U is restricted to those such that $U^{\mathrm{T}} x_i = 0$ $(1 \le i \le \ell)$, then the minimum in (3.2) is $\sum_{i=1}^{k} \theta_{\ell+i}$, and (3.3) becomes $\theta_{\ell+i} \le \mu_i \le \theta_{i+m-k}$. The next theorem gives similar results for H.

Theorem 3.6. *Suppose that one of K, $M \in \mathbb{R}^{n\times n}$ is definite. Denote by $z_i = \begin{pmatrix} y_i \\ x_i \end{pmatrix}$ $(1 \le i \le \ell)$ the linear independent eigenvectors of H corresponding to eigenvalues λ_i, respectively, where all x_i, $y_i \in \mathbb{R}^n$. Set $Y_1 = (y_1, y_2, \ldots, y_\ell)$ and $X_1 = (x_1, x_2, \ldots, x_\ell)$.*

1. *We have*
$$\sum_{i=1}^{k} \lambda_{\ell+i} = \frac{1}{2} \inf_{\substack{U^{\mathrm{T}}V = I_k \\ U^{\mathrm{T}}Y_1 = 0, V^{\mathrm{T}}X_1 = 0}} \operatorname{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV). \tag{3.25}$$
If also $0 < \lambda_{\ell+1}$ and $\lambda_{\ell+k} < \lambda_{\ell+k+1}$, then for any U and V that attain the minimum, $\{\operatorname{span}(U), \operatorname{span}(V)\}$ is a pair of deflating subspaces of $\{K, M\}$ corresponding to the eigenvalues $\pm\lambda_{\ell+i}$ $(1 \le i \le k)$ of H.

2. *Let $U, V \in \mathbb{R}^{n\times k}$ such that $U^{\mathrm{T}}V$ is nonsingular, $U^{\mathrm{T}}Y_1 = 0$ and $V^{\mathrm{T}}X_1 = 0$. Write $W = U^{\mathrm{T}}V = W_1^{\mathrm{T}}W_2$, where $W_i \in \mathbb{R}^{k\times k}$ are nonsingular, and define H_{SR} by (2.13). Denote by $\pm\mu_i$ $(1 \le i \le k)$ the eigenvalues of H_{SR}, where $0 \le \mu_1 \le \cdots \le \mu_k$. Then*
$$\lambda_{\ell+i} \le \mu_i \le \frac{\sqrt{\min\{\kappa(K), \kappa(M)\}}}{\cos\angle(\mathcal{U}, \mathcal{V})} \lambda_{i+n-k} \quad \text{for } 1 \le i \le k. \tag{3.26}$$
If also $0 < \lambda_{\ell+1}$ and $\lambda_{\ell+k} < \lambda_{\ell+k+1}$ and if $\lambda_{\ell+i} = \mu_i$ for $1 \le i \le k$, then $\{\operatorname{span}(U), \operatorname{span}(V)\}$ is a pair of deflating subspaces of $\{K, M\}$ corresponding to the eigenvalues $\pm\lambda_{\ell+i}$ $(1 \le i \le k)$ of H.

Proof. See appendix A. □

4 Concluding remarks

We have obtained new minimization principles and Cauchy-like interlacing inequalities for the LR (a.k.a. RPA) eigenvalue problem in computational quantum chemistry and physics. Also obtained is a structure-preserving projection H_{SR} of H onto a pair of subspaces. The role of H_{SR} for the LR eigenvalue problem (1.1) in many ways is the same as that of the Rayleigh quotient matrix for the symmetric eigenvalue problem. These new results mirror the three well-known results for the eigenvalue problem of a real symmetric matrix. They lay the foundation for our numerical investigation in the second paper of this sequel where new efficient numerical methods will be devised for computing the first few smallest eigenvalues with the positive sign and corresponding eigenvectors simultaneously.

Although, throughout this paper and its following one, it is assumed both K and M are real matrices, all results are valid for Hermitian positive semi-definite K and M with one of them

being definite after minor changes: replacing all $\mathbb{R}$ by $\mathbb{C}$ and all superscripts $(\cdot)^{\mathrm{T}}$ by complex conjugate transposes $(\cdot)^{\mathrm{H}}$.

The second inequalities in Theorem 3.4 and Corollary 3.2 that mirror Cauchy's interlacing inequalities for the standard symmetric eigenvalue problem are not as satisfactory as we would like. We demonstrated that the factor $[\cos\angle(\mathcal{U},\mathcal{V})]^{-1}$ is in general not removable, but the factor $\sqrt{\min\{\kappa(K),\kappa(M)\}}$ could be an artifact of our proof and thus might be removed. No proof has been found yet.

A Proofs of Theorems 3.2 – 3.6

Lemma A.1. *Let $\omega_i \in \mathbb{R}$ for $1 \le i \le n$ be arranged in ascending order, i.e., $\omega_1 \le \omega_2 \le \cdots \le \omega_n$, and let $\alpha_i \in \mathbb{R}$ for $1 \le i \le n$. Denote by $\alpha_i^{\downarrow}$ $(i = 1, \ldots, n)$ the rearrangement of α_i $(i = 1, \ldots, n)$ in descending order, i.e., $\alpha_1^{\downarrow} \ge \cdots \ge \alpha_n^{\downarrow}$. Then*

$$\sum_{i=1}^{n} \omega_i \alpha_i \ge \sum_{i=1}^{n} \omega_i \alpha_i^{\downarrow}. \tag{A.1}$$

If (A.1) *is an equality and if $\alpha_k > \alpha_{k+1}$ and $\omega_k < \omega_{k+1}$ for some $1 \le k < n$, then*

$$\{\alpha_j^{\downarrow},\, j = 1, \ldots, k\} = \{\alpha_j,\, j = 1, \ldots, k\}, \tag{A.2}$$

i.e., α_j, $j = 1, \ldots, k$ give the largest k values among all α_i's.

Proof. Inequality (A.1) is well-known. See, for example, [7, (II.37) on p.49]. We now prove (A.2), under the conditions that (A.1) is an equality, $\alpha_k^{\downarrow} > \alpha_{k+1}^{\downarrow}$, and $\omega_k < \omega_{k+1}$. Suppose, to the contrary, that (A.2) did not hold. Then there would exist

$$\begin{aligned} &\ell_1 \le k \text{ and } \ell_2 > k \text{ such that } \alpha_{\ell_1} = \alpha_{\ell_2}^{\downarrow}, \\ &j_1 \le k \text{ and } j_2 > k \text{ such that } \alpha_{j_1}^{\downarrow} = \alpha_{j_2}. \end{aligned}$$

Since

$$\begin{aligned} \omega_{\ell_1}\alpha_{\ell_1} + \omega_{j_2}\alpha_{j_2} - (\omega_{\ell_1}\alpha_{j_2} + \omega_{j_2}\alpha_{\ell_1}) &= (\alpha_{j_2} - \alpha_{\ell_1})(\omega_{j_2} - \omega_{\ell_1}) \\ &= (\alpha_{j_1}^{\downarrow} - \alpha_{\ell_2}^{\downarrow})(\omega_{j_2} - \omega_{\ell_1}) \\ &\ge (\alpha_k^{\downarrow} - \alpha_{k+1}^{\downarrow})(\omega_{k+1} - \omega_k) \\ &> 0, \end{aligned}$$

we have

$$\sum_{i=1}^{n} \omega_i\alpha_i = \sum_{i \ne \ell_1, j_2} \omega_i\alpha_i + \omega_{\ell_1}\alpha_{\ell_1} + \omega_{j_2}\alpha_{j_2} > \sum_{i \ne \ell_1, j_2} \omega_i\alpha_i + \omega_{\ell_1}\alpha_{j_2} + \omega_{j_2}\alpha_{\ell_1} \ge \sum_{i=1}^{n} \omega_i\alpha_i^{\downarrow},$$

contradicting that (A.1) is an equality. This proves (A.2). □

Lemma A.2. *Let $U \in \mathbb{R}^{n\times k}$ and $\Omega = \mathrm{diag}(\omega_1, \omega_2, \ldots, \omega_n)$, where $\omega_1 \le \omega_2 \le \cdots \le \omega_n$. Then*

$$\mathrm{trace}(U^{\mathrm{T}}\Omega U) \ge \sum_{i=1}^{k} \sigma_i^2\, \omega_i, \tag{A.3}$$

where σ_i $(i = 1, \ldots, k)$ are the k singular values of U in descending order, i.e., $\sigma_1 \ge \cdots \ge \sigma_k \ge 0$. If (A.3) *is an equality, $\omega_k < \omega_{k+1}$, and $\sigma_k > 0$, then $U_{(k+1:n,:)} = 0$, i.e., the last $n-k$ rows of U are zeros.*

Proof. Write $\alpha_i = (UU^{\mathrm{T}})_{(i,i)}$, the ith diagonal entry of UU^{T}. By Lemma A.1,

$$\operatorname{trace}(U^{\mathrm{T}}\Omega U) = \operatorname{trace}(UU^{\mathrm{T}}\Omega) = \sum_{i=1}^{n} \omega_i \alpha_i \geq \sum_{i=1}^{n} \omega_i \alpha_i^{\downarrow}, \tag{A.4}$$

where $\alpha_i^{\downarrow}$ $(i = 1, \ldots, n)$ are defined as in Lemma A.1. Since UU^{T} is symmetric positive semidefinite, its diagonal entries: α_i $(i = 1, \ldots, n)$ are majorized by its n eigenvalues: σ_i^2 $(i = 1, \ldots, k)$ and $\sigma_i^2 = 0$ $(i = k+1, \ldots, n)$ [7, (II.14) on p.35], meaning

$$t_j \stackrel{\text{def}}{=} \sum_{i=1}^{j} \alpha_j^{\downarrow} \leq s_j \stackrel{\text{def}}{=} \sum_{i=1}^{j} \sigma_i^2 \text{ for } 1 \leq j \leq n-1, \text{ and } t_n = s_n. \tag{A.5}$$

Therefore, by [16, Lemma 2.3],

$$\sum_{i=1}^{n} \omega_i \alpha_i^{\downarrow} \geq \sum_{i=1}^{k} \omega_i \sigma_i^2 \tag{A.6}$$

which, combined with (A.4), lead to (A.3). But in order to characterize those matrices U that make (A.3) an equality, we need to look into when (A.6) becomes an equality. To that end, we still have to give a proof of (A.6), despite of [16, Lemma 2.3]. Let $t_0 = s_0 = 0$. We have

$$\begin{aligned}
\sum_{i=1}^{n} \omega_i \alpha_i^{\downarrow} &= \sum_{i=1}^{n} \omega_i (t_i - t_{i-1}) \\
&= \omega_n t_n + \sum_{i=1}^{n-1} (\omega_i - \omega_{i+1}) t_i \\
&\geq \omega_n s_n + \sum_{i=1}^{n-1} (\omega_i - \omega_{i+1}) s_i \\
&= \sum_{i=1}^{n} \omega_i \sigma_i^2 \\
&= \sum_{i=1}^{k} \omega_i \sigma_i^2. \qquad (\sigma_i = 0 \text{ for } i > k)
\end{aligned} \tag{A.7}$$

This is (A.6).

Now if (A.3) is an equality and if $\omega_k < \omega_{k+1}$, then the equal sign in (A.7) must hold and thus $t_k = s_k$ because $\omega_k - \omega_{k+1} < 0$. It follows from $\sigma_i^2 = 0$ $(i = k+1, \ldots, n)$ that $t_k = s_k = \cdots = s_n = t_n$; so $\alpha_j^{\downarrow} = 0$ for $j > k$ by (A.5). Because (A.4) must be an equality, $\alpha_k^{\downarrow} > 0 = \alpha_{k+1}^{\downarrow}$ (since $\sigma_k > 0$) and $\omega_k < \omega_{k+1}$, we conclude by Lemma A.1 that (A.2) holds, and thus $\alpha_j = (UU^{\mathrm{T}})_{(j,j)} = 0$ for $j > k$ which implies

$$(UU^{\mathrm{T}})_{(i,j)} = 0 \quad \text{for } \max\{i, j\} > k$$

because UU^{T} is symmetric positive semi-definite. In particular

$$U_{(k+1:n,:)} U_{(k+1:n,:)}^{\mathrm{T}} = (UU^{\mathrm{T}})_{(k+1:n,k+1:n)} = 0$$

which implies $U_{(k+1:n,:)} = 0$, as expected. □

***Proof* of Theorem 3.2.** Suppose that M is definite. Equations in (2.4) hold for some nonsingular $Y \in \mathbb{R}^{n\times n}$ and $X = Y^{-\mathrm{T}}$. We have by (2.4)

$$\begin{aligned} U^{\mathrm{T}}KU + V^{\mathrm{T}}MV &= U^{\mathrm{T}}Y\Lambda^2Y^{\mathrm{T}}U + V^{\mathrm{T}}XX^{\mathrm{T}}V \\ &= \hat{U}^{\mathrm{T}}\Lambda^2\hat{U} + \hat{V}^{\mathrm{T}}\hat{V}, \end{aligned} \tag{A.8}$$

where $\hat{U} = Y^{\mathrm{T}}U$ and $\hat{V} = X^{\mathrm{T}}V$. It can be verified that $\hat{U}^{\mathrm{T}}\hat{V} = U^{\mathrm{T}}V$ and that the correspondences between U and $\hat{U}$ and between V and $\hat{V}$ are one-one. Therefore

$$\inf_{U^{\mathrm{T}}V=I_k} \operatorname{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV) = \inf_{\hat{U}^{\mathrm{T}}\hat{V}=I_k} \operatorname{trace}(\hat{U}^{\mathrm{T}}\Lambda^2\hat{U} + \hat{V}^{\mathrm{T}}\hat{V}). \tag{A.9}$$

For any given $\hat{U}$ and $\hat{V}$, denote their singular values, respectively, by α_i $(i = 1, \ldots, k)$ and β_i $(i = 1, \ldots, k)$ in descending order. Then by Lemma A.2

$$\begin{aligned} \operatorname{trace}(\hat{U}^{\mathrm{T}}\Lambda^2\hat{U} + \hat{V}^{\mathrm{T}}\hat{V}) &\geq \sum_{i=1}^{k} \alpha_i^2\lambda_i^2 + \sum_{i=1}^{k} \beta_i^2 && \text{(A.10)} \\ &= \sum_{i=1}^{k} (\alpha_i^2\lambda_i^2 + \beta_{k-i+1}^2) \\ &\geq 2\sum_{i=1}^{k} \alpha_i\beta_{k-i+1}\lambda_i && \text{(A.11)} \\ &\geq 2\sum_{i=1}^{k} \lambda_i. && \text{(A.12)} \end{aligned}$$

The last inequality holds because of [12, (3.3.18) on p.178] which says $\alpha_i\beta_{k-i+1}$ is greater or equal to the kth largest singular value of $U^{\mathrm{T}}V = I_k$ which is 1. Combine (A.9) and (A.12) to get

$$\frac{1}{2}\inf_{U^{\mathrm{T}}V=I_k} \operatorname{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV) \geq \sum_{i=1}^{k} \lambda_i. \tag{A.13}$$

Now if all $\lambda_i > 0$ (i.e., K is also definite), then it can be seen that picking U and V such that

$$\widehat{U} = \left(\begin{array}{c} \operatorname{diag}(\lambda_1^{-1/2}, \ldots, \lambda_k^{-1/2}) \\ \hline 0 \end{array}\right), \quad \widehat{V} = \left(\begin{array}{c} \operatorname{diag}(\lambda_1^{1/2}, \ldots, \lambda_k^{1/2}) \\ \hline 0 \end{array}\right),$$

gives $\frac{1}{2}\operatorname{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV) = \sum_{i=1}^{k} \lambda_i$ which, together with (A.13), yield (3.10) with "inf" replaced by "min".

When K is singular, $\lambda_1 = 0$ and (A.11) is always a strict inequality. So

$$\frac{1}{2}\operatorname{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV) > \sum_{i=1}^{k} \lambda_i \quad \text{for any } U^{\mathrm{T}}V = I_k. \tag{A.14}$$

Suppose $0 = \lambda_1 = \cdots = \lambda_\ell < \lambda_{\ell+1} \leq \cdots \leq \lambda_k$. We pick U and V such that

$$\widehat{U} = \left(\begin{array}{c|c} \epsilon^{-1}I_\ell & \\ \hline & \operatorname{diag}(\lambda_{\ell+1}^{-1/2}, \ldots, \lambda_k^{-1/2}) \\ \hline \multicolumn{2}{c}{0} \end{array}\right), \quad \widehat{V} = \left(\begin{array}{c|c} \epsilon I_\ell & \\ \hline & \operatorname{diag}(\lambda_{\ell+1}^{1/2}, \ldots, \lambda_k^{1/2}) \\ \hline \multicolumn{2}{c}{0} \end{array}\right).$$

Then $\frac{1}{2}\operatorname{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV) = \sum_{i=1}^{k}\lambda_i + \ell\epsilon^2$ which goes to $\sum_{i=1}^{k}\lambda_i$ as $\epsilon \to 0$. So we have (3.10) by (A.14), and "inf" cannot be replaced by "min".

Now suppose $0 < \lambda_1$ and $\lambda_k < \lambda_{k+1}$ and suppose that U and V attain the minimum, i.e.,

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

For this to happen, all equal signs in (A.10), (A.11), and (A.12) must take place. For the equality sign in (A.10) to take place, by Lemma A.2 we have $\hat{U}_{(k+1:n,:)} = 0$. Partition

$$\hat{U} = \begin{pmatrix}\hat{U}_1\\ 0\end{pmatrix}, \quad \hat{V} = \begin{pmatrix}\hat{V}_1\\ \hat{V}_2\end{pmatrix}, \quad \hat{U}_1,\, \hat{V}_1 \in \mathbb{R}^{k\times k}.$$

We claim $\hat{V}_2 = 0$, too. Here is why. For the equality sign in (A.12) to take place, we have $\alpha_i\beta_{k-i+1} = 1$ for $1 \le i \le k$. Now $I_k = \hat{U}^{\mathrm{T}}\hat{V} = \hat{U}_1^{\mathrm{T}}\hat{V}_1$ implies $\alpha_i\gamma_{k-i+1} \ge 1$ [12, (3.3.18) on p.178], where γ_i $(i = 1, \ldots, k)$ are the singular values of $\hat{V}_1$ in descending order. Since $\hat{V}^{\mathrm{T}}\hat{V} = \hat{V}_1^{\mathrm{T}}\hat{V}_1 + \hat{V}_2^{\mathrm{T}}\hat{V}_2$, we have $\gamma_i \le \beta_i$ for $1 \le i \le k$ and thus

$$1 \le \alpha_i\gamma_{k-i+1} \le \alpha_i\beta_{k-i+1} = 1$$

which implies $\gamma_i = \beta_i$ for $1 \le i \le k$. So $\hat{V}_2 = 0$. Now use $U = X\hat{U}$ and $V = Y\hat{V}$ to conclude that $\{\operatorname{span}(U), \operatorname{span}(V)\}$ is the pair of deflating subspaces of $\{K, M\}$ corresponding to the eigenvalues $\pm\lambda_i$ $(1 \le i \le k)$ of H. □

Remark **A.1.** The first part of Theorem 3.2 – equation (3.10) – for the case when both K and M are definite has a quick proof upon using the results of Kovač-Striko and Veselić [14]. the equivalence between the eigenvalue problem (1.1) and the one for (1.14). Since $\boldsymbol{B} - \lambda\boldsymbol{A}$ is diagonalizable if both K and M are definite, we have by Theorem 3.1 and Corollary 3.3 of [14]

$$\sum_{i=1}^{k}\lambda_i = \min_{Z^{\mathrm{T}}\boldsymbol{A}Z = I_k}\operatorname{trace}(Z^{\mathrm{T}}\boldsymbol{B}Z).$$

Write $Z = \begin{pmatrix}\hat{V}\\ \hat{U}\end{pmatrix}$, where $U,\, V \in \mathbb{R}^{n\times k}$, to get

$$\sum_{i=1}^{k}\lambda_i = \min_{U^{\mathrm{T}}V + V^{\mathrm{T}}U = I_k}\operatorname{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV) \tag{A.15}$$

$$= \frac{1}{2}\min_{U^{\mathrm{T}}V + V^{\mathrm{T}}U = 2I_k}\operatorname{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV) \tag{A.16}$$

$$\le \frac{1}{2}\min_{U^{\mathrm{T}}V = I_k}\operatorname{trace}(U^{\mathrm{T}}KU + V^{\mathrm{T}}MV). \tag{A.17}$$

The equal sign in (A.16) is due to scaling both U and V by $1/\sqrt{2}$ and the inequality (A.17) is due to $\{(U, V) : U^{\mathrm{T}}V = I_k\} \subseteq \{(U, V) : U^{\mathrm{T}}V + V^{\mathrm{T}}U = 2I_k\}$. Finally we notice the equal sign in (A.17) is attainable using Theorem 2.3. This gives (3.10) for the case when both K and M are definite. While this does seem to provide a short and quick proof of (3.10) for the definite case, we point out that the argument in [14] that leads to (A.15) is nontrivial and lengthy (no shorter than ours that leads to the complete proof of Theorem 3.2). ◇

***Proof* of Theorem 3.4.** Assume that M is definite. Without loss of generality, we may simply assume $U^{\mathrm{T}}V = I_k$ and $W_1 = W_2 = I_k$; otherwise substitutions:

$$U \leftarrow UW_1^{-1}, \quad V \leftarrow VW_2^{-1}, \quad I_k \leftarrow W_1, \quad I_k \leftarrow W_2,$$

will give new U and V with $U^{\mathrm{T}}V = I_k$ and at the same time the same H_{SR}.

Equations in (2.4) hold for some nonsingular $Y \in \mathbb{R}^{n\times n}$ and $X = Y^{-\mathrm{T}}$. Then

$$U^{\mathrm{T}}KU = U^{\mathrm{T}}Y\Lambda^2Y^{\mathrm{T}}U = \hat{U}^{\mathrm{T}}\Lambda^2\hat{U}, \tag{A.18a}$$

$$V^{\mathrm{T}}MV = V^{\mathrm{T}}XX^{\mathrm{T}}V = \hat{V}^{\mathrm{T}}\hat{V}, \tag{A.18b}$$

where $\hat{U} = Y^{\mathrm{T}}U$ and $\hat{V} = X^{\mathrm{T}}V$. Still $\hat{U}^{\mathrm{T}}\hat{V} = U^{\mathrm{T}}V = I_k$. Decompose $\hat{V}$ as

$$\widetilde{V} \stackrel{\mathrm{def}}{=} Q^{\mathrm{T}}\hat{V} = \begin{pmatrix} \widetilde{V}_1 \\ 0 \end{pmatrix}, \quad Q^{\mathrm{T}}Q = I_n, \quad \widetilde{V}_1 \text{ nonsingular.} \tag{A.19}$$

This can be proved, for example, using SVD of $\hat{V}$. Then $\hat{V}^{\mathrm{T}}\hat{V} = \widetilde{V}_1^{\mathrm{T}}\widetilde{V}_1$. Partition

$$\widetilde{U} \stackrel{\mathrm{def}}{=} Q^{\mathrm{T}}\hat{U} = \begin{pmatrix} \widetilde{U}_1 \\ \widetilde{U}_2 \end{pmatrix}, \quad \widetilde{U}_1 \in \mathbb{R}^{k\times k}. \tag{A.20}$$

Then $\hat{U}^{\mathrm{T}}\hat{V} = (Q^{\mathrm{T}}\hat{U})^{\mathrm{T}}Q^{\mathrm{T}}\hat{V} = \widetilde{U}_1^{\mathrm{T}}\widetilde{V}_1 = I_k$ which implies $\widetilde{U}_1^{\mathrm{T}} = \widetilde{V}_1^{-1}$. Set

$$A = Q^{\mathrm{T}}\Lambda^2Q, \quad E = \widetilde{U}_2\widetilde{V}_1^{\mathrm{T}} \tag{A.21}$$

to get

$$\hat{U}^{\mathrm{T}}\Lambda^2\hat{U} = \widetilde{U}^{\mathrm{T}}A\widetilde{U}, \quad \widetilde{U}\widetilde{V}_1^{\mathrm{T}} = \begin{pmatrix} I_k \\ E \end{pmatrix}. \tag{A.22}$$

By Theorem 2.1, μ_i^2 $(1 \le i \le k)$ are all the eigenvalues of

$$(U^{\mathrm{T}}KU)(V^{\mathrm{T}}MV) = (\hat{U}^{\mathrm{T}}\Lambda^2\hat{U})(\hat{V}^{\mathrm{T}}\hat{V}) = (\widetilde{U}^{\mathrm{T}}A\widetilde{U})(\widetilde{V}_1^{\mathrm{T}}\widetilde{V}_1) \tag{A.23}$$

whose eigenvalues are the same as $\widetilde{V}_1(\widetilde{U}^{\mathrm{T}}A\widetilde{U})\widetilde{V}_1^{\mathrm{T}}$, a real symmetric positive semi-definite matrix. Set

$$P = \widetilde{U}\widetilde{V}_1^{\mathrm{T}}(I_k + E^{\mathrm{T}}E)^{-1/2}.$$

Then $P^{\mathrm{T}}P = I_k$ by (A.22). Denote by ν_i $(1 \le i \le k)$ the eigenvalues of $P^{\mathrm{T}}AP$ in ascending order. We have

$$\lambda_i^2 \le \nu_i \le \lambda_{i+n-k}^2 \quad \text{for } 1 \le i \le k \tag{A.24}$$

by Cauchy's interlacing theorem [25, 30]. For any $\hat{u} \in \mathbb{R}^k$, letting $u = (I_k + E^{\mathrm{T}}E)^{1/2}\hat{u}$ gives

$$(1 + \|E\|_2^2)\,\frac{u^{\mathrm{T}}(P^{\mathrm{T}}AP)u}{u^{\mathrm{T}}u} \ge \frac{\hat{u}^{\mathrm{T}}\left[\widetilde{V}_1(\widetilde{U}^{\mathrm{T}}A\widetilde{U})\widetilde{V}_1^{\mathrm{T}}\right]\hat{u}}{\hat{u}^{\mathrm{T}}\hat{u}} \ge \frac{u^{\mathrm{T}}(P^{\mathrm{T}}AP)u}{u^{\mathrm{T}}u} \tag{A.25}$$

since

$$\hat{u}^{\mathrm{T}}\hat{u} \le u^{\mathrm{T}}u = \hat{u}^{\mathrm{T}}\hat{u} + \hat{u}^{\mathrm{T}}E^{\mathrm{T}}E\hat{u} \le (1 + \|E\|_2^2)\hat{u}^{\mathrm{T}}\hat{u}.$$

Denote by $\hat{\mathcal{U}}_i$ and $\mathcal{U}_i$ subspaces of $\mathbb{R}^k$ of dimension i. Using the Courant-Fischer min-max principle (see [25, p.206], [30, p.201]), we have

$$\mu_i^2 = \min_{\hat{\mathcal{U}}_i}\max_{\hat{u}\in\hat{\mathcal{U}}_i} \frac{\hat{u}^{\mathrm{T}}\left[\widetilde{V}_1(\widetilde{U}^{\mathrm{T}}A\widetilde{U})\widetilde{V}_1^{\mathrm{T}}\right]\hat{u}}{\hat{u}^{\mathrm{T}}\hat{u}}$$

$$
\begin{aligned}
&\geq \min_{\mathcal{U}_i=(I_k+E^{\mathrm{T}}E)^{1/2}\hat{\mathcal{U}}_i} \max_{u\in\mathcal{U}_i} \frac{u^{\mathrm{T}}(P^{\mathrm{T}}AP)u}{u^{\mathrm{T}}u} && \text{(by (A.25))}\\
&= \min_{\mathcal{U}_i} \max_{u\in\mathcal{U}_i} \frac{u^{\mathrm{T}}(P^{\mathrm{T}}AP)u}{u^{\mathrm{T}}u}\\
&= \nu_i \geq \lambda_i^2, && \text{(by (A.24))}\\
\mu_i^2 &\leq (1+\|E\|_2^2) \min_{\mathcal{U}_i=(I_k+E^{\mathrm{T}}E)^{1/2}\hat{\mathcal{U}}_i} \max_{u\in\mathcal{U}_i} \frac{u^{\mathrm{T}}(P^{\mathrm{T}}AP)u}{u^{\mathrm{T}}u} && \text{(by (A.25))}\\
&= (1+\|E\|_2^2)\,\nu_i\\
&\leq (1+\|E\|_2^2)\,\lambda_{i+n-k}^2. && \text{(by (A.24))}
\end{aligned}
$$

It remains to bound $1+\|E\|_2^2$. We have from (A.19) – (A.22)

$$
\begin{aligned}
\sqrt{1+\|E\|_2^2} &= \|\widetilde{U}\widetilde{V}_1^{\mathrm{T}}\|_2\\
&\leq \|\widetilde{U}\|_2\|\widetilde{V}_1^{\mathrm{T}}\|_2\\
&= \|\hat{U}\|_2\|\hat{V}\|_2\\
&= \|Y^{\mathrm{T}}U\|_2\|X^{\mathrm{T}}V\|_2\\
&\leq \|Y^{\mathrm{T}}\|_2\|Y^{-1}\|_2\|U\|_2\|V\|_2\\
&= \sqrt{\kappa(M)}\,\|U\|_2\|V\|_2. \qquad \text{(A.26)}
\end{aligned}
$$

In Theorem 2.7, we proved that the eigenvalues of H_{SR} do not changes with respect to the choices of basis matrices. Which means, in proving this theorem, we can use H_{SR} constructed from different basis matrices for $\mathcal{U}$ and $\mathcal{V}$. What we are going to do is to pick new U and V such that the right hand side of (A.26) is

$$
\frac{\sqrt{\kappa(M)}}{\cos\angle(\mathcal{U},\mathcal{V})}.
$$

To this end, we compute QR decompositions

$$
U = Q_1R_1, \quad V = Q_2R_2,
$$

where Q_1, $Q_2 \in \mathbb{R}^{n\times k}$ have orthonormal columns. By [30, Theorem 5.2 on p.40], there are orthogonal matrices $P \in \mathbb{R}^{n\times n}$ and S_1, $S_2 \in \mathbb{R}^{k\times k}$ such that

$$
PQ_1S_1 = \begin{array}{c} \\ k \\ k \\ n-2k \end{array}\!\!\begin{array}{c} k \\ \begin{pmatrix} I \\ 0 \\ 0 \end{pmatrix} \end{array}, \qquad PQ_2S_2 = \begin{array}{c} \\ k \\ k \\ n-2k \end{array}\!\!\begin{array}{c} k \\ \begin{pmatrix} \Gamma \\ \Sigma \\ 0 \end{pmatrix} \end{array} \qquad \text{if } 2k \leq n, \qquad \text{(A.27a)}
$$

$$
PQ_1S_1 = \begin{array}{c} \\ n-k \\ 2k-n \\ n-k \end{array}\!\!\begin{array}{c} \begin{array}{cc} n-k & 2k-n \end{array} \\ \begin{pmatrix} I & 0 \\ 0 & I \\ 0 & 0 \end{pmatrix} \end{array}, \; PQ_2S_2 = \begin{array}{c} \\ n-k \\ 2k-n \\ n-k \end{array}\!\!\begin{array}{c} \begin{array}{cc} n-k & 2k-n \end{array} \\ \begin{pmatrix} \Gamma & 0 \\ 0 & I \\ \Sigma & 0 \end{pmatrix} \end{array} \text{ if } 2k > n, \qquad \text{(A.27b)}
$$

where $\Gamma = \mathrm{diag}(\gamma_1,\ldots,\gamma_\ell)$ and $\Sigma = \mathrm{diag}(\sigma_1,\ldots,\sigma_\ell)$, $\ell = k$ or $n-k$, all γ_i, $\sigma_i \geq 0$ and $\gamma_i^2+\sigma_i^2 = 1$. With (A.27), we pick new U and V to be

$$
P^{\mathrm{T}}\begin{pmatrix} \Gamma^{-1} \\ 0 \\ 0 \end{pmatrix}, \qquad P^{\mathrm{T}}\begin{pmatrix} \Gamma \\ \Sigma \\ 0 \end{pmatrix} \qquad \text{if } 2k \leq n,
$$

$$P^{\mathrm{T}}\begin{pmatrix}\Gamma^{-1} & 0\\ 0 & I_{2n-k}\\ 0 & 0\end{pmatrix}, \quad P^{\mathrm{T}}\begin{pmatrix}\Gamma & 0\\ 0 & I_{2n-k}\\ \Sigma & 0\end{pmatrix} \quad \text{if } 2k > n,$$

respectively. These new U and V span the same space as the old U and V and satisfy $U^{\mathrm{T}}V = I_k$ and $\|U\|_2\|V\|_2 = [\cos\angle(\mathcal{U},\mathcal{V})]^{-1}$. The proof of (3.19) is completed for the case when M is definite.

Now if $\lambda_k < \lambda_{k+1}$ and $\lambda_i = \mu_i$ for all $i = 1, 2, \ldots, k$, then $\nu_i = \lambda_i^2$ for all $i = 1, 2, \ldots, k$ since $\mu_i^2 \geq \nu_i \geq \lambda_i^2$. In particular, $\mathrm{trace}(P^{\mathrm{T}}AP) = \sum_{i=1}^k \lambda_i^2$. Apply [16, Theorem 2.2] or [14, Theorem 4] on $-A = Q^{\mathrm{T}}(-\Lambda^2)Q$ to conclude that $(QP)_{(1:k,:)}$ is orthogonal and $(QP)_{(k+1:n,:)} = 0$. Write

$$\hat{U} = \begin{pmatrix}\hat{U}_1\\ \hat{U}_2\end{pmatrix}, \quad \hat{V} = \begin{pmatrix}\hat{V}_1\\ \hat{V}_2\end{pmatrix}, \quad \hat{U}_1,\, \hat{V}_1 \in \mathbb{R}^{k\times k}, \quad \Lambda_1^2 = \mathrm{diag}(\lambda_1^2, \ldots, \lambda_k^2).$$

Since $QP = \hat{U}\widetilde{V}_1^{\mathrm{T}}(I_k + E^{\mathrm{T}}E)^{-1/2}$ by (A.20), we conclude that $\hat{U}_2 = 0$ and thus $\mathcal{U} = \mathrm{span}(X_{(1:k,:)})$. Use $\hat{U}^{\mathrm{T}}\hat{V} = I_k$ to get $\hat{U}_1^{\mathrm{T}}\hat{V}_1 = I_k$ or equivalently $\hat{U}_1^{\mathrm{T}} = \hat{V}_1^{-1}$. Note, by (A.23),

$$(U^{\mathrm{T}}KU)(V^{\mathrm{T}}MV) = \hat{U}_1^{\mathrm{T}}\Lambda_1^2\hat{U}_1\hat{V}^{\mathrm{T}}\hat{V}$$

which has the same eigenvalues as $\Lambda_1^2\hat{U}_1\hat{V}^{\mathrm{T}}\hat{V}\hat{U}_1^{\mathrm{T}}$ which has the same eigenvalues as

$$\Lambda_1\hat{U}_1\hat{V}^{\mathrm{T}}\hat{V}\hat{U}_1^{\mathrm{T}}\Lambda_1 = \Lambda_1^2 + \Lambda_1\hat{U}_1\hat{V}_2^{\mathrm{T}}\hat{V}_2\hat{U}_1^{\mathrm{T}}\Lambda_1.$$

Since by assumption the eigenvalues of $(U^{\mathrm{T}}KU)(V^{\mathrm{T}}MV)$ are λ_i^2 $(1 \leq i \leq k)$, we have

$$\sum_{i=1}^k \lambda_i^2 = \mathrm{trace}(\Lambda_1^2 + \Lambda_1\hat{U}_1\hat{V}_2^{\mathrm{T}}\hat{V}_2\hat{U}_1^{\mathrm{T}}\Lambda_1) = \sum_{i=1}^k \lambda_i^2 + \mathrm{trace}(\Lambda_1\hat{U}_1\hat{V}_2^{\mathrm{T}}\hat{V}_2\hat{U}_1^{\mathrm{T}}\Lambda_1)$$

which implies $\mathrm{trace}(\Lambda_1\hat{U}_1\hat{V}_2^{\mathrm{T}}\hat{V}_2\hat{U}_1^{\mathrm{T}}\Lambda_1) = 0$ and thus if $\lambda_1 > 0$, then $\hat{V}_2\hat{U}_1^{\mathrm{T}} = 0 \Rightarrow \hat{V}_2 = 0$. Therefore

$$U = X\hat{U} = X_{(1:k,:)}\hat{U}_1, \quad V = Y\hat{V} = Y_{(1:k,:)}\hat{V}_1,$$

as expected. □

***Proof* of Theorem 3.6.** Equations in (2.4) holds for some nonsingular $Y \in \mathbb{R}^{n\times n}$ and $X = Y^{-\mathrm{T}}$. Since the columns of $Z = \begin{pmatrix}Y\Lambda\\ X\end{pmatrix}$ are the eigenvectors of H corresponding to λ_i $(i = 1, 2, \ldots, n)$ and the eigenvectors corresponding to a multiple λ_i can be picked as any $\langle\cdot,\cdot\rangle_{\mathscr{I}}$-orthogonal basis vectors of the associated invariant subspace, we may assume that z_i is parallel to $Z_{(:,i)}$, the ith column of Z. Now for any $U^{\mathrm{T}}X_1 = 0$ and $V^{\mathrm{T}}Y_1 = 0$, $\hat{U}^{\mathrm{T}}\Lambda^2\hat{U}$ and $\hat{V}^{\mathrm{T}}\hat{V}$ in (A.8) and (A.18) become

$$\hat{U}^{\mathrm{T}}\Lambda^2\hat{U} = \hat{U}_2^{\mathrm{T}}\Lambda_2^2\hat{U}_2, \quad \hat{V}^{\mathrm{T}}\hat{V} = \hat{V}_2^{\mathrm{T}}\hat{V}_2,$$

where

$$\hat{U} = \begin{array}{c}\ell\\ n-\ell\end{array}\begin{pmatrix}0\\ \hat{U}_2\end{pmatrix}, \quad \hat{V} = \begin{array}{c}\ell\\ n-\ell\end{array}\begin{pmatrix}0\\ \hat{V}_2\end{pmatrix}, \quad \Lambda_2 = \mathrm{diag}(\lambda_{\ell+1}, \ldots, \lambda_n).$$

The rest of the proof are the same as the corresponding parts in the proofs of Theorems 3.2 and 3.4. □

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