

SpectrUW: a laboratory for the numerical exploration of spectra of linear operators

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Abstract

Spectra of linear operators play an important role in various aspects of applied mathematics. For all but the simplest operators, the spectrum cannot be determined analytically and as such it is difficult to build up any intuition about the spectrum. One way to obtain such intuition is to consider many examples numerically and observe emerging patterns. This is feasible using an efficient black-box numerical method, *i.e.*, a method that requires no conceptual changes for different examples. Hill's method satisfies these requirements. It is the mathematical foundation of SpectrUW (pronounced "spectrum"), mathematical black-box software that serves as a laboratory for the numerical approximation of spectra of one-dimensional linear operators.

1 Introduction

For many problems in applied mathematics, it is necessary to determine the spectrum of a linear operator. Three instances of this are (i) the linear stability analysis of equilibrium solutions of dynamical systems (finite or infinite dimensional) [14], (ii) the forward scattering problem for an integrable differential equation [1], and (iii) the theory of vibrating strings and membranes [21]. Nevertheless, for all but the simplest cases, it is impossible to determine the spectrum analytically. Because of this scarcity of examples, it is difficult to build up any intuition about spectra. For instance, one might be interested in their topology (*i.e.*, their appearance in the complex plane), or in their elements with largest real part (for stability problems), or their asymptotic behavior near infinity.

Such intuition can be obtained by considering many examples numerically. By doing this, emerging patterns may be observed, and in some cases conjectures about specific spectra can be made, perhaps resulting in a statement that can be rigorously proven. Such an approach is only feasible if one has available an efficient black-box method for the computation of spectra, *i.e.*, a method that applies to many examples without any conceptual changes to its algorithm. Hill's method is such a method. It was examined in detail in [8]. In this paper we review the method, emphasizing its algorithmic nature, and its implementation as a black-box method. Specifically, we introduce SpectrUW (pronounced "spectrum"), a Java-based mathematical freeware package for the numerical computation of spectra of one-dimensional linear operators. SpectrUW relies on either Maple or Mathematica as its computational engine. In this context, we show how SpectrUW may be used to examine spectra and their corresponding eigenfunctions. More

examples of the use of Hill's method are found in [8]. Those examples focus on the performance of the algorithm (exponential convergence, *etc.*), whereas those given here focus on the use of the software.

2 Problem statement

The problem considered here is that of determining the spectrum of a one-dimensional linear operator of order M

$$\mathcal{L} = \sum_{k=1}^M f_k(x) \partial_x^k. \quad (1)$$

The spectrum $\sigma(\mathcal{L})$ is the set of all numbers λ in the complex plane such that the equation

$$\mathcal{L}\psi = \lambda\psi \quad (2)$$

has solutions ψ , bounded in some norm, denoted $\|\psi\|$. Here $x \in [a, b]$ and boundary conditions have to be imposed. Depending on whether \mathcal{L} is a square matrix operator or a scalar operator, (2) is either a vector or a scalar problem. Thus

$$\sigma(\mathcal{L}) = \{\lambda \in \mathbb{C} : \text{there is a } \psi \text{ such that } \mathcal{L}\psi = \lambda\psi \text{ and } \|\psi\| < \infty\}. \quad (3)$$

As mentioned above, (2) can originate from a variety of problems. For generic operators \mathcal{L} few concrete statements about their spectrum can be made. There are a few large classes of examples where some properties are known. For instance for self-adjoint operators, the spectrum is confined to the real line. For infinitesimally skew-symmetric operators, the spectrum is reflection symmetric around both the real and imaginary axes [7, 17, 18].

3 Hill's method

The method discussed here originates with Hill [13], who used it to study the equation that now bears his name. It has been rediscovered several times, by different groups working on specific problems, *e.g.*, see [3, 6, 10, 12, 20, 22]. Only in [22] did the authors hint at the generality of the method. Its generality and properties as a numerical method were treated in detail in [8]. We review the method briefly here. For the sake of simplicity, we restrict ourselves to the scalar case. The more general case where \mathcal{L} is a matrix operator and (2) is a vector problem is discussed below. Also, we start by considering coefficient functions that are periodic in x , with common period L :

$$f_k(x + L) = f_k(x), \quad \text{for } k = 0, \dots, M. \quad (4)$$

Different classes of coefficient functions are commented on below.

There are 5 steps to Hill's method:

1. **Determine the Fourier coefficients of the coefficient functions** $f_k(x)$, $k = 0, \dots, N$.

Since the coefficient functions are periodic with period L , we have

$$f_k(x) = \sum_{j=-\infty}^{\infty} \hat{f}_{k,j} e^{i2\pi jx/L}, \quad k = 0, \dots, M, \quad (5)$$

with

$$\hat{f}_{k,j} = \frac{1}{L} \int_{-L/2}^{L/2} f_k(x) e^{-i2\pi jx/L} dx, \quad k = 0, \dots, M, \quad j \in \mathbb{Z}, \quad (6)$$

where i denotes the imaginary unit.

2. **Represent the eigenfunctions using Floquet theory.** The eigenfunctions are by definition bounded. It follows from Floquet theory that they may be represented as

$$\psi(x) = e^{i\mu x} \sum_{j=-\infty}^{\infty} \hat{\psi}_j e^{i\pi jx/L} = \sum_{j=-\infty}^{\infty} \hat{\psi}_j e^{ix(\mu + \pi j/L)}, \quad (7)$$

for some set of (possibly complex-valued) coefficients $(\dots, \hat{\psi}_{-1}, \hat{\psi}_0, \hat{\psi}_1, \dots)$. Here μ is the Floquet exponent,

$$\mu \in (-\pi/2L, \pi/2L]. \quad (8)$$

A complete justification of the representation (7) is given in [8].

3. **Construct the bi-infinite Floquet-Fourier difference equation.** Next, (7) is substituted in (2) using (5). An overall factor $e^{i\mu x}$ is eliminated, and the n th Fourier coefficient the left- and right-hand sides of the remaining expression are equated. This results in a bi-infinite difference equation

$$\hat{\mathcal{L}}(\mu)\hat{\psi} = \lambda\hat{\psi}, \quad (9)$$

with $\hat{\psi} = (\dots, \hat{\psi}_{-2}, \hat{\psi}_{-1}, \hat{\psi}_0, \hat{\psi}_1, \hat{\psi}_2, \dots)^T$ and where the μ -dependence of $\hat{\mathcal{L}}$ is explicitly indicated. The entries of the bi-infinite matrix $\hat{\mathcal{L}}(\mu)$ are given by

$$\hat{\mathcal{L}}(\mu)_{nm} = \begin{cases} 0 & \text{if } n - m \text{ is odd,} \\ \sum_{k=0}^M \hat{f}_{k, \frac{n-m}{2}} [i(\mu + \frac{\pi m}{L})]^k & \text{if } n - m \text{ is even.} \end{cases} \quad (10)$$

Note that no approximations were introduced to obtain the difference equation (9). Thus (9) is *equivalent* to the original problem (2).

4. **Truncate the difference equation.** At this point, the difference equation (9) is truncated, so that only N Fourier modes ($N > 0$) of the eigenfunctions are kept, in addition to the zero mode:

$$\hat{\psi}_N = (\hat{\psi}_{-N}, \dots, \hat{\psi}_{-2}, \hat{\psi}_{-1}, \hat{\psi}_0, \hat{\psi}_1, \hat{\psi}_2, \dots, \hat{\psi}_N)^T \quad (11)$$

This is the only approximation in the application of Hill's method. As a result, (9) is now reduced to a matrix eigenvalue-eigenvector problem, of dimension $(2N + 1) \times (2N + 1)$:

$$\hat{\mathcal{L}}_N(\mu)\hat{\psi}_N = \lambda_N\hat{\psi}_N, \quad (12)$$

where the eigenvalues λ_N are approximations to elements of the spectrum of \mathcal{L} , in the sense that all $\lambda_N \in \sigma(\hat{\mathcal{L}}_N(\mu)) \rightarrow \lambda \in \sigma(\mathcal{L})$ as $N \rightarrow \infty$. Similarly, for any fixed μ , the knowledge of the eigenvectors $\hat{\psi}_N$ allows for the reconstruction of an approximation to the eigenfunction $\psi(x)$, using (7).

5. **Determine the eigenvalues.** Using the QR algorithm (see *e.g.* [24]), the eigenvalue problem (12) is solved numerically, for any given $\mu \in (-\pi/2L, \pi/2L]$.

In summary, the application of Hill's method to compute an approximation of the spectrum of a one-dimensional linear operator requires three pieces of input: (i) the linear operator, specified by its coefficient functions $(f_0(x), \dots, f_M(x))$, (ii) the number N determining the dimension of the eigenvalue problem (12), and (iii) the number D of equally-spaced μ values in $(-\pi/2L, \pi/2L]$ for which (12) is constructed.

Remarks

- **Function space:** Typical eigenfunctions of the form (7) are quasi-periodic due to the presence of two typically non-commensurate periods $2L$ and $2\pi/\mu$. Nevertheless, the eigenfunctions are square-integrable on $[-L, L]$, since the $2\pi/\mu$ -periodicity disappears from the integration:

$$\frac{1}{2L} \int_{-L}^L |\psi|^2 dx = \sum_{j=-\infty}^{\infty} |\hat{\psi}_j|^2 < \infty.$$

In addition, all these eigenfunctions are bounded on the real line.

- **Different periods:** In [8] a more general form of the eigenfunctions (7) was used, with the period of the sum being PL , for some integer P . In doing so, the case $\mu = 0$ results in eigenfunctions that are periodic with period PL . Here we are restricting ourselves to $P = 2$, which is advantageous from a computational point of view as discussed in [8]. Further, in the important case of self-adjoint second-order operators, this results in the eigenfunctions with $\mu = 0$ corresponding to the edge points of the bands of the spectrum [19].
- **Boundary conditions:** These can be made more explicit at this point. The eigenfunctions satisfy

$$\psi(x + 2L) = e^{2i\mu L} \psi(x),$$

which follows from (7) immediately. Such boundary conditions are known as Bloch boundary conditions [2]. Due to the attention devoted to second-order self-adjoint problems, it has been customary to focus especially on periodic (with period L) and anti-periodic (with period $2L$) eigenfunctions, which correspond to $\mu = 0$. This results in only a discrete subset of the spectrum we wish to capture. By considering eigenfunctions of larger periods (for instance by choosing $P > 2$), a larger discrete subset is found. As the period of the eigenfunctions approaches infinity, an increasingly larger discrete subset of the spectrum we consider is found. That spectrum may be obtained as the limit spectrum of these discrete spectra, for sequences of eigenfunctions with increasing periods. The linear operator \mathcal{L} with these boundary conditions is referred to as the maximal extension [16] of L . In contrast, our approach is to compute the spectrum of L for a variety of μ values.

- **Problems defined on the whole line:** Problems with *bounded coefficients that are not periodic*, but are instead defined on all of \mathbb{R} may be treated effectively by considering them as the limit of periodic problems with increasing period. This was illustrated for the quantum harmonic oscillator in [8]. A research-level problem with such boundary conditions is found in [9].
- **Vector problems:** If \mathcal{L} is a square matrix of size $M \times M$ with elements that are scalar linear operators, approximate solutions to the equation (2) and thus an approximation to

$\sigma(\mathcal{L})$ may be found by using Hill’s method as well. To this end, the bi-infinite Floquet-Fourier difference equation is replaced by an $M \times M$ block matrix eigenvalue problem, where every block is bi-infinite and contains the Floquet-Fourier difference equation of the corresponding scalar linear operator. A finite-dimensional eigenvalue problem of size $M(2N + 1) \times M(2N + 1)$ is obtained by imposing a modal truncation with N modes, as before.

4 SpectrUW

Hill’s method is algorithmic and implemented in our black-box package for the computation of spectra of linear operators. SpectrUW (pronounced “spectrum”) is such a package. It is being developed in the Department of Applied Mathematics at the University of Washington with assistance from the Mathematics Department at Seattle University. This section describes SpectrUW and its features.

SpectrUW is written in Java, and can be used on any platform. Although the user only interacts with the Java interface, the software requires the presence of either Maple (version 9.5 or higher) or Mathematica (version 5.0 or higher) on the user’s machine, as the internal calculations are done in one of these software packages.

Remarks

- We have not built an implementation of SpectrUW which calls on Matlab, because a number of the calculations require symbolic manipulation at a level that is not conveniently done with Matlab.
- For typical examples, we have found that choosing Mathematica as the computational engine is a factor of 4-6 faster than choosing Maple.
- We intend to incorporate two- and three-dimensional eigenvalue problems as a future extension.
- To our knowledge, no other software packages exist that compute spectra of linear operators with the same combination of generality and user-friendliness of SpectrUW. Various researchers are using finite-difference codes that are easily adapted to different problems, but no user-friendly package exists that we are aware of. Finite-difference methods are compared with Hill’s method in [8]. Hill’s method itself is used as the algorithm for BandSolve [11]. BandSolve is used to solve the linear Schrödinger equation by using Bloch theory, as in solid state physics [2]. Using the Floquet parameter as a continuation parameter, Rademacher *et al.* [23] have an algorithm which compares well with Hill’s method in terms of speed and accuracy. However, they have not developed a general package: using their algorithm requires the user to implement it in AUTO [15].

4.1 Installation

SpectrUW is freeware and may be downloaded from

<http://www.amath.washington.edu/hill/spectruw.html>.

Self-extracting installations for Mac, Linux and Windows platforms are available.

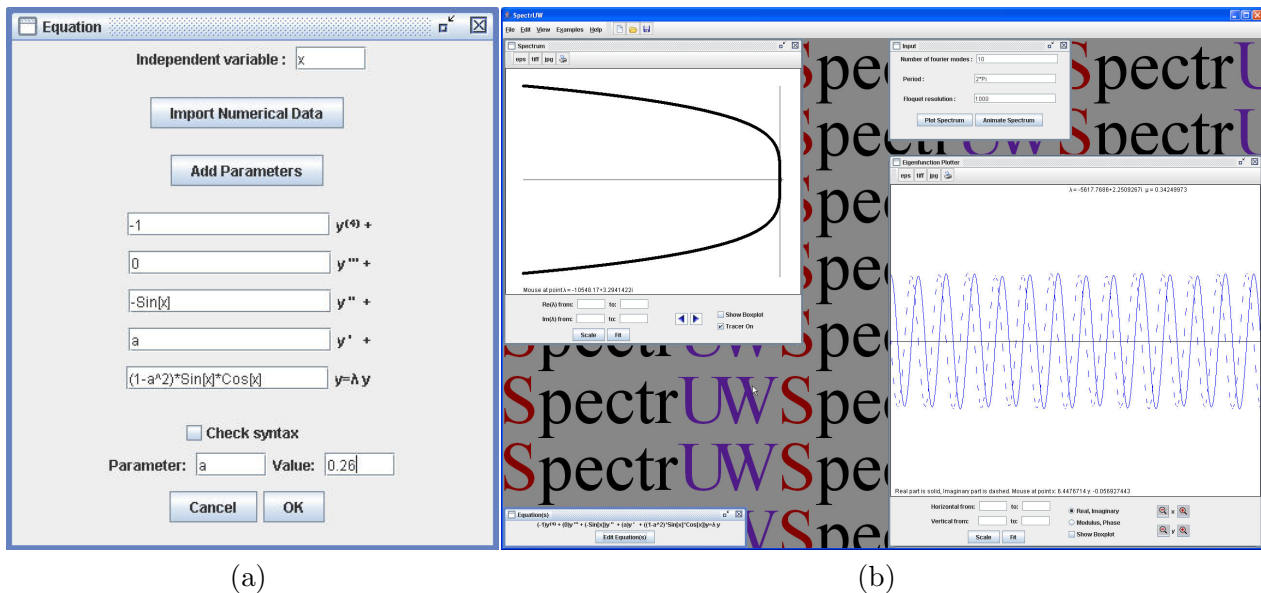


Figure 1: (a) A screen capture of the input (using Mathematica syntax) of the scalar linear eigenvalue problem $-y'''' - y'' \sin x + ay' + (1 - a^2)y \sin x \cos x = \lambda y$, with parameter value $a = 0.26$. (b) The SpectrUW desktop, displaying the spectrum window (upper left), the eigenfunction window (lower right), the equation panel (lower left; hard to read at this resolution), and the numerical settings panel (upper right).

4.2 Input

1. Once installed, SpectrUW is started by double-clicking its desktop icon. The first choice the user is prompted to make is whether to use Maple or Mathematica as the computational kernel. This choice can only be altered by exiting SpectrUW and restarting it.
2. The second choice is whether the user wants to examine a scalar or a vector problem. For vector problems, the vector size is entered at this point.
3. The third choice is that of which linear operator to study. This is done by (i) specifying the order of the operator, and (ii) entering the functional forms of the coefficient functions, using either Maple or Mathematica syntax. This is the only point in the use of SpectrUW where the user is required to be familiar with Maple or Mathematica syntax. For vector problems, this process has to be repeated for every scalar operator in the square matrix \mathcal{L} . If the linear operator depends on any parameters, they may be entered at this point. An input window for a scalar operator is shown in Fig. 1a. In the case that one or more of the coefficient functions are only available numerically, a data file may be uploaded for each such function. This data file contains either a discrete sampling of the coefficient function, or else a list of Fourier coefficients.
4. The last choices remaining are those for Hill's method: the model truncation number N and the number D of equally-spaced Floquet exponents to consider. The truncation number N should be chosen so that the coefficient functions are well represented using a Fourier series with N modes. Clicking "plot spectrum" proceeds to use Hill's method to compute the spectrum and the associated eigenfunctions. The time required for this computation increases linearly with N^3 (due to the use of the QR algorithm) and D .

Alternatively, if one or more parameters are present, the user can click "animate spectrum", which uses Hill's method to compute a range of spectra for a equispaced sequence of chosen

parameter values.

4.3 Computation

During the computation, SpectrUW is minimized and a “busy” indicator is shown at the bottom of the screen.

4.4 Output

Single spectrum

Once the computation is finished, the user is returned to the SpectrUW desktop, shown in Fig. 1b, where one of the windows displays the location of the spectrum in the complex plane. By using the mouse or by specifying plot ranges, the user can zoom in on any part of the spectrum. All points plotted are the result of a computation. No interpolation is done on any part of the spectrum. Clicking on any point of the spectrum displays the eigenfunction constructed from the Fourier series with N modes in a separate window. All plots and data sequences can be saved for future use or for inclusion in reports.

Spectrum animations

The main window on this desktop is the animation window. The user can run the animation, display all spectra combined (color coded by parameter value), or display the positive real parts of the spectrum as a function of the parameter (for stability problems the positive real part indicates unstable growth). By using the mouse or by specifying plot ranges, the user can zoom in on any part of these figures. All points plotted are the result of a computation. No interpolation is done on any part of the spectrum. All animations, plots and data sequences can be saved for future use or for inclusion in reports

5 Examples

In this section, we describe how SpectrUW may be used as a laboratory for the numerical exploration of spectra of linear operators. Specifically, we study two examples that are presumably not exactly solvable. We show how the use of SpectrUW allows us to (i) understand the structure of the spectrum and its associated eigenfunctions, and (ii) formulate precise statements about the nature of the spectrum, which may be the starting point for a verification using perturbative or other methods.

A scalar example

The first example is

$$-y'''' - y'' \sin x + ay' + (1 - a^2) \sin x \cos x y = \lambda y, \quad (13)$$

where a is a parameter. In Fig. 2, six successive zooms of the spectrum of (13) are shown, for $a = 0.26$. This numerical experiment took 98 seconds using the Mathematica kernel on a 3GHz processor machine with 2GB memory, running Windows XP Professional. The numerical parameters used in Fig. 2 are $N = 10$ and $D = 1000$. This large number of Floquet exponents is the reason for the near-continuous appearance of the spectrum. Only the last two panels show the discreteness of the approximation. More points may be computed by considering even more Floquet exponents, *i.e.*, a larger value of D . Once the spectrum is computed, simple mouse

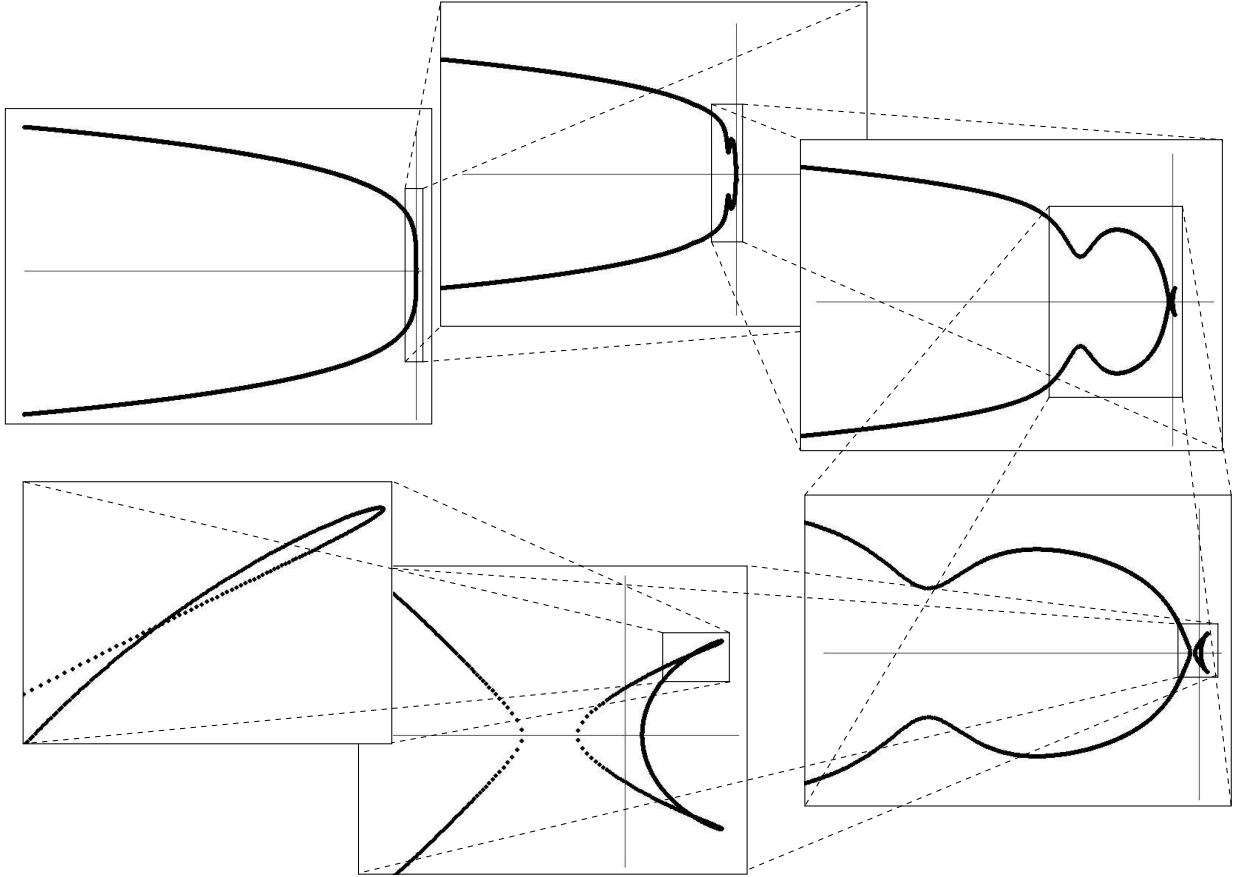


Figure 2: Six successive zoom-ins of the spectrum corresponding to (13) with $a = 0.26$. The zoom sequence starts with the upper-left panel and ends with the lower-left one. The horizontal and vertical axes are the real and imaginary axes of the complex λ plane.

controls allow the user to explore specific regions of the spectrum by zooming in, or to explore eigenfunctions by panning over the spectrum.

By letting the parameter a vary, changes in the spectral structure may be observed by using the animation feature. Such animations are viewed using the built-in animation panel. They may be saved as animated .gif files. As discussed before, two other options are available. Figure 3a displays all spectra for different a -values. Different colors correspond to different values of a , shown using gray scale here. Lastly, if (13) may be interpreted as a linear stability problem, Fig. 3b shows the unstable growth rates as a function of the parameter a . It follows from this that larger values of a result in lower growth rates, but instabilities are present for all values of $a \in [0, 1]$. The nature of these instabilities could be examined by investigating the eigenfunctions corresponding to the spectral elements with positive real part.

A vector example

The second example is

$$\begin{pmatrix} \sqrt{B(B+V_0)} \sin(2x) & -\frac{1}{2} \partial_x^2 - \frac{1}{2} + (B+V_0)(1 - \cos(2x)) \\ \frac{1}{2} \partial_x^2 + \frac{1}{2} - B(1 + \cos(2x)) & -\sqrt{B(B+V_0)} \sin(2x) \end{pmatrix} \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix} = \lambda \begin{pmatrix} \varphi_1 \\ \varphi_2 \end{pmatrix}. \quad (14)$$

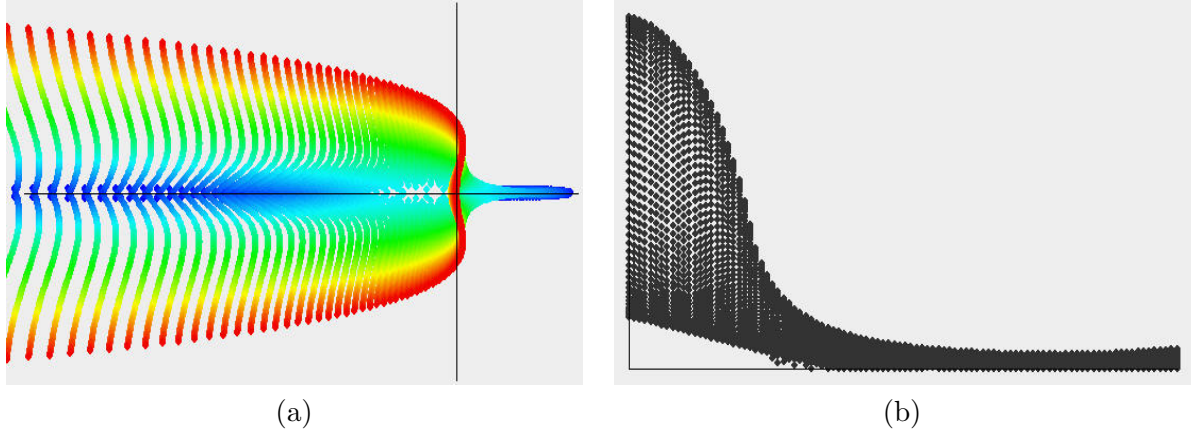


Figure 3: (a) All spectra corresponding to (13) for 100 equally spaced values of a in $[0, 1]$, shown in different gray scales. The region $\text{Re}\lambda \in [-1, 0.2]$ (horizontal axis), $\text{Im}\lambda \in [-1, 1]$ (vertical axis) is shown. (b) The unstable growth rates (vertical axis) corresponding to (13) for these same a values (vertical axis). The region $(\text{Re}\lambda, a) \in [0, 0.2] \times [0, 1]$ is shown.

Here V_0 and B are positive parameters. This is the linear stability problem for the solution

$$\psi = e^{-(1/2+B)t} \left(\sqrt{B} \cos x + i\sqrt{B-V_0} \sin x \right) \quad (15)$$

of the Gross-Pitaevskii equation with optical lattice potential

$$i\psi_t = -\frac{1}{2}\psi_{xx} + |\psi|^2\psi - \psi V_0 \sin^2 x. \quad (16)$$

This equation describes the dynamics of a repulsive Bose-Einstein condensate in an external optical lattice potential. As a result of direct numerical simulations on (16), it was conjectured in [4, 5] that this solution with $V_0 = 1$ is unstable for $B < 1/2$, but stable for $B > 1$. We reexamine this problem here, by considering (14) with $V_0 = 1$, but for a variety of B values, ranging from 0 to 1, using SpectrUW's animation feature. Different panels of this animation are shown in Fig. 4. Based on this animation (and zooms of individual panels) it appears that the transition from unstable solutions (the spectrum has a component with positive real part) to spectrally stable solutions (no spectral elements with positive real part) occurs in the B -interval $[0.96, 0.97]$, confirming the statements made in [4, 5].

6 Summary

We have presented SpectrUW, a software package for the numerical computation of spectra of linear operators using Hill's method [8]. The package may be used to examine specific problems originating from stability analysis, or other applications of spectral theory. In addition, it provides a convenient and efficient numerical laboratory to investigate spectra of linear operators and build up intuition about their behavior.

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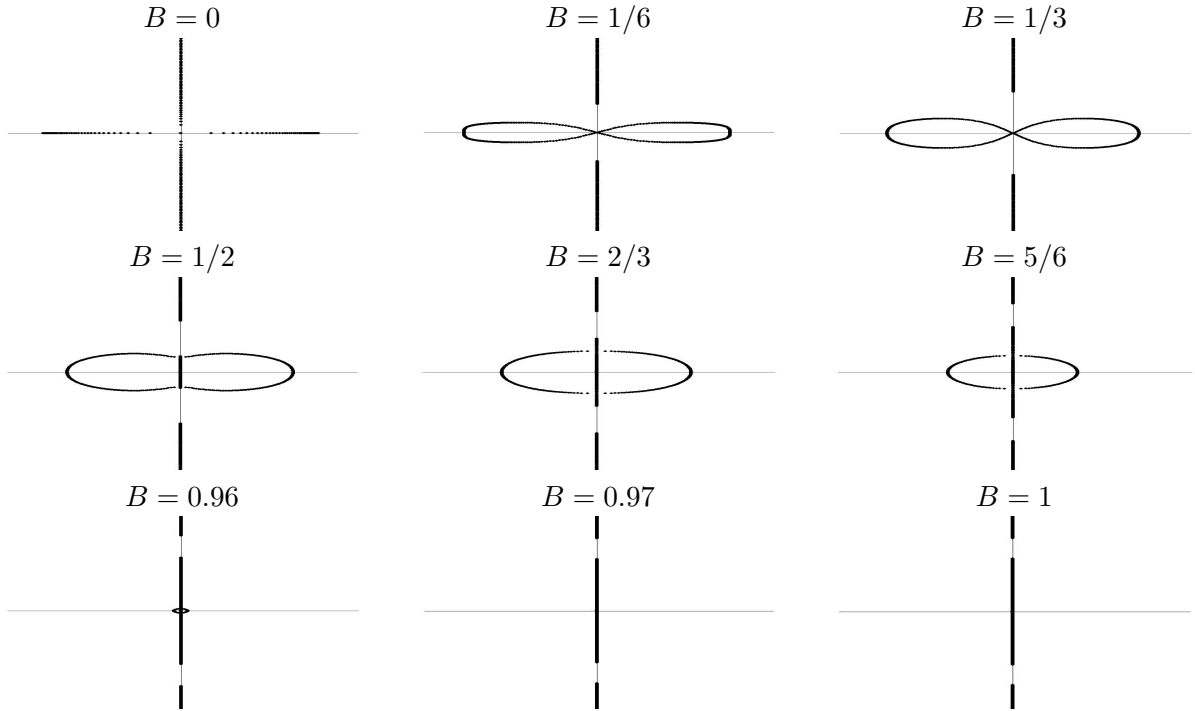


Figure 4: Nine panels of an animation of the spectrum of (14) with $V_0 = 1$. For all panels, $\text{Re}\lambda \in [-1/2, 1/2]$ (horizontal axis) and $\text{Im}\lambda \in [-1, 1]$ (vertical axis). This allows us to establish that the transition from unstable to stable solutions occurs for $B \in (0.96, 0.97)$.

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