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ERROR REPRESENTATION FORMULA FOR EIGENVALUE APPROXIMATIONS FOR POSITIVE DEFINITE OPERATORS

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Abstract. The main contribution of this paper is an error representation formula for eigenvalue approximations for positive definite operators defined as quadratic forms. The formula gives an operator theoretic framework for treating discrete eigenvalue approximation/estimation problems for unbounded positive definite operators independent of the multiplicity. Furthermore, by the use of the error representation formula, we give computable lower and upper estimates for discrete eigenvalues of such operators. The estimates could be seen as being of the Kato–Temple type. Our estimates can be applied to the Rayleigh–Ritz approximation on the test subspace which is a subset of the corresponding form domain of the operator. We present several completely soluble prototype examples for an application of the presented theory and argue the optimality of our approach in this context.

1. Introduction

The purpose of this paper is to establish estimates for discrete eigenvalues of positive definite operators in a Hilbert space which have the following three properties:

- they are of relative type, which means that the estimates are scaled with respect to the magnitude of the approximated eigenvalues,
- the test subspace from which we are approximating the eigenvalues need not be a subset of the domain of the operator; it is sufficient that it is a subset of the domain of the corresponding form of the operator,
- the estimates take into account the multiplicity of the eigenvalues.

The main contribution of the paper is the new eigenvalue error representation formula which is given as an operator identity to facilitate the treatment of eigenvalue multiplicity, cf. Theorem 6.

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To illustrate the power of the new error representation formula we will show how they can be used to obtain tight asymptotical estimates for the eigenvalues of two classes of spectral problems.

Our approach uses the theory of quadratic forms from [18, Chapters VI–VIII] and an adaptation of the matrix relative perturbation theory. As a result we establish the same high performance residual type estimates from [9] in our more general setting, cf. [5] for most recent matrix results. For a review of the matrix relative perturbation theory see [23] and the references therein.

We emphasize that we are interested solely in residual based eigenvalue estimation techniques for unbounded positive definite operators which are defined by quadratic forms. On the other hand, there have been several recent studies of similar estimates in other contexts. Most notable are reference [3] and recent surveys [25, 26] which contain a large list of references. Such methods are frequently proved for bounded operators, and then applied to unbounded operators by a suitable regularization.

The rest of the present paper is organized as follows. In Section 2 we give basic definitions of the objects of study together with some useful properties, and give a precise formulation of the problem. In Section 3 we prove the main result, and in Section 4 we compare our approach with other estimation techniques. In Section 5 we apply our result to three problems: spectral convergence in the large coupling limit for an analytically solvable 1D model, finite element computations for an analytically solvable 1D model and spectral convergence in the large coupling limit for a model problem in higher dimensions.

2. Formulation of the problem

Let $\mathfrak{h}$ be a closed, symmetric and positive form in a Hilbert space $\mathscr{H}$ which has a dense domain $\mathrm{Dom}(\mathfrak{h})$. Here by positive form we mean that there exists $\gamma > 0$ such that $\mathfrak{h}(\psi,\psi) > \gamma\|\psi\|$ for all $\psi \in \mathscr{H} \setminus \{0\}$.

We know by the Kato's second representation thorem [18] that such form defines in $\mathscr{H}$ the self–adjoint postitive definite operator H which has the following properties: $\mathrm{Dom}(H^{1/2}) = \mathrm{Dom}(\mathfrak{h})$ and $\mathfrak{h}(\phi,\psi) = (H^{1/2}\phi, H^{1/2}\psi)$ for all $\phi,\psi \in \mathrm{Dom}(\mathfrak{h})$.

Let $\overline{P}$ be an orthogonal projector such that $\dim \mathsf{Ran}(\overline{P}) = m$ and $\mathsf{Ran}(\overline{P}) \subset \mathrm{Dom}(\mathfrak{h})$ We will call $\mathsf{Ran}(\overline{P})$ a *test subspace* of dimension m. The operator M defined by the form $\mathfrak{h}(\overline{P}\cdot,\overline{P}\cdot)$ in $\mathsf{Ran}(\overline{P})$ will be called (generalized) *Rayleigh quotient*. Its eigenvalues $\mu_1 \leqslant \ldots \leqslant \mu_m$ will be called *the Ritz values* from the test subspace $\mathsf{Ran}(\overline{P})$ and the vectors $u_i \in \mathsf{Ran}(\overline{P})$ such that $Mu_i = \mu_i u_i$, $\|u_i\| = 1$ will be called the *Ritz vectors*. Since $\mathfrak{h}$ is positive it follows $\mu_1 > 0$.

Let $\underline{P} = I - \overline{P}$. We define the operator $W : \mathsf{Ran}(\underline{P}) \to \mathsf{Ran}(\underline{P})$ as the one defined by the form $\mathfrak{h}(\underline{P}\cdot,\underline{P}\cdot)$ on $\mathsf{Ran}(\underline{P})$.

We will need the following result to compare the eigenvalues of H and W.

LEMMA 1. (Stenger's inequality, [34]) [1] *Let us assume that the lower parts of the spectra of H and W consist of isolated eigenvalues $\lambda_1 \leqslant \lambda_2 \leqslant \ldots$ and $\lambda'_1 \leqslant \lambda'_2 \leqslant \ldots$*

[1]The use of Stenger's inequality has been suggested to the authors by an anonymous referee. The authors are thankful for this suggestion.

each having finite multiplicity. Then we have

$$\lambda_1 + \lambda_{i+j} \leqslant \mu_i + \lambda'_j. \tag{1}$$

We now construct the positive form $\widetilde{\mathfrak{h}}(\phi,\psi) := \mathfrak{h}(\overline{P}\phi,\overline{P}\psi) + \mathfrak{h}(\underline{P}\phi,\underline{P}\psi)$, $\phi,\psi \in \mathrm{Dom}(\mathfrak{h})$. This form — called the $(\overline{P},\underline{P})$-*diagonal* part of $\mathfrak{h}$ — defines the positive definite self-adjoint operator $\widetilde{H}$.

We define the operator $K : \mathsf{Ran}(\overline{P}) \to \mathsf{Ran}(\underline{P})$ as the unique operator which satisfies

$$(\psi, K\phi) = \mathfrak{h}(\widetilde{H}^{-1/2}\psi, \widetilde{H}^{-1/2}\phi), \text{ for all } \psi \in \mathrm{Dom}(\mathfrak{h}) \cap \mathsf{Ran}(\underline{P}), \phi \in \mathsf{Ran}(\overline{P}).$$

We call K the scaled residual.

We also define the form $\widetilde{\mathfrak{r}}(\phi,\psi) = \mathfrak{h}(\overline{P}\phi,\underline{P}\psi) + \mathfrak{h}(\underline{P}\phi,\overline{P}\psi)$, $\phi,\psi \in \mathrm{Dom}(\mathfrak{h})$, which is an approximation defect in $\mathsf{Ran}(\overline{P})$, since $\mathsf{Ran}(\overline{P})$ is an invariant subspace of H if and only if $\widetilde{\mathfrak{r}} \equiv 0$. For a proof see [15]. Furthermore, it was shown in [13] that

P1. $\mathsf{Ran}(\overline{P})$ reduces $\widetilde{H}$

P2. $M = \overline{P}\widetilde{H}\overline{P}$

P3. $\mathsf{Ran}(H^{-1} - \widetilde{H}^{-1})$ is finite dimensional which implies $\mathrm{Spec}_{\mathrm{ess}}(H) = \mathrm{Spec}_{\mathrm{ess}}(\widetilde{H})$.

Here Spec denotes the spectrum and $\mathrm{Spec}_{\mathrm{ess}}$ denotes the essential spectrum.

The properties P1, P2 and P3 imply that $\mu_i \in \mathrm{Spec}(\widetilde{H})$. We set the scene for an application of the relative perturbation theory from [18, Chapters VI–VIII] and so we will be able, regardless of the fact that $\mathrm{Dom}(H) \neq \mathrm{Dom}(\widetilde{H})$, to interpret H as a perturbation of $\widetilde{H}$ and thus bring μ_i's in connection with some component of $\mathrm{Spec}(H)$.

Let us now look into the structure of this construction in more detail. According to [13, Theorem 4.5] the form $\widetilde{\mathfrak{s}}(\cdot,\cdot) := \widetilde{\mathfrak{r}}(\widetilde{H}^{-1/2}\cdot, \widetilde{H}^{-1/2}\cdot)$ defines the bounded operator $\widetilde{S}$ and $\dim \mathsf{Ran}(\widetilde{S}) < \infty$. The standard perturbation result from [18] implies that the estimates

$$\omega_i(1 - \|\widetilde{S}\|) \leqslant \lambda_i \leqslant \omega_i(1 + \|\widetilde{S}\|)$$

hold for all discrete eigenvalues $\omega_1 \leqslant \cdots \leqslant \omega_q \leqslant \cdots < \lambda_{\mathrm{ess}}(H) = \lambda_{\mathrm{ess}}(\widetilde{H})$ of $\widetilde{H}$. Here $\lambda_{\mathrm{ess}}(H)$ denotes the infinum of the essential spectrum of the operator H. The property P1 implies that some ω_i — together with multiplicities — are identical with the Ritz values $\mu_1 \leqslant \cdots \leqslant \mu_m$. This results yields a computable estimates of a collection of eigenvalues of joint multiplicity m. To turn this into a practical estimate we need to localize this subset in $\mathrm{Spec}(H)$, e.g. if we assume that m and $\overline{P}$ are such that $\|\widetilde{S}\| < \frac{1}{2}\frac{\lambda_{m+1}-\lambda_m}{\lambda_{m+1}+\lambda_m}$ holds then

$$\frac{|\lambda_i - \mu_i|}{\mu_i} \leqslant \|\widetilde{S}\|, \quad i = 1,\cdots,m\,. \tag{2}$$

As is given our definition of $\widetilde{S}$ is not constructive. The properties of the operator $\widetilde{S}$ have been analyzed in detail in [13] and we point an interested reader there for further discussion. We collect the relevant properties for this paper in the following lemma.

LEMMA 2. *Define*

$$\eta_i := \Big[\max_{\substack{\mathscr{S}\subset \mathsf{Ran}(\overline{P}),\\ \dim(\mathscr{S})=m-i+1}} \min\Big\{ \frac{(\psi,H^{-1}\psi)-(\psi,\widetilde{H}^{-1}\psi)}{(\psi,H^{-1}\psi)} \mid \psi\in\mathscr{S}, \|\psi\|=1 \Big\}\Big]^{1/2}, \qquad (3)$$

$i=1,\cdots,m$. Then $\eta_i<1$, $i=1,\cdots,m$ and there exists $r\leqslant m$ such that $\eta_{r+1},\ldots,\ \eta_m$ are all the nonzero singular values of $\widetilde{S}$. Furthermore, $\eta_{r+1},\ldots,\ \eta_m$ are all non-zero singular values of the scaled residual K.

At this point we note that for every $\psi\in\mathsf{Ran}(\overline{P})$ we have the following identity

$$(\psi,H^{-1}\psi)-(\psi,\widetilde{H}^{-1}\psi)=\|HM^{-1}\psi-\psi\|_{H^{-1}}^2=\|H^{-1}\psi-M^{-1}\psi\|_H^2. \qquad (4)$$

Here $\|\cdot\|_H=\|H^{1/2}\cdot\|$ and $\|\cdot\|_{H^{-1}}=\|H^{-1/2}\cdot\|$.

Assume that the eigenvalues of H which are below the infimum of its essential spectrum $\lambda_{\mathrm{ess}}(H)$ are ordered according to multiplicity and that for some $q,m\in\mathbb{N}$ we have

$$\lambda_1\leqslant\cdots\leqslant\lambda_{q-1}<\lambda_q=\lambda_{q+m-1}<\lambda_{q+m}\leqslant\cdots<\lambda_{\mathrm{ess}}(H)\,.$$

The singular values of the operator $I-\lambda_q M^{-1}$ are the relative errors $\frac{|\lambda_q-\mu_i|}{\mu_i}$, $i=1,\ldots,m$ for the Ritz values μ_i. Our aim is to find a lower and upper bound on $I-\lambda_q M^{-1}$ in terms of the scaled residual K. From Lemma 2 it follows that our bounds can (and henceforth will) be written in terms of numbers η_i.

REMARK 3. The definition of η_i indicates that the problem of computing (or estimating) η_i requires the solution of the $m\times m$ positive definite generalized eigenvalue problem, cf. (4). Since m is the multiplicity of the eigenvalue of interest, the computational cost of the solution of such problem is negligible. The main problem is how to evaluate or estimate the moments $(u_i,H^{-1}u_j)$, $i,j=1,\ldots,m$ without actually inverting the operator H^{-1}. For some possibilities to do this see [1, Section 3.], [11, Section 5.] or [8, Remark 8].

3. Main result

We now present the main contribution of this article, the relative eigenvalue estimates in the presence of Ritz value clusters. Our technique is based on the Wilkinson's trick from matrix analysis, cf. [27, p. 183], which we now present in the context of operator matrices.

THEOREM 4. (Wilkinson's trick) *Let $A:\mathscr{H}_1\to\mathscr{H}_1$ and $X:\mathscr{H}_2\to\mathscr{H}_1$ be bounded operators and let A be self-adjoint. Assume further that $B:\mathscr{H}_2\to\mathscr{H}_2$ is self-adjoint and that it has a bounded inverse and define $T=\begin{bmatrix} A & X\\ X^* & B\end{bmatrix}$, to be understood as operator on $\mathscr{H}_1\oplus\mathscr{H}_2$. If $\dim\mathsf{Null}(T)=\dim\mathscr{H}_1<\infty$ then*

$$A=XB^{-1}X^*.$$

Proof. We shall adapt the Schur-complement technique from [27, p. 183]. Since B^{-1} is assumed to be bounded we can write

$$T = \begin{bmatrix} I & XB^{-1} \\ 0 & I \end{bmatrix} \begin{bmatrix} A - XB^{-1}X^* & 0 \\ 0 & B \end{bmatrix} \begin{bmatrix} I & 0 \\ B^{-1}X^* & I \end{bmatrix} =: L^*DL. \tag{5}$$

Both of the operator matrices L and L^{-1} define bounded operators on $\mathscr{H}_1 \oplus \mathscr{H}_2$, and so $D = L^{-*}TL^{-1}$. This implies that $\mathrm{Dom}(T) = \mathrm{Dom}(D)$ and as a consequence of a simple dimension counting we obtain that $\dim \mathsf{Null}(T) = \dim \mathsf{Null}(D) < \infty$. Since B has a bounded inverse this can only be true if $A - XB^{-1}X^* = 0$. $\square$

REMARK 5. Note that the theorem remains valid if we only assume that B is injective and $B^{-1}X^*$ is bounded. In this case we conclude that $A = X(B^{-1}X^*)$. In the case when $\mathscr{H}_1$ is infinite dimensional the dimension counting cannot be used to prove the result. Some spectral properties of Schur complements in a general situation can be found in [22].

THEOREM 6. (Representation formula for the relative error in λ_q) *If there exists $q \in \mathbb{N}$ such that $\lambda_{q-1} < \lambda_q = \lambda_{q+m-1} < \lambda_{q+m}$ and*

$$\frac{\eta_m}{1-\eta_m} < \min\left\{ \frac{\lambda_{q+m} - \mu_m}{\lambda_{q+m} + \mu_m}, \frac{\mu_1 - \lambda_{q-1}}{\mu_1 + \lambda_{q-1}} \right\}$$

holds, then

$$I - \lambda_q M^{-1} = K^*(I - \lambda_q W^{-1})^{-1} K \tag{6}$$

$$= K^*K + \lambda_q K^* W^{-1/2}(I - \lambda_q W^{-1})^{-1} W^{-1/2} K. \tag{7}$$

Proof. A modification of [13, Theorems 5.1 and 5.2] implies that the form

$$\mathfrak{h}(\widetilde{H}^{-1/2}\cdot, \widetilde{H}^{-1/2}\cdot) - \lambda_q(\widetilde{H}^{-1/2}\cdot, H^{-1/2}\cdot)$$

defines the bounded operator $I + \widetilde{S} - \lambda_q \widetilde{H}^{-1}$, which allows the operator matrix representation

$$I + \widetilde{S} - \lambda_q \widetilde{H}^{-1} = \begin{bmatrix} I - \lambda_q M^{-1} & K^* \\ K & I - \lambda_q W^{-1} \end{bmatrix}, \tag{8}$$

with respect to $\mathscr{H} = \mathsf{Ran}(\overline{P}) \oplus \mathsf{Ran}(\underline{P})$. Now, [13, Theorem 5.1] implies that $I - \lambda_q W^{-1}$ is invertible and we may use the Wilkinson's trick to derive the quadratic estimates. Now set $B_{\mathrm{rel}} := (I - \lambda_q W^{-1})$. Then

$$I + \widetilde{S} - \lambda_q \widetilde{H}^{-1} = \begin{bmatrix} I & K^* B_{\mathrm{rel}}^{-1} \\ 0 & I \end{bmatrix} \begin{bmatrix} (I - \lambda_q M^{-1}) - K^* B_{\mathrm{rel}}^{-1} K & 0 \\ 0 & B_{\mathrm{rel}} \end{bmatrix} \begin{bmatrix} I & 0 \\ B_{\mathrm{rel}}^{-1} K & I \end{bmatrix},$$

and Theorem 4 yields $I - \lambda_q M^{-1} = K^*(I - \lambda_q W^{-1})^{-1} K$, hence we obtained (6). By the simple manipulation the last equation can be rewritten as

$$I - \lambda_q M^{-1} = K^*K + \lambda_q K^* W^{-1/2}(I - \lambda_q W^{-1})^{-1} W^{-1/2} K. \quad \square$$

Set

$$\delta_q = \left(\min\{|\lambda_q - \mu|\mu^{-1} : \mu \in \operatorname{Spec}(\widetilde{H}) \setminus \{\mu_1, \dots, \mu_m\}\}\right)^{-1},$$

as the measure of the relative gap in the spectrum and let $|||\cdot|||$ be any unitary invariant norm.

COROLLARY 7. *Assume the setting of Theorem 6. Then we have*

$$|||\, I - \lambda_q M^{-1} \,||| \leqslant \eta_m \delta_q \,|||\, \operatorname{diag}(\eta_1, \cdots, \eta_m) \,|||. \tag{9}$$

Proof. From (6) and the definition of δ_q it immediately follows

$$|||\, I - \lambda_q M^{-1} \,||| \leqslant \delta_q \,|||\, K^* K \,|||.$$

Now (9) can be obtained by the use of the relation $|||\, K^*K \,||| \leqslant \|K^*\| \,|||\, K \,|||$ (cf. [33]). We also use that for the singular values η_i, $i = 1, \dots, m$ of K we have $|||\, K \,||| = |||\operatorname{diag}(\eta_1, \cdots, \eta_m) \,|||$, where $\operatorname{diag}(\eta_1, \cdots, \eta_m)$ is the $m \times m$ diagonal matrix with η_i on the diagonal. $\square$

COROLLARY 8. *Assume the setting of Theorem 6. If $\mu_m < \lambda_{m+1}$, $q = 1$ and the minimum of the spectrum of W is an isolated eigenvalue of finite multiplicity. Then we have:*

$$|||\operatorname{diag}(\eta_1^2, \cdots, \eta_m^2) \,||| \leqslant |||\, I - \lambda_1 M^{-1} \,||| \leqslant \frac{\lambda_{m+1}}{\lambda_{m+1} - \mu_m} \,|||\operatorname{diag}(\eta_1^2, \cdots, \eta_m^2) \,|||, \tag{10}$$

$$\sum_{i=1}^m \eta_i^2 \leqslant \sum_{i=1}^m \frac{\mu_i - \lambda_i}{\mu_i} \leqslant \frac{\lambda_{m+1}}{\lambda_{m+1} - \mu_m} \sum_{i=1}^m \eta_i^2. \tag{11}$$

Proof. To prove the right hand side of (10) it is sufficient to prove that

$$|||\, (I - \lambda_m W^{-1})^{-1} \,||| \leqslant \frac{\lambda_{m+1}}{\lambda_{m+1} - \mu_m}. \tag{12}$$

To prove (12) we will use Lemma 1 with $i = m$, $j = 1$ which implies

$$W \geqslant (\lambda_m + \lambda_{m+1} - \mu_m) I. \tag{13}$$

Now we can use functional calculus and the fact that $\lambda_1 = \lambda_m \leqslant \mu_1 \leqslant \mu_m$ (Rayleigh–Ritz bound, see eg. [30]) to prove (12). The left hand side in (10) follows from the fact that $I - \lambda_q W^{-1}$ is positive definite which follows from (13). Analogously one can prove — using (7) —

$$K^* K \leqslant I - \lambda_q M^{-1} \leqslant \frac{\lambda_{m+1}}{\lambda_{m+1} - \mu_m} K^* K. \tag{14}$$

The bound (11) now readily follows by an application of the trace operator $\mathrm{tr}(\cdot)$ on (14). $\square$

The relation (11) indicates that the size of the approximation error $\sum_{i=1}^{m} \frac{\mu_i - \lambda_i}{\mu_i}$ is essentially related to the singular values of K plus a correction term. This result is a mixture of the measure of the relative gap — which is expressed by the quantity δ_q — and the measure of the approximation defects η_i^2, since $\overline{P}$ is the eigenprojection of H if and only if $\eta_i = 0$, $i = 1, \ldots, m$.

A lower bound for the approximation error similar to the left hand side in (11) can be obtained even when some of the assumptions of Corollary 8 do not hold. Indeed, let $\lambda_m < \lambda_{m+1}$ and let $\mathsf{Ran}(\overline{P})$ be the test space such that $2\eta_m < 1$. Then

$$\frac{\mu_1}{2\mu_m} \sum_{i=1}^{m} \eta_i^2 \leqslant \sum_{i=1}^{m} \frac{\mu_i - \lambda_i}{\mu_i}. \tag{15}$$

The proof follows from

$$\begin{aligned} \sum_{i=1}^{m} \left[(u_i, H^{-1} u_i) - (u_i, M^{-1} u_i) \right] &= \sum_{i=1}^{m} \left[(u_i, H^{-1} u_i) - \frac{1}{\mu_i} \right] \\ &\leqslant \sum_{i=1}^{m} \left[\frac{1}{\lambda_i} - \frac{1}{\mu_i} \right] = \sum_{i=1}^{m} \frac{\mu_i - \lambda_i}{\lambda_i \mu_i} \end{aligned} \tag{16}$$

and the relation — guaranteed by the assumption $2\eta_m < 1$ —

$$\frac{1}{2}(u, Mu) \leqslant (u, Hu) \leqslant \frac{3}{2}(u, Mu), \qquad u \in \mathsf{Ran}(\overline{P}).$$

The upper estimate in (15) can be achieved by a repeated application of the trace operator and to the identity (6). The estimate is rather technical and we leave it out. However, we emphasize that we can recreate the framework of [10, Proposition 2.3] completely.

4. A comparison with other estimates

The standard form of Kato–Temple inequality (originally proved in [17]) says that if λ is the unique eigenvalue in some interval (α, β) of a self–adjoint operator H, then

$$\mu - \frac{r^2}{\beta - \mu} \leqslant \lambda \leqslant \mu + \frac{r^2}{\mu - \alpha}, \tag{17}$$

where $\mu = (u, Hu)$ and $r = \|(H - \mu)u\|$, under the assumptions $\mu \in (\alpha, \beta)$, $r^2 \leqslant (\beta - \mu)(\mu - \alpha)$.

For the proof we can consider — without reducing the level of generality — the case $\mu = 0$ and simply observe that $(H - \alpha I)(H - \lambda I)$ and $(H - \beta I)(H - \lambda I)$ are positive definite operators. We can then apply this positivity property for the vector u.

Temple inequality is a special case of the left hand side of (17) when λ is additionally the smallest element from the spectrum.

In the case of clustered eigenvalues, one needs a generalization of this result and Kato's original paper [17] contains such a result which however is not suitable for computational practice (but there are modifications which are developed precisely for the purposes of practical eigenvalue bracketing, see [3], [29] and [28] for details).

Now we will show that under some additional assumptions, we can recover a form of the standard Kato–Temple inequality for the clustered eigenvalues given in Theorem 6 and Corollaries 7 and 8.

Let us assume $\mathsf{Ran}(\overline{P}) \subset \mathrm{Dom}(H)$ then $H : \mathrm{Dom}(H) \to \mathscr{H}$ can be written as

$$H = \begin{bmatrix} M & R^* \\ R & W \end{bmatrix},$$

with R a bounded operator. Under these assumptions and the assumptions of Theorem 6 we can prove, again using the Wilkinson's trick, that we have

$$M - \lambda I = R^*(W - \lambda I)^{-1} R. \tag{18}$$

If we assume $\mu_m < \lambda_{m+1}$, we can use Lemma 1 to obtain $\|(W-\lambda I)^{-1}\| \leqslant (\lambda_{m+1} - \mu_m)^{-1}$.

If we denote the norm of the (single) Ritz vector residuals by $r_i := \|Hu_i - \mu_i u_i\|$ and apply the trace operator $\mathrm{tr}(\cdot)$ on (18), we obtain

$$\sum_{i=1}^{m} |\mu_i - \lambda| \leqslant \frac{1}{\lambda_{m+1} - \mu_m} \sum_{i=1}^{m} r_i^2. \tag{19}$$

Estimate (19) can be regarded as a generalization of the Temple inequality. Indeed, if we take $m = 1$, $\beta = \lambda_{m+1}$, $\lambda = \lambda_m$, $\mu = \mu_m$, then the left hand side of (17) can be written as $|\lambda - \mu| \leqslant \frac{r^2}{\lambda_{m+1} - \mu}$.

Inequality (19) is of the same vein as the inequality in [24], in fact it is an unbounded variant of the result in [24].

If we apply (18) to the operator $\widetilde{H}^{-1/2} H \widetilde{H}^{-1/2}$ we obtain the equation (6), which means we can formally think of (6) as a Kato–Temple inequality in the norm $\|\cdot\|_{\widetilde{H}^{-1}}$. But we stress that, in general, (6) cannot be obtained from (18) without additional assumptions. For an alternative way to utilize (17) to approximate the eigenvalue by the Ritz value from the form domain of the operator see Remark 10.

5. Kato–Temple bounds in the asymptotic regime

The main contribution of this paper is the error representation formula (7). Its main feature is that the contribution of the scaled residual K is separated from the contribution of the relative gap operator B_{rel}. Furthermore, unlike in the approach from [24] — which is directly generalized in (18) — the operator B_{rel} is both bounded and has — unlike the operator $(W - \lambda I)^{-1}$ a bounded inverse. This makes the formula (7) particularly suitable for the study of asymptotic processes. So far this has been successfully applied in the design of high performance stopping criteria for modern mathematical software in [10]. We apply our generalization of those techniques to study several infinite dimensional prototype eigenvalue approximation problems.

More to the point, it is the aim of this section to demonstrate a way to use the error representation formula (7) to prove

$$\|\| I-\lambda_q M^{-1} \|\| = \|\| \operatorname{diag}(\eta_1^2,\cdots,\eta_m^2) \|\| + o(\|\| \operatorname{diag}(\eta_1^2,\cdots,\eta_m^2) \|\|). \tag{20}$$

This formula is to be read in the context of η_i's being the computable (in the sense of Remark 3) first order correctors (as $\eta_i \to 0$) for μ_i's as approximations of λ_q. Rather than to present general proofs, which would require too much additional technical detail for the intended scope of this article, we prove this fact for two concrete prototype model problems. The significance of this formula is that it indicates that as $\eta_i \to 0$, the contribution of the distance to the unwanted component of the spectrum is asymptotically of higher order and the behavior of the eigenvalue approximations are effectively controlled by the computable quantities η_i. An interested reader can look up further technical details in [12].

5.1. Spectral convergence in the large coupling limit: analytically solvable 1D model problem

The main feature of the matrix eigenvalue algorithms from [10] is that they are robust when applied to extremely badly scaled input matrices. We bring this in correspondence with the behavior of the spectrum of stiffly/singularly perturbed operators from [6, 7, 32]. To be more precise let us consider a class of eigenvalue problems which is given by the family of positive definite forms

$$\mathfrak{h}_\kappa(u,v) = \mathfrak{h}_b(u,v) + \kappa^2 \mathfrak{h}_e(u,v), \quad \kappa \text{ large}. \tag{21}$$

Without affecting the generality of our results, we assume that $\mathfrak{h}_b$ is positive definite and densely defined and that $\operatorname{Dom}(\mathfrak{h}_e)$ satisfies $\operatorname{Dom}(\mathfrak{h}_b) \subset \operatorname{Dom}(\mathfrak{h}_e)$. An extensive study of non-inhibited stiff families of operators has been performed, with the help of the results from this article, in [12, 16]. We will now consider a very simple problem of this form. Let $H_0^1[0,1]$ and $H_0^1(\mathbb{R}_+)$, $\mathbb{R}_+ := [0,\infty)$ be the standard Sobolev spaces. We also identify the functions from $H_0^1[0,1]$ with their extension by zero to the whole of $\mathbb{R}_+$ and write $H_0^1[0,1] \subset H_0^1(\mathbb{R}_+)$. Consider the family of positive definite forms

$$\mathfrak{h}_\kappa(u,v) = \int_0^\infty u'v' + \kappa^2 \int_1^\infty uv, \quad u,v \in H_0^1(\mathbb{R}_+). \tag{22}$$

By H_κ we denote the positive definite operator defined by $\mathfrak{h}_\kappa$ in (22). The operators H_κ converge in the generalized sense to the operator H_∞, which is defined by the form $h_\infty(u,v) = \int_0^1 u'v'$, $u,v \in H_0^1[0,1]$. Such operators are representative for those which appear in the modeling of semiconductor nano-devices, cf. [21]. We also formally write $H_\kappa = -\partial_{xx} + \kappa^2 \chi_{[1,\infty\rangle}$ and $H_\infty = -\partial_{xx}$. As a test function(s) we chose

$$u_q(x) = \begin{cases} \sqrt{2}\sin(q\pi x), & 0 \leqslant x \leqslant 1 \\ 0, & 1 \leqslant x \end{cases}, q \in \mathbb{N}. \tag{23}$$

Note that here $u_q \in \mathrm{Dom}(\mathfrak{h}_\kappa) = H_0^1(\mathbb{R}_+)$ but $u_q \notin \mathrm{Dom}(H_\kappa)$. The space $\mathrm{Dom}(H_\kappa)$ is the space of all functions $\psi \in H^2(\mathbb{R}_+)$ which satisfy the boundary condition $\psi(0) = 0$ and we have used $H_0^1(\mathbb{R}_+)$ and $H^2(\mathbb{R}_+)$ to denote the usual Sobolev spaces with the Hilbert space structure. The eigenvalues of the operator H_κ have to be described implicitly, cf. [36]. Let $H_\kappa v^\kappa = \lambda^\kappa v^\kappa$. Then v^κ is a smooth function given by the formula

$$v^\kappa(x) = \begin{cases} \sin(\sqrt{\lambda^\kappa}x), & 0 \leqslant x \leqslant 1 \\ \frac{\sin\sqrt{\lambda^\kappa}}{e^{-\sqrt{\kappa^2-\lambda^\kappa}}}\, e^{-\sqrt{\kappa^2-\lambda^\kappa}\,x}, & 1 \leqslant x \end{cases}$$

and λ^κ is a solution of the equation

$$\sqrt{\kappa^2 - \lambda^\kappa} = -\sqrt{\lambda^\kappa}\cot(\sqrt{\lambda^\kappa}). \tag{24}$$

The smallest eigenvalue of H_κ is given as the smallest positive root λ_1^κ of (24), whereas $\lambda_1^\infty = \pi^2$ is the smallest eigenvalue of H_∞. The quotient $\frac{\lambda_1^\infty - \lambda_1^\kappa}{\lambda_1^\infty}$ can be represented (for $\kappa \to \infty$) by a convergent Taylor series

$$\frac{\lambda_1^\infty - \lambda_1^\kappa}{\lambda_1^\infty} = 2\frac{1}{\kappa} - 3\frac{1}{\kappa^2} + 8\left(\frac{1}{2!} + \frac{1}{4!}\pi^2\right)\frac{1}{\kappa^3} - 10\left(\frac{1}{2!} + \frac{4}{4!}\pi^2\right)\frac{1}{\kappa^4} + O\left(\frac{1}{\kappa^5}\right). \tag{25}$$

We directly compute

$$\begin{aligned}(u_q, H_\kappa^{-1}u_q - H_\infty^{-1}u_q) &= \int_0^1 \left[\int_0^x 2\left(\frac{y(1+\kappa(1-x))}{1+\kappa} - y(1-x)\right)\sin(q\pi y)\sin(q\pi x)\, dy\right. \\ &\quad \left. + \int_x^1 2\left(\frac{x(1+\kappa(1-y))}{1+\kappa} - x(1-y)\right)\sin(q\pi y)\sin(q\pi x)\, dy\right] dx \\ &= \frac{2}{(1+\kappa)\pi^2 q^2}, \end{aligned} \tag{26}$$

where we have abused the notation for the action of H_∞^{-1} onto the function defined on the whole $\mathbb{R}_+$. Similarly, we obtain

$$\begin{aligned}(u_q, H_\kappa^{-1}u_q) &= \int_0^1 \left[\int_0^x \frac{y\,(1+\kappa\,(1-x))}{1+\kappa}\, 2\sin(q\pi y)\sin(q\pi x)\, dy\right. \\ &\quad \left. + \int_x^1 \frac{x\,(1+\kappa\,(1-y))}{1+\kappa}\, 2\sin(q\pi y)\sin(q\pi x)\, dy\right] dx \\ &= \frac{3+\kappa}{(1+\kappa)\pi^2 q^2}. \end{aligned} \tag{27}$$

Now, definition (3) and identities (26)–(27) yield that for the given κ and independently of $q \in \mathbb{N}$ we have

$$\eta_1^2 = \frac{2}{3+\kappa}.$$

We now combine $\eta_1^2 = \frac{2}{3+\kappa}$ with (24) and the first order estimate from [13, Theorem 4.5] to obtain $\left(1 - \sqrt{\frac{2}{3+\kappa}}\right)4\pi^2 =: D(\kappa) \leqslant \lambda_2(H)$, $\kappa \geqslant 5$. Corollary 8 now yields

$$\frac{2}{3+\kappa} \leqslant \frac{\lambda_1^\infty - \lambda_1^\kappa}{\lambda_1^\infty} \leqslant \frac{D(\kappa)}{D(\kappa)-\pi^2}\frac{2}{3+\kappa} = \frac{8}{3\kappa} - \frac{8\sqrt{2}}{9}\frac{1}{\kappa^{3/2}} + O\left(\frac{1}{\kappa^2}\right), \qquad \kappa \geqslant 5, \quad (28)$$

which is a tight estimate on the behavior of $\frac{\lambda_1^\infty - \lambda_1^\kappa}{\lambda_1^\infty}$. Similar estimates hold for other eigenvalues, too. This example illustrates the "efficiency" of this *a posteriori* estimator. Furthermore, it indicates the role which is played by the first order estimates from [13] in the general theory. For some further details of the computation see [12]. In our κ dependent problem we can improve (20) and prove (cf. (25) and (28))

$$\lim_{\kappa\to\infty} \frac{\frac{\lambda_q^\infty - \lambda_q^\kappa}{\lambda_q^\infty}}{\eta_1^2} = \lim_{\kappa\to\infty} \frac{\frac{\lambda_q^\infty - \lambda_q^\kappa}{\lambda_q^\infty}}{\frac{2}{3+\kappa}} = 1, \quad q \in \mathbb{N}. \tag{29}$$

Furthermore, we can check that this convergence is pretty rapid.

REMARK 9. The general proof of (29) follows from the fact that $\|W_\kappa^{-1/2}K\|^2 = o(\eta_m^2)$, since we have that

$$\sup\{\|W_\kappa^{-1/2}\psi\| \;:\; \psi,\ \mathfrak{h}_b(\psi,\phi) = 0, \forall\phi \in \mathsf{Null}(\mathfrak{h}_e)\} \to 0 \tag{30}$$

as $\kappa \to \infty$.

REMARK 10. It should be noted here that the estimate (28) can be obtained from the standard Kato–Temple inequality (17). To do this we have to apply the standard inequality to the operator H_κ^{-1} in the H_κ scalar product[2], and then utilize the formulae (4) and (17).

Let us assume we want to assess the accuracy of the approximation of the eigenvalue λ_1^κ by the Ritz value $\lambda_1^\infty = (H_\kappa^{1/2}u_1, H_\kappa^{1/2}u_1) = \pi^2$. In this case we have for the vector $v_1 = \frac{1}{\pi}u_1$ the following

$$(v_1, H_\kappa^{-1}v_1)_{H_\kappa} = (H_\kappa^{1/2}v_1, H_\kappa^{1/2}H_\kappa^{-1}v_1) = \frac{1}{\|H_\kappa^{1/2}u_1\|^2} = \frac{1}{\lambda_1^\infty},$$

$$r^2 = \frac{(u_1, H_\kappa^{-1}u_1)}{(H_\kappa^{1/2}u_1, H_\kappa^{1/2}u_1)}\ \eta_1^2 = \frac{\frac{3+\kappa}{(1+\kappa)\pi^2}}{\pi^2}\frac{2}{3+\kappa}.$$

Setting $\alpha = 1/D(\kappa)$ and using the inequality $\lambda_1^\kappa \leqslant \pi^2$ we obtain from (17)

$$\frac{1}{\lambda_1^\kappa} \leqslant \frac{1}{\lambda_1^\infty} + \frac{r^2}{\frac{1}{\lambda_1^\infty} - \frac{1}{D(\kappa)}},$$

[2]The use of the Kato–Temple formula in the changed scalar product has been suggested to the authors by an anonymous referee. Authors are thankful for this suggestion.

and then the error estimate

$$\frac{\lambda_1^\infty - \lambda_1^\kappa}{\lambda_1^\infty} \leqslant \frac{8(\sqrt{2}-\sqrt{3+\kappa})}{(1+\kappa)(4\sqrt{2}-3\sqrt{3+\kappa})} = \frac{8}{3\kappa} - \frac{8\sqrt{2}}{9}\frac{1}{\kappa^{3/2}} + O\left(\frac{1}{\kappa^2}\right). \tag{31}$$

follows. The estimates (28) and (31) are identical in the first two terms. However, the terms hidden in the notation $O\left(\frac{1}{\kappa^2}\right)$ differ. Since both formulae are explicitly available, a more detailed analysis shows that (28) is sharper than (31) for $\kappa \geqslant 5$. We point out that (29) together with the estimate

$$\lambda_1^\kappa \leqslant (1-\eta_1^2)\lambda_1^\infty = \left(1 - \frac{2}{3+\kappa}\right)\pi^2 < \pi^2 = \lambda_1^\infty$$

yields an improvement over the standard Rayleigh estimate. This indicates that (7) provides a framework for computing first order corrections — as $\kappa \to \infty$ — to the Ritz value λ_1^∞. Examining the optimality of various approaches in the case of the multiple eigenvalue λ is technically much more involved and — in the authors' opinion — would not bring further understanding to the main topic of this paper. If such comparison is to be attempted, then one approach might be to use an adaptation of the majorization technique from [19].

5.1.1. A model problem in higher dimensions.

Schroedinger like operators in higher dimensions can also been studied using our framework. The estimate for η_i^2 can in this case be computed by the use of the advanced probabilistic techniques from [7] or by the use of the boundary layer techniques from [6] (naturally, under the assumption that the domain is finite). In this section, we concentrate on the similar higher dimensional problems which can be treated by algebraic techniques in higher dimensional setting, too. Let us consider the differential operator H_κ which is defined by the expression

$$H_\kappa u = \nabla \cdot \left[(1+\kappa^2\chi_{\mathscr{C}})\nabla\right]u, \qquad u \in C_0^\infty(\Omega) \tag{32}$$

in $H_0^1(\Omega)$. Here we use $\chi_{\mathscr{C}}$ to denote the characteristic function of the bounded domain $\mathscr{C}$ and $C_0^\infty(\Omega)$ denotes the space of infinitely differentiable functions with compact support in the domain $\Omega \subset \mathbb{R}^d$, $d > 1$. It is assumed that the boundary $\partial\mathscr{C}$ is Lipschitz and that closure of $\mathscr{C}$ is subset of Ω.

In the quadratic form formulation we have — assuming $\mathscr{O} = \Omega \setminus \mathscr{C}$ —

$$\begin{aligned}
\mathfrak{h}_\kappa(u,v) &= \int_\Omega \nabla u \cdot \nabla v + \kappa^2 \int_\Omega \chi_{\mathscr{C}} \nabla u \cdot \nabla v, \qquad u,v \in H_0^1(\Omega) \\
\mathfrak{h}_\infty(u,v) &= \int_{\mathscr{O}} \nabla u \cdot \nabla v, \qquad u,v \in H_0^1(\mathscr{O})\,.
\end{aligned}$$

Let H_κ and H_∞ be the self-adjoint operators which are defined by these expressions in the appropriate Hilbert spaces in the sense of Kato's second representation theorem. The standard monotone convergence theory of [35] implies that H_κ converges to H_∞ in the generalized strong resolvent sense and that the corresponding spectral projections converge in norm. See also [2, 4, 6, 7, 16, 32] for further references.

Let $\lambda_1^\kappa \leqslant \cdots \leqslant \lambda_i^\kappa \leqslant \cdots$ be the eigenvalues of H_κ and let $\lambda_1^\infty \leqslant \cdots \leqslant \lambda_i^\infty \leqslant \cdots$ be the eigenvalues of H_∞. We assume that we are counting the eigenvalues by multiplicity. Under the assumption that $\partial\mathscr{C}$ is Lipschitz we can apply the theory from [20, Section 2 and 3] to estimate the speed of the convergence of the resolvents. Let u_i^∞, $i \in \mathbb{N}$ be eigenvectors of H_∞ which are associated to λ_i^∞ and span an orthonormal basis of $H_0^1(\mathscr{O})$. Using [20, Lemma 3.6] and [16] we can conclude

$$(u, \widetilde{H}_\kappa^{-1} v) = O\left(\frac{(u,v)}{\kappa^2}\right), \qquad u, v \perp_1 H_0^1(\mathscr{O})$$
$$\sum_{i=1}^m \eta_i^2 = O\left(\frac{1}{\kappa^2}\right), \qquad i = 1, \ldots, m,$$

were we use $\overline{P}$ to denote the projection onto the span of $\{u_1^\infty, \ldots u_m^\infty\}$ and $\perp_1$ to denote the relation of being perpendicular in the scalar product induced by the form $(u,v)_1 = \int_\Omega \nabla u \cdot \nabla v$. To apply [20, Lemma 3.6] we note that — in the notation of [20, Lemma 3.6] — we have $\omega = 1$ and $\tilde{c} = O(\kappa^2)$. We put together these two results and (11) to obtain

$$\sum_{i=1}^m \eta_i^2 \leqslant \sum_{i=1}^m \frac{\lambda_i^\infty - \lambda_i^\kappa}{\lambda_i^\infty} \leqslant \sum_{i=1}^m \eta_i^2 + O\left(\frac{\sum_{i=1}^m \eta_i^2}{\kappa^2}\right)$$
$$\leqslant \sum_{i=1}^m \eta_i^2 + O\left(\frac{1}{\kappa^4}\right).$$

The values of η_i^2 cannot be computed explicitly in a general higher dimensional case. Efficient finite element algorithm for the numerical approximation of η_i^2 — which is sharp enough to be used in this correction formulae — has been developed and described in [14]. Instead of presenting practical details of that algorithm, for this report we concentrate on the academic explicitly solvable finite element example in the next section.

5.2. Finite element computations: analytically solvable 1D model problem

Let us consider the family of eigenvalue problems which are given in the weak formulation by: Find all $\lambda_i \in \mathbb{R}$ and $v_i \in \mathrm{Dom}(\mathfrak{h})$, $\|v_i\| = 1$, $i \in \mathbb{N}$ such that

$$\mathfrak{h}(\psi, v_i) = \int_0^{2\pi} (\overline{\psi'}\phi' - \alpha\overline{\psi}\phi) = \lambda_i(\psi, v_i), \quad \psi \in \mathrm{Dom}(\mathfrak{h}), \tag{33}$$
$$\mathrm{Dom}(\mathfrak{h}) = \left\{\psi \mid \psi, \psi' \in L^2(0, 2\pi), e^{\mathrm{i}\theta}\psi(0) = \psi(2\pi)\right\}. \tag{34}$$

The eigenvalues of the problem (33) as well as the Green function of the operator H, which is defined by $\mathfrak{h}(\cdot,\cdot)$ are known explicitly, see [31, 36] (also cf. [12, Section 2.7.2 pp. 57] for computational details). Let us now choose $\theta = \pi$ and $\alpha = 0.2499$ for our numerical experiment. With this choice of parameter all eigenvalues have the multiplicity two and in particular it holds that $\lambda_1 = \lambda_2 = \frac{1}{4} - \alpha = 10^{-4}$. For $N \in \mathbb{N}$ define the finite element space

$$\mathscr{V}_N^1 = \Big\{ \psi \mid \psi \in C[0,2\pi], -\psi(0) = \psi(2\pi), \psi \text{ is linear in } \mathscr{I}_p, p = 1,\dots,N \Big\},$$

where $\mathscr{I}_p := \left\langle \frac{(p-1)2\pi}{N}, \frac{p\,2\pi}{N} \right\rangle$, and use

$$\mu_i^N := \max_{\substack{\mathscr{S} \subset \mathscr{V}_N^1 \\ \dim \mathscr{S} = \dim \mathscr{V}_N^1 - i}} \min_{\psi \in \mathscr{S} \setminus \{0\}} \frac{\mathfrak{h}(\psi,\psi)}{(\psi,\psi)}, \qquad i = 1,2$$

to define the Rayleigh-Ritz approximations to the eigenvalue $\lambda_1 = \lambda_2$. Let also $u_i^N \in \mathscr{V}_N^1$, $i = 1,2$ be two vectors of norm one for which $\mu_i^N = \mathfrak{h}(u_i^N, u_i^N)$, $i = 1,2$ holds. Now, let $\overline{P}^N$ be an orthogonal projection onto the linear span of $\{u_1^N, u_2^N\}$. We now apply Corollary 8 on $\overline{P}^N$ and display the results in Table 1.

N	estimate (10)	$\vert\vert\vert I - \lambda_1 M^{-1} \vert\vert\vert_{HS}$	estimate (10)
40	7.9540e-001	7.9540e-001	7.9558e-001
60	5.1413e-001	5.1413e-001	5.1422e-001
80	3.4389e-001	3.4389e-001	3.4393e-001
100	2.4120e-001	2.4120e-001	2.4123e-001
120	1.7671e-001	1.7671e-001	1.7673e-001

Table 1: *The performance of the estimates (10) on the family of test spaces* $\mathsf{Ran}(\overline{P}^N)$ *and for the choice of the norm* $\vert\vert\vert\cdot\vert\vert\vert = \vert\vert\vert\cdot\vert\vert\vert_{HS}$. *Here* $\vert\vert\vert\cdot\vert\vert\vert_{HS}$ *denotes the Hilbert–Schmidt norm. The computational details can be found in* [12, Section 2.7.3, pp. 64].

The results from Table 1 show that η_1, η_2 accurately capture the behavior of the relative error as $\frac{1}{N} \to 0$. However, the explicit knowledge of the Green function is most certainly an information which cannot in general be assumed when considering higher dimensional eigenvalue problems. A possibility to use these estimates in the context of finite element computations for higher dimensional eigenvalue problems has been presented in [14]. To summarize, the arguments of Remark 3 indicate that it is possible to estimate the H^{-1} norm of the residual cheaper than it takes to solve the linear system (i.e. approximately solve the associated boundary value problem). This numerical example illustrates the sharpness of this approach in case of degenerate or clustered eigenvalues. Using the Green functions and the recursion formulae for the Ritz vectors from [12, Section 2.7.3] we can now prove (20) — as $N \to \infty$ — for the sequence which is generated by $\overline{P}^N$. In this case this reads

$$\lim_{N\to\infty} \frac{\sqrt{\left[\frac{\lambda_1 - \mu_1^N}{\mu_1^N}\right]^2 + \left[\frac{\lambda_2 - \mu_2^N}{\mu_2^N}\right]^2}}{\eta_1^2 + \eta_2^2} = 1,$$

and as can be seen from Table 1, the convergence can be rapid. Similar behavior has been proved (and observed in experiments) in [14] for higher dimensional operators.

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REFERENCES

[1] M. ARIOLI, *A stopping criterion for the conjugate gradient algorithms in a finite element method framework*, Numer. Math. **97**, 1 (2004), 1–24.

[2] H. BAUMGÄRTEL AND M. DEMUTH, *Decoupling by a projection*, Rep. Math. Phys. **15**, 2 (1979), 173–186.

[3] C. BEATTIE AND F. GOERISCH, *Methods for computing lower bounds to eigenvalues of self-adjoint operators*, Numer. Math. **72**, 2 (1995), 143–172.

[4] A. BEN AMOR AND J. F. BRASCHE, *Sharp estimates for large coupling convergence with applications to Dirichlet operators*, J. Funct. Anal. **254**, 2 (2008), 454–475.

[5] N. BOSNER AND Z. DRMAČ, *Subspace gap residuals for Rayleigh-Ritz approximations*, SIAM J. Matrix Anal. Appl. **31**, 1 (2009), 54–67.

[6] V. BRUNEAU AND G. CARBOU, *Spectral asymptotic in the large coupling limit*, Asymptot. Anal. **29**, 2 (2002), 91–113.

[7] M. DEMUTH, F. JESKE, AND W. KIRSCH, *Rate of convergence for large coupling limits by Brownian motion*, Ann. Inst. H. Poincaré Phys. Théor. **59**, 3 (1993), 327–355.

[8] Z. DRMAČ, *On relative residual bounds for the eigenvalues of a Hermitian matrix*, Linear Algebra Appl. **244** (1996), 155–163.

[9] Z. DRMAČ AND V. HARI, *Relative residual bounds for the eigenvalues of a Hermitian semidefinite matrix*, SIAM J. Matrix Anal. Appl. **18**, 1 (1997), 21–29.

[10] Z. DRMAČ AND K. VESELIĆ, *New fast and accurate Jacobi SVD algorithm. II*, SIAM Journal on Matrix Analysis and Applications **29**, 4 (2008), 1343–1362.

[11] G. H. GOLUB AND G. MEURANT, *Matrices, moments and quadrature*, In Numerical analysis 1993 (Dundee, 1993), volume 303 of Pitman Res. Notes Math. Ser., pages 105–156, Longman Sci. Tech., Harlow, 1994.

[12] L. GRUBIŠIĆ, Ritz value estimates and applications in Mathematical Physics, PhD thesis, Fernuniversität in Hagen, dissertation.de Verlag im Internet, 2005.

[13] L. GRUBIŠIĆ, *On eigenvalue estimates for nonnegative operators*, SIAM J. Matrix Anal. Appl. **28**, 4 (2006), 1097–1125.

[14] L. GRUBIŠIĆ AND J. S. OVALL, *On estimators for eigenvalue/eigenvector approximations*, Math. Comp. **78** (2009), 739–770.

[15] L. GRUBIŠIĆ AND K. VESELIĆ, *On Ritz approximations for positive definite operators I*, (theory), Linear Algebra and its Applications **417**, 2-3 (2006), 397–422.

[16] L. GRUBIŠIĆ, *Relative convergence estimates for the spectral asymptotic in the large coupling limit*, Integral Equations Operator Theory **65**, 1 (2009), 51–81.

[17] T. KATO, *On the upper and lower bounds of eigenvalues*, J. Phys. Soc. Japan **4** (1949), 334–339.

[18] T. KATO, *Perturbation theory for linear operators*, Grundlehren der Mathematischen Wissenschaften, Band 132, Springer-Verlag, Berlin, second edition, 1976.

[19] A. V. KNYAZEV AND M. E. ARGENTATI, *Rayleigh-Ritz majorization error bounds with applications to FEM*, SIAM J. Matrix Anal. Appl. **31**, 3 (2009), 1521–1537.

[20] A. V. KNYAZEV AND O. WIDLUND, *Lavrentiev regularization + Ritz approximation = uniform finite element error estimates for differential equations with rough coefficients*, Mathematics of Computation **72** (2003), 17–40. Posted on July 13, 2001, S0025-5718-01-01378-3.
[21] T. KOPRUCKI, R. EYMARD, AND J. FUHRMANN, *Convergence of a finite volume scheme to the eigenvalues of a Schrödinger operator*, WIAS Preprint No. 1260, 2007.
[22] M. KRAUS, M. LANGER, AND C. TRETTER, *Variational principles and eigenvalue estimates for unbounded block operator matrices and applications*, J. Comput. Appl. Math. **171**, 1-2 (2004), 311–334.
[23] R.-C. LI, *Relative perturbation theory. I. Eigenvalue and singular value variations*, SIAM J. Matrix Anal. Appl. **19**, 4 (1998), 956–982 (electronic).
[24] R. MATHIAS, *Quadratic residual bounds for the Hermitian eigenvalue problem*, SIAM J. Matrix Anal. Appl. **19**, 2 (1998), 541–550 (electronic).
[25] E. OVTCHINNIKOV, *Cluster robust error estimates for the Rayleigh–Ritz approximation II: Estimates for eigenvalues*, Linear Algebra Appl. **415**, 1 (2006).
[26] E. OVTCHINNIKOV, *Cluster robust error estimates for the Rayleigh-Ritz approximation. I. Estimates for invariant subspaces*, Linear Algebra Appl. **415**, 1 (2006), 167–187.
[27] B. N. PARLETT, *The symmetric eigenvalue problem*, Prentice-Hall Series in Computational Mathematics, Prentice-Hall Inc., Englewood Cliffs, N.J., 1980.
[28] M. PLUM, *Bounds for eigenvalues of second–order elliptic differential operators*, ZAMP **42** (1991), 848–863.
[29] M. PLUM, *Bounds for eigenvalues of second–order ordinary differential operators by a numerical homotopy method*, ZAMP **41** (1990), 205–226.
[30] M. PLUM, *Guaranteed numerical bounds for eigenvalues*, In Spectral theory and computational methods of Sturm–Liouville problems, volume 191 of Lecture notes in pure and applied mathematics, pages 313–332. Marcel Dekker Inc., New York, 1997.
[31] M. REED AND B. SIMON, *Methods of modern mathematical physics. I–IV*. Academic Press [Harcourt Brace Jovanovich Publishers], New York, 1978.
[32] E. SÁNCHEZ-PALENCIA, *Asymptotic and spectral properties of a class of singular-stiff problems*, J. Math. Pures Appl. (9) **71**, 5 (1992), 379–406.
[33] B. SIMON, *Trace ideals and their applications*, volume 35 of London Mathematical Society Lecture Note Series, Cambridge University Press, Cambridge, 1979.
[34] W. STENGER, *An inequality for the eigenvalues of a class of self–adjoint operators*, Bull. Amer. Math. Soc. **73**, 3 (1967), 487–490.
[35] J. WEIDMANN, *Stetige Abhängigkeit der Eigenwerte und Eigenfunktionen elliptischer Differentialoperatoren vom Gebiet*, Math. Scand. **54**, 1 (1984), 51–69.
[36] J. WEIDMANN, *Spectral theory of ordinary differential operators*, volume 1258 of Lecture Notes in Mathematics, Springer-Verlag, Berlin, 1987.

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