

# THE ROTATION OF EIGENSPACES OF PERTURBED MATRIX PAIRS

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ABSTRACT. We revisit the relative perturbation theory for invariant subspaces of positive definite matrix pairs. As a prototype model problem for our results we consider parameter dependent families of eigenvalue problems. We show that new estimates are a natural way to obtain sharp — as functions of the parameter indexing the family of matrix pairs — estimates for the rotation of spectral subspaces.

## 1. INTRODUCTION AND MOTIVATION

This paper is concerned with the notion of the optimality of bounds on the rotation of spectral subspaces of positive definite Hermitian matrix pairs under the influence of additive perturbations. Precisely, given positive definite Hermitian matrix pairs  $(H, M)$  and  $(\tilde{H}, \tilde{M}) = (H + \delta H, M + \delta M)$  and their spectral subspaces  $\mathcal{E}$  and  $\tilde{\mathcal{E}}$  of the same dimensionality we provide estimates

$$(1) \quad \|\sin \Theta_M(\mathcal{E}, \tilde{\mathcal{E}})\| \leq \text{Gap}_1 \frac{\eta_H}{\sqrt{1 - \eta_H}} + \text{Gap}_2 \frac{\eta_M}{\sqrt{1 - \eta_M}}$$

where  $\eta_A = \|A^{-1/2}(A - \tilde{A})A^{-1/2}\|$  is the usual relative distance between positive definite Hermitian matrices  $A$  and  $\tilde{A}$ ,  $\text{Gap}_i$  measure the gaps in the spectrum and  $\|\sin \Theta_M(\mathcal{E}, \tilde{\mathcal{E}})\|$  measures the size of the rotation in the scalar product  $(x, y)_M = x^* M y$  dependent on the matrix  $M$ . For more on  $\sin \Theta$  theorems see [5, 9, 12, 13, 15]. In comparison, we approach the problem of the changing scalar product by presenting our estimates in the  $M$ -scalar product, whereas the standard approach yields estimates in the Euclidean scalar product.

Let us now consider the notion of the optimality of perturbation estimates in the context of parameter dependent perturbation families. In this setting we analyze rotations of eigenspaces of positive definite Hermitian matrix pairs  $(H, M)$  under the influence of a parameter dependent family of perturbations. The allowed families of perturbations  $\delta H_\kappa$  and  $\delta M_\kappa$  — where  $\kappa$  is some indexing parameter — are assumed to satisfy the restrictions

$$(2) \quad |x^* \delta H_\kappa y| \leq \mathcal{F}(\kappa) \sqrt{x^* H x y^* H y} \quad |x^* \delta M_\kappa y| \leq \mathcal{G}(\kappa) \sqrt{x^* M x y^* M y}$$

$$(3) \quad \lim_{\kappa \rightarrow \infty} \mathcal{F}(\kappa) = 0 \quad \lim_{\kappa \rightarrow \infty} \mathcal{G}(\kappa) = 0.$$

Here the matrix valued functions  $\delta H_\kappa$  and  $\delta M_\kappa$  are assumed to take value in the space of Hermitian matrices of appropriate size, and by a convention  $x^*$  denotes the transpose or Hermitian transpose of an object  $x$  — be it matrix or vector — as is given by the context. We also assume that  $\mathcal{F}$  and  $\mathcal{G}$  are some real valued functions and we apply (1) by setting  $H_\kappa := H + \delta H_\kappa$  and  $M_\kappa := M + \delta M_\kappa$  and noting the estimates  $\eta_{H_\kappa} \leq \mathcal{F}(\kappa)$  and  $\eta_{M_\kappa} \leq \mathcal{G}(\kappa)$  if we set  $\tilde{H} = H_\kappa$  and  $\tilde{M} = M_\kappa$ .

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It is our aim to argue that matrix dependent scalar product gives a natural environment to obtain optimal convergence estimates as functions of the parameter  $\kappa$ . Further feature of our theory is that our estimates are invariant<sup>1</sup> to the “inversion of the problem”, so we can also obtain estimates in the  $H$  based scalar product by switching the roles of  $H$  and  $M$ . In this context the reader should also note that the identity (2), under the assumption that  $\kappa$  is such that  $\mathcal{F}(\kappa) < 1$  and  $\mathcal{G}(\kappa) < 1$  yields the estimates (cf. equation (63))

$$(4) \quad |x^*(H_\kappa^{-1} - H^{-1})y| \leq \frac{\mathcal{F}(\kappa)}{1 - \mathcal{F}(\kappa)} \sqrt{x^*H^{-1}x y^*H^{-1}y}$$

$$(5) \quad |x^*(M_\kappa^{-1} - M^{-1})y| \leq \frac{\mathcal{G}(\kappa)}{1 - \mathcal{G}(\kappa)} \sqrt{x^*M^{-1}x y^*M^{-1}y}.$$

Let us now give more insight into the applications which are covered by the assumptions (2). This structure is rich enough to include discretization matrices approximating several singularly perturbed families of problems appearing in mathematical physics. Among other applications, the penalty methods for Stokes and Maxwell equations from [16] can be analyzed in this context, too. The parameter  $\kappa$  is then called the penalty parameter, and it is of interest what happens to the eigenvalues and eigenspaces as  $\kappa \rightarrow \infty$ . In [16, Section 4] the authors have studied the perturbation of eigenvalues by a very elegant Gerschgorin type argument and in this paper we give an eigenspace counterpart of such a result. For more details see A and the explicitly solved academic model problems from Section 4.1.

Also, the effect of numerical integration on the rotation of eigenspaces, when assembling finite element mass and stiffness matrices, is covered by (2). In this context  $\kappa$  is the parameter describing the effect of increasing accuracy of the integration formula. This approach is also used for “mass lumping” which amounts to constructing a diagonal matrix  $D = M + \delta M$ , with  $\delta M$  small in some sense. For further information and references see the paper [1], A and the academic example from Section 4.2 where we rather favorably compare our results with those that follow from the standard reference [15].

We end this discussion by noting that similar energy norm estimates for eigenvectors have been obtained in [10] in the context of the analysis of Lanczos method. Furthermore, the authors show how to efficiently compute the ingredients of the estimator in the context of computationally competitive numerical linear algebra procedures. We extend some of those results by giving a subspace version of some of the estimates, e.g. see appropriate parts of [10, Proposition 3.3 and 3.4] and compare with our numerical results from Section 4. It is possible that our subspace results could be of technical help when developing a similar analysis of the block Lanczos method.

We now turn to the main question of this paper. What is the real nature of the sharpness claim of a  $\sin \Theta$  theorem? Many of such theorems are obtained under essentially different spectral assumptions. Each is claimed to be sharp by constructing an appropriate example where the bound is attained. The results cannot be readily compared, even though one class of results can be seen to be following from the other, since their optimality depends on the set of assumption which were necessary to obtain the results. Quantitatively, transforming one class of results into the other type of estimates changes the quantitative performance of the results so considerably that a direct comparison is no longer fair. In a sense, each result

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<sup>1</sup>The value of  $\text{Gap}_i$  does not change under this transformation of the problem.

is “sharp” given the setting in which it has been obtained so discussion is more about which set of assumptions are more appropriate than the others.

We do not further address this fundamental questions. Instead, we opt to normalize the estimates by dividing the measure of the rotation which is being estimated with the estimator and then compare various estimates on specially tailored model problems. A first logical candidate — in a single matrix case — for a competing estimate would be a  $\sin \Theta$  theorem from [5, 13, 9]. However, it turns out that this estimate — as the function of  $\kappa$  — is overly pessimistic. Our aim is in particular to derive sharp estimates for the rotation of eigenspaces for this class of problems given by the parameter dependent family  $H_\kappa = H + \delta H_\kappa$ . The solution is to look for the rotation of eigenspaces in the energy norm, that is  $H$  based. In our setting this boils down to the analysis of the matrix pair  $(H_\kappa^{-1}, H_\kappa)$ . Let us also point out that we will discuss sharpness, or lack of it, in the various  $\sin \Theta$  results by comparing the residual type estimates which can be obtained for matrix pairs

$$(H_\kappa, I), (I, H_\kappa), (H_\kappa^{-1}, H_\kappa), (H_\kappa^{-1}, I), (I, H_\kappa^{-1}).$$

We will conclude that any estimate of an eigenspace rotation under the assumptions (2) is actually meant to be in a matrix dependent scalar product and that it will under-perform if used to measure rotations in the Euclidean scalar product.

## 2. NOTATIONS, DEFINITIONS AND THE GENERAL SETTING

The optimal setting to consider all of the above eigenvector problems is an analysis of the whole class of positive definite matrix pairs  $(H, M)$ , where  $H$  and  $M$  are positive definite. More to the point, we consider the following generalized eigenvector problem

$$(6) \quad Hx = \lambda Mx,$$

and the corresponding perturbed one

$$(7) \quad (H + \delta H)\tilde{x} = \tilde{\lambda}(M + \delta M)\tilde{x},$$

where  $H, M, \tilde{H} \equiv H + \delta H, \tilde{M} \equiv M + \delta M \in \mathbb{C}^{n \times n}$  are Hermitian positive definite.

**2.1. Spectral theorem and block operator matrix notation.** Under these assumptions matrix pairs  $(H, M)$  can be simultaneously diagonalized, that is there exists a non-singular matrix  $X$  such that

$$(8) \quad X^* H X = \Lambda, \quad X^* M X = I,$$

where  $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$   $\lambda_i \in \mathbb{R}$  for  $i = 1, \dots, n$  and we use  $X^*$  to denote the Hermitian adjoint.

We will represent our perturbation problem by block operator matrices and will use the following notation for the perturbation problems which will be needed in the analysis. Let us decompose  $X$  and  $\tilde{X}$  as

$$X = [X_1 \quad X_2] \quad \tilde{X} = [\tilde{X}_1 \quad \tilde{X}_2],$$

where  $X_1, \tilde{X}_1 \in \mathbb{C}^{n \times k}$  and  $X_2, \tilde{X}_2 \in \mathbb{C}^{n \times n-k}$ . The eigen-decomposition (8) can now be written as

$$(9) \quad \begin{bmatrix} X_1^* \\ X_2^* \end{bmatrix} H [X_1 \quad X_2] = \begin{bmatrix} \Lambda_1 & 0 \\ 0 & \Lambda_2 \end{bmatrix}, \quad \begin{bmatrix} X_1^* \\ X_2^* \end{bmatrix} M [X_1 \quad X_2] = \begin{bmatrix} I_k & 0 \\ 0 & I_{n-k} \end{bmatrix}.$$

Similarly as above, for perturbed quantities one can write

$$(10) \quad \begin{bmatrix} \tilde{X}_1^* \\ \tilde{X}_2^* \end{bmatrix} \tilde{H} [\tilde{X}_1 \quad \tilde{X}_2] = \begin{bmatrix} \tilde{\Lambda}_1 & 0 \\ 0 & \tilde{\Lambda}_2 \end{bmatrix}, \quad \begin{bmatrix} \tilde{X}_1^* \\ \tilde{X}_2^* \end{bmatrix} \tilde{M} [\tilde{X}_1 \quad \tilde{X}_2] = \begin{bmatrix} I_k & 0 \\ 0 & I_{n-k} \end{bmatrix}.$$

and

$$(11) \quad \begin{bmatrix} \hat{X}_1^* \\ \hat{X}_2^* \end{bmatrix} \hat{H} [\hat{X}_1 \quad \hat{X}_2] = \begin{bmatrix} \hat{\Lambda}_1 & 0 \\ 0 & \hat{\Lambda}_2 \end{bmatrix}, \quad \begin{bmatrix} \hat{X}_1^* \\ \hat{X}_2^* \end{bmatrix} M [\hat{X}_1 \quad \hat{X}_2] = \begin{bmatrix} I_k & 0 \\ 0 & I_{n-k} \end{bmatrix},$$

where  $\hat{X}_1 \in \mathbb{C}^{n \times k}$  and  $\hat{X}_2 \in \mathbb{C}^{n \times n-k}$  and  $\hat{X} = [\hat{X}_1 \quad \hat{X}_2]$ .

**2.2. Measuring perturbations of positive definite matrices.** The size of the perturbations  $\delta H$  and  $\delta M$  will be measured in the relative sense. This means that we assume that we have information on the singular values of the matrices

$$(12) \quad H^{-1/2}(H - \tilde{H})\tilde{H}^{-1/2} \text{ and } M^{-1/2}(M - \tilde{M})\tilde{M}^{-1/2}$$

or

$$(13) \quad H^{-1/2}(H - \tilde{H})H^{-1/2} \text{ and } M^{-1/2}(M - \tilde{M})M^{-1/2}.$$

Typically we only use the maximal singular value, that is the spectral norm estimate of these relative perturbations. More to the point we will use the quantities defined in the lemma below in most of our arguments. In this paper we use  $\|\cdot\|_2$  to denote the spectral matrix norm, and  $\|\cdot\|$  to denote any unitary invariant matrix norm, when there is no danger of confusion.

**Lemma 2.1.** *Let  $H$  be a positive definite matrix and let  $\Psi_H = \|H^{-1/2}(H - \tilde{H})\tilde{H}^{-1/2}\|$  and  $\eta_H = \|H^{-1/2}(H - \tilde{H})H^{-1/2}\|_2$ . Then for any  $x, y \in \mathbb{C}^n$*

$$(14) \quad |x^*(H - \tilde{H})x| \leq \eta_H x^*Hx,$$

$$(15) \quad |x^*(H - \tilde{H})y| \leq \frac{\eta_H}{\sqrt{1 - \eta_H}} \sqrt{x^*Hx x^*\tilde{H}x},$$

$$(16) \quad \|H^{-1/2}(H - \tilde{H})\tilde{H}^{-1/2}\| \leq \frac{1}{\sqrt{1 - \eta_H}} \|H^{-1/2}(H - \tilde{H})H^{-1/2}\|.$$

*In particular, relation (16) reduces to  $\Psi_H \leq \frac{\eta_H}{\sqrt{1 - \eta_H}}$  in the case  $\|\cdot\| = \|\cdot\|_2$ .*

The proof is by direct computation, see also [9]. Let us note that our theory is not limited to the use of spectral norm only. We allow for the consideration of any unitary invariant norm of the perturbations (12) and (13).

**Remark 2.2.** *When there is a danger of confusion we will use the notation*

$$(17) \quad \Psi_H^{\|\cdot\|} = \|H^{-1/2}(H - \tilde{H})\tilde{H}^{-1/2}\|$$

*to denote the dependence of the perturbation measure on the unitary invariant norm.*

**Remark 2.3.** *Let us note that in an application of this theory in the setting of the mass lumping finite element methods we consider the perturbations of the  $M$  matrix. The constant  $\eta_M$  for such a perturbation typically depends on mesh parameters. Furthermore, let us note that if there exist constants  $\delta_1, \delta_0, 0 < \delta_0 \leq \delta_1$  such that*

$$\delta_0 x^*Dx \leq x^*Mx \leq \delta_1 x^*Dx$$

holds for some symmetric positive definite matrices  $D$  and  $M$ , then  $\widetilde{M} = \frac{\delta_1 + \delta_0}{2}D$  has the property

$$\frac{2\delta_0}{\delta_0 + \delta_1}x^*\widetilde{M}x \leq x^*Mx \leq \frac{2\delta_1}{\delta_0 + \delta_1}x^*\widetilde{M}x$$

which can be written as

$$|x^*(M - \widetilde{M})x| \leq \frac{\delta_1 - \delta_0}{\delta_1 + \delta_0}x^*\widetilde{M}x.$$

**2.3. Relations between subspaces in the changing scalar product.** Let us now define the basic tools which will be used to compare subspaces of  $\mathbb{C}^n$ . Let  $\mathcal{X}$  and  $\mathcal{Y}$  be some generic  $m$ -dimensional subspaces of  $\mathbb{C}^n$ . For any of such subspaces there are bases<sup>2</sup>  $X, Y \in \mathbb{C}^{n \times m}$  such that  $\mathcal{X} = \text{Ran}(X)$  and  $\mathcal{Y} = \text{Ran}(Y)$ . Let us choose  $X$  and  $Y$  such that  $X^*X = Y^*Y = I_m$  then  $P_{\mathcal{X}} = XX^*$  and  $P_{\mathcal{Y}} = YY^*$  are orthogonal projections onto  $\mathcal{X}$  and  $\mathcal{Y}$ . Typically, one compares the subspaces  $\mathcal{X}$  and  $\mathcal{Y}$  by analyzing the spectral properties of the product  $S_{(\mathcal{X}, \mathcal{Y})} = (I - P_{\mathcal{X}})P_{\mathcal{Y}}$ . The  $m$ -singular values of  $S_{\mathcal{X}, \mathcal{Y}}|_{\mathcal{X}}$ —the restriction of  $S_{\mathcal{X}, \mathcal{Y}}$  on  $\mathcal{X}$ —are called the sines of the angle between the subspaces  $\mathcal{X}$  and  $\mathcal{Y}$ . In the matrix notation they are exactly the  $m$ -singular values of the matrix

$$S_{\mathcal{X}, \mathcal{Y}} = (I - XX^*)Y.$$

This is the measure of the size of the rotation<sup>3</sup> in  $\mathbb{C}^n$  which would move the subspace  $\mathcal{X}$  onto  $\mathcal{Y}$ .

In this note we analyze the angles between the subspaces  $\mathcal{X}$  and  $\mathcal{Y}$  in the scalar product  $(x, y)_M = x^*My$ ,  $x, y \in \mathbb{C}^n$  which is defined by the positive definite matrix  $M$ . To this end let  $X^*MX = Y^*MY = I_m$ , which is to say let  $X$  and  $Y$  be  $M$ -unitary. Then the sines of the angle between  $\mathcal{X}$  and  $\mathcal{Y}$  in the  $M$ -scalar product are the  $m$ -singular values of the matrix product

$$S_{\mathcal{X}, \mathcal{Y}}^M = M^{1/2}(I - XX^*M)Y$$

For more on angles between the subspaces of  $\mathbb{C}^n$  see [5, 11].

Let us not that since both  $M$  and  $H$  are subject to perturbation particular care is needed because the underlying space geometry changes with  $M$ . We shall therefore simplify the subsequent discussion of the  $M$ -product dependent subspace angles.

In order to be definite we shall concentrate—and give explicit formulae for the angles—only on the relationship between the subspaces of interest for our analysis. That is we consider the relationship between the subspaces  $\text{Ran}(X_1)$ ,  $\text{Ran}(\widetilde{X}_1)$  and  $\text{Ran}(\widehat{X}_1)$ .

The columns of  $X_1$  and  $\widehat{X}_1$  are  $M$ -orthogonal, then we use the following characterization of the sines of the canonical angles between the  $M$  orthogonal subspaces  $\mathcal{X}_1 = \text{Ran}(X_1)$  and  $\widehat{\mathcal{X}}_1 = \text{Ran}(\widehat{X}_1)$  induced by weighted  $M$ -inner product:

$$(18) \quad \sin \Theta_M(\mathcal{X}_1, \widehat{\mathcal{X}}_1) = \widehat{X}_1^*MX_1.$$

Let us now consider the problem of the changing scalar product. Since  $\widetilde{M} = M + \delta M$ , it follows from (10) that

$$\widetilde{X}^*M\widetilde{X} = I - \widetilde{X}^*\delta M\widetilde{X}.$$

<sup>2</sup>By saying the basis  $Y$  we mean “the basis given by the columns of  $Y$ ”.

<sup>3</sup>Such rotation exists if all of the sines of the angle between  $\mathcal{X}$  and  $\mathcal{Y}$  are strictly smaller than one.

Assume that  $I - \tilde{X}^* \delta M \tilde{X}$  is positive definite. Then  $\hat{X}$  and  $\tilde{X}Y^{-*}$  are  $M$ -orthogonal, where  $Y$  is Cholesky factor such that  $YY^* = I - \tilde{X}^* \delta M \tilde{X}$ . We can now use a similar characterization of the sines of canonical angles as in (18). We show that the sines of the canonical angles between the eigenspaces  $\hat{\mathcal{X}}_1 = \text{Ran}(\hat{X}_1)$  and  $\tilde{\mathcal{X}}_1 = \text{Ran}(\tilde{X}_1)$  induced by weighted  $M$ -inner product are given by:

$$(19) \quad \sin \Theta_M(\hat{\mathcal{X}}_1, \tilde{\mathcal{X}}_1) = \hat{X}_2^* M \tilde{X}_1 Y_{11}^{-*}, \quad \text{where} \quad Y = \begin{bmatrix} Y_{11} & Y_{12} \\ 0 & Y_{22} \end{bmatrix}.$$

Finally, let  $P_{\mathcal{X}} = XX^*$  be orthogonal projector onto  $m$ -dimensional subspace  $\mathcal{X} = \text{Ran}(X)$ , where  $X$  satisfies  $X^*X = I_m$ . Using the [15, Theorem II 4.10.], one can write

$$(20) \quad \|\sin \Theta(\mathcal{X}, \mathcal{Y})\| = \|P_{\mathcal{X}} - P_{\mathcal{Y}}\| = \|(I - P_{\mathcal{X}})P_{\mathcal{Y}}\| = \|(I - P_{\mathcal{Y}})P_{\mathcal{X}}\|,$$

for any unitary invariant norm  $\|\cdot\|$ . Further, note that the columns of the matrices  $X_1^M = M^{1/2}X_1$ ,  $\hat{X}_1^M = M^{1/2}\hat{X}_1$  and  $\tilde{X}_1^M = M^{1/2}\tilde{X}_1Y_{11}^{-*}$  are unitary, thus using (20), one can write

$$(21) \quad \left\| \sin \Theta_M(\mathcal{X}_1, \hat{\mathcal{X}}_1) \right\| = \|P_{\mathcal{X}_1} - P_{\hat{\mathcal{X}}_1}\| = \left\| \hat{X}_2^* M X_1 \right\|.$$

where  $P_{\mathcal{X}_1} = X_1^M (X_1^M)^*$  and where  $P_{\hat{\mathcal{X}}_1} = \hat{X}_1^M (\hat{X}_1^M)^*$ , and similarly

$$\left\| \sin \Theta_M(\hat{\mathcal{X}}_1, \tilde{\mathcal{X}}_1) \right\| = \|P_{\hat{\mathcal{X}}_1} - P_{\tilde{\mathcal{X}}_1}\| = \left\| \hat{X}_2^* M \tilde{X}_1 Y_{11}^{-*} \right\|,$$

where  $P_{\tilde{\mathcal{X}}_1} = \tilde{X}_1^M (\tilde{X}_1^M)^*$  and  $P_{\hat{\mathcal{X}}_1} = \hat{X}_1^M (\hat{X}_1^M)^*$ .

The results above imply the upper bound for the sines of the canonical angles between the eigenspaces  $\mathcal{X}_1 = \mathcal{R}(X_1)$  and  $\tilde{\mathcal{X}}_1 = \text{Ran}(\tilde{X}_1)$ , can be obtained in any unitary invariant norm  $\|\cdot\|$ , using the simple triangle inequality. We have

$$(22) \quad \left\| \sin \Theta_M(\mathcal{X}_1, \tilde{\mathcal{X}}_1) \right\| \leq \left\| \sin \Theta_M(\mathcal{X}_1, \hat{\mathcal{X}}_1) \right\| + \left\| \sin \Theta_M(\hat{\mathcal{X}}_1, \tilde{\mathcal{X}}_1) \right\|,$$

that is  $\left\| \sin \Theta_M(\mathcal{X}_1, \tilde{\mathcal{X}}_1) \right\|$  can be estimated as the sum of the upper bounds for the norms of the sines matrices from (18) and (19).

### 3. THE MAIN RESULT

Our aim is to derive a bound for the sines of the canonical angles between eigenspaces  $\mathcal{X}_1 = \text{Ran}(X_1)$  and  $\tilde{\mathcal{X}}_1 = \text{Ran}(\tilde{X}_1)$  from (9) and (10).

This will be done with the two steps procedure as suggested by the form of the inequality (22). This approach is in the line with the pioneering analysis of the relative sensitivity of the eigenvalues of a positive-definite matrix pair from [2].

The road-map for the proof is outlined in the following list. For each preparatory step we will prove a theorem to justify the procedure and at the end we will combine the conclusion in the main theorem. The preparatory steps can be classified as follows:

(1)  $H$  perturbed,  $M$  unchanged

$$(23) \quad X^*HX = \Lambda, \quad X^*MX = I, \quad \hat{X}^* \tilde{H} \hat{X} = \hat{\Lambda}, \quad \hat{X}^* M \hat{X} = I,$$

where  $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$ ,  $\hat{\Lambda} = \text{diag}(\hat{\lambda}_1, \dots, \hat{\lambda}_n)$ ,  $\lambda_i, \hat{\lambda}_i \in \mathbb{R}$ , for  $i = 1, \dots, n$ .

(2)  $M$  perturbed,  $H$  unchanged

$$(24) \quad X^* \tilde{H} X = \hat{\Lambda}, \quad X^* M \hat{X} = I, \quad \tilde{X}^* \tilde{H} \tilde{X} = \tilde{\Lambda}, \quad \tilde{X}^* \tilde{M} \tilde{X} = I,$$

where  $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$ , and  $\tilde{\Lambda} = \text{diag}(\tilde{\lambda}_1, \dots, \tilde{\lambda}_n)$ , and  $\lambda_i, \tilde{\lambda}_i \in \mathbb{R}$ , for  $i = 1, \dots, n$ .

The main tools in our analysis will be sharp estimates for the solution of the structured Sylvester equations from [13, Lemma 2.4] and [13, Lemma 2.3]. That is, we consider the structured Sylvester equations<sup>4</sup>

$$(25) \quad AX - XB = A^{1/2}CB^{1/2}$$

$$(26) \quad AX - XB = CB.$$

**3.1. The first step.** Now we will state our first theorem. We will use the notation and the conclusions of Lemma 2.1 without further comments.

**Theorem 3.1.** *Let  $(H, M)$  be a Hermitian pair defined by (6) and let  $(\tilde{H}, M)$  be perturbed pair defined by*

$$(H + \delta H)\hat{x} = \hat{\Lambda}M\hat{x}.$$

Let  $X = [X_1 \ X_2]$  and  $\hat{X} = [\hat{X}_1 \ \hat{X}_2]$ , be non-singular matrices which simultaneously diagonalize the pairs  $(H, M)$  and  $(\tilde{H}, M)$ , as in (23). By setting  $\Psi_H = \|H^{-1/2}(H - \tilde{H})\tilde{H}^{-1/2}\|$  we have

$$(27) \quad \|\sin \Theta_M(\mathcal{X}_1, \hat{\mathcal{X}}_1)\| \leq \frac{\Psi_H}{\text{RelGap}},$$

where

$$(28) \quad \text{RelGap} = \min_{\substack{\lambda_i \in \Lambda_2 \\ \hat{\lambda}_j \in \hat{\Lambda}_1}} \frac{|\lambda_i - \hat{\lambda}_j|}{\sqrt{|\lambda_i| |\hat{\lambda}_j|}} \quad \Lambda_2 = \text{diag}(\lambda_{k+1}, \dots, \lambda_n), \quad \hat{\Lambda}_1 = \text{diag}(\hat{\lambda}_1, \dots, \hat{\lambda}_k).$$

*Proof.* Since, according to (18),

$$\sin \Theta_M(\mathcal{X}_1, \hat{\mathcal{X}}_1) = X_2^* M \hat{X}_1,$$

we have to bound  $\|X_2^* M \hat{X}_1\|$ . By the definition we have  $X^* H X = \Lambda$ , and so one can write

$$(29) \quad H^{1/2} X = U \Lambda^{1/2},$$

where  $U = [U_1 \ U_2] = H^{1/2} X \Lambda^{-1/2}$  is unitary and has the block structure conforming to the structure of  $X$ . A similar identity also holds for perturbed quantities. On the other hand, for perturbed quantities it also holds

$$(H + \delta H)\hat{X}_1 = M\hat{X}_1\hat{\Lambda}_1,$$

where  $\hat{\Lambda}_1 = \text{diag}(\hat{\lambda}_1, \dots, \hat{\lambda}_r)$ , and similarly for unperturbed quantities. We multiply the above equality by  $X_2^*$  from the left, and get

$$X_2^* H \hat{X}_1 - X_2^* M \hat{X}_1 \hat{\Lambda}_1 = -X_2^* \delta H \hat{X}_1.$$

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<sup>4</sup>The solution of (25) is presented in [13, Lemma 2.4]. This equation has also been analyzed in infinite dimensional setting in [9]. The equation (26) has been analyzed in [13, Lemma 2.3], see also [12].

Using the fact that  $HX_2 = MX_2\Lambda_2$ , this identity can be transformed into

$$(30) \quad \Lambda_2 X_2^* M \widehat{X}_1 - X_2^* M \widehat{X}_1 \widehat{\Lambda}_1 = -X_2^* \delta H \widehat{X}_1.$$

We will proceed by rearranging the right-hand side of (30). For that purpose note that one can rewrite the right-hand side of (30) as

$$(31) \quad X_2^* \delta H \widehat{X}_1 = X_2^* H^{1/2} H^{-1/2} \delta H \widetilde{H}^{-1/2} \widetilde{H}^{1/2} \widehat{X}_1,$$

which together with (29) gives

$$X_2^* \delta H \widehat{X}_1 = \Lambda_2^{1/2} U_2^* H^{-1/2} \delta H \widetilde{H}^{-1/2} \widehat{U}_1 \widehat{\Lambda}_1^{1/2}.$$

The above equality and (30) give

$$(32) \quad \Lambda_2 X_2^* M \widehat{X}_1 - X_2^* M \widehat{X}_1 \widehat{\Lambda}_1 = -\Lambda_2^{1/2} U_2^* H^{-1/2} \delta H \widetilde{H}^{-1/2} \widehat{U}_1 \widehat{\Lambda}_1^{1/2}.$$

This identity can be recognized as the structured Sylvester equation from (25). This equation is even meaningful when  $H$  and  $M$  are unbounded operators. In this setting it is called the weak Sylvester equation and it has been analyzed in [9].

Applying [13, Lemma 2.4] to obtain the bounds on the solution of the structured Sylvester equation (see also [12]), on (32) one gets, see (17):

$$(33) \quad \|X_2^* M \widehat{X}_1\| \leq \frac{\Psi_H^{\|\cdot\|}}{\text{RelGap}}, \quad \text{where} \quad \text{RelGap} = \min_{\lambda_i \in \Lambda_2, \widehat{\lambda}_j \in \widehat{\Lambda}_1} \frac{|\lambda_i - \widehat{\lambda}_j|}{\sqrt{\lambda_i \widehat{\lambda}_j}},$$

for any unitary invariant norm  $\|\cdot\|$ .  $\blacksquare$

**3.2. The second step—the change in scalar product.** Here we will derive the upper bound for the sines of the canonical angles between the eigenspaces  $\widehat{\mathcal{X}}_1 = \text{Ran}(\widehat{X}_1)$  and  $\widetilde{\mathcal{X}}_1 = \text{Ran}(\widetilde{X}_1)$  induced by weighted  $M$ -inner product, defined by

$$(34) \quad \sin \Theta_M(\widehat{\mathcal{X}}_1, \widetilde{\mathcal{X}}_1) = \widehat{X}_2^* M \widetilde{X}_1 Y_{11}^{-*},$$

where

$$(35) \quad \begin{bmatrix} Y_{11} & 0 \\ Y_{21} & Y_{22} \end{bmatrix} \begin{bmatrix} Y_{11}^* & Y_{21}^* \\ 0 & Y_{22}^* \end{bmatrix} = I - \widetilde{X}^* \delta M \widetilde{X}.$$

**Remark 3.2.** Note that one of possibilities to chose  $Y_{11}$  in (35) can be obtained by Block Cholesky elimination applied on the right-hand side in (35). This choice yields the block  $Y_{11} = \sqrt{I - \widetilde{X}_1^* \delta M \widetilde{X}_1}$ .

We now consider the problem of the perturbation of the matrix pair  $(\widetilde{H}, M)$  to  $(\widetilde{H}, \widetilde{M})$ . The following theorem contains the upper bound for the  $\|\widehat{X}_2^* M \widetilde{X}_1\|$ , where  $\|\cdot\|$  stands for any unitary invariant norm.

**Theorem 3.3.** Let  $(\widetilde{H}, M)$  be a Hermitian pair and let  $(\widetilde{H}, \widetilde{M})$  be perturbed pair defined by

$$(H + \delta H)\widetilde{y} = \widetilde{\lambda} \widetilde{M} \widetilde{y}.$$



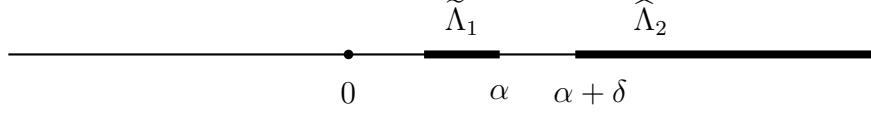


FIGURE 1. Spectral configuration for Theorem 3.3.

Let  $\widehat{X} = [\widehat{X}_1 \ \widehat{X}_2]$  and  $\widetilde{X} = [\widetilde{X}_1 \ \widetilde{X}_2]$ , be non-singular matrices which simultaneously diagonalize the pairs  $(\widehat{H}, M)$  and  $(\widetilde{H}, \widetilde{M})$ , as in (24). If

$$(36) \quad \|\widehat{\Lambda}_2\| \leq \alpha \quad \text{and} \quad \|\widetilde{\Lambda}_1^{-1}\|^{-1} \geq \alpha + \delta \quad \text{or}$$

$$(37) \quad \|\widehat{\Lambda}_2^{-1}\|^{-1} \geq \alpha + \delta \quad \text{and} \quad \|\widetilde{\Lambda}_1\| \leq \alpha$$

where  $\widehat{\Lambda}_2 = \text{diag}(\widehat{\lambda}_{k+1}, \dots, \widehat{\lambda}_n)$ ,  $\widetilde{\Lambda}_1 = \text{diag}(\widetilde{\lambda}_1, \dots, \widetilde{\lambda}_k)$ , see Figure 1, then

$$(38) \quad \left\| \widehat{X}_2^* M \widetilde{X}_1 \right\| \leq \frac{\Psi_M}{\text{RelGap}_p}.$$

Here we have used  $\Psi_M = \|M^{-1/2}(M - \widetilde{M})\widetilde{M}^{-1/2}\|$  and for all  $1 \leq p \leq \infty$  and we have

$$(39) \quad \frac{\delta}{\alpha + \delta} \geq \min_{\substack{\widehat{\lambda}_i \in \widehat{\Lambda}_2 \\ \widetilde{\lambda}_j \in \widetilde{\Lambda}_1}} \frac{|\widehat{\lambda}_i - \widetilde{\lambda}_j|}{(\widehat{\lambda}_i^p + \widetilde{\lambda}_j^p)^{1/p}} =: \text{RelGap}_p.$$

*Proof.* For the perturbed quantities it holds that

$$(H + \delta H)\widetilde{X}_1 = \widetilde{M}\widetilde{X}_1\widetilde{\Lambda}_1,$$

where  $\widetilde{\Lambda}_1 = \text{diag}(\widetilde{\lambda}_1, \dots, \widetilde{\lambda}_r)$ , and similarly for the unperturbed quantities. Now, by multiplying the above equality by  $\widehat{X}_2^*$  from the left, we get

$$\widehat{X}_2^* \widetilde{H} \widetilde{X}_1 - \widehat{X}_2^* \widetilde{M} \widetilde{X}_1 \widetilde{\Lambda}_1 = 0.$$

Using the fact  $\widetilde{H}\widehat{X}_2 = M\widehat{X}_2\widehat{\Lambda}_2$  (see (24)) this gives

$$(40) \quad \widehat{\Lambda}_2 \widehat{X}_2^* M \widetilde{X}_1 - \widehat{X}_2^* M \widetilde{X}_1 \widetilde{\Lambda}_1 = -\widehat{X}_2^* \delta M \widetilde{X}_1 \widetilde{\Lambda}_1.$$

We will proceed by rearranging the right-hand side of (40). For that purpose note that one can rewrite the right-hand side of (40) as

$$(41) \quad \widehat{X}_2^* \delta M \widetilde{X}_1 = \widehat{X}_2^* M^{1/2} M^{-1/2} \delta M \widetilde{M}^{-1/2} \widetilde{M}^{1/2} \widetilde{X}_1 \widetilde{\Lambda}_1.$$

Recall, that from (24) it follows that  $\widehat{Q}_2^* \equiv \widehat{X}_2^* M^{1/2}$  and  $\widetilde{Q}_1 \equiv \widetilde{M}^{1/2} \widetilde{X}_1$  have unitary columns, which together with (41) gives

$$\widehat{X}_2^* \delta M \widetilde{X}_1 = \widehat{Q}_2^* M^{-1/2} \delta M \widetilde{M}^{-1/2} \widetilde{Q}_1.$$

Applying [13, Lemma 2.3] to obtain the bounds on the solution of a structured Sylvester equation (see also [12]), on (32) one gets:

$$(42) \quad \left\| \widehat{X}_2^* \delta M \widetilde{X}_1 \right\| \leq \frac{1}{\text{RelGap}_p} \cdot \|M^{-1/2} \delta M \widetilde{M}^{-1/2}\|$$

where  $\|\cdot\|$  stands for any unitary invariant norm, and  $\text{RelGap}_p$  is defined as in (39). Now from (42) directly follows bound (38). ■

**3.3. The main result.** As we have mentioned in our road-map, from (22) follows that the upper bound for

$$\|\sin \Theta_M(\mathcal{X}_1, \tilde{\mathcal{X}}_1)\|$$

will be obtained as the sum of the bounds for  $\|\sin \Theta_M(\mathcal{X}_1, \hat{\mathcal{X}}_1)\|$  and  $\|\sin_M \Theta(\hat{\mathcal{X}}_1, \tilde{\mathcal{X}}_1)\|$ . Thus we have the following theorem:

**Theorem 3.4.** *Let  $(H, M)$  be a Hermitian pair and let  $(\tilde{H}, \tilde{M})$  be the perturbed pair. Let  $X = [X_1 \ X_2]$  and  $\tilde{X} = [\tilde{X}_1 \ \tilde{X}_2]$ , be non-singular matrices which simultaneously diagonalize the pairs  $(H, M)$  and  $(\tilde{H}, \tilde{M})$ , as in (9) and (10), respectively. If*

$$\eta_M := \|M^{-1/2} \delta M M^{-1/2}\|_2 < \frac{1}{2},$$

and if (36) or (37) hold, then

$$(43) \quad \|\sin \Theta_M(\mathcal{X}_1, \tilde{\mathcal{X}}_1)\| \leq \frac{1}{\text{RelGap}} \cdot \Psi_H + \frac{1}{\text{RelGap}_p} \cdot \frac{\sqrt{1 - \eta_M}}{\sqrt{1 - 2\eta_M}} \cdot \Psi_M,$$

where  $\|\sin \Theta_M(\mathcal{X}_1, \tilde{\mathcal{X}}_1)\|$  — the sine of the angle between the subspaces in  $M$  scalar product — is defined by (21), and  $\text{RelGap}$  and  $\text{RelGap}_p$  are defined by (28) and (39), respectively.

*Proof.* Using (22), (27), (34) and (38) and the multiplicative properties of unitary invariant matrix norms one gets

$$(44) \quad \|\sin \Theta_M(\mathcal{X}_1, \tilde{\mathcal{X}}_1)\| \leq \frac{1}{\text{RelGap}} \cdot \Psi_H + \frac{1}{\text{RelGap}_p} \cdot \Psi_M \cdot \|Y_{11}^{-1}\|_2,$$

where  $Y_{11} = \sqrt{I - \tilde{X}_1^* \delta M \tilde{X}_1}$  is defined as in (35). It left us to compute the bound for  $\|Y_{11}^{-1}\|_2$ . Using the  $\tilde{M}$ -orthogonality of  $\tilde{X}$  it can be easily seen that  $\tilde{X}$  and  $M^{-1/2}(I + M^{-1/2} \delta M M^{-1/2})^{-1/2}$  are unitarily similar, that is that exists unitary matrix  $Q$  such that

$$(45) \quad \tilde{X} = M^{-1/2}(I + M^{-1/2} \delta M M^{-1/2})^{-1/2} Q$$

Now we can proceed, note that

$$(46) \quad \|(I - \tilde{X}_1^* \delta M \tilde{X}_1)^{-1/2}\|_2 \leq \frac{1}{\sqrt{1 - \|\tilde{X}_1^* \delta M \tilde{X}_1\|_2}} \leq \frac{1}{\sqrt{1 - \|\tilde{X}^* \delta M \tilde{X}\|_2}}.$$

Set  $W = M^{-1/2} \delta M M^{-1/2}$ , then from (45) follows

$$(47) \quad \|\tilde{X}^* \delta M \tilde{X}\|_2 = \|(I + W)^{-1/2} W (I + W)^{-1/2}\|_2 \leq \frac{\eta_M}{1 - \eta_M}.$$

Finally inserting (47) in (46) one gets

$$(48) \quad \|(I - \tilde{X}_1^* \delta M \tilde{X}_1)^{-1/2}\| \leq \frac{\sqrt{1 - \eta_M}}{\sqrt{1 - 2\eta_M}}.$$

Now, insert (48) in (44) to get (43), which completes the proof. ■

An alternative version—that is to say a version where alternative relative perturbation sizes feature—can be obtained using Lemma 2.1.

**Corollary 3.5.** *Under the assumptions of Theorem 3.4 we have the estimate*

$$(49) \quad \|\sin \Theta_M(\mathcal{X}_1, \tilde{\mathcal{X}}_1)\| \leq \frac{1}{\text{RelGap}} \cdot \frac{\Phi_H}{\sqrt{1-\eta_H}} + \frac{1}{\text{RelGap}_p} \cdot \frac{\Phi_M}{\sqrt{1-2\eta_M}},$$

where  $\Phi_M = \|M^{-1/2}\delta MM^{-1/2}\|$  and  $\Phi_H = \|H^{-1/2}\delta HH^{-1/2}\|$ .

3.3.1. *Weakening the assumption on the spectral dichotomy.* Note that theorem 3.3 requires the special structure on specters of  $\tilde{\Lambda}_1$  and  $\tilde{\Lambda}_2$ . The reason for this lies in the more involved analysis of the structures Sylvester equation (26), see the comment in the introduction to [12].

This limitation can be overcome by the use of the Frobenius norm instead of spectral norm. Thus, the next theorem contains the perturbation bound similar to the one from Theorem 3.3 given for  $\left\| \hat{X}_2^* M \tilde{X}_1 \right\|_F$ , without any additional assumptions on spectral configuration of the pair  $(H, M)$ .

**Theorem 3.6.** *Let  $(\tilde{H}, M)$ ,  $(\tilde{H}, \tilde{M})$ ,  $\hat{X} = [\hat{X}_1 \ \hat{X}_2]$  and  $\tilde{X} = [\tilde{X}_1 \ \tilde{X}_2]$ , be as in Theorem 3.3. Then*

$$(50) \quad \left\| \hat{X}_2^* M \tilde{X}_1 \right\|_F \leq \frac{\Psi_M^{\|\cdot\|_F}}{\text{RelGap}_{\text{comp}}},$$

where we remember the definition  $\Psi_M^{\|\cdot\|_F} = \|M^{-1/2}\delta M \tilde{M}^{-1/2}\|_F$  from (17) and we assume that

$$(51) \quad \text{RelGap}_{\text{comp}} := \min_{\substack{\tilde{\lambda}_i \in \tilde{\Lambda}_2 \\ \tilde{\lambda}_j \in \tilde{\Lambda}_1}} \frac{|\hat{\lambda}_i - \tilde{\lambda}_j|}{\tilde{\lambda}_j}$$

is strictly larger than zero.

*Proof.* The first part of the proof is similar to the proof of theorem 3.3 up to the equality (41). Thus we continue the proof from there, that is one can write:

$$(52) \quad \hat{\Lambda}_2 \hat{X}_2^* M \tilde{X}_1 - \hat{X}_2^* M \tilde{X}_1 \tilde{\Lambda}_1 = -\hat{X}_2^* \delta M \tilde{X}_1 \tilde{\Lambda}_1,$$

and

$$(53) \quad \hat{X}_2^* \delta M \tilde{X}_1 = \hat{Q}_2^* M^{-1/2} \delta M \tilde{M}^{-1/2} \tilde{Q}_1,$$

where  $\hat{Q}_2^* \equiv \hat{X}_2^* M^{1/2}$  and  $\tilde{Q}_1 \equiv \tilde{M}^{1/2} \tilde{X}_1$  have unitary columns.

By interpreting (52) and (53) component-wise it follows

$$(\hat{\Lambda}_2)_{ii} (\hat{X}_2^* M \tilde{X}_1)_{ij} - (\hat{X}_2^* M \tilde{X}_1)_{ij} (\tilde{\Lambda}_1)_{jj} = -(\hat{Q}_2^* M^{-1/2} \delta M \tilde{M}^{-1/2} \tilde{Q}_1)_{ij} (\tilde{\Lambda}_1)_{jj},$$

or

$$(54) \quad (\hat{X}_2^* M \tilde{X}_1)_{ij} = -\frac{(\tilde{\Lambda}_1)_{jj}}{(\hat{\Lambda}_2)_{ii} - (\tilde{\Lambda}_1)_{jj}} \left( (\hat{Q}_2)_{(:,i)}^* M^{-1/2} \delta M \tilde{M}^{-1/2} (\tilde{Q}_1)_{(:,j)} \right),$$

where  $(Q)_{(:,j)}$  denotes  $j$ -th column of the matrix  $Q$ .

By computing the Frobenius norm from (54) we have

$$(55) \quad \|\widehat{X}_2^* M \widetilde{X}_1\|_F^2 = \sum_{i=k+1}^n \sum_{j=k+1}^n \frac{1}{\left| \frac{(\widehat{\Lambda}_2)_{ii} - (\widetilde{\Lambda}_1)_{jj}}{(\widehat{\Lambda}_1)_{jj}} \right|^2} \left( (\widehat{Q}_2)_{(:,i)}^* M^{-1/2} \delta M \widetilde{M}^{-1/2} (\widetilde{Q}_1)_{(:,j)} \right)^2,$$

which gives

$$(56) \quad \|\widehat{X}_2^* M \widetilde{X}_1\|_F \leq \frac{1}{\text{RelGap}_{\text{comp}}} \cdot \|\widehat{Q}^* M^{-1/2} \delta M \widetilde{M}^{-1/2} \widetilde{Q}\|_F.$$

Now from (56), noting that  $\widehat{Q}$  and  $\widetilde{Q}$  are both unitary, we obtain (50). ■

We can now give a Frobenius norm version of Theorem 3.4.

**Theorem 3.7.** *Let  $(H, M)$  be a Hermitian pair and let  $(\widetilde{H}, \widetilde{M})$  be the perturbed pair. Let  $X = [X_1 \ X_2]$  and  $\widetilde{X} = [\widetilde{X}_1 \ \widetilde{X}_2]$ , be non-singular matrices which simultaneously diagonalize the pairs  $(H, M)$  and  $(\widetilde{H}, \widetilde{M})$ , as in (9) and (10), respectively. If the spectra are separated so that  $\text{RelGap}_{\text{comp}} > 0$  then*

$$(57) \quad \|\sin \Theta_M(\mathcal{X}_1, \widetilde{\mathcal{X}}_1)\|_F \leq \frac{1}{\text{RelGap}} \cdot \Psi_H^{\|\cdot\|_F} + \frac{1}{\text{RelGap}_{\text{comp}}} \cdot \Psi_M^{\|\cdot\|_F},$$

where  $\|\sin \Theta_M(\mathcal{X}_1, \widetilde{\mathcal{X}}_1)\|_F$  — the sine of the angle between the subspaces in  $M$  scalar product — is defined by (21), and  $\text{RelGap}$  and  $\text{RelGap}_{\text{com}}$  are defined by (28) and (51), respectively.

#### 4. NUMERICAL EXAMPLES

It is not easy to numerically compare the eigenvector estimates for the perturbations of matrix pencils. The reason is that there is no canonical norm for the analysis of the eigenvector problem. For instance, assume that we have a positive definite symmetric pencil  $(H, M)$ , then any of the matrix dependent norms (and the associated scalar products)

$$\|x\|_{\alpha, \beta} = \sqrt{\alpha x^* H x + \beta x^* M x}, \quad \alpha \geq 0, \beta \geq 0, \text{ and } \alpha\beta \neq 0$$

is a meaningful candidate as well as is the standard Euclidean norm  $\|\cdot\|$ .

Applying any of the competing estimates in a situation for which they were not designed, is only possible after a nontrivial intervention which often severely affects the sharpness of the result. To this end we use the same set of problems for various approaches and compare them by comparing how well they are doing a job they were designed for. More to the point, the estimate of the type  $\text{Left}(\kappa) \leq \text{Right}(\kappa)$  — where  $\kappa \in \mathbb{R}$  is a parameter — is considered asymptotically sharp if

$$(58) \quad \lim_{\kappa \rightarrow \infty} \frac{\text{Left}(\kappa)}{\text{Right}(\kappa)} = 1.$$

Such property of an estimator is sometimes called the asymptotic exactness of an estimator, see [8] and relation (58) below.

**Remark 4.1.** *If we were to adopt the philosophy of [10], we would consider the family of eigenvalue problems  $(H, \alpha H + \beta M)$  — assuming  $\alpha, \beta \in \mathbb{R}$  are such that  $\alpha H + \beta M$  is hermitian positive definite — and ask for such  $\alpha$  and  $\beta$  which are in some sense optimal. We cannot give an answer to the question of the choice the optimal energy norm now, but*

we might return to the question in future work. Instead, we note that given  $\alpha, \beta \in \mathbb{R}$  such that  $\alpha H + \beta M$  and  $H$  are Hermitian positive definite reduces the problem to the one we can handle. The eigenvalues  $\lambda_i$  of the matrix pair  $(H, M)$  and  $\lambda_i^{\alpha, \beta}$  of the pair  $(H, \alpha H + \beta M)$  are related by the transformation  $\mu_i = \lambda_i / (\alpha \lambda_i + \beta)$ .

**4.1. Perturbations of eigenspaces in the energy norm.** We will now use the theory from the preceding section to study the rotation of eigenvectors of a parameter dependent family of eigenvalue problems

$$H_\kappa = H_b + \kappa H_e, \quad \kappa \gg 1.$$

Here  $H_b$  is positive definite,  $H_e$  is a positive semi-definite matrix and we are interested in the estimate of the rotation of eigenvectors in the changing energy norm

$$\|x\|_{H_\kappa} = \sqrt{x^* H_\kappa x}.$$

For some further motivation for studying these problems see the Appendix

To this end we note that eigenvector problems

$$(59) \quad H_\kappa v = \lambda v, \quad v = \frac{1}{\lambda} H_\kappa v, \quad v = \lambda H_\kappa^{-1} v$$

$$(60) \quad H_\kappa^{-1} v = \frac{1}{\lambda} v, \quad H_\kappa^{-1} v = \frac{1}{\lambda^2} H_\kappa v$$

have the same eigenvectors. Furthermore, it is known, [7, 16] that as  $\kappa$  tends to infinity the eigenvalues of  $H_\kappa$  either tend to infinity or, they converge to the nonzero eigenvalues of

$$L_b := P_{\text{Ker}(H_e)} H_\kappa \Big|_{\text{Ker}(H_e)}.$$

Subsequently, we decompose the space  $\mathbb{R}^n = \text{Ker}(H_e) \oplus (\text{Ker}(H_e))^\perp$  and, without reducing the level of generality—see [16, Formula (12)]—think of  $H_\kappa$  as the block operator matrix

$$(61) \quad H_\kappa = \begin{bmatrix} L_b & R_b^* \\ R_b & W_b \end{bmatrix} + \kappa \begin{bmatrix} 0 & 0 \\ 0 & H_e \end{bmatrix}.$$

We also denote the block diagonal of  $H_\kappa$  with

$$D_\kappa = \begin{bmatrix} L_b & \\ & W_b + \kappa H_e \end{bmatrix}$$

and compute

$$\begin{aligned} \|D_\kappa^{-1/2} (D_\kappa - H_\kappa) D_\kappa^{-1/2}\| &= \left\| \begin{bmatrix} 0 & L_b^{-1/2} R_b^* (W_b + \kappa H_e)^{-1/2} \\ (W_b + \kappa H_e)^{-1/2} R_b L_b^{-1/2} & 0 \end{bmatrix} \right\| \\ &= \frac{1}{\sqrt{\kappa}} \left\| \begin{bmatrix} 0 & L_b^{-1/2} R_b^* (\frac{1}{\kappa} W_b + H_e)^{-1/2} \\ (\frac{1}{\kappa} W_b + H_e)^{-1/2} R_b L_b^{-1/2} & 0 \end{bmatrix} \right\| \\ &= O\left(\frac{1}{\sqrt{\kappa}}\right). \end{aligned}$$

Let us introduce the perturbation estimate  $\eta_{H_\kappa} := \|D_\kappa^{-1/2}(D_\kappa - H_\kappa)D_\kappa^{-1/2}\|$ . With this we note the following inequalities

$$(62) \quad |x^* H_\kappa x - x^* D_\kappa x| \leq \eta_{H_\kappa} x^* D_\kappa x$$

$$(63) \quad |x^* H_\kappa^{-1} x - x^* D_\kappa^{-1} x| \leq \frac{\eta_{H_\kappa}}{1 - \eta_{H_\kappa}} x^* D_\kappa^{-1} x.$$

Obviously, with this analysis we can chose

$$(64) \quad \eta_{H_\kappa^{-1}} = \frac{\eta_{H_\kappa}}{1 - \eta_{H_\kappa}}$$

and so we can apply Theorem 3.4 directly.

**Remark 4.2.** *This discussion indicates that it is easy, within this theory, to switch the roles of  $H$  and its inverse  $H^{-1}$ . This is so because an estimate on the perturbation of the one implies the relative estimate for the perturbation of the other. A similar feature is shared by the relative gap from (57) since*

$$\frac{|\frac{1}{\lambda} - \frac{1}{\mu}|}{\sqrt{\frac{1}{\lambda\mu}}} = \frac{|\lambda - \mu|}{\sqrt{\lambda\mu}}.$$

*It is pleasing and useful — when switching the roles of  $H$  and  $M$  — that both ingredients of an estimate like (57) are robust with respect to inversion of the eigenvalues.*

For first simple experiments we consider the family of problems

$$(65) \quad H_\kappa = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & -1 \\ 0 & -1 & 2 + \kappa \end{bmatrix}, \quad \mathbb{H}_\kappa = \begin{bmatrix} 2 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 2 + \kappa \end{bmatrix} \quad \kappa \gg 1.$$

In the first experiment we will see how do the ingredients of the estimates—relative gap and the residual—feature in their performance.

By  $\lambda_1^{H_\kappa} < \lambda_2^{H_\kappa} < \lambda_3^{H_\kappa}$  we denote the eigenvalues of  $H_\kappa$  and by  $\lambda_1^{\mathbb{H}_\kappa} < \lambda_2^{\mathbb{H}_\kappa} < \lambda_3^{\mathbb{H}_\kappa} < \lambda_4^{\mathbb{H}_\kappa}$  the eigenvalues of  $\mathbb{H}_\kappa$ . We also use for eigenvectors the following notation

$$\begin{aligned} H_\kappa v_i^{H_\kappa} &= \lambda_i^{H_\kappa} v_i^{H_\kappa}, & i &= 1, 2, 3, \\ \mathbb{H}_\kappa v_i^{\mathbb{H}_\kappa} &= \lambda_i^{\mathbb{H}_\kappa} v_i^{\mathbb{H}_\kappa}, & i &= 1, 2, 3, 4. \end{aligned}$$

The behavior of the family of problems (65) has been analyzed in [16] with the help of the Gerschgorin theorem. Let us consider the eigenspace which belongs to the eigenvalues  $\lambda_1^{H_\kappa} < \lambda_2^{H_\kappa}$  and  $\lambda_1^{\mathbb{H}_\kappa} < \lambda_2^{\mathbb{H}_\kappa}$ . to this end we write the implicit partial diagonalization of  $H_\kappa$  and  $\mathbb{H}_\kappa$  in the generic block matrix form

$$\begin{bmatrix} L_b & R_b^* \\ R_b & W_b + \kappa H_e \end{bmatrix} \begin{bmatrix} V_\kappa \\ \widehat{W}_\kappa \end{bmatrix} = \begin{bmatrix} V_\kappa \\ \widehat{W}_\kappa \end{bmatrix} \Lambda_\kappa$$

where  $L_b$ ,  $W_b$ ,  $R_b$  and  $H_e$  are as in (61) and  $\Lambda_\kappa$  is the diagonal matrix containing the targeted eigenvalues. The orthogonality property  $V_\kappa^* V_\kappa + \widehat{W}_\kappa^* \widehat{W}_\kappa = I$  together with the Gerschgorin theorem implies, see [16, pg. 3209], the estimates

$$(66) \quad \|L_b V_\kappa - V_\kappa \Lambda_\kappa\| = O\left(\frac{1}{\kappa}\right), \quad \|V_\kappa^* V_\kappa - I\| = O\left(\frac{1}{\kappa^2}\right), \quad \|\widehat{W}_\kappa\| = O\left(\frac{1}{\kappa}\right).$$

In the example that follows we show this explicitly on the model problem and indicate a possible dependence on  $\kappa$  of the otherwise inaccessible matrix  $V_\kappa$ .

**Example 4.3.** In this example we show that the estimates are *asymptotically sharp*—for the definition of this notion see (58) below and reference [8] for a discussion of its significance in finite element computations—for the matrix  $H_\kappa$ . For this problem we have for eigenvalues and eigenvectors

$$\begin{aligned}\lambda_1^\kappa &= 1 - \frac{1}{2\kappa} + \frac{3}{8\kappa^2} - \frac{55}{128\kappa^4} + \frac{1}{2\kappa^5} + O\left(\frac{1}{\kappa^6}\right) \\ \lambda_2^\kappa &= 3 - \frac{1}{2\kappa} - \frac{3}{8\kappa^2} + \frac{55}{128\kappa^4} + \frac{1}{2\kappa^5} + O\left(\frac{1}{\kappa^6}\right) \\ \lambda_3^\kappa &= \kappa + 2 + \frac{1}{\kappa} - \frac{1}{\kappa^5} + O\left(\frac{1}{\kappa^6}\right)\end{aligned}$$

$$\begin{aligned}v_1^\kappa &= \begin{bmatrix} 1 + \frac{1}{2\kappa} + \frac{5}{8\kappa^2} - \frac{1}{2\kappa^3} + \frac{7}{128\kappa^4} + \frac{1}{2\kappa^5} - \frac{675}{1024\kappa^6} + O\left(\frac{1}{\kappa^7}\right) \\ 1 + \frac{1}{\kappa} + \frac{1}{2\kappa^2} - \frac{3}{8\kappa^3} + \frac{55}{128\kappa^5} - \frac{1}{2\kappa^6} + O\left(\frac{1}{\kappa^7}\right) \\ \frac{1}{\kappa} \end{bmatrix}, \\ v_2^\kappa &= \begin{bmatrix} -1 + \frac{1}{2\kappa} - \frac{5}{8\kappa^2} - \frac{1}{2\kappa^3} - \frac{7}{128\kappa^4} + \frac{1}{2\kappa^5} + \frac{675}{1024\kappa^6} + O\left(\frac{1}{\kappa^7}\right) \\ 1 - \frac{1}{\kappa} + \frac{1}{2\kappa^2} + \frac{3}{8\kappa^3} - \frac{55}{128\kappa^5} - \frac{1}{2\kappa^6} + O\left(\frac{1}{\kappa^7}\right) \\ \frac{1}{\kappa} \end{bmatrix}, \\ v_3^\kappa &= \begin{bmatrix} \left(\frac{1}{\kappa}\right)^2 - \left(\frac{1}{\kappa}\right)^4 + O\left(\frac{1}{\kappa^6}\right) \\ -\frac{1}{\kappa} + \left(\frac{1}{\kappa}\right)^5 + O\left(\frac{1}{\kappa^6}\right) \\ 1 \end{bmatrix}\end{aligned}$$

and  $\eta_{H_\kappa} = \sqrt{\frac{2}{6+3\kappa}}$ . Note that the matrix  $\left[V_\kappa \widehat{W}_\kappa\right]^*$  has columns given by  $v_1^\kappa$  and  $v_2^\kappa$ , and so we can see the dependence  $V_\kappa$  on the penalty parameter in this example explicitly. Using (64) we obtain

$$\text{Right}_\kappa := \frac{1}{\text{RelGap}} \cdot \frac{\eta_{H_\kappa^{-1}}}{\sqrt{1 - \eta_{H_\kappa^{-1}}}} + \frac{1}{\text{RelGap}_p} \cdot \frac{\eta_{H_\kappa}}{\sqrt{1 - 2\eta_{H_\kappa}}} = O\left(\frac{1}{\sqrt{\kappa}}\right).$$

On the other hand, a simple computation and Theorem 3.4 yield, cf. (66) that

$$\text{Left}_\kappa := \sin \Theta_{H_\kappa}(\text{Ran}[v_1^\kappa \ v_2^\kappa], \text{Ran}[v_1^\infty \ v_2^\infty]) = O\left(\frac{1}{\sqrt{\kappa}}\right).$$

Here we have used the symbol  $v_i^\infty$ ,  $i = 1, 2, 3$  to denote the limit eigenvectors of  $v_i^\kappa$ ,  $i = 1, 2, 3$  as  $\kappa \rightarrow \infty$ . They are also the eigenvectors of the limit matrix

$$H_\infty = \begin{bmatrix} 2 & -1 & 0 \\ -1 & 2 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

This shows that the energy norm estimate is sharp when viewed as the function of  $\kappa$ . On the other hand a simple computation reveals that any of the  $\sin \Theta$  theorems from [5, 9, 13]

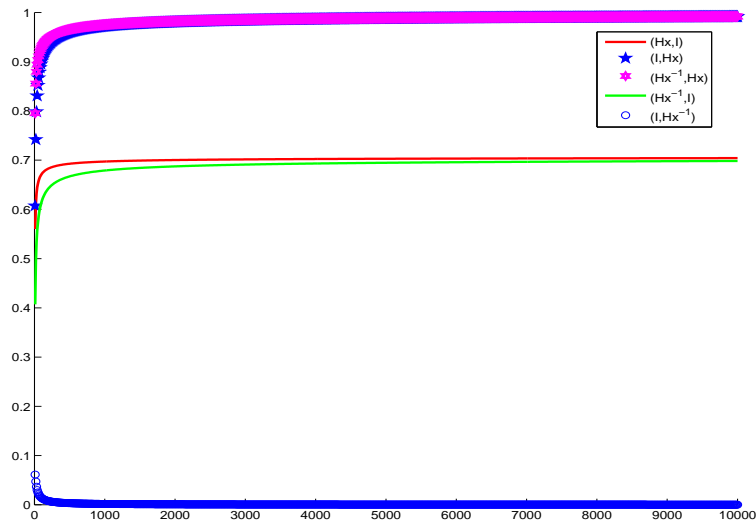


FIGURE 2. Numerical experiment for Example 4.3. The experiment demonstrates the notion of the *asymptotic sharpness*. In this plot we have depicted the effectivity quotient against the penalty parameter, see Example 4.3 for the definition.

yields a similar  $O(\frac{1}{\sqrt{\kappa}})$ —or even worse<sup>5</sup> for the  $O(1)$ —upper estimate for the

$$\sin \Theta(\text{Ran}[v_1^\kappa \ v_2^\kappa], \text{Ran}[v_1^\infty \ v_2^\infty]) = O\left(\frac{1}{\kappa}\right).$$

We now turn our attention to the study of the asymptotic sharpness — in the sense of (58) — of our estimates on concrete examples This can be proved by direct computation for the case of our estimate applied to the matrix pairs  $(H_\kappa^{-1}, H_\kappa)$  and  $(I, H_\kappa)$ , cf. Example 4.4 for further discussion. This shows that a notion of sharpness—a  $\sin \Theta$  theorem is considered to be sharp if there is a perturbation in the allowed class of perturbations such that the bound is attained—for the estimates of the rotation of eigenvectors is a delicate question. Let us note that we will call  $\frac{\text{Left}_\kappa}{\text{Right}_\kappa}$  the *effectivity quotient*.

**Example 4.4.** In this example we perform a Matlab experiment in which we evaluate the estimate of Corollary 3.5 for the matrix pairs

$$(\mathbb{H}_\kappa, I), (I, \mathbb{H}_\kappa), (\mathbb{H}_\kappa^{-1}, \mathbb{H}_\kappa), (\mathbb{H}_\kappa^{-1}, I), (I, \mathbb{H}_\kappa^{-1}).$$

The results are presented on Figure 3. The results further illustrate the delicacy of the issue of the sharpness of  $\sin \Theta$  theorems. Namely, the estimates are not asymptotically sharp for any of the considered matrix pairs, but the energy norm estimates—that is estimates for the pairs  $(I, \mathbb{H}_\kappa)$  and  $(\mathbb{H}_\kappa^{-1}, \mathbb{H}_\kappa)$ — are of the same order of the magnitude as the error—this can be seen from the fact that the effectivity quotients converge to a constant—where es in the case of the estimates for the other norms the effectivity quotients converge to zero. These

<sup>5</sup>The residual estimate (66) gets spoilt when we chose the orthonormal basis for  $\text{Ran}[v_1^\infty \ v_2^\infty]$  as the columns of  $V_\kappa$  are not orthonormal.



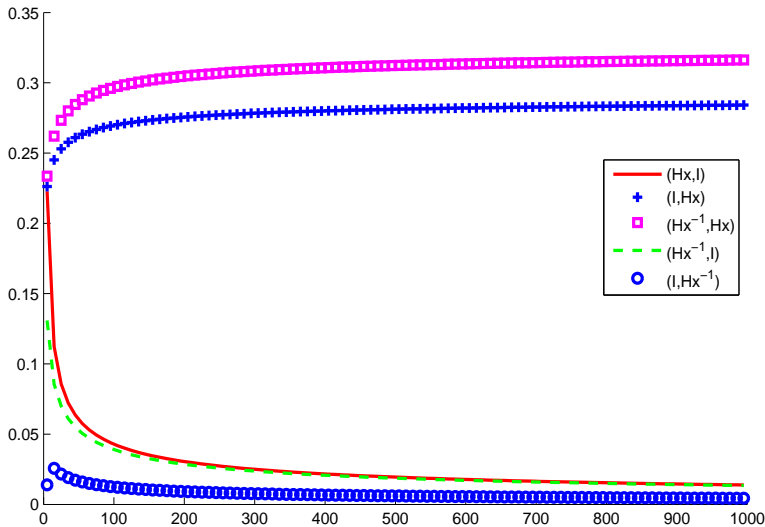


FIGURE 3. Numerical experiment for Example 4.4. In this plot we have depicted the effectivity quotient against the penalty parameter, see Example 4.3 for the definition.

convergence claims can be verified by a direct symbolic computation. This example shows that both the choice of a measure of the spectral gap as well as the choice of the measure of the residual play a role in obtaining high performance estimators, since it was the influence of the measure of the relative gap which guaranteed the asymptotic sharpness in Example 4.3, compare Figures 2 and 3.

**4.2. A Matrix Market example.** For a further illustration of an effect similar to mass lumping we will consider the generalized eigenvalue problem

$$Hx = \lambda Mx,$$

where the matrix  $H$  is taken from the Matrix Market basis, see [14]. We choose  $H$  from the set CYLSHELL: Finite element analysis of cylindrical shells matrices. From this test set we took the matrix `s1rmq4m1.mtx` which is real symmetric positive definite,  $5489 \times 5489$  matrix with 143300 entries. This matrix is obtained by finite element discretization of an octant of a cylindrical shell. The ends of the cylinder are free.

For the matrix  $M$  we took diagonal matrix with—in Matlab notation—`diag(1 : n)` and we consider random perturbations  $\delta H$  and  $\delta M$ , which satisfy

$$|(\delta H)_{ij}| \leq \eta_H |H_{ij}|, \quad |(\delta M)_{ij}| \leq \eta_M |M_{ij}|,$$

where  $\eta_H = \eta_M = 10^{-8}$ . The above assumption means that zeros remain unperturbed and we have chosen the  $M$  matrix whose norm explodes as  $n \rightarrow \infty$ . This is a reasonable choice for our method, since the technique of our proof can readily be adapted to yield the same result for some unbounded pair of operators in a Hilbert space.

As a comparison we consider one of the well known the standard perturbation bound for matrix pairs is given by the theorem of Stewart and Sun from [15, Chapter VI]. To this end,

let  $(H, M)$  be a symmetric definite pair, such that (9) holds. That is, let  $X = [X_1 \ X_2]$  be such that

$$(67) \quad \begin{bmatrix} X_1^* \\ X_2^* \end{bmatrix} H [X_1 \ X_2] = \begin{bmatrix} \Lambda_1 & \\ & \Lambda_2 \end{bmatrix} \quad \begin{bmatrix} X_1^* \\ X_2^* \end{bmatrix} M [X_1 \ X_2] = \begin{bmatrix} I_k & \\ & I_{n-k} \end{bmatrix},$$

where

$$\Lambda_1 = \text{diag}(\lambda_1, \dots, \lambda_k), \quad \Lambda_2 = \text{diag}(\lambda_{k+1}, \dots, \lambda_n),$$

and  $X_1 \in \mathbb{C}^{n \times k}$ ,  $X_2 \in \mathbb{C}^{n \times n-k}$ . The following theorem contains a bound for the Frobenius norm of the diagonal matrix which contains the sines of the canonical angles between eigenspace  $\text{Ran}(X_1)$  and corresponding perturbed eigenspace  $\mathcal{R}(\tilde{X}_1)$ .

**Theorem 4.5** (Sun). *Let the definite pair  $(H, M)$  be decomposed as in (67) where  $X_1$  and  $X_2$  have orthonormal columns. Let the analogous decomposition be given for the pair  $(\tilde{H}, \tilde{M}) \equiv (H + \delta H, M + \delta M)$ . If*

$$\delta = \min \left\{ \frac{|\tilde{\lambda} - \lambda|}{\sqrt{1 + \tilde{\lambda}^2} \sqrt{1 + \lambda^2}}; \lambda \in \varrho(\Lambda_1), \tilde{\lambda} \in \varrho(\tilde{\Lambda}_2) \right\},$$

then

$$(68) \quad \|\sin \Theta[\text{Ran}(X_1), \text{Ran}(\tilde{X}_1)]\|_F \leq \frac{\sqrt{\|H^2 + M^2\|} \sqrt{\|\delta H X_1\|_F^2 + \|\delta M X_1\|_F^2}}{\gamma(H, M) \gamma(\tilde{H}, \tilde{M}) \delta},$$

where

$$(69) \quad \gamma(H, M) = \min_{\substack{x \in \mathbb{C}^n \\ \|x\|=1}} |x^*(H + iM)x| = \min_{\substack{x \in \mathbb{C}^n \\ \|x\|=1}} \sqrt{(x^* H x)^2 + (x^* M x)^2} > 0.$$

We estimate the perturbation of invariant subspace which corresponds with first four smallest eigenvalues of the matrix pair  $(H, M)$ . The experiment is to be understood in the context of the testing of the asymptotic sharpness of the estimator as in the definition (58).

**Example 4.6** (The performance of our estimate). The exact perturbation gives:

$$\|\sin \Theta_M(\mathcal{X}_1, \tilde{\mathcal{X}}_1)\| \approx 6.727 \cdot 10^{-7},$$

while our bound (43) gives

$$\|\sin \Theta_M(\mathcal{X}_1, \tilde{\mathcal{X}}_1)\| \leq 8.6721 \cdot 10^{-4}.$$

**Example 4.7** (The performance of the Stewart-Sun bound). The bound (68) here is not satisfactory due the fact that  $\gamma(H, M) = 1$ , and  $\gamma(H + \delta H, M + \delta M) \approx 1 + \varepsilon$ . On the other hand the gap  $\delta \sim 10^{-6}$  and  $\sqrt{\|H^2 + M^2\|} \sim 10^5$ . Together with

$$\sqrt{\|\delta H X_1\|_F^2 + \|\delta M X_1\|_F^2} = 3.872 \cdot 10^{-6},$$

we have

$$\|\sin \Theta[\text{Ran}(X_1), \text{Ran}(\tilde{X}_1)]\|_F \leq 6 \cdot 10^5.$$

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## APPENDIX A. A MOTIVATION TO STUDY THE PROBLEMS OF THE LARGE COUPLING LIMIT

Consider positive definite eigenvector problems of the following type: find  $\psi$ ,  $\|\psi\| = 1$  and  $\lambda \in \mathbb{R}$  such that

$$(70) \quad H_\kappa \psi = H_b \psi + \kappa H_e \psi = \lambda \psi,$$

where  $H_b$  is positive definite matrix and  $H_e$  is a semidefinite perturbation which has a significant null space and  $\kappa \gg 1$ . The presence of a large coupling constant  $\kappa$  the singular perturbation  $H_e$  causes the appearance of spurious, that is nonphysical, eigenvalues due to

the non-zero component of  $H_e$ . It is our aim to obtain bounds on the rotation of eigenspaces which is caused by this perturbation.

When considering the families of matrices/operators like  $H_\kappa = H_b + \kappa H_e$ ,  $\kappa \gg 1$ . the parameter  $\kappa$  is called the coupling — or depending on the context the penalty — parameter. The family of perturbations  $\kappa H_e$  splits the spectrum of  $H_\kappa$  into a bounded and an unbounded component as  $\kappa \rightarrow \infty$ .

One typical example of a problem in this setting are the penalty methods for Maxwell or Stokes' eigenvalue problems. For more information and further references see [16]. There, the authors analyze the dependence of the spectrum of the discretization matrix of the Maxwell's eigenvalue problem on the large coupling parameter and show—by a very elegant Gerschgorin type argument—that as  $\kappa \rightarrow \infty$  the eigenvalues of interest converge with the rate proportional to  $\kappa^{-1}$ .

Let us note that the models where one considers the limits of the large penalty are representative for a larger class of parameter dependent singularly perturbed eigenvalue problems. These problems typically appear in the study of optical nano-devices, hard core scattering theory and in the analysis of lower dimensional approximations to the 3D elasticity (like Arches and Plates), see [3, 4, 6, 7]. Another example is the so called “lumped mass approximation” in which an auxiliary diagonal mass matrix  $\tilde{M}$  is constructed which generates an equivalent scalar product. Such matrices are typically constructed by using quadrature formulae and pseudo  $L^2$  projections, see [1]. The analysis from [3, 7] shows that the eigenvalue estimates from [16] are sharp when viewed in terms of the dependence on the coupling constant, cf. Example 4.3. <sup>6</sup>

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<sup>6</sup>Explicit constants and their physical interpretations are explicitly given in [3, 7].