On approximation of the eigenvalues of perturbed periodic Schrödinger operators

2007 J. Phys. A: Math. Theor. 40 9319

(http://iopscience.iop.org/1751-8121/40/31/010)

IOP Publishing Journal of Physics A: Mathematical and Theoretical

J. Phys. A: Math. Theor. **40** (2007) 9319–9329 doi:10.1088/1751-8113/40/31/010

On approximation of the eigenvalues of perturbed periodic Schrödinger operators*

Lyonell Boulton and Michael Levitin

Maxwell Institute for Mathematical Sciences and Department of Mathematics, Heriot-Watt University, Riccarton, Edinburgh EH14 4AS, UK

E-mail: L.Boulton@ma.hw.ac.uk and M.Levitin@ma.hw.ac.uk

Received 14 February 2007, in final form 21 June 2007
Published 19 July 2007
Online at stacks.iop.org/JPhysA/40/9319

Abstract

This paper addresses the problem of computing the eigenvalues lying in the gaps of the essential spectrum of a periodic Schrödinger operator perturbed by a fast decreasing potential. We use a recently developed technique, the so-called *quadratic projection method*, in order to achieve convergence free from spectral pollution. We describe the theoretical foundations of the method in detail and illustrate its effectiveness by several examples.

PACS numbers: 02.30.Jr, 02.60.Lj
Mathematics Subject Classification: 35B27, 65N25

(Some figures in this article are in colour only in the electronic version)

1. Introduction

It is well known that the problem of approximating the eigenvalues lying in the gaps of the essential spectrum of a self-adjoint operator by a sequence of finite-dimensional problems (e.g. for numerical analysis) is far from trivial. The presence of essential spectrum both above and below an eigenvalue means that there is no obvious variational principle (cf, e.g., [DoEsSe]), so an approximation/computation by a standard projection method is not always possible. The main difficulty is due to the existence of sequences of eigenvalues of the (finite-dimensional) approximate operators, accumulating at points in the gaps which do not belong to the spectrum. These points are called *spurious eigenvalues*, and the phenomenon itself is often referred to as *spectral pollution*.

It has been shown, for general unbounded self-adjoint operators, that spectral pollution in a projection method may occur at any real point of the resolvent set located between two parts of the essential spectrum (see [LeSh, theorem 2.1]). This is a consequence of the fact that the resolvent is not compact. A substantial amount of research has been devoted to finding ways

* This research is supported by the Leverhulme Trust grant F/00 276/F.

of choosing the projectors, in order to achieve a 'safe' method for particular problems, see, e.g., [RaSa2Va] and [BoBr]. Techniques vary considerably according to the problem and are by no means universal.

In this paper, we address the question of spectral pollution and its avoidance for a perturbed periodic Schrödinger operator

$$H := -\Delta + V, \tag{1.1}$$

acting in the Hilbert space $L^2(\mathbb{R}^N)$, where $V = V_p + V_d$, with V_p being purely periodic with respect to some lattice of $\mathbb{R}^N$ and V_d being fast decaying at infinity. The essential spectrum of H is determined by V_p. It consists of bands of absolutely continuous spectrum, separated by gaps in the resolvent set. If $V_d = 0$, the spectrum is purely essential. If $V_d \neq 0$, discrete eigenvalues may appear in the gaps, see [DeHe].

A usual method for finding the essential spectrum of H analytically, the so-called Floquet–Bloch technique, has been well studied (see, e.g., [ReSi], [Ku] and the references therein). It gives a decomposition of the periodic part of the operator into a direct integral of operators on a basic periodic cell. This reduces the problem of finding the endpoints of the bands in the essential spectrum, to the problem of finding the eigenvalues of differential operators in a compact domain with regular boundary conditions.

Much less in known about the discrete spectrum of H, which has to be either estimated numerically or studied by means of asymptotic techniques (for the latter see, e.g., [DeHe], [Bi] and [Su]). As we shall see below, the natural approach of truncating $\mathbb{R}^N$ to a large compact domain and applying the projection method to the corresponding Dirichlet problem is prone to spectral pollution. This makes the numerical localization of these eigenvalues particularly difficult.

The purpose of this paper is to describe an alternative procedure for finding eigenvalues, the so-called *quadratic projection method*, recently studied in an abstract setting in [Sh], [LeSh], [Bo1] and [Bo2]. The distinctive feature of our method is that the underlying discretized eigenvalue problem is quadratic in the spectral parameter (rather than linear) and has non-real eigenvalues. Its main advantage over a standard projection method lies in its robustness: it *never* pollutes and it always provides *a posteriori two-sided estimates* of the error of computed eigenvalues.

The paper is organized as follows. In section 2, we discuss the phenomenon of spectral pollution in a standard projection method and discuss the quadratic projection in an abstract context. Our corollary 2.6 is an improvement upon previously known non-pollution results for the general quadratic method. In section 3, we provide details on how to implement the quadratic projection method for the numerical localization of the eigenvalues of operator H. We also discuss some concrete numerical examples, but deliberately avoid including the full account of the numerical procedures we have used, in order not to overload the text with unnecessary technical details. These will appear elsewhere.

2. The quadratic projection method

2.1. Spectral pollution in an ordinary projection method

Before proceeding to describe our method, we want to give a rigorous motivation why it is needed at all, and why spectral pollution is intrinsic in the standard projection method.

Let A be a self-adjoint operator in a Hilbert space $\mathcal{H}$ with a dense domain, $\mathrm{Dom}(A)$. The spectrum of A, $\mathrm{Spec}(A)$, can be decomposed into the discrete spectrum, $\mathrm{Spec}_{\mathrm{disc}}(A)$, consisting of isolated eigenvalues of finite multiplicity, and the essential spectrum, $\mathrm{Spec}_{\mathrm{ess}}(A) := \mathrm{Spec}(A)\backslash\mathrm{Spec}_{\mathrm{disc}}(A) = \{\lambda : A - \lambda I \text{ is not Fredholm}\}$.

Take a finite-dimensional subspace $\mathcal{L} \subset \mathrm{Dom}(A)$, and let $\Pi_{\mathcal{L}} : \mathcal{H} \longrightarrow \mathcal{L}$ be the orthogonal projection onto $\mathcal{L}$. Let $A_{\mathcal{L}} := \Pi_{\mathcal{L}} A \restriction \mathcal{L}$.

The *projection* method, also known as the *Galerkin* method, consists in truncating the (infinite-dimensional) spectral problem $Au = \lambda u$ to

$$A_{\mathcal{L}} u = \lambda u \qquad \text{for some} \quad u \in \mathcal{L}\backslash\{0\}. \tag{2.1}$$

If the operator A is bounded from below and has a compact resolvent, this provides an effective way of numerically estimating the eigenvalues of A. The kth eigenvalue of (2.1) will always be above the kth eigenvalue of A, counting multiplicity, [ReSi, section XIII.1]. Furthermore, if $\mathcal{L}$ approximates $\mathrm{Dom}(A)$ reasonably well, then the first few eigenvalues of (2.1) will be close to the corresponding ones of A.

A precise statement can be easily obtained from the minimax principle:

Lemma 2.1. *Let $\mathcal{L}_n$ be a sequence of finite-dimensional subspaces of* $\mathrm{Dom}(A)$. *Assume that A is bounded below and has a compact resolvent. Let $\lambda_1 \leqslant \cdots \leqslant \lambda_m$ be the first m eigenvalues of A. Let*

$$\mathcal{E} = \mathrm{Span}\{u \in \mathrm{Dom}(A) : Au = \lambda_k u,\ 1 \leqslant k \leqslant m\}$$

be the spectral subspace associated with $\{\lambda_1, \ldots, \lambda_m\}$. If

$$\lim_{n\to\infty} \left\| A^p \left(u - \Pi_{\mathcal{L}_n} u\right)\right\| = 0 \tag{2.2}$$

holds for $p = 0, 1$ and all $u \in \mathcal{E}$, then the kth eigenvalue of (2.1) approaches the kth eigenvalue of A as $n \to \infty$ for $1 \leqslant k \leqslant m$.

We omit the proof.

In some particular cases it is also possible to estimate the convergence rate of the eigenvalues [StFi].

Similar results can be established if the resolvent of A is non-compact, for eigenvalues outside the extrema of $\mathrm{Spec}_{\mathrm{ess}}(A)$. However, the situation changes if we want to approximate an eigenvalue in a gap of $\mathrm{Spec}_{\mathrm{ess}}(A)$. There is no easy minimax principle, and spectral pollution may happen at any point of the gap.

The difficulties involved in the computation of these eigenvalues are well known for particular operators, see, e.g., [BoBr] or [RaSa2Va]. Moreover, in a generic situation we have

Lemma 2.2. *If $\lambda \notin \mathrm{Spec}_{\mathrm{ess}}(A)$ is such that $\alpha < \lambda < \beta$ where $\alpha, \beta \in \mathrm{Spec}_{\mathrm{ess}}(A)$, there exists a sequence of subspaces $\mathcal{L}_n$ satisfying (2.2) for all $p \in \mathbb{N}$ and all $u \in \mathrm{Dom}(A)$, such that $\lambda \in \mathrm{Spec}(A_{\mathcal{L}_n})$ for all $n \in \mathbb{N}$.*

This lemma directly follows from [LeSh, theorem 2.1].

2.2. The abstract quadratic projection method

Let, as before, $\mathcal{L}$ be a finite-dimensional subspace of $\mathrm{Dom}(A)$, and let $E = \{e_1, \ldots, e_n\}$ be a basis of $\mathcal{L}$. This basis need not be orthogonal.

Consider the quadratic matrix polynomial

$$P_{\mathcal{L}}(z) := Q_{\mathcal{L}} - 2zA_{\mathcal{L}} + z^2 B_{\mathcal{L}}, \tag{2.3}$$

where

$$[B_{\mathcal{L}}]_{jk} = \langle e_j, e_k\rangle \qquad [A_{\mathcal{L}}]_{jk} = \langle Ae_j, e_k\rangle \qquad [Q_{\mathcal{L}}]_{jk} = \langle Ae_j, Ae_k\rangle. \tag{2.4}$$

In numerical analysis, $A_{\mathcal{L}}$ is called the *stiffness* matrix, $B_{\mathcal{L}}$ is a *mass* matrix and $Q_{\mathcal{L}}$ is a *bending* matrix. If E is an orthonormal basis, then $A_{\mathcal{L}} = \Pi_{\mathcal{L}} A \restriction \mathcal{L}$ and $B_{\mathcal{L}} = \mathrm{Id} \restriction \mathcal{L}$. Additionally, if $E \subseteq \mathrm{Dom}(A^2)$, then $Q_{\mathcal{L}} = \Pi_{\mathcal{L}} A^2 \restriction \mathcal{L}$ and $P_{\mathcal{L}}(z) = \Pi_{\mathcal{L}}(A - z)^2 \restriction \mathcal{L}$.

We define the spectrum of the matrix polynomial $P_{\mathcal{L}}$, $\mathrm{Spec}(P_{\mathcal{L}})$, as the set of $\mu \in \mathbb{C}$ such that

$$P_{\mathcal{L}}(\mu)u = 0 \qquad \text{for some} \quad u \in \mathcal{L}\backslash\{0\}. \tag{2.5}$$

Since $B_{\mathcal{L}}$ is non-singular, $\det(P_{\mathcal{L}}(z))$ is a polynomial in z of degree $2\dim(\mathcal{L})$. Moreover, if $\mu \in \mathrm{Spec}(P_{\mathcal{L}})$, then also $\overline{\mu} \in \mathrm{Spec}(P_{\mathcal{L}})$. Therefore, $\mathrm{Spec}(P_{\mathcal{L}})$ is a set of at most $2\dim(\mathcal{L})$ complex points, symmetric with respect to the real axis.

The core idea of the quadratic projection method lies in the fact that $\mathrm{Spec}(A)$ can be well estimated if one knows the points of $\mathrm{Spec}(P_{\mathcal{L}})$ which are 'close' to the real line, see corollary 2.5 and theorem 2.7. In [Sh], [LeSh] and [Bo1], $\mathrm{Spec}(P_{\mathcal{L}})$ is called the *second-order spectrum of A relative to $\mathcal{L}$*. This set was first studied in connection with the spectrum of A in [Da], where the name originated.

Remark 2.3. Intuitively, the quadratic projection method arises from the following simple observation. Let $\zeta \in \mathbb{R}$ lie in a gap of the essential spectrum. By virtue of the spectral theorem, the discrete eigenvalues of $(\zeta - A)$ inside the corresponding shifted gap of $(\zeta - A)$ containing the origin are also the discrete eigenvalues of $(\zeta - A)^2$ lying below the bottom of the essential spectrum of $(\zeta - A)^2$. This suggests that the truncations of the latter operator must provide information about the localization of a portion of $\mathrm{Spec}_{\mathrm{disc}}(A)$ near ζ. The quadratic projection method is a rigorous realization of a similar idea.

The main reason for preferring (2.5) over (2.1) for estimating the spectrum of A lies in the following observation. Let $D(a, b)$ be the open disc in the complex plane with an interval $[a, b]$ as a diameter:

$$D(a, b) := \left\{ w \in \mathbb{C} : \left| w - \frac{a+b}{2} \right| < \frac{b-a}{2} \right\}.$$

Theorem 2.4 ([LeSh, lemma 5.2])**.** *Suppose that $(a, b) \cap \mathrm{Spec}(A) = \varnothing$. If $z \in D(a, b)$, then the matrix $P_{\mathcal{L}}(z)$ is non-singular.*

Proof. Our proof is slightly different from that of [LeSh]. Let $z \in D(a, b)$. Let

$$\Sigma_z := \{(\lambda - z)^2 : \lambda \in (-\infty, a] \cup [b, \infty)\}.$$

We first show that $0 \notin \overline{\mathrm{Conv}\Sigma_z}$ (here $\mathrm{Conv}\Omega$ denotes the convex hull of the set $\Omega \subset \mathbb{C}$). Indeed, let θ be the angle at z of the triangle T whose vertexes are a, b, z. Elementary geometric arguments show that $\theta > \pi/2$. Then the transformation $m : \lambda \mapsto (\lambda - z)^2$ maps the angular region

$$B = \{(w - z) : \rho w \in T \text{ for some } \rho \geqslant 0\}$$

into another angular sector centred at the origin with angle $2\theta > \pi$. Since $(-\infty, a) \cup (b, \infty) \subset \mathbb{C}\backslash B$ and

$$m : (-\infty, a] \cup [b, \infty) \longmapsto \Sigma_z,$$

there exist $-\pi < \theta_0 \leqslant \pi$ and $c > 0$, such that $\mathrm{Re}(\mathrm{e}^{\mathrm{i}\theta_0} w) \geqslant c$ for all $w \in \Sigma_z$. This ensures that $0 \notin \overline{\mathrm{Conv}\Sigma_z}$ as required.

Since $A = A^*$, $(A - z)^2$ with domain $\mathrm{Dom}(A^2)$ is a normal operator, [Ka]. As we have for the numerical range

$$\mathrm{Num}(A - z)^2 \subseteq \overline{\mathrm{Conv}[\mathrm{Spec}(A - z)^2]} \subseteq \overline{\mathrm{Conv}\Sigma_z},$$

and $\mathrm{Dom}(A^2)$ is a core for A, we have

$$\mathrm{Re}[e^{i\theta_0}\langle (A-z)u, (A-\overline{z})u\rangle] \geqslant c$$

for all $u \in \mathrm{Dom}(A)$ with $\|u\| = 1$. In particular this holds true for all $u \in \mathcal{L}$ with $\|u\| = 1$, so that $P_{\mathcal{L}}(z)$ cannot be a singular matrix. □

As a consequence of theorem 2.4, the points of $\mathrm{Spec}(P_{\mathcal{L}})$ which are close to the real line are *necessarily* close to $\mathrm{Spec}(A)$. In other words, the method never pollutes. We also have two immediate corollaries.

Corollary 2.5. *If $\mu \in \mathrm{Spec}(P_{\mathcal{L}})$, then*

$$\inf\{|\mathrm{Re}\,\mu - \lambda| : \lambda \in \mathrm{Spec}(A)\} \leqslant |\mathrm{Im}\,\mu|. \tag{2.6}$$

If $\lambda \in \mathrm{Spec}(A)$ is isolated from other point of the spectrum, (2.6) provides a two-sided estimate of λ, with an error explicitly determined without the need for computing eigenfunctions. In case this error is small, we can actually improve it by a square.

Corollary 2.6. *Let $\lambda \in \mathrm{Spec}(A)$. Assume that λ is isolated from other points of the spectrum and let*

$$\begin{aligned}\delta &:= \min\{|\lambda - \nu| : \nu \neq \lambda, \nu \in \mathrm{Spec}(A)\} \\ &= \mathrm{dist}(\lambda, \mathrm{Spec}(A)\backslash\{\lambda\}).\end{aligned} \tag{2.7}$$

If $|\mu - \lambda| < \delta/2$ for $\mu \in \mathrm{Spec}(P_{\mathcal{L}})$, then

$$|\mathrm{Re}\,\mu - \lambda| < \frac{2(\mathrm{Im}\,\mu)^2}{\delta}. \tag{2.8}$$

Proof. Theorem 2.4 yields

$$\left|\mu - \left(\lambda \pm \frac{\delta}{2}\right)\right| > \frac{\delta}{2}. \tag{2.9}$$

Using the assumption $|\mu - \lambda| < \delta/2$, we can rewrite (2.9) as

$$|\mathrm{Re}\,\mu - \lambda| < \frac{\delta}{2} - \sqrt{\frac{\delta^2}{4} - (\mathrm{Im}\,\mu)^2}.$$

Thus

$$|\mathrm{Re}\,\mu - \lambda| < \frac{(\mathrm{Im}\,\mu)^2}{\frac{\delta}{2} + \sqrt{\frac{\delta^2}{4} - (\mathrm{Im}\,\mu)^2}} < \frac{2(\mathrm{Im}\,\mu)^2}{\delta}.$$

□

Corollary 2.6 supersedes corollary 2.5 once we have found points of $\mathrm{Spec}(P_{\mathcal{L}})$ sufficiently close to an isolated point of the spectrum of A. Note that $\lambda \in \mathrm{Spec}(A)$ does not have to be a discrete eigenvalue.

The above 'non-pollution' results are useful as long as there are points of $\mathrm{Spec}(P_{\mathcal{L}})$ near to the real line. It is not immediately clear, however, whether or not the eigenvalues of A are approximated by some points in $\mathrm{Spec}(P_{\mathcal{L}})$ when the dimension of $\mathcal{L}$ goes to infinity. The results of [Bo1] and [Bo2] show that this is indeed the case, under a condition analogous to (2.2).

Theorem 2.7 ([Bo2, theorem 2.2])**.** *Let $\lambda \in \mathrm{Spec}_{\mathrm{disc}}(A)$, and let $\tilde{\mathcal{E}}_\lambda := \{u : Au = \lambda u\}$ be the corresponding eigenspace. Let $\mathcal{L}_n \subset \mathrm{Dom}(A^2)$ be subspaces with corresponding orthogonal projections $\Pi_{\mathcal{L}_n}$, such that (2.2) holds for $p = 0, 1, 2$ and all $u \in \tilde{\mathcal{E}}_\lambda$. Then there exist eigenvalues $\lambda_n \in \mathrm{Spec}(P_{\mathcal{L}_n})$ such that $\lambda_n \to \lambda$ as $n \to \infty$.*

3. The quadratic projection method for perturbed periodic Schrödinger operators

Let H be the differential expression defined by (1.1) acting on the dense domain $W^{2,2}(\mathbb{R}^N)$.

Let

$$\begin{array}{ll} p=2 & \text{if} \quad N\leqslant 3,\\ p>2 & \text{if} \quad N=4,\\ p>N/2 & \text{if} \quad N\geqslant 5. \end{array}$$

Below and elsewhere we assume that the potential $V:\mathbb{R}^N\longrightarrow\mathbb{R}$ is *uniformly locally* L^p in the sense that

$$\int_C |V(x)|^p\,\mathrm{d}^N x\leqslant M \tag{3.1}$$

for any unit hyper-cube C, where the constant M is independent of C.

Condition (3.1) ensures that the operator of multiplication by V is $(-\Delta)$-bounded with relative bound equal to 0, so that H is a self-adjoint operator and $C_0^\infty(\mathbb{R}^N)$ is a core for H (cf [ReSi, theorem XIII.96]). Furthermore, H is bounded below.

3.1. Approximating subspaces in the quadratic projection method for the Schrödinger operator

We have already established, in the abstract setting of theorem 2.4, that, for any choice of a subspace $\mathcal{L}\subset W^{2,2}(\mathbb{R}^N)$, the eigenvalues of the matrix polynomial $P_{\mathcal{L}}(z)$ lying close to the real axis will be close to the spectrum of H (and those 'far away' from the real axis do not matter). In other words, the quadratic projection method does not pollute. In order, however, to achieve a small error and approximate as many eigenvalues as possible, the choice of $\mathcal{L}$ (or of a sequence of such spaces) is absolutely crucial, see theorem 2.7. Two main difficulties here are the infinite geometry and the extra smoothness requirements needed for $Q_{\mathcal{L}}$ to make sense, see (2.4).

Let $\Omega_s:=[-s,s]^N$. Let $\mathcal{M}_s:=W_0^{2,2}(\Omega_s)$ be a nested family of Sobolev spaces. Let $\mathcal{M}_{s,n}$, $n\in\mathbb{N}$, be a sequence of n-dimensional subspaces of $\mathcal{M}_s$. Let $\{\phi_{s,n,k}\}_{k=1}^n$ be a basis for $\mathcal{M}_{s,n}$. Set, for $j,k=1,\dots,n$,

$$\begin{aligned} [B_{s,n}]_{j,k}&:=\int_{\Omega_s}\phi_{s,n,j}\phi_{s,n,k},\\ [A_{s,n}]_{j,k}&:=\int_{\Omega_s}\nabla\phi_{s,n,j}\cdot\nabla\phi_{s,n,k}+V\phi_{s,n,j}\phi_{s,n,k},\\ [Q_{s,n}]_{j,k}&:=\int_{\Omega_s}\Delta\phi_{s,n,j}\Delta\phi_{s,n,k}+2V\phi_{s,n,j}\Delta\phi_{s,n,k}+V^2\phi_{s,n,j}\phi_{s,n,k}. \end{aligned} \tag{3.2}$$

and consider a quadratic $(n\times n)$-matrix polynomial

$$P_{s,n}(z):=Q_{s,n}-2zA_{s,n}+B_{s,n}. \tag{3.3}$$

Now, let s_n be a monotonically increasing unbounded sequence of positive real numbers, let $\mathcal{L}_n=\mathcal{M}_{s_n,n}$ and let $P_n(z)=P_{s_n,n}(z)$. Then theorem 2.7 still holds as long as one can verify (2.2) for $p=0,1,2$.

If the potential V is sufficiently smooth, a natural choice of the basis functions $\phi_{s,n,k}$ are piecewise C^2 splines on Ω_s satisfying $\phi|_{\partial\Omega_s}=\partial\phi/\partial n|_{\partial\Omega_s}=0$. However, even for this simple choice, verifying (2.2) is still highly technical, and we omit the details.

Even fixing *both* parameters s and n and not imposing *any* condition on $\mathcal{M}_{s,n}$ except $\mathcal{M}_{s,n}\subset W_0^{2,2}(\Omega_s)$ still usually provides some useful information about the spectrum,

with *a posteriori* two-sided estimates: if $\lambda_n \in \mathrm{Spec}(P_{s,n})$ and $\mathrm{dist}(\mathrm{Re}\,\lambda_n, \mathrm{Spec}_{\mathrm{ess}}(H)) \geqslant |\mathrm{Im}\,\lambda_n|$, then there exists $\lambda \in \mathrm{Spec}_{\mathrm{disc}}(H)$ which lies in the same spectral gap as $\mathrm{Re}\,\lambda_n$. See corollary 2.6 for a sharper estimate.

On the other hand, to achieve approximation it is crucial that both parameters n and s go to infinity in our choice of approximate spaces $\mathcal{L}_n$. If we fix an arbitrarily large s and let $n \to \infty$, then though we still do not have pollution (unlike a standard projection method), neither we have approximation.

3.2. The quadratic matrix polynomial problem

The quadratic projection method prescribes finding the spectrum $\mathrm{Spec}(P)$ of the quadratic matrix polynomial of the form

$$P(z) = Q + 2zA + z^2 B,$$

cf section 2.2. In applications, the matrix coefficients Q, A and B are expected to be sparse and real. They are always Hermitian, so $P(z)$ is a self-adjoint matrix polynomial in the sense of [Go].

The standard way of finding $\mathrm{Spec}(P)$ is to construct a suitable companion linear pencil eigenvalue problem,

$$Lv = \mu K v \qquad \text{for some} \quad 0 \neq v \in \mathcal{L} \oplus \mathcal{L}, \tag{3.4}$$

such that $\mu \in \mathrm{Spec}(P)$ if and only if (3.4) holds true. The coefficients, L, K, of the companion form, $(L - zK)$, are twice the size of the coefficients of $P(z)$. They are not unique. Two possible companion forms are given by

$$L = \begin{pmatrix} 0 & N \\ -Q & A \end{pmatrix} \qquad K = \begin{pmatrix} N & 0 \\ 0 & B \end{pmatrix}$$

and

$$L = \begin{pmatrix} -Q & 0 \\ 0 & N \end{pmatrix} \qquad K = \begin{pmatrix} A & B \\ N & 0 \end{pmatrix},$$

where N is a non-singular matrix.

Different companion forms lead to different stability properties of the linear pencil problem to be solved once the matrices have been assembled. It is desirable finding a companion form that does not worsen the condition numbers of the original matrix polynomial spectral problem. For a thorough account on this issue see [HiMaTi] and references therein.

3.3. Examples

One-dimensional example—Gaussian perturbation of the Mathieu potential. Let

$$N = 1, \qquad V_p(x) = \cos(x), \qquad V_d(x) = -\mathrm{e}^{-x^2},$$

and H as in (1.1) with potential $V = V_p + V_d$. We now illustrate how to implement the theoretical discussion carried out in the previous sections to the study of $\mathrm{Spec}(H)$.

The essential spectrum of H is determined by V_p. It comprises an infinite number of non-intersecting bands $[\alpha_n, \beta_n]$ of absolutely continuous spectrum whose endpoints are determined by the Mathieu characteristic values [In, section 7.4]. The approximate endpoints of the first five bands are given in table 1.

Addition of the negative Gaussian potential yields a non-empty discrete spectrum. By implementing the quadratic projection method (3.3) into a finite element scheme, we detect three eigenvalues of H with high accuracy:

$$\lambda_1 \approx -0.409\,61, \qquad \lambda_2 \approx 0.377\,63, \qquad \lambda_3 \approx 1.182\,16.$$

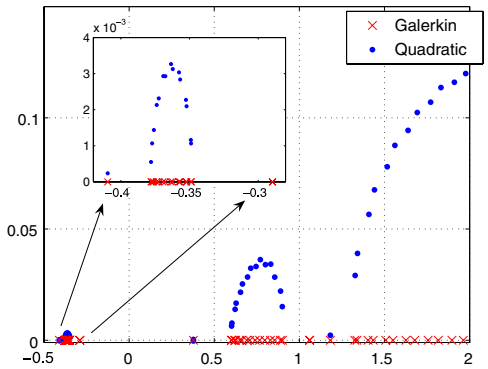

Figure 1. The quadratic projection method versus the Galerkin projection method. Here $s = 49$. Inset: zoom near $\lambda \approx -0.35$.

Table 1. Endpoints of the first five bands of the essential spectrum for the Gaussian perturbation of the Mathieu potential, cf [AbSt].

n	α_n	β_n
1	−0.378 490	−0.347 670
2	0.594 800	0.918 058
3	1.293 17	2.285 16
4	2.342 58	4.031 92
5	4.035 30	6.270 82

The eigenvalue λ_1 is below the bottom of the essential spectrum, whereas λ_2 and λ_3 lie in the first and the second gap, respectively.

Figure 1 illustrates the main ideas discussed in the previous sections. The spectrum of $P(z)$ is shown as blue dots, while the eigenvalues of the standard Galerkin eigenvalue problem (2.1) are shown as red crosses. The picture shows a narrow strip of the complex plane with the bottom edge being the interval $[-0.5, 2]$. Note that there are eigenvalues of $P(z)$ close to each of the eigenvalues λ_1, λ_2 and λ_3. According to corollary 2.5, these eigenvalues are not spurious: the real part of a complex number $z \in \mathrm{Spec}(P)$ is *always* an approximation of points in $\mathrm{Spec}(H)$, with a two-sided error estimate depending on $\mathrm{Im}\, z$. There are also eigenvalues of the linear problem (2.1) near to $\mathrm{Spec}_{\mathrm{disc}}(H)$. These eigenvalues also provide one-sided approximation (from above) for λ_j. However, one should be careful when using the Galerkin method, as spectral pollution may happen. For this particular set of parameters there are two spurious eigenvalues: one near -0.3 and the other near 1.1.

Two-dimensional examples. We now consider a family of case studies with $N = 2$. For $f \in W^{2,2}(\mathbb{R}^2)$, let

$$H_0 f(x, y) = -\Delta f(x, y) + (\cos(x) + \cos(y)) f(x, y)$$
$$H_1 f(x, y) = H_0 f(x, y) - c\, \mathrm{e}^{-(x^2+y^2)} f(x, y)$$
$$H_2 f(x, y) = H_0 f(x, y) - cx\, \mathrm{e}^{-(x^2+y^2)} f(x, y),$$

where $c > 0$. A straightforward argument involving separation of variables shows that

$$\mathrm{Spec}(H_0) = \bigcup_{\lambda \in \mathrm{Spec}(\tilde{H})} \{\lambda + \mu : \mu \in \mathrm{Spec}(\tilde{H})\},$$

Table 2. Endpoints of $\mathrm{Spec}_{\mathrm{ess}}(H_0)$.

n	α_n	β_n
1	−0.756 978	−0.695 338
2	0.216 310	0.570 389
3	0.914 677	∞

Table 3. Approximated eigenvalues of H_1 and H_2.

Eigenvalues of H_1			Eigenvalues of H_2		
c	λ_1	λ_2	c	λ_1	λ_2
5.0		$-0.096\,97 \pm 3.39 \times 10^{-4}$	10	$0.137\,7 \pm 6.61 \times 10^{-3}$	$0.755\,9 \pm 7.07 \times 10^{-2}$
5.2		$-0.171\,33 \pm 2.03 \times 10^{-4}$	11	$0.086\,5 \pm 2.79 \times 10^{-3}$	$0.681 \pm 1.05 \times 10^{-1}$
5.4		$-0.252\,55 \pm 1.45 \times 10^{-4}$	12	$0.011\,5 \pm 1.28 \times 10^{-3}$	
5.6		$-0.339\,05 \pm 1.44 \times 10^{-4}$	13	$-0.091\,90 \pm 8.19 \times 10^{-4}$	
5.8		$-0.429\,02 \pm 1.71 \times 10^{-4}$	14	$-0.222\,50 \pm 7.77 \times 10^{-4}$	
6.0	$-0.769\,46 \pm 2.85 \times 10^{-3}$	$-0.519\,78 \pm 2.52 \times 10^{-4}$	15	$-0.373\,0 \pm 1.17 \times 10^{-3}$	
6.2	$-0.786\,12 \pm 8.43 \times 10^{-4}$	$-0.605\,27 \pm 5.21 \times 10^{-4}$	16	$-0.527\,9 \pm 1.97 \times 10^{-3}$	

where $\tilde{H} = -\partial_x^2 + \cos(x)$ is the one-dimensional Mathieu Hamiltonian. Furthermore, as both H_1 and H_2 are relatively compact perturbations of H_0,

$$\mathrm{Spec}_{\mathrm{ess}}(H_1) = \mathrm{Spec}_{\mathrm{ess}}(H_2) = \mathrm{Spec}(H_0).$$

An approximation of the endpoints of the bands comprising the essential spectrum is given in table 2. Unlike the one-dimensional model, we now have a finite number of gaps. Note that the perturbation associated with H_1 is radially symmetric and sign definite, while that associated with H_2 is sign indefinite and not radially symmetric.

With the quadratic projection method we have been able to detect some discrete eigenvalues of H_1 and H_2 for different values of the coupling constant c. These results are presented in table 3. As we increase the value of c, eigenvalues of H_1 are moving from right to left. From the numerical results, the same seems to be true for eigenvalues of H_2. Note that if an eigenvalue is close to an endpoint of a band of the essential spectrum, the estimate (2.6) does not allow us to distinguish between this eigenvalue and the endpoint of the band—thus the gaps in table 3.

Note that an eigenvalue λ_1 of the Hamiltonian H_1 is below the bottom of the essential spectrum for $c \gtrapprox 6$. The Galerkin method could actually be implemented to approximate this eigenvalue. The quadratic projection, however, works whether an eigenvalue is in a gap or not and also provides a good approximation in this case.

In figure 2, we show the portion of $\mathrm{Spec}(P)$ lying in the box $[-1, 1/2] \times [-3/2, 3/2]$ for $H \equiv H_2, c = 14$ and $s = 60$. Corresponding pictures for H_1 and other choices of c and s are qualitatively similar. This graph clearly indicates approximation to an eigenvalue $\lambda_1 \approx -0.2225$ (see the right-hand picture). A large portion of $\mathrm{Spec}(P)$ forms an annular cloud around the spectral gap (β_1, α_2) and is sufficiently away from $\mathbb{R}$ to indicate that there are no other eigenvalues in this gap. Note also that some eigenvalue of $P(z)$ are close to $\mathrm{Spec}_{\mathrm{ess}}(H_2)$.

4. Final remarks

Other procedures exist for computing the eigenvalues of perturbed periodic partial differential operators such as H, see [Do]. These include a method based on finding the eigenvalues of

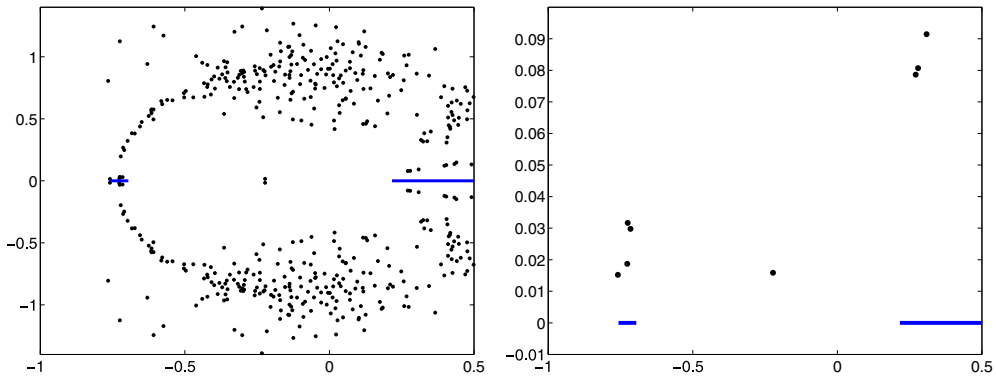

Figure 2. The quadratic projection method for our two-dimensional models. Left: typical output in the computation of Spec(P) for the operator H_2 when $c = 14$ (here $s = 60$). Right: zoom in the left picture on a narrow strip near the real line.

the matrix pencil problem

$$A_{s,n}u = \lambda B_{s,n}u \qquad \text{for some} \quad u \in \mathcal{L}\backslash\{0\}, \tag{4.1}$$

where the matrix coefficients are defined by (3.2) (that is applying the projection method) for several values of s and n, and observing the dynamics of the eigenvalues of (4.1) as s increases. Some of the eigenvalues of (4.1) will be spurious and some will be close to the true spectrum of H. The spurious eigenvalues will typically be unstable as functions of the parameter s. The approximate eigenvalues close to the true spectrum of H will be, on the other hand, very stable. Thus, by increasing s, and tracking the evolution of the eigenvalues of (4.1), one would be able to obtain some information about Spec(H).

This method, however, is quite inaccurate and it becomes useless when $N \geqslant 2$, and we are interested in finding large eigenvalues. Furthermore, it very much depends upon the choice of approximating subspaces $\mathcal{L}_s$. We are not aware of any rigorous treatment of the effectiveness of this approach.

As the chosen subspaces $W_0^{2,2}(\Omega_s)$ are naturally nested for increasing values of $s > 0$ and they are all embedded in $W^{2,2}(\mathbb{R}^N)$, every point in Spec(H) is approximated (always from above) by the spectrum of $\overline{\left(H \restriction W_0^{2,2}(\Omega_s)\right)}$. Note that compactly supported functions form a core for the operator and satisfy *any* boundary condition if the boundary is far enough away. Spectral pollution in the projection method is a consequence of high eigenvalues of $\overline{\left(H \restriction W_0^{2,2}(\Omega_s)\right)}$ accumulating at the bottom of the essential spectrum of H, and this effect is unavoidable.

We suggest using instead (or in addition to standard techniques) the quadratic projection method, which never pollutes.

Acknowledgments

We are grateful to Marco Marletta for useful discussions and helpful advice.

References

[Bi] Birman M 1995 The discrete spectrum in gaps of the perturbed periodic Schrödinger operator: I. Regular perturbations *Boundary Value Problems, Schrödinger Operators, Deformation Quantization (Math. Top.)* vol 8 (Berlin: Akademie Verlag) pp 334–52

[AbSt] Abramowitz M and Stegun I 1964 *Handbook of Mathematical Functions with Formulas, Graphs and Mathematical Tables* (National Bureau of Standards)

[BoBr] Boffi D, Brezzi F and Gastaldi L 1999 On the problem of spurious eigenvalues in the approximation of linear elliptic problems in mixed form *Math. Comput.* **69** 121–40

[Bo1] Boulton L 2006 Limiting set of second order spectrum *Math. Comput.* **75** 1367–82

[Bo2] Boulton L 2007 Non-variational approximation of discrete eigenvalues of self-adjoint operators *IMA J. Numer. Anal.* **27** 102–21

[Da] Davies E B 1998 Spectral enclosures and complex resonances for general self-adjoint operators *LMS J. Comput. Math.* **1** 42–74

[DeHe] Deift P A and Hempel R 1986 On the existence of eigenvalues of the Schrödinger operator $H - \lambda W$ in a gap of $\sigma(H)$ *Commun. Math. Phys.* **103** 461–90

[DoEsSe] Dolbeault J, Esteban M J and Séré E 2000 On the eigenvalues of operators with gaps. Application to Dirac operators *J. Funct. Anal.* **174** 208–26

[Do] Dowling J P *Photonic & Sonic Band-Gap Bibliography* http://phys.lsu.edu/jdowling/pbgbib.html

[Go] Gohberg I, Lancaster P and Rodman L 1982 *Matrix Polynomials* (New York: Academic)

[HiMaTi] Higham N, Mackey S and Tisseur F 2006 The Conditioning of Linearizations of Matrix Polynomials *SIAM J. Matrix Anal. Appl.* **28** 1005–28

[In] Ince E 1956 *Ordinary Differential Equations* (New York: Dover)

[Ka] Kato T 1980 *Perturbation Theory for Linear Operators* 2nd edn (Berlin: Springer)

[Ku] Kuchment P 1993 *Floquet Theory For Partial Differential Equations* (Basel: Birkhauser)

[LeSh] Levitin M and Shargorodsky E 2004 Spectral pollution and second order relative spectra for self-adjoint operators *IMA J. Numer. Anal.* **24** 393–416

[RaSa2Va] Rappaz J, Hubert J Sanchez, Palencia E Sanchez and Vassiliev D 1997 On spectral pollution in the finite element approximation of thin elastic 'membrane' shell *Numer. Math.* **75** 473–500

[ReSi] Reed M and Simon B 1978 *Methods of Modern Mathematical Physics, Vol 4: Analysis of Operators* (New York: Academic)

[Sh] Shargorodsky E 2000 Geometry of higher order relative spectra and projection methods *J. Oper. Theor.* **44** 43–62

[StFi] Strang G and Fix G 1973 *An Analysis of the Finite Element Method* (NJ: Prentice-Hall)

[Su] Suslina T 2003 The discrete spectrum of a two-dimensional second-order periodic elliptic operator perturbed by a decaying potential: II. Inner gaps *Algebra Analiz* **15** 128–89
Suslina T 2004 *St. Petersburg Math. J.* **15** 249–87 (Engl. Transl.)