NON-VARIATIONAL APPROXIMATION OF DISCRETE EIGENVALUES OF SELF-ADJOINT OPERATORS

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ABSTRACT. We establish sufficiency conditions in order to achieve approximation to discrete eigenvalues of self-adjoint operators in the second-order projection method suggested recently by Levitin and Shargorodsky. We find explicit estimates for the eigenvalue error and study in detail two concrete model examples. Our results show that, unlike the majority of the standard methods, second-order projection strategies combine non-pollution and approximation at a very high level of generality.

1. INTRODUCTION

Let $M$ be a self-adjoint operator acting on a dense domain, $\text{Dom} M$, in a separable Hilbert space $\mathcal{H}$. Let the spectrum of $M$ be split into isolated eigenvalues of finite multiplicity (discrete spectrum) and degenerate points (essential spectrum), in symbols $\text{Spec} M = \text{Spec}_{\text{disc}} M \cup \text{Spec}_{\text{ess}} M$. In order to approximate discrete eigenvalues $\lambda$ of $M$, we may consider using the following projection method: choose an orthonormal basis of $\mathcal{H}$, $\{\phi_k\}_{k=1}^{\infty} \subset \text{Dom} M$, and find the spectrum of large matrices $M_n$ resulting from compressing $M$ to the finite dimensional subspaces $\mathcal{L}_n = \text{span}\{\phi_1, \ldots, \phi_n\}$.

The successful outcomes of this strategy is illustrated by the well known Rayleigh-Ritz theorem for the approximation of variational eigenvalues, see e.g. [18, Theorem XIII.4]. Assume that $M$ has a non-degenerate ground eigenvalue $\lambda = \min[\text{Spec} M] < \min[\text{Spec}_{\text{ess}} M]$. Let $\Pi_n$ be the orthogonal projection onto $\mathcal{L}_n$ and $M_n := \Pi_n M |_{\mathcal{L}_n}$. If

\[ \lim_{n \to \infty} \|M_n \Pi_n \psi - \lambda \psi\| = 0 \quad \text{for all} \ M \psi = \lambda \psi, \]

then the first eigenvalue of $M_n$ converges from above to $\lambda$ (i.e. approximation is achieved) and the second eigenvalue of $M_n$, counting multiplicity, can not be smaller than $\min[\text{Spec} M \setminus \{\lambda\}]$ (i.e. no chance

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of spurious eigenvalues). Conditions such as (1) are useful in applications because they can sometimes be verified on abstract grounds, [18, Ex. XIII.2.1 and XIII.2.2]. Similar results hold for any other variational eigenvalue (i.e. those below the minimum of the essential spectrum or above the maximum of this set) simple or otherwise.

Although this technique is proven to be valuable in the study of spectral properties of self-adjoint operators, think e.g. of Galerkin approximation, two main difficulties are in place when we extend it to the analysis of non-variational eigenvalues:

- **Lack of approximation**: no eigenvalue of $M_n$ is close to $\lambda$ in the limit $n \to \infty$, and

- **Spectral pollution**: there are eigenvalues $z_n$ of $M_n$ which appear to converge to some $\mu$ not in the spectrum of $M$.

In fact any $\mu \in \text{conv}[\text{Spec}_{\text{ess}}M] \setminus \text{Spec}M$ is potentially an accumulation point of $\text{Spec}M_n$ in the limit $n \to \infty$. This is known to occur in several important applications such as elasticity, electromagnetism and hydrodynamics, see e.g. [1], [2], [6], [16] and the references therein. Widely available commercial packages such as FEMLAB are known to produce spectacularly incorrect results even in cases of the simplest one-dimensional Stokes’ type systems, [15]. Actually one may construct simple examples of bounded $M$ and natural orthonormal basis $\{\phi_k\}$ with the property that every $\mu \in \text{conv}[\text{Spec}_{\text{ess}}M] \setminus \text{Spec}M$ is an accumulation point of $\text{Spec}M_n$ in the limit $n \to \infty$, see [15] and [4].

The standard approach to deal with pollution around non-variational eigenvalues, aims at choosing $L_n$ sufficiently close to the spectral subspaces of $M$ in order to capture the eigenfunctions associated to $\lambda$, see e.g. [1], [2] and [16]. Unfortunately no universal device is known for constructing such subspaces.

A different approach hinges on the spectral theorem and it exploits the fact that for $\zeta$ lying in a gap of $\text{Spec}_{\text{ess}}M$, the eigenvalues of $\zeta - M$ inside the corresponding shifted gap enclosing the origin, become variational eigenvalues of $(\zeta - M)^2$. In [15] Levitin and Shargorodsky consider this idea in a concrete manner. They propose complementing the usual projection method with *a posteriori* estimates found by computing the eigenvalues of the matrix polynomial

\[
P_n(z) := \Pi_n(z - M)^2|L_n = z^2 - 2M_nz + [M^2]_n.
\]

Usually $\text{Spec}P_n$ contains non-real points (see the definitions in Section 2). Their result is based on a remarkable property [15, Theorem 2.6] guaranteeing that for $z \in \text{Spec}P_n$,

\[
[\text{Re } z - |\text{Im } z|, \text{Re } z + |\text{Im } z|] \cap \text{Spec}M \neq \emptyset.
\]
Hence the strategy would be finding points in \( \text{Spec } P_n \). If these points are close to \( \mathbb{R} \), they must also be close to the spectrum of \( M \).

Numerical evidence found in [3] and [15] suggests that approximation occurs for concrete operators and natural basis \( \{ \phi_k \} \). The aim of the present paper is to discuss in detail this complementary problem of approximation in this “second-order” projection method. Our main contribution summarizes in the following statement: if \( \lambda \in \text{Spec}_{\text{disc}} M \) and

\[
\lim_{n \to \infty} \| \Pi_n M^k \Pi_n \psi - \lambda^k \psi \| = 0, \quad k = 0, 1, 2, \text{ whenever } M \psi = \lambda \psi,
\]

then there exists \( z_n \in \text{Spec } P_n \) such that \( z_n \to \lambda \) as \( n \to \infty \). See Theorems 1 and 2 below and also [4]. Hence, discrete eigenvalues satisfying (4) will always be approached no matter their location relative to \( \text{Spec}_{\text{ess}} M \). Notice that condition (4) here plays the role of (1) in the “linear” projection method.

In Section 2 we establish the main theoretical contribution. Theorem 1 finds explicit estimates for the eigenvalue error \( |z_n - \lambda| \) in terms of bounds for the difference in the left side of (4). This result depends on knowing exactly the entries of the matrices \( M_n \) and \( [M^2]_n \), hence its scope is mainly theoretical. Theorem 2 on the other hand, demonstrates that introducing noise to the entries of \( P_n(z) \) within a certain tolerance, does not affect approximation. This result is better suited for applications. We give precise bounds for this tolerance in terms of invariants of the problem.

Section 3 illustrates the scope of the theoretical results by means of two model examples. The first one corresponds to finite rank perturbations of multiplication operators by a bounded symbol. We find explicit estimates for the error \( |z_n - \lambda| \) when \( \{ \phi_k \} \) is of Fourier type and report on numerical outputs. The second model is unbounded, the Schrödinger operator with band gap essential spectrum. We choose \( \{ \phi_k \} \) to be the Hermite functions, then find explicit upper bounds for eigenvalue error in terms of smoothness properties of the potential.

In order to make the paper more readable, the proofs of Theorems 1 and 2 are to be found in Section 5 while Section 4 introduces and describes a convenient notation in order to simplify the presentation of most arguments. Being of obvious interest, in Section 6 we discuss the question of whether approximation also occurs for the essential spectrum.
2. Speed of convergence and stability: general results

We begin this section by fixing some notation. Let $\lambda \in \text{Spec}_{\text{disc}} M$. Throughout this paper $\{\Pi_n\}$ denotes a family of orthogonal projections onto $\mathcal{H}$ satisfying (4) such that $L_n := \text{Ran} \Pi_n \subset \text{Dom} M^2$. The sequence $\delta(n) > 0$ shall always denote an upper bound for the left side of (4) such that $\delta(n) \to 0$ as $n \to \infty$: for all $\psi \in \text{Dom} M$ satisfying $M\psi = \lambda \psi$ and $\|\psi\| = 1$, 

$$\|\Pi_n M^k \Pi_n \psi - \lambda^k \psi\| \leq \delta(n) \quad \text{for } n \in \mathbb{N} \text{ and } k = 0, 1, 2.$$ 

Below we shall always assume that $\psi$ is an eigenvector associated to $\lambda$ normalized by $\|\psi\| = 1$.

Let $P(z) = \sum_{k=0}^m A_k z^k$ where $z$ is a complex variable, $A_k \in \mathbb{C}^{n \times n}$ and $\det A_m \neq 0$. The spectrum of $P$ is, by definition, the set of eigenvalues 

$$\text{Spec } P := \{ z \in \mathbb{C} : \det P(z) = 0 \}.$$ 

The hypothesis $\det A_m \neq 0$ ensures that Spec $P$ comprises no more than $mn$ finite points.

We are concerned with the spectrum of the quadratic matrix polynomial $P_n(z)$ given by (2). The determinant of $P_n(z)$ is a scalar polynomial in $z$ of degree $(2 \dim L_n)$, so that Spec $P_n$ is a finite set comprising at most $(2 \dim L_n)$ different complex numbers. In general these points do not intersect the real line, unless $L_n$ contains an eigenfunction of $M$. Furthermore, since $\det P_n(z) = \det P_n(\bar{z})$, $\mathbb{R}$ is an axis of symmetry for Spec $P_n$. In Section 4 we characterize Spec $P_n$ as the poles of a certain positive-valued subharmonic function. Other descriptions of the spectrum of matrix polynomials better suited for computation, e.g. as the eigenvalues of block matrices, may be found in the literature, see [10] or [11, Part II].

The goal of the procedure suggested by Levitin and Shargorodsky in [15] is finding the points in Spec $P_n$ which are close to $\mathbb{R}$. Statement (3) ensures that these points will necessarily be close to Spec $M$. A complementary assertion guarantees that discrete eigenvalues satisfying (4) will always be approached no matter their location relative to Spec_{ess} $M$.

Our first theorem in this direction establishes that the rate of convergence $|z_n - \lambda| \to 0$ for $z_n \in \text{Spec } P_n$ is at least a power $1/2$ the rate at which the $L_n$ approximate $M^k \psi$, $k = 0, 1, 2$. It is unclear whether the claimed power $1/2$ is sharp for general choices of $L_n$. In Section 3.2 below, we provide specific numerical evidence suggesting that for particular cases the actual eigenvalue error is $|z_n - \lambda| = O(\delta(n)^a)$ for $a \approx 1$. 
**Theorem 1.** Let $\lambda \in \text{Spec}_{\text{disc}}M$ and assume that $[\ref{5}]$ holds. There exists $b > 0$ independent of $n$ and $z_n \in \text{Spec} P_n$, such that

$$|z_n - \lambda| < b[\delta(n)]^{1/2}, \quad n \in \mathbb{N}.$$  \hspace{1cm} (6)

The scope of Theorem 1 is mainly theoretical. Computing $\text{Spec} P_n$ usually requires estimating the coefficients of $P_n(z)$. Since $P_n(z)$ is Hermitian for all $z \in \mathbb{R}$, a well known result in the theory of matrix polynomials (cf. [11, Theorem II.2.6]), ensures that we can always find a factorization

$$P_n(z) = (z - A_n)(z - A_n^*), \quad z \in \mathbb{C},$$  \hspace{1cm} (7)

where $A_n$ are square matrices of size $\dim L_n$ constant in $z$. Clearly $\text{Spec} P_n = (\text{Spec} A_n) \cup (\text{Spec} A_n^*)$. A small perturbation in the coefficients of $P_n$ will change the coefficients of $A_n$. Typically the eigenvalues of $A_n$ are not semi-simple. In fact their condition number might, in principle, be large as $n$ is large, forcing $\text{Spec} P_n$ to be sensitive to small changes in the entries of $M_n$ and $[M^2]_n$, see [12]. Our next result establishes that this sensitivity can be controlled uniformly in neighbourhoods of $\text{Spec}_{\text{disc}}M$. To be more specific, approximation to a small $\delta$-neighbourhood of $\lambda$ is always achieved, if we estimate the coefficients of $P_n$ within an error smaller than some prescribed tolerance, $w_k \varepsilon$.

Below and elsewhere we shall write $\mu := \text{dist} [\lambda, \text{Spec} M \setminus \{\lambda\}] > 0$. The norm $\|\cdot\|$ for matrices shall always refer to the uniform operator norm. Let $\varepsilon \geq 0$ and $\bar{w} = (w_0, w_1)$ where $w_k \geq 0$. We denote by $\mathcal{P}_{\varepsilon, \bar{w}}$ the set of sequences of linear matrix polynomials $(Q_n)_{n=1}^{\infty}$ such that $Q_n(z) = F_nz - G_n$, where $F_n$ and $G_n$ are square matrices constant in $z$ of size $(\dim L_n)$ satisfying $\|G_n\| \leq w_0 \varepsilon$ and $\|F_n\| \leq w_1 \varepsilon$.

**Theorem 2.** Let $\lambda \in \text{Spec}_{\text{disc}}M$. Assume that $[\ref{11}]$ holds and that $w_0, w_1 \geq 0$ do not vanish simultaneously. Let $0 < \delta < \mu/4$ be fixed. Let

$$0 \leq \varepsilon < \frac{\delta^2 \mu^2}{2(2\delta^2 + 3\mu^2)[w_0 + w_1(\mu/4 + |\lambda|)]}.$$  \hspace{1cm} (8)

There exists $N > 0$ only dependant upon $\delta$, $w_0$ and $w_1$, such that for all $(Q_n)_{n=1}^{\infty} \in \mathcal{P}_{\varepsilon, \bar{w}}$,

$$\text{Spec} (P_n + Q_n) \cap \{\delta \leq |z - \lambda| \leq \mu/4\} = \emptyset \quad \text{and} \quad \text{Spec} (P_n + Q_n) \cap \{|z - \lambda| < \delta\} \neq \emptyset \quad \text{for } n > N.$$  \hspace{1cm} \text{Moreover, if we count multiplicities, the number of eigenvalues of } P_n \text{ and } P_n + Q_n \text{ in } \{|z - \lambda| < \delta\} \text{ coincide.}$$
In other words, if we aim at detecting \( \lambda \) with an error of \( \delta \), it is enough to consider estimations

\[
P_n(z) + Q_n(z) = z^2 - (2M_n - F_n)z + ([M^2]_n - G_n)
\]

with sufficiently small \( \|F_n\| \) and \( \|G_n\| \), and find the spectrum of \( P_n + Q_n \) for sufficiently large \( n \). The weights \( w_0 \) and \( w_1 \) are introduced in order to allow independent control on how perturbations are measured in the truncations of \( M \) and \( M^2 \). For instance, two possibilities are: the absolute weights \( w_0 = w_1 = 1 \) and the relative weights

\[
w_0 = \frac{\mu^2}{4(2\delta^2 + 3\mu^2)} \quad \text{and} \quad w_1 = \frac{w_0}{(\mu/4 + |\lambda|)}.
\]

3. Speed of convergence: examples

In the examples presented below we find \( \delta(n) \) explicitly for concrete operators \( M \). Among other results, we illustrate how the error \( |z_n - \lambda| \) depends strongly on the correct choice of \( L_n \). We also provide numerical evidence suggesting that, in cases, the power 1/2 of \( \delta(n) \) predicted by Theorem 1 can actually be improved to a power \( \alpha \approx 1 \).

3.1. Finite rank perturbations of multiplication operators. As a first example we consider \( M = S + K \) acting on \( f \in L^2(-\pi, \pi) =: L^2 \), where

\[
Sf(x) = s(x)f(x), \quad Kf(x) = \sum_{j=1}^{\ell} \langle f, g_j \rangle g_j(x),
\]

\( s(x) \) is a bounded real-valued function and \( g_j \in L^2 \). Since \( K \) has finite rank, Weyl’s theorem ensures that Spec\(_{\text{ess}}(S + K) = \) Spec\(_{\text{ess}} S = \) Spec \( S = \) essRange \( s(x) \). We aim at finding asymptotic upper bounds for \( \delta(n) \) in the limit \( n \to \infty \) in terms of invariants of \( s(x) \) and \( g_j(x) \), for suitable \( L_n \) specified later. The discrete Schrödinger operator studied in [3, 15, Example I] and the example discussed in [4, Section 4], all satisfy the hypothesis of Lemma 3 below.

Let \( \mathcal{B}_1 := \{e^{inx}\}_{n=-\infty}^{\infty} \). By declaring the inner product normalized as

\[
\langle f, g \rangle := \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x)g(x)dx,
\]

clearly \( \mathcal{B}_1 \) is an orthonormal basis of \( L^2 \). Denote by \( \hat{h}(n) := \langle h, e^{inx} \rangle \) the Fourier coefficient of a complex-valued real function \( h \). The following notation is in place for the examples of this section. For \( q \geq 1 \),

\[
\mathcal{O}^q := \{h : 2\pi - \text{periodic in } \mathbb{R} \text{ s.t. } |\hat{h}(n)| = O(|n|^{-q}) \text{ as } n \to \pm \infty\}.
\]

The well known rules relating Fourier coefficients and differentiation, easily show that if \( h' \in \mathcal{O}^q \), then \( h \in \mathcal{O}^{q+1} \). Hence, \( h \in \mathcal{O}^{r+1} \) whenever
$h \in C^r(\mathbb{R})$ is $2\pi$-periodic. Furthermore, $h \in \mathcal{O}^1$ for functions $h$ of bounded variation, cf. e.g. [9 §2.3.6].

**Lemma 3.** Let $M = S + K$ and $\mathcal{L}_n = \text{Span} \{e^{-inx}, \ldots, e^{inx}\}$. If $\frac{g_j(x)}{\lambda - s(x)} \in \mathcal{O}^q$ for all $j = 1, \ldots, l$, then we may choose $\delta(n) = O(n^{-q + 1/2})$ as $n \to \infty$ in (5).

**Proof.** Since $M = S + K$ is bounded, it is enough estimating the left hand side of (5) for $k = 0$. Indeed,

$$\|\Pi_n M^k \Pi_n \psi - \lambda^k \psi\| \leq \|\Pi_n M^k \Pi_n \psi - \Pi_n M^k \psi\| + \|\lambda^k \Pi_n \psi - \lambda^k \psi\| \leq (\|M^k\| + |\lambda|^k) \|\Pi_n \psi - \psi\|.$$ 

Now, since $M \psi = \lambda \psi$, then $(\lambda - s(x)) \psi(x) = \sum_{j=1}^l (\langle \psi, g_j \rangle) g_j(x)$ and so the hypothesis guarantees that $\psi(x) \in \mathcal{O}^q$. The estimate

$$\|\Pi_n \psi - \psi\|^2 = \sum_{|j| > n} |\hat{\psi}(j)|^2 \leq c_1 \sum_{|j| > n} \frac{1}{|j|^{2q}} = O(|n|^{1-2q}), \quad n \to \infty,$$

completes the proof.

In particular we may formulate the following conclusions for $M = S + K$ and $\mathcal{L}_n = \text{Span} \{e^{-inx}, \ldots, e^{inx}\}$.

a) If $s(x)$ and $g_j(x)$ are $2\pi$-periodic functions in $C^r(\mathbb{R})$, then we may choose $\delta(n) = O(|n|^{-r-1/2})$ in (5).

b) If $s'(x)$ and $g'_j(x)$ are of bounded variation, then we may choose $\delta(n) = O(|n|^{-3/2})$ in (5).

c) If $s(x)$ and $g_j(x)$ are of bounded variation, then we may choose $\delta(n) = O(|n|^{-1/2})$ in (5).

All these assertions follow from the fact that if $\lambda \in \text{Spec}_{\text{disc}} (S + K)$, then necessarily $\lambda \notin \text{essRange} s(x)$ and so $\frac{1}{\lambda - s(x)}$ is of the same degree of smoothness as $s(x)$. The interesting case in our current discussion is c), because gaps in the essential spectrum only occur if $s(x)$ is discontinuous.

### 3.2. A numerical example.

Let $M = S + K$ be as in the previous section. Assume that

$$s(x) = \begin{cases} 
-2 + \sin(2x), & -\pi < x \leq 0, \\
2 + \sin(2x), & 0 < x \leq \pi,
\end{cases}$$

then $l = 1$ and $g_1(x) \equiv \sqrt{2}$, so that $K f(x) = 2 \hat{f}(0)$. We may find $\text{Spec} M$ in closed form. Clearly $\text{Spec}_{\text{ess}} M = [-3, -1] \cup [1, 3]$. On the other
hand, according to [4, Lemma 7], we know that \( \lambda \) is an eigenvalue in the discrete spectrum of \( M \) if and only if
\[
\int_{-\pi}^{0} \frac{dx}{(\lambda + 2) - \sin(2x)} + \int_{0}^{\pi} \frac{dx}{(\lambda - 2) - \sin(2x)} = \pi.
\]
The explicit computation of the integrals reveals that \( \text{Spec}_{\text{disc}} M \) consists of two eigenvalues, the variational \( \lambda_+ \approx 3.5796 \) and the pollution-prone \( \lambda_- \approx -0.7674 \).

A direct calculation yields
\[
\hat{s}(j) = \begin{cases} 
\frac{4}{ij\pi}, & j \text{ odd}, \\
\left(\delta_{2,j} - \delta_{-2,j}\right) \frac{1}{2\pi}, & j \text{ even}, 
\end{cases}
\]
so that \( |\hat{s}(j)| \sim |j|^{-1} \) as \( j \to \pm\infty \) (here \( \delta_{j,l} \) denotes the Kronecker symbol). Thus, by Lemma 3 we can choose \( \delta(n) = O(n^{1/2}) \) and, according to Theorem 1 the existence of \( z_{n}^{\pm} \in \text{Spec} P_n \) such that \( |z_{n}^{\pm} - \lambda_{\pm}| = O(n^{-1/4}) \) in the limit \( n \to \infty \) is predicted.

From the explicit expression for \( \hat{s}(j) \) it is not difficult to find \( P_n(z) \). In Table 1 we report on the numerical approximations of \( |z_{n}^{\pm} - \lambda_{\pm}| \)

| \( n \) | \( z_{n}^{\pm} - \lambda_{\pm} \) | \( \log(|z_{n}^{\pm} - \lambda_{\pm}|) \) | \( \log(n) \) | Slope |
|-----|-----------------|-----------------|-----------------|-------|
| 190 | 0.040879        | -3.1971         | 5.247           | -0.50849 |
| 235 | 0.036961        | -3.3052         | 5.4596          | -0.48708 |
| 280 | 0.033689        | -3.3906         | 5.6348          | -0.50956 |
| 325 | 0.031226        | -3.4665         | 5.7838          | -0.4876 |
| 370 | 0.029312        | -3.5297         | 5.9135          | -0.50963 |
| 415 | 0.027647        | -3.5882         | 6.0283          | -0.48918 |
| 460 | 0.025071        | -3.6385         | 6.1312          | -0.50928 |
| 505 | 0.022406        | -3.6860         | 6.2246          | -0.48918 |
| 550 | 0.020873        | -3.7278         | 6.3099          | -0.50875 |
| 595 | 0.023103        | -3.7678         | 6.3866          | -0.49003 |
| 640 | 0.022292        | -3.8035         | 6.4615          | -0.50813 |
| 685 | 0.021535        | -3.8381         | 6.5294          | -0.49086 |
| 730 | 0.020873        | -3.8693         | 6.5933          | -0.50748 |
| 775 | 0.020249        | -3.8997         | 6.6529          | -0.49167 |
| 820 | 0.019695        | -3.9274         | 6.7093          | -0.50682 |
| 865 | 0.019169        | -3.9545         | 6.7627          | -0.49244 |
| 910 | 0.018696        | -3.9795         | 6.8134          | -0.50617 |
| 955 | 0.018245        | -4.0039         | 6.8617          | -0.49318 |
| 1000| 0.017835         | -4.0266         | 6.9078          | -0.49167 |

Table 1. Estimation of the exponent of \( \delta(n) \) for approximations of \( \lambda_- \) using \( B_1 \).
for different values of $n = 190 : 1000$ and the corresponding pairwise slopes between the steps $n$ and $n + 45$ of the graph $\log |z_n^+ - \lambda| \ vs \ \log(n)$. We have found the numerical data by writing explicitly $M_n$ and $[M^2]_n$, and computing the eigenvalue of the companion matrix of $P_n(z)$ that is nearer to $\lambda$. For calculations we use the standard eigs routine available in the MATLAB package. The last column strongly suggests that $|z_n^+ - \lambda| = O(n^{-\alpha})$ for $\alpha \approx 1/2$. Similar numbers are found for the variational $\lambda_+$. Table 1 suggests that there is generally a significant gap between the approximation predicted by (6) and the actual rate of convergence $|z_n^+ - \lambda| \to 0$. An obvious conjecture is that, perhaps, the bound $\delta(n)^{1/2}$ in Theorem 1 can actually be improved to $\delta(n)$.

3.3. Direct sum of multiplication operators. Choosing the right basis is crucial for achieving efficient approximation. In the example discussed above, this choice should be made attending the nature of the symbol, i.e. piecewise continuity. Below we introduce the correct basis to deal with symbols such as (9). The following results have obvious extensions to direct sum of any finite number of operators, i.e. many gaps in the essential spectrum. In order to keep our notation simple, we only consider two summing terms.

Assume now that $M = S + K$ is an operator acting on $L^2 \oplus L^2$, where

\begin{equation}
S \begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix} := \begin{pmatrix} s_1(x) f_1(x) \\ s_2(x) f_2(x) \end{pmatrix}, \quad K \begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix} := \sum_{j=1}^l \left\langle \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, G_j \right\rangle G_j(x),
\end{equation}

$s_1$, $s_2$ are real-valued bounded symbols and $G_j = (g_{j,1}, g_{j,2})^t \in L^2 \oplus L^2$. The difference with the previous model lies on the fact that $\text{Spec}_{\text{ess}} M = \text{essRange } s_1(x) \cup \text{essRange } s_2(x)$, so gaps in the essential spectrum may occur even when $s_1$ and $s_2$ are continuous and $2\pi$-periodic.

The following lemma is the natural adaptation of Lemma 3 to the present situation. Let $e_n(x) := (e^{inx}, 0)^t$ and $h_n(x) = (0, e^{inx})^t$. Then $\{e_n, h_n\}_{n=-\infty}^{\infty}$ is an orthonormal basis of $L^2 \oplus L^2$ with the usual inner product.

**Lemma 4.** Let $M = S + K$ where $S$ and $K$ are as in (10). Let $L_n := \text{Span } \{ e_{-n}, h_{-n}, \ldots, e_n, h_n \}$. If $g_{j,m}(x) \in \mathcal{O}^q$ for all $j = 1, \ldots, l$ and $m = 1, 2$, then we may choose $\delta(n) = O(n^{-q+1/2})$ as $n \to \infty$ in (5).

The proof is analogous to that of Lemma 3.
As an application of Lemma 4, we now consider a better suited basis for estimating the eigenvalues of the symbol discussed in Section 3.2. The crucial observation is that $L^2$ is isometrically isomorphic to $L^2 \oplus L^2$ via the unitary map
\[ f(x) \mapsto \begin{pmatrix} f(\frac{x-\pi}{2}) \\ f(\frac{x+\pi}{2}) \end{pmatrix}. \]

The orthonormal basis $\{e_n, h_n\}$ maps under $U^*$ onto an orthonormal basis $B_2 = \{U^*e_n, U^*h_n\} \subset L^2$ in such manner that $U^*e_n$ span all functions with support contained in $[-\pi, 0]$ and $U^*h_n$ all those with support in $[0, \pi]$. When $s(x)$ is as in (9),
\[ UMU^* \begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix} = \begin{pmatrix} -2 + \sin x & 0 \\ 0 & 2 + \sin x \end{pmatrix} \begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix} + 2 \langle \begin{pmatrix} f_1 \\ f_2 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \end{pmatrix} \rangle \begin{pmatrix} 1 \\ 1 \end{pmatrix}. \]

Then, Lemma 4 along with Theorem 1 predict that the basis $B_2$ would produce sequences approaching to $\lambda_\pm$ whose speed of convergence is faster than any power of $n$. That is, if $M$ is as in Section 3.2 and
\[ \mathcal{L}_n = \text{Span} \{U^*e_{-n}, U^*h_{-n}, \ldots, U^*e_n, U^*h_n\}, \]
then for all $q > 0$ there is $c(q) > 0$ independent of $n$ such that $|z_n^\pm - \lambda_\pm| \leq c(q)n^{-q}$ for all $n \in \mathbb{N}$.

In Table 2 we report on computations of the nearest point in Spec $P_n$ to $\lambda_-$ and list the values analogous to Table 1. In this case we only consider $n = 12 : 78$. Notice that the approximation of $\lambda_-$ using $B_2$ at $n = 12$ is already more accurate than the one obtained using the basis $B_1$ at $n = 1000$. The super-polynomial speed of approximation holds true for $B_2$ as well.
predicted by Lemma 4 and Theorem 1 is already evidenced by the first few entries of the last column.

3.4. Schrödinger operators with band gap essential spectrum. For our last example we consider an unbounded operator. Let $M$ be the one-dimensional Schrödinger operator

$$(11) \quad Mf(x) = -\partial_x^2 f(x) + V(x)f(x), \quad f \in \text{Dom } M := W^{2,2}(\mathbb{R})$$

acting on $L^2(\mathbb{R})$, where the potential $V = V_1 + V_2$, $V_1 \in W^{2,2}(\mathbb{R})$ and $V_2 \in W^{2,\infty}(\mathbb{R})$. Here $W^{n,p}(\mathbb{R})$ denotes the $n$th derivative $L^p$ Sobolev space: $V \in W^{n,p}(\mathbb{R})$ if and only if $V \in L^p(\mathbb{R})$ and $\partial^q_x V \in L^p(\mathbb{R})$ for $q = 1, \ldots, n$.

Since, in particular, $V \in L^2(\mathbb{R}) + L^\infty(\mathbb{R})$, multiplication by $V$ is $\partial_x^2$ bounded with relative bound 0 [18, Theorem XIII.96]. Recall that the operator $L$ is said to be $L^0$ bounded, if and only if $\text{Dom } L^0 \subseteq \text{Dom } L$ and

$$\|L f\| \leq \alpha \|L_0 f\| + \beta \|f\|, \quad f \in \text{Dom } L_0$$

for suitable non-negative constants $\alpha$ and $\beta$. The infimum of all $\alpha$ allowing the above for some $\beta$ is called the relative bound of $L$ (with respect to $L_0$). By virtue of Kato-Rellich theorem [17, Theorem X.12], the above choice of $\text{Dom } M$ guarantees $M = M^*$. Notice that $\text{Dom } M^2 = W^{4,2}(\mathbb{R})$.

Furthermore, since $V_1$ is relatively compact with respect to $-\partial_x^2$, $V_2$ is bounded, $V_1$ is also relatively compact with respect to $-\partial_x^2 + V_2$. Hence, by Weyl’s theorem, the essential spectrum of $H$ is characterized completely by $V_2$, that is $\text{Spec}_{\text{ess}} M = \text{Spec}_{\text{ess}} (-\partial_x^2 + V_2)$. If $V_2$ is periodic [18, Chapter XIII.16], the essential spectrum is bounded below, it lies in bands and it extends to infinity. In general, $V_1$ may produce non-empty discrete spectrum.

We put

$$(12) \quad \mathcal{L}_n = \text{span}\{\phi_0, \ldots, \phi_n\}$$

where $\phi_j(x) = c_k h_j(x) e^{-x^2/2}$, $c_j = \frac{1}{\sqrt{2^j j! \sqrt{\pi}}}$, and $h_j(x)$ is the $j$th Hermite polynomial given by Rodriguez’s formula

$$h_j(x) = (-1)^j e^{x^2} (\partial_x^j e^{-x^2}).$$

The choice of $c_j$ ensures that $\|\phi_j\| = 1$ for all $j = 0, 1, \ldots$. It is well known that $\psi_j(x)$ are the eigenvectors of the quantum mechanical harmonic oscillator $H := -\partial_x^2 + x^2$, so that $\{\phi_j\}_{j=0}^\infty$ is an orthonormal basis of $L^2(\mathbb{R})$. 

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Theorem 5. Let $M$ be given by (11) and $L_n$ be given by (12). Then for all $\lambda \in \text{Spec}_{\text{disc}}M$ there is $z_n \in \text{Spec}P_n$ such that $z_n \to \lambda$ as $n \to \infty$. Furthermore, if $\partial_x^q V(x)$ is continuous and bounded for some $q \geq 3$, then $|z_n - \lambda| = o(n^{\frac{3}{4q-1}})$ as $n \to \infty$.

The proof of this result will be a consequence of three technical lemmas.

Lemma 6. If $\partial_x^q V(x)$ is continuous and bounded for some $q \geq 1$, then $\psi \in C^{q+2}(\mathbb{R})$ and $|\partial_x^{q+2} \psi(x)| < d_1 e^{-a_1|x|}$, $x \in \mathbb{R}$, for suitable constants $d_1, a_1 > 0$.

Proof. Since $V \in W^{2,2}(\mathbb{R})$, then $V'(x)$ is a continuous function. By hypothesis, $\psi'' = (V - \lambda)\psi$, showing that $\psi''(x)$ is also continuous. By repeating recursively this argument $q$ times, the equality

$$\partial_x^{q+2} \psi = \psi \partial_x^q (V - \lambda) + \ldots + (V - \lambda) \partial_x^q \psi$$

implies the existence and the needed continuity of $\partial_x^{q+2} \psi(x)$.

By virtue of the results of [19, §C.3], the hypothesis on $V$ ensures that

$$|\psi(x)| < d_2 e^{-a_2|x|}, \quad x \in \mathbb{R},$$

for some positive constants $d_2, a_2$. Since $V(x) - \lambda$ is continuous and bounded, then $|\psi''(x)| < d_3 e^{-a_3|x|}$. By repeating recursively this argument $q$ times, (13) and the hypothesis, yield the desired upper bound for $|\partial_x^{q+2} \psi(x)|$.

Lemma 7. Let $M$ be given by (11). Then any eigenfunction of $M$ lies in $\text{Dom} H^2$.

Proof. From the inclusion $\psi \in \text{Dom} M^2 = W^{4,2}(\mathbb{R})$ and (11) (which do not require any smoothness property on $V$), it follows that $\psi \in W^{2,2}(\mathbb{R}) \cap \text{Dom} (x^2) = \text{Dom} H$ and $(-\psi'' + x^2 \psi) \in \text{Dom} H$. This ensures the desired property. The only non-trivial facts in the latter assertions are, perhaps, the inclusions $x^2 \psi \in W^{2,2}(\mathbb{R})$ and $\psi'' \in \text{Dom} (x^2)$. The first follows from the second, by differentiating twice the term $x^2 \psi$ and noticing that $(x\psi')' \in L^2(\mathbb{R})$. The second one is achieved as follows. Since $M\psi$ is an eigenvector of $M$, $| - \psi''(x) + V(x)\psi(x)| \leq d_3 e^{-a_3|x|}$. 

Then
\[ \|x^2\psi''\| \leq \|x^2(-\psi'' + V\psi)\| + \|x^2V\psi\| \]
\[ \leq d_4 + \left( \int x^4|V(x)|^2|\psi(x)|^2dx \right)^{1/2} \]
\[ \leq d_4 + d_2^2 \left( \int x^4e^{-2a_2|x|}|V(x)|^2dx \right)^{1/2}. \]

The latter integral is bounded because of \( V \in L^2(\mathbb{R}) + L^\infty(\mathbb{R}) \), therefore \( \psi'' \in \text{Dom}(x^2) \).

**Lemma 8.** Let \( M \) be given by [□□]. Then both \( M \) and \( M^2 \) are \( H^2 \) bounded.

**Proof.** Multiplication by \( V \) is \( \partial_x^2 \) bounded with bound 0. Then \( M \) is \( \partial_x^4 \) bounded with relative bound 0. Similarly, from the identity
\[ (-\partial_x^2 + V)^2u = \partial_x^4u - 2V\partial_x^2u - 2V'\partial_xu + (V^2 - V'')u \]
and the fact that \( V, V', V'' \) lie in \( L^2(\mathbb{R}) + L^\infty(\mathbb{R}) \), one may deduce that \( M^2 \) is \( \partial_x^4 \) bounded with relative bound 1. Then the proof reduces to showing that \( \partial_x^4 \) is \( H^2 \) bounded. For this, let
\[ A := 2^{-1/2}(x + \partial_x) \quad \text{and} \quad A^* = 2^{-1/2}(x - \partial_x). \]
Then \((-\partial_x^2 + x^2) = 2(AA^* - 1) \) and \( \partial_x^4 = (A - A^*)^4 \). Thus the desired property follows from the identity (cf. [□□ eq.(X.28)])
\[ \|A^{#1} \cdots A^{#q}u\| \leq c\|(-\partial_x^2 + x^2)^{q/2}u\|, \quad q = 1, 2, \ldots \]
where \( A^{#k} \) is either \( A \) or \( A^* \). This is easily shown by induction and using the estimate
\[ \|(-\partial_x^2 + x^2)^{p/2}u\| \leq \|(-\partial_x^2 + x^2)^{p/2}u\|, \quad p < q. \]
This completes the proof of the lemma.

We may now complete the proof of Theorem [□□]. Let \( \phi := H^2\psi \). The crucial point lies in the following observation. According to Lemma 8, there exist non-negative constants \( \alpha \) and \( \beta \), such that
\[ \|\Pi_nM^k\Pi_n\psi - \lambda^k\psi\| \leq \|\Pi_nM^k\Pi_n\psi - \Pi_nM^k\psi\| + \|\Pi_nM^k\psi - \lambda^k\psi\| \]
\[ \leq \|M^k(\Pi_n\psi - \psi)\| + \|\lambda^k(\Pi_n\psi - \psi)\| \]
\[ \leq \alpha\|H^2(\Pi_n\psi - \psi)\| + (\beta + |\lambda|^k)\|\Pi_n\psi - \psi\| \]
\[ = \alpha\|\Pi_n\phi - \phi\| + (\beta + |\lambda|^k)\|\Pi_n\phi - \phi\|. \]
This ensures directly the first part of the theorem. For the second part we only require estimating \( \|\Pi_n\psi - \psi\| \) and \( \|\Pi_n\phi - \phi\| \) as \( n \to \infty \).
A straightforward application of lemma 6 shows that, if ∂^q_x V(x) is continuous and bounded for q ≥ 2, then for any set of polynomials \{p_0(x), \ldots, p_{q+2}(x)\}, the functions \(\sum_{j=0}^{q+2} p_j(x)\psi^{(j)}(x)\) and \(\sum_{j=0}^{q-2} p_j(x)\phi^{(j)}(x)\) are continuous and square integrable. By virtue of the fundamental relation

\[ h_j(x) = \frac{h_{j+1}'(x)}{2(j + 1)}, \quad j = 0, 1, \ldots, \]

integration by parts yields

\[
\langle \psi, \phi_k \rangle = c_k \int_{-\infty}^{\infty} \psi(x)h_k(x)e^{-x^2/2} \, dx = c_k \int_{-\infty}^{\infty} \psi(x) \left( \frac{h_{k+1}'(x)}{2(k + 1)} \right) e^{-x^2/2} \, dx
\]

\[
= -\frac{c_k}{2(k + 1)} \int_{-\infty}^{\infty} \left[ \psi(x)e^{-x^2/2}\right]'h_{k+1}(x) \, dx
\]

\[
= -\frac{c_k}{2(k + 1)} \int_{-\infty}^{\infty} \left[ \psi'(x) - x\psi(x) \right] e^{-x^2/2}h_{k+1}(x) \, dx = \ldots
\]

\[
= \frac{(-1)^q c_k}{2^q + 2(k + 1) \cdots (k + q + 2)} \int_{-\infty}^{\infty} \left[ \sum_{j=0}^{q+2} p_j(x)\psi^{(j)}(x) \right] e^{-x^2/2}h_{k+q+2}(x) \, dx
\]

\[
= \frac{(-1)^q c_k}{2^q + 2 \sqrt{(k + 1) \cdots (k + q + 2)}} \int_{-\infty}^{\infty} \left( \sum_{j=0}^{q+2} p_j(x)\psi^{(j)}(x) \right) e^{-x^2/2}h_{k+q+2}(x) \, dx
\]

where \(\zeta(x) = \sum_{j=0}^{q+2} p_j(x)\psi^{(j)}(x)\) is continuous and square integrable. Thus

\[
\|\Pi_n \psi - \psi\|^2 = \sum_{k=n+1}^{\infty} |\langle \psi, \phi_k \rangle|^2
\]

\[
\leq \sum_{k=n}^{\infty} \frac{|\langle \zeta, \phi_{k+q+2} \rangle|^2}{2^q + 2 \sqrt{(k + 1) \cdots (k + q + 2)}}
\]

\[
\leq \frac{1}{2^q + 2} \sum_{k=n}^{\infty} |\langle \zeta, \phi_{k+q+2} \rangle|^2 = o(n^{-(q+2)}),
\]

as \(n \to \infty\). A similar calculation with \(\phi\) instead of \(\psi\), gives

\[
\|\Pi_n \phi - \phi\|^2 = o(n^{-(q-2)}),\quad n \to \infty,
\]

completing the proof of Theorem 5.

We remark that Theorem 5 may be extended to higher dimension without much effort.
4. Distance to singularity, the spectral function

In order to simplify the notation in the proof of Theorems 11 and 24 we first discuss the notion of distance from $P(z)$ to the nearest singular matrix. For convenience, all the ideas in this section refer to general matrix polynomials of arbitrary degree $P(z) = \sum_{k=0}^{m} A_k z^k$, where $A_k \in \mathbb{C}^{j \times j}$ and $\det A_m \neq 0$. Some of the results below are related to the recent electronic manuscript by Davies [7] and the paper by Lancaster and Psarrakos [14].

For all $z \in \mathbb{C}$, we define

$$\sigma_P(z) := \inf_{v \neq 0} \frac{\|P(z)v\|}{\|v\|}.$$  

Four different characterizations of this function are,

a) $\sigma_P(z)$ equals the smallest singular value of $P(z)$,

b) $\sigma_P(z)^{-1} = \|P(z)^{-1}\|$ whenever $\det P(z) \neq 0$,

c) $\sigma_P(z)^{-1} = \sup_{u,v \neq 0} \frac{\text{Re} \langle P(z)^{-1}u, v \rangle}{\|u\| \|v\|}$ whenever $\det P(z) \neq 0$,

d) $\sigma_P(z) = \min\{\|E\| : \det[P(z) + E] = 0, E \in \mathbb{C}^{j \times j}\}$

$$= \min\{\|E\| : \det[P(z) + E] = 0, \text{Rank } E = 1\}.$$  

Since

$$\text{Spec } P = \{z \in \mathbb{C} : \sigma_P(z) = 0\},$$

we may call the scalar quantity $\sigma_P(z)$ a “spectral function” of the matrix polynomial $P$.

The proofs of a), b) and c) are straightforward and property d) holds trivially when $\sigma_P(z) = 0$. In order to prove d) when $\sigma_P(z) \neq 0$, we use b). If $\|E\| < \|P(z)^{-1}\|^{-1}$, then $\|P(z)^{-1}E\| < 1$ and $P(z) + E = P(z)(I + P(z)^{-1}E)$ so that $\det(P(z) + E) \neq 0$. This shows that $\|P(z)^{-1}\|^{-1}$ cannot be greater than the right sides of d). Conversely, let $v \in \mathbb{C}^j$ be such that $\|P(z)^{-1}v\| = \|P(z)^{-1}\|$ and $\|v\| = 1$, and let $u := \|P(z)^{-1}\|^{-1}P(z)^{-1}v$. Then $\|u\| = 1$. Put $Ew := -\|P(z)^{-1}\|^{-1}\langle w, u \rangle v$ for all $w \in \mathbb{C}^j$. Then the linear operator $E$ has rank one, it satisfies $\|E\| = \|P(z)^{-1}\|^{-1}$ and $Eu = -\|P(z)^{-1}\|^{-1}v$. Thus $(P(z) + E)u = 0$ so that $\det[P(z) + E] = 0$. This ensures that the bottom right side of d) is not greater than $\|P(z)^{-1}\|^{-1}$.

The following lemma will play a fundamental role in the sequel. See [14] Lemma 2] and [7] Section 3.4).

**Lemma 9.** The non-negative function $\sigma_P(z)$ is Lipschitz continuous in every compact subset of the complex plane. Furthermore $\sigma_P(z)^{-1}$ is subharmonic in $\mathbb{C} \setminus \text{Spec } P$, so that $z_0$ is a local minimum of $\sigma_P$ if and only if $z_0 \in \text{Spec } P$.  

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Proof. The first part of the lemma follows easily from the triangle inequality once we have proven the estimate
\begin{equation}
|\sigma_P(z) - \sigma_P(w)| \leq \|P(z) - P(w)\| \quad \text{for all } z, w \in \mathbb{C}. 
\end{equation}
We show the latter by considering two separated cases. If \(z \in \text{Spec } P\) and \(w \not\in \text{Spec } P\), since \(P(z) = P(w) + (P(z) - P(w))\) is not invertible, d) ensures \((15)\). If \(z, w \not\in \text{Spec } P\), then
\[ P(z)^{-1} - P(w)^{-1} = P(z)^{-1}[P(w) - P(z)]P(w)^{-1}. \]
By the triangle inequality,
\[ \|P(z)^{-1} - P(w)^{-1}\| \leq \|P(z)^{-1}\|\|P(w) - P(z)\|\|P(w)^{-1}\| \]
and so \((15)\) is consequence of b). The second part of the lemma follows from c) and the elementary properties of subharmonic functions.

We now consider weighted perturbations of \(P(z)\) in the sense studied recently in [13] and [14]. We will require these results in the proof of Theorem 2. Below, \(Q(z) = \sum_{k=0}^{m} E_k z^k\) shall always refer to a small perturbation of \(P\). Let \(\varepsilon \geq 0\) and \(\tilde{w} = (w_0, \ldots, w_n)\) where \(w_k \geq 0\). The (weighted) \(\varepsilon\)-pseudospectra of \(P\) are the set given by
\[ \text{Spec}_{\varepsilon, \tilde{w}} P : = \left\{ z \in \mathbb{C} : \det[P(z) + Q(z)] = 0, \text{ for some } Q(z) = \sum_{k=0}^{m} E_k z^k, \text{ such that } \|E_k\| \leq w_k \varepsilon, k = 0, \ldots, m \right\}. \]
This definition was studied by Higham and Tisseur in [13] and it extends the standard definition of pseudospectra of a matrix \(A\) in the obvious manner, by considering \(P(z) = (z - A)\) and \(\tilde{w} = (1,0)\). The weight \(\tilde{w}\) is introduced in order to allow freedom in controlling the perturbation of each individual coefficient of \(P\), e.g. this may be given in an absolute sense \((w_k = 1)\) or in a relative sense \((w_k = \|A_k\|)\). Observe that \(\text{Spec}_{0, \tilde{w}} P = \text{Spec } P\).

By combining the remarkable result [13, Lemma 2.1] with b), we achieve the useful characterization
\[ \text{Spec}_{\varepsilon, \tilde{w}} P = \left\{ z \in \mathbb{C} : \sigma_P(z) \leq \varepsilon \left( w_0 + w_1 |z| + \ldots + w_m |z|^m \right) \right\}. \]
Notice that we do not require \(\|E_m\|\) to be small, so \(\text{Spec}_{\varepsilon, \tilde{w}} P\) is not guaranteed to be bounded. This shall not be an important point here. Necessary and sufficient conditions for these set to be bounded may be found in [14, Theorem 2.2].

The following lemma is relevant in the proof of Theorem 2. This has also been established by Lancaster and Psarrakos in the more sophisticated [14, Theorem 2.3].

**Lemma 10.** Let \(\varepsilon > 0\). Let \(\Omega\) be a connected component of \(\text{Spec}_{\varepsilon, \tilde{w}} P\) such that \(\Omega \cap \text{Spec } P \neq \emptyset\). If \(\|E_k\| \leq w_k \varepsilon\) for all \(k = 1, \ldots, m\), then
Lemma 11. \( \Omega \cap \text{Spec} (P + Q) \neq \emptyset \). Furthermore \( P + Q \) has the same number of eigenvalues in \( \Omega \), counting multiplicity, than \( P \) has.

\textbf{Proof.} Let \( P_\delta (z) := \sum_{k=0}^m (A_k + \delta E_k) z^k \) for \( 0 \leq \delta \leq 1 \). Then \( P_0(z) = P(z) \) and \( P_1(z) = P(z) + Q(z) \). Since these eigenvalues are the zeros of a certain family of scalar polynomials whose coefficients depend continuously upon \( \delta \), the eigenvalues of \( P_\delta (z) \) depend continuously on \( \delta \).

Let \( \mu_\delta \in \text{Spec} P_\delta \), be such that \( \mu_0 \in \Omega \). Since \( ||\delta E_k|| \leq ||E_k|| \leq w_k \varepsilon \), then \( \mu_\delta \in \text{Spec}_{\varepsilon, \bar{\varepsilon}} P \) for all \( 0 \leq \delta \leq 1 \). Being a continuous trajectory, necessarily \( \mu_\delta \in \Omega \) for all \( 0 \leq \delta \leq 1 \).

5. \textbf{Proof of theorems 1 and 2}

Throughout this section we shall write \( \sigma_n \equiv \sigma_{P_n} \).

Let \( b_1 := 2 + 2|\lambda| + 3|\lambda|^2 \). By virtue of the triangle inequality,

\[
\|\Pi_n (\lambda - M)^2 \Pi_n \psi\| = \|\lambda^2 \Pi_n \psi - 2\lambda \Pi_n M \Pi_n \psi + \Pi_n M^2 \Pi_n \psi\|
\leq \|\Pi_n M^2 \Pi_n \psi - \lambda^2 \Pi_n \psi\| + \|2\lambda \Pi_n \psi - 2\lambda \Pi_n M \Pi_n \psi\|
\leq \|\Pi_n M^2 \Pi_n \psi - \lambda^2 \psi\| + 2|\lambda| \|\lambda \psi - \Pi_n M \Pi_n \psi\| + 3|\lambda|^2 \|\psi - \Pi_n \psi\|
< (b_1 - 1/2) \delta(n).
\]

Then, from the definition of \( \sigma_n \), by choosing \( v = \Pi_n \psi \), we achieve the following.

\textbf{Lemma 11.} There exists \( N_1 > 0 \) such that \( \sigma_n (\lambda) < b_1 \delta(n) \) for all \( n > N_1 \).

The proof of both theorems depends heavily on applying the second part of Lemma 10. For this we combine Lemma 11 with lower bounds for \( \sigma_n (z) \) along the boundary of small neighbourhoods of \( \lambda \). Our first step towards computing these bounds, involves finding estimates for \( \|P_n (z)^{-1}\| \) in subspaces that are orthogonal to the eigenspace associated to \( \lambda \).

Let \( \mathcal{E} := \text{span} \{ \psi \in \text{Dom} M : M \psi = \lambda \psi \} \), \( d_\lambda := \dim \mathcal{E} \) and \( \Pi_\mathcal{E} \) be the orthogonal projection onto \( \mathcal{E} \). Let \( \tilde{\mu} = \pm \mu \) be such that \( \lambda - \tilde{\mu} \in \text{Spec} M \) and

\[
A := M (I - \Pi_\mathcal{E}) + (\lambda - \tilde{\mu}) \Pi_\mathcal{E}, \quad \text{Dom} A = \text{Dom} M.
\]

Then, by construction, \( A = A^* \) and \( \text{Spec} A = \text{Spec} M \setminus \{\lambda\} \).

For \( z \in \mathbb{C} \), we write \( A(z) := (z - A)^2 \) with \( \text{Dom} A(z) = \text{Dom} M^2 \), \( K(z) = \tilde{\mu}(2\lambda - 2z - \tilde{\mu}) \Pi_\mathcal{E} \), so that

\[
A(z)x = (z - M)^2 x - K(z)x \quad \text{for} \quad x \in \text{Dom} M^2;
\]

\[
A_n (z) := \Pi_n A(z)|\mathcal{L}_n, \quad K_n (z) = \Pi_n K(z)|\mathcal{L}_n \quad \text{and} \quad A_n (z)^{-1} = [A_n (z)]^{-1}.
\]
Let $D := \{ |z - \lambda| \leq \mu/4 \}$. Then $D$ does not intersect Spec $A$ and $\lambda$ is the closest point in Spec $M$ to the boundary of $D$. Furthermore, if $z \in D$, then

$$\inf_{w \in \mathbb{R} \setminus [\lambda - \mu, \lambda + \mu]} \Re (z - w)^2 = \inf_{w \in \mathbb{R} \setminus [\lambda - \mu, \lambda + \mu]} (w - \lambda - \Re z)^2 - (\Im z)^2 \geq \frac{\mu^2}{2} > 0.$$  

Put $\gamma := \mu^2/2$. Since $\langle \Pi_n(z - A)^2 | L_n v, v \rangle = \langle (z - A)^2 v, v \rangle$ for all $v \in L_n$ and $A(z)$ is a normal operator, then the following inclusion for the numerical range of $A_n(z)$ holds for all $z \in D$,

$$\text{Num } A_n(z) \subseteq \text{Num } A(z) \subseteq \text{Conv}\{\text{Spec } (z - A)^2\}
\subseteq \{ (z - w)^2 : w \in [\lambda - \mu, \lambda + \mu] \} \subseteq \{ \Re (z) \geq \gamma > 0 \}.$$

Thus $A_n(z)$ is invertible and

$$||A_n^{-1}(z)|| \leq [\text{dist } (0, \text{Num } A_n(z))]^{-1} \leq \gamma^{-1}$$

for all $z \in D$ and $n \in \mathbb{N}$.

Let

$$b_2 := 1 + 2(\mu/4 + |\lambda|) + (\mu/4 + |\lambda|)^2 + 2\mu(4|\lambda| + 3\mu/2).$$

The triangle inequality ensures that

$$||A_n(z) \Pi_n \psi - A(z) \psi|| = ||\Pi_n(z - M)^2 \Pi_n \psi - (z - M)^2 \psi - \mu(2\lambda - 2z - \mu)[\psi - \Pi_n \Pi_\xi \Pi_n \psi]||$$

$$\leq ||\Pi_n M^2 \Pi_n \psi - \lambda^2 \psi|| + 2|z| ||\Pi_n M \Pi_n \psi - \lambda \psi|| + (2|\mu(2\lambda - 2z - \mu)| + |z|^2) ||\psi - \Pi_n \psi||$$

$$\leq (1 + 2|z| + |z|^2 + 2\mu(2\lambda - 2z - \mu)) \delta(n) \leq b_2 \delta(n)$$

for all $z \in D$ and $n \in \mathbb{N}$. Let $\nu := (\lambda - \bar{\mu} - z)^2$, so that $A(z) \psi = \nu \psi$. Then

$$||A_n(z)^{-1} \Pi_n \psi - A(z)^{-1} \psi|| = ||A_n(z)^{-1} \Pi_n \psi - \nu^{-1} \psi||$$

$$\leq ||A_n(z)^{-1} \Pi_n \psi - \nu^{-1} \Pi_n \psi|| + ||\nu^{-1} \Pi_n \psi - \nu^{-1} \psi||$$

$$\leq \gamma^{-1} ||\nu^{-1}|| \nu \Pi_n \psi - A_n(z) \Pi_n \psi|| + ||\nu^{-1}|| \Pi_n \psi - \psi||$$

$$= \gamma^{-1} ||\nu^{-1}|| \Pi_n A(z) \psi - A_n(z) \Pi_n \psi|| + ||\nu^{-1}|| \Pi_n \psi - \psi||$$

$$\leq \gamma^{-1} ||\nu^{-1}|| A(z) \psi - A_n(z) \Pi_n \psi|| + ||\nu^{-1}|| \Pi_n \psi - \psi||$$

$$\leq (\gamma^{-1} b_2 + 1) ||\nu^{-1}|| \delta(n)$$

$$\leq (4(\gamma^{-1} b_2 + 1) \mu/3) \delta(n) =: b_3 \delta(n)$$
for all \( z \in D \) and \( n \in \mathbb{N} \). Hence, a straightforward computation shows that
\[
\|A_n(z)^{-1}\Pi_nK(z) - A(z)^{-1}K(z)\| < d_3b_3\delta(n)
\]
for all \( z \in D \) and \( n \in \mathbb{N} \).

The following estimate, which is a direct consequence of the definition of \( K(z) \), will be needed below:
\[
\|K(z)\| \leq \mu(2|z - \lambda| + \mu) \leq 3\mu^2/2 =: b_4 \quad \text{for all } z \in D.
\]

5.1. **Proof of Theorem II** By virtue of Lemma \( \text{II} \) the only local minima of \( \sigma_n(z) \) are those points in Spec \( P_n \). Then the proof of Theorem II reduces to finding \( \tilde{b} > 0 \) and \( N_2 > 0 \), both independent of \( z \) and \( n \), such that
\[
\sigma_n(z) > \sigma_n(\lambda) \quad \text{for all } \{z - \lambda| = \tilde{b}\delta(n)^{1/2}\} \text{ and } n > N_2.
\]

Since Spec \( P_n \) is finite, the existence of \( b > 0 \) as we require in the thesis part of the theorem becomes obvious.

Inequality (17) is a consequence of Lemma III and the following.

**Lemma 12.** Let \( \tilde{b} := (4b_4 \max \{d_3b_3, \gamma^{-1}b_1\} + 1)^{1/2} \) and let \( N_2 \in \mathbb{N} \) be such that
\[
\delta(n) < \min\{\tilde{b}^{-2}(\mu/4)^2, (4d_3b_3)^{-1}, \gamma(4b_1)^{-1}\}, \quad n > N_2.
\]
Then \( \sigma_n(z) > b_4\delta(n) \) for all \( |z - \lambda| = \tilde{b}\delta(n)^{1/2} \) and \( n > N_2 \).

**Proof.** Throughout the proof we assume that \( n > N_2 \) and \( |z - \lambda| = \tilde{b}\delta(n)^{1/2} \). Since \( \tilde{b}\delta(n)^{1/2} < \mu/4 \), then \( A(z) + K(z) = (z - M)^2 \) is invertible and
\[
\|[I + A(z)^{-1}K(z)]^{-1}\| = \|[z - M]^{-2}A(z)\|
\]
\[
= \|[z - M]^{-2}((z - M)^2 - K(z))\|
\]
\[
= \|I - (z - M)^{-2}K(z)\| \leq 1 + b_4\|(z - M)^{-2}\|
\]
\[
\leq 1 + b_4[\text{dist}(z, \text{Spec } M)]^{-2} = \frac{\tilde{b}^2\delta(n) + b_4}{\tilde{b}^2\delta(n)} =: [c(n)]^{-1}.
\]
Thus, given \( v \in \mathcal{L}_n \),
\[
c(n)\|v\| \leq \|v + A(z)^{-1}K(z)v\|
\]
\[
\leq \|v + A_n(z)^{-1}\Pi_nK(z)v\| + \|A_n(z)^{-1}\Pi_nK(z) - A(z)^{-1}K(z)\|\|v\|.
\]
Since $\tilde{b}^2 > 4b_1d_3b_3$ and $\delta(n) < (4d_3b_3)^{-1}$, then $\tilde{b}^2 > \frac{2b_3b_3\delta(n)}{1 - 2b_3\delta(n)}$ so that (16) and an easy calculation yield $\|A_n(z)^{-1}\Pi_n K(z) - A(z)^{-1}K(z)\| < c(n)/2$. Hence

$$\frac{c(n)n}{2}\|v\| \leq \|v + A_n(z)^{-1}\Pi_n K(z)v\|$$

$$\leq \|A_n(z)^{-1}\|\|A_n(z)v + \Pi_n K(z)v\|$$

$$\leq \gamma^{-1}\|\Pi_n(z - M)^2|\mathcal{L}_n||$$

Therefore $\Pi_n(z - M)^2|\mathcal{L}_n$ is invertible and

$$\sigma_n(z) = \|(|\Pi_n(z - M)^2|\mathcal{L}_n))^{-1}\|^{-1} \leq \frac{\gamma c(n)}{2}.$$ 

Since $\tilde{b}^2 > \gamma^{-1}4b_4b_1$ and $\delta(n) < (4b_1)^{-1}$, it is easy to see that $\tilde{b}^2 > \frac{2b_4b_1}{\gamma - 2b_4\delta(n)}$. Thus $\sigma_n(z) > b_4\delta(n)$ as claimed in the lemma.

This completes the proof of Theorem 1. Explicit expressions for $\tilde{b}$ in terms of $\lambda$ and $\mu$ might be useful in applications. A direct substitution yields $\tilde{b} = (\max \{b_5, 12b_1\} + 1)^{1/2}$ where

$$b_5 := d_\lambda \frac{16 + 16|\lambda|^2 + 8\mu + 57\mu^2 + 8|\lambda|(4 + 17\mu)}{\mu}. $$

5.2. Proof of Theorem 2. The proof will be a consequence of lemmas 10, 11 and the following.

Lemma 13. For all $0 < \delta < \mu/4$, there exists $N_3 > 0$ independent of $z$ or $n$, such that

$$\sigma_n(z) > \frac{\delta^2\gamma}{2(\delta^2 + b_4)}$$

for all $n > N_3$ and $\delta \leq |z - \lambda| \leq \mu/4$.

Proof. Let $C := \{\delta \leq |z - \lambda| \leq \mu/4\}$. Throughout the proof we assume $z \in C$. Since $C \subset D$, then $A(z) + K(z) = (z - M)^2$ is invertible. By virtue of the third line of (18),

$$\|\|I + A(z)^{-1}K(z)\|^{-1}\| \leq 1 + b_4[\text{dist}(z, \text{Spec} M)]^{-2} \leq \frac{\delta^2 + b_4}{\delta^2} =: c_2^{-1}. $$

Let $N_3 > 0$ be such that $d_3b_3\delta(n) < c_2/2$ for all $n > N_3$. Then a straightforward computation along with (16) yield

$$\|A_n(z)^{-1}\Pi_n K(z) - A(z)^{-1}K(z)\| < \frac{c_2}{2}$$

for all $n > N_3$. Given $v \in \mathcal{L}_n$, then

$$c_2\|v\| \leq \|v + A_n(z)^{-1}\Pi_n K(z)v\| + \|A_n(z)^{-1}\Pi_n K(z) - A(z)^{-1}K(z)||v||.$$
Thus $c_2\|v\|/2 \leq \|P_n(z)v\|/\gamma^2$, so that $P_n(z)$ is invertible and $\sigma_n(z) \geq \gamma c_2/2$ for all $n > N_3$.

We now complete the proof of Theorem 2. Notice that the case $\varepsilon = 0$ is an obvious corollary of Theorem 1. Let $\varepsilon > 0$ be as in the hypothesis of Theorem 2 and let $\tilde{w} = (w_0, w_1, 0)$. A straightforward argument yields

$$D \cap \text{Spec}_{\varepsilon, \tilde{w}} P_n = \{ z \in D : \sigma_n(z) < \varepsilon (w_0 + w_1|z|) \}$$

Thus, if $n > N_3$, by virtue of Lemma 13, $C \cap \text{Spec}_{\varepsilon, \tilde{w}} P_n = \emptyset$ guaranteeing the first conclusion of the claimed result.

On the other hand, Lemma 14 ensures the existence of $N_4 \geq N_1$ such that $\sigma_n(\lambda) < \delta^2 \gamma/2(\delta^2 + b_4)$ for all $n > N_4$. Let $N := \max\{N_3, N_4\}$ and assume that $n > N$. By Lemma 15 there exists $z_n \in \text{Spec} P_n$ such that $|z_n - \lambda| < \delta$. Furthermore, the connected component $\Omega_n \subset \text{Spec}_{\varepsilon, \tilde{w}} P_n$ such that $z_n \in \Omega_n$, satisfies $\Omega_n \subset D \setminus C$. Hence, the second and third conclusions of the theorem follow directly from Lemma 10.

6. THE ESSENTIAL SPECTRUM

The essential spectrum of $M$ is usually found by means of analytical methods. Nonetheless, besides of being a natural question per se, the numerical evidence in all the examples discussed in [3], [15], [4] and
suggest that approximation of this portion of the spectrum may also occur in the “second-order” projection method described above. In this final section, we discuss some results and open questions related to this issue.

Ideally, we would like to know where does the whole set \( \text{Spec} P_n \) accumulates in the limit \( n \to \infty \). To this end, we may consider the following two limiting set and then study the connection between them as well as their relationship with \( \text{Spec} M \). Given \( \varepsilon \geq 0 \), let

\[
\Lambda_\varepsilon := \{ \zeta \in \mathbb{C} : \text{there exists } z_n \to \zeta \text{ such that } \sigma_n(z_n) \leq \varepsilon \}
\]

and

\[
\Sigma_\varepsilon := \{ \zeta \in \mathbb{C} : \limsup_{n \to \infty} \sigma_n(\zeta) \leq \varepsilon \}.
\]

Theorem 1 ensures that \( \text{Spec} \text{disc} M \subseteq R \cap \Lambda_0 \). We now ask, which conditions yield a similar property for \( \text{Spec} \text{ess} M \). We do not intend to answer this question here. Nevertheless, elementary properties of these set might provide an insight towards further investigations in this direction. Notice that \( \Lambda_\varepsilon \) is the (uniform) limit set of \( \text{Spec} \varepsilon \), \((1, 0, 0) P_n\) as \( n \to \infty \).

For simplicity we assume from now on that \( M \) is bounded. Thus

\[
\Lambda_0 \subseteq \Sigma_0 = \bigcap_{\delta > 0} \Sigma_\delta = \bigcap_{\delta > 0} \Lambda_\delta.
\]

Indeed, directly from the definition, it follows that

\[
\sigma_n(z) \leq \min_{\|v\| > 0} \frac{\|P_n(w)v\| + |z - w|\|\Pi_n(2M - z - w)\|}{\|v\|}
\]

\[
\leq \sigma_n(w) + |w - z| \sup_{\|v\|} \frac{\|\Pi_n(2M - z - w)v\|}{\|v\|}
\]

\[
\leq \sigma_n(w) + |w - z| c
\]

for all \( |w - z| < \tilde{\varepsilon} < 1 \), where \( c > 0 \) is chosen independently from \( \tilde{\varepsilon}, n, z \) and \( w \), because of \( M \) is bounded. Now, assume on the one hand that \( z \not\in \Sigma_\varepsilon \). Then there exists \( n(j) \in \mathbb{N} \) and \( a > 0 \), such that \( \sigma_{n(j)}(z) > \varepsilon + a \) for all \( j \in \mathbb{N} \). According to \((20)\),

\[
\sigma_{n(j)}(w) \geq \sigma_{n(j)}(z) - c|w - z| > \varepsilon + a - c\tilde{\varepsilon}
\]

for all \( |w - z| < \tilde{\varepsilon} \). Hence, by choosing \( \tilde{\varepsilon} = a/(2c) \), it becomes evident that \( \sigma_{n(j)}(w) > \varepsilon \) whenever \( |w - z| < \tilde{\varepsilon} \) for all \( j \in \mathbb{N} \), so that \( z \not\in \Lambda_\varepsilon \).

Thus

\[
\Lambda_\varepsilon \subseteq \Sigma_\varepsilon \quad \text{for all } \varepsilon \geq 0.
\]

On the other hand, it is not difficult to prove that

\[
\Sigma_\varepsilon \subseteq \Lambda_{\varepsilon + \delta} \quad \text{for all } \varepsilon \geq 0 \text{ and } \delta > 0
\]

and that \( \bigcap_{\delta > 0} \Sigma_\delta \subseteq \Sigma_0 \). These three inclusions ensure \((19)\).
The following proposition is crucial in the method suggested recently by Davies and Plum in [3].

**Proposition 14.** If $M$ is bounded, then $\Sigma_0 \cap \mathbb{R} = \text{Spec } M$.

**Proof.** Indeed, if $\lambda \in \text{Spec } M$, for each $k > 0$ there is $\psi_k \in \mathcal{H}$, $\|\psi_k\| = 1$, such that $\|(\lambda - M)^2\psi_k\| < 1/k$. Then

$$
\lim_{n \to \infty} \frac{\|P_n(\lambda)\Pi_n\psi_k\|}{\|\Pi_n\psi_k\|} < 1/k
$$

and so $\sigma_n(\lambda) \to 0$ as $n \to \infty$. Conversely, notice that if $\lambda \in \mathbb{R}$ but $\lambda \not\in \text{Spec } M$, then $\text{Num } P_n(\lambda) \subset \text{Num } (\lambda - M)^2 \subset [\mu, \infty)$. Hence

$$
\sigma_n(\lambda) \geq \text{dist } [0, \text{Num } P_n(\lambda)] \geq \mu,
$$

so that $\lambda \not\in \Sigma_0 \cap \mathbb{R}$.

In other words, the inclusion $\Sigma_0 \subseteq \Lambda_0$ complementary to the first one in (19), will automatically imply approximation to the whole spectrum, in particular to $\text{Spec } \text{ess } M$. For instance, [4] Proposition 3, if $M^2 = \text{Id}$, then $\Sigma_0 = \Lambda_0 \subseteq \{|\zeta| = 1\}$. The validity of this inclusion is closely related to the problem of whether there is an upper bound independent of $n$ for the size of the blocks in the Jordan canonical form of $A_n$, in the factorization $P_n(z) = (z - A_n)(z - A_n^*)$. Indeed, let $R_n(z) = (z - S_n)(z - S_n^*)$, where

$$
S_n = \begin{pmatrix}
0 & 0 & \cdots & 0 \\
1 & 0 & \cdots & 0 \\
& \ddots & \ddots & \ddots \\
& & 1 & 0
\end{pmatrix} \in \mathbb{C}^{n \times n}.
$$

Then $\text{Spec } R_n = \text{Spec } S_n \cup \text{Spec } S_n^* = \{0\}$ for all $n \in \mathbb{N}$. Thus $\Lambda_0 = \{0\}$. By choosing $v = (z^{n-1}, \ldots, z, 1)^t$, $R_n(z)v = (z^{n+1}, 0, \ldots, 0)$ so $\sigma_{R_n}(z) \leq |z|^{n+1}$. Hence $\Sigma_0 = \{|z| \leq 1\}$. Of course, although strict inclusion holds in this case, it not clear whether $R_n(z) = P_n(z)$ for some $M = M^*$ and $\{\Pi_n\}$.

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