Numerical Methods 2: Hill's Method

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1 Introduction and motivation

In this talk, I will discuss how to compute a numerical approximation to the spectrum of a linear operator with periodic coefficients. This is useful for several reasons. In the framework of this workshop, it tells us something about the spectral stability of periodic equilibrium solutions of partial differential equations.

Spectral stability

Consider the evolution system

$$\boldsymbol{u}_t = \boldsymbol{N}(\boldsymbol{u}). \qquad (*)$$

with an equilibrium solution $\boldsymbol{u}_e$:

$$\boldsymbol{N}(\boldsymbol{u}_e) = \boldsymbol{0}.$$

Is this solution stable or unstable? Start with linear stability analysis first: let

$$\boldsymbol{u} = \boldsymbol{u}_e + \boldsymbol{\epsilon\psi}.$$

Substitute in $(*)$ and retain first-order terms in $\boldsymbol{\epsilon}$:

$$\boldsymbol{\psi}_t = \boldsymbol{\mathcal{L}}[\boldsymbol{u}_e(\boldsymbol{x})]\boldsymbol{\psi}.$$

Separation of variables: $\psi(x,t) = e^{\lambda t}\phi(x)$:

$$\boxed{\mathcal{L}[u_e(x)]\phi = \lambda\phi.}$$

- This is a spectral problem.
- If $\Re(\lambda) \leq 0$ for all bounded $\phi(x)$, then u_e is spectrally stable.

2 Spectra of linear operators with periodic coefficients

Let's look at scalar problems in one spatial dimension:

Our starting point is

$$\mathcal{L}\phi = \lambda\phi,$$

with

$$\mathcal{L} = \sum_{k=0}^{M} f_k(x)\partial_x^k, \qquad f_k(x+L) = f_k(x).$$

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We wish to determine

- The spectrum $\sigma(\mathcal{L}) = \{\lambda \in \mathbb{C} : ||\phi|| < \infty\}$.
- For any $\lambda \in \sigma(\mathcal{L})$: what are the corresponding eigenfunctions $\phi(\lambda, x)$?

What space do the eigenfunctions live in? There are several natural options:

1. The eigenfunctions are periodic with the same period as the coefficients
2. The period of the eigenfunctions is an integer multiple of that of the coefficients
3. The eigenfunctions are bounded

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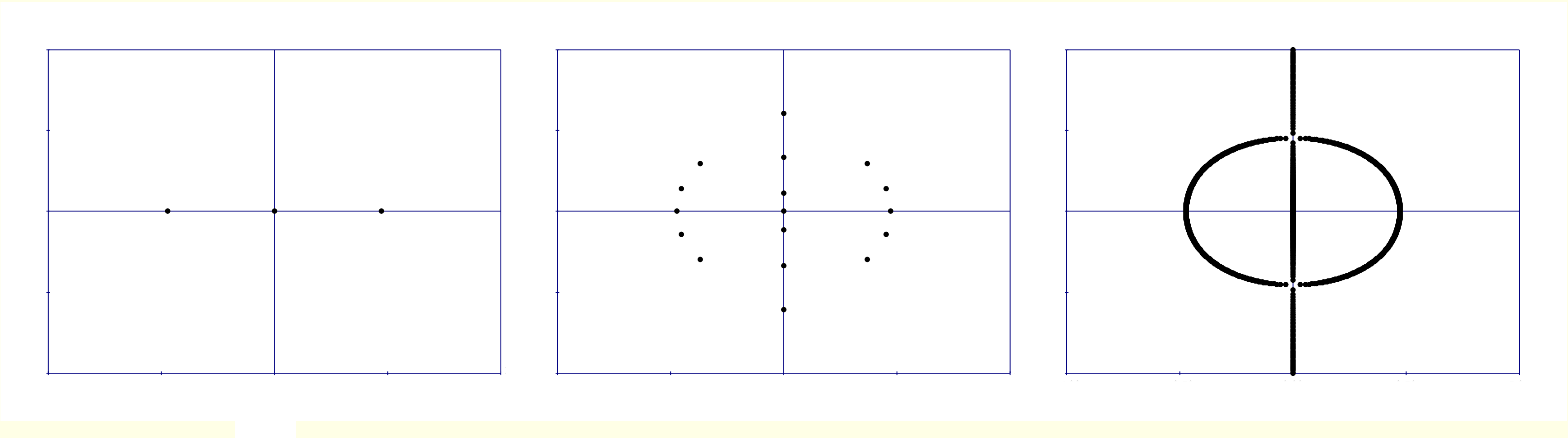

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- (1) or (2) are easy to do numerically, but are not always justified by the applications.
- All three approaches would lead us to conclude "instability" in the previous example. They do not always lead to the same conclusion.

3 Hill's method for scalar 1-D problems

Let's return to our original spectral problem:

$$\mathcal{L}\phi = \lambda\phi,$$

with

$$\mathcal{L} = \sum_{k=0}^{M} f_k(x)\partial_x^k, \qquad f_k(x+L) = f_k(x).$$

We have

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

with

$$\hat{f}_{k,j} = \frac{1}{L}\int_{-L/2}^{L/2} f_k(x)\, e^{-i2\pi jx/L}\, dx.$$

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Floquet's theorem: Consider

$$\boldsymbol{\phi_x = A(x)\phi, \quad A(x+L) = A(x).} \qquad (*)$$

Floquet's theorem states that the fundamental matrix $\boldsymbol{\Phi}$ for this system has the decomposition

$$\boldsymbol{\Phi(x) = P(x)e^{Rx}},$$

with $\boldsymbol{P(x+L) = P(x)}$ and $\boldsymbol{R}$ constant.

Conclusion: all bounded solutions of $(*)$ are of the form

$$\phi = e^{i\mu x} \sum_{j=-\infty}^{\infty} \hat{\phi}_j \, e^{i2\pi jx/L},$$

with $\mu \in [0, 2\pi/L)$.

Conclusion: all bounded solutions of $(*)$ are of the form

$$\boldsymbol{\phi = e^{i\mu x} \sum_{j=-\infty}^{\infty} \hat{\phi}_j \, e^{i2\pi jx/L},}$$

with $\boldsymbol{\mu \in [0, 2\pi/L)}$.

Thus the eigenfunctions are expanded as

$$\boldsymbol{\phi = e^{i\mu x} \sum_{j=-\infty}^{\infty} \hat{\phi}_j \, e^{i2\pi jx/PL},}$$

with $\boldsymbol{\mu \in [0, 2\pi/PL)}$

Next:

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This gives

$$\Rightarrow \qquad \boxed{\hat{\mathcal{L}}(\mu)\hat{\phi} = \lambda\hat{\phi}},$$

with $\hat{\phi} = (\cdots, \hat{\phi}_{-2}, \hat{\phi}_{-1}, \hat{\phi}_0, \hat{\phi}_1, \hat{\phi}_2, \cdots)^T$ and

$$\hat{\mathcal{L}}(\mu)_{nm} = \begin{cases} 0 & \text{if} \quad P \not| \, n-m \\ \displaystyle\sum_{k=0}^{M} \hat{f}_{k,\frac{n-m}{P}} \left[i\left(\mu + \frac{2\pi m}{PL}\right)\right]^k & \text{if} \quad P \mid n-m \end{cases}$$

More transparently:

$$\boldsymbol{f_k(x)\partial_x^k} \leftrightarrow \begin{pmatrix} * & & & * & & & * & & \\ & * & & & * & & & * & \\ & & * & & & * & & & * \\ * & & & * & & & * & & \\ & * & & & * & & & * & \\ & & * & & & * & & & * \\ * & & & * & & & * & & \\ & * & & & * & & & * & \\ & & * & & & * & & & * \end{pmatrix}$$

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with $P-1$ zero "diagonals" between any pair of successive non-zero "diagonals".

Note:
so far, no approximations have been made. At this point: **Cut off at N modes** $\longrightarrow (2N+1)\times(2N+1)$ matrix.

Algorithm:

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- Reconstruct eigenfunctions corresponding to eigenvalues

History

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4 Vector, Multi-D, whole-line or nonlocal problems

Vector problems

For vector problems

$$\mathcal{L}\phi = \lambda\phi,$$

where $\mathcal{L}$ is a matrix of linear operators, replace every matrix entry $\mathcal{L}_{ij}$ by $\hat{\mathcal{L}}_{ij}$

Multidimensional problems

- Expand the coefficient functions in a multidimensional Fourier series.
- Expand the eigenfunctions using Bloch theory. For instance, in 2-D:

$$\phi = e^{i\mu_1 x + i\mu_2 y} \sum_{j_1, j_2 = -\infty}^{\infty} \hat{\phi}_{j_1 j_2} \, e^{i2\pi j_1 x/P_1 L_1 + i2\pi j_2 x/P_2 L_2},$$

with $\mu_1 \in [0, 2\pi/P_1 L_1)$, $\mu_2 \in [0, 2\pi/P_2 L_2)$.

Whole-line problems

Note: this is not supposed to work... Let's push our luck!

- Restrict the coefficient functions to large period boxes.
- Proceed as before.
- Some bands will degenerate to isolated points (eigenvalues), so one may judge the accuracy of this limiting process.

Nonlocal problems

If the spectral problem contains convolutions

$$\int_{-\infty}^{\infty} R(x-y)\phi(y)dy,$$

or antiderivatives

$$\int_{a}^{x} \phi(y)dy,$$

these are easily incorporated to the Fourier-series based approach.

5 Examples

the return of the algorithm:

- Find Fourier coefficients of all functions
- Choose a number of $\boldsymbol{\mu}$ values $\boldsymbol{\mu_1, \mu_2, \ldots}$
- For all chosen $\boldsymbol{\mu}$ values, construct $\hat{\boldsymbol{\mathcal{L}}}_N(\boldsymbol{\mu})$
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5.1 The Mathieu equation

The Mathieu equation is

$$\boxed{-y'' + 2q\cos(2x)y = ay.}$$

We have: $\mathcal{L} = -\partial_x^2 + 2q\cos(2x)$, $L = \pi$, $M = 2$

$$\begin{aligned}
f_2(x) &= -1 & &\longrightarrow & \hat{f}_2 &= (-1),\\
f_1(x) &= 0 & &\longrightarrow & \hat{f}_1 &= (),\\
f_0(x) &= 2q\cos(2x) & &\longrightarrow & \hat{f}_0 &= (q, 0, q).
\end{aligned}$$

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\end{aligned}$$

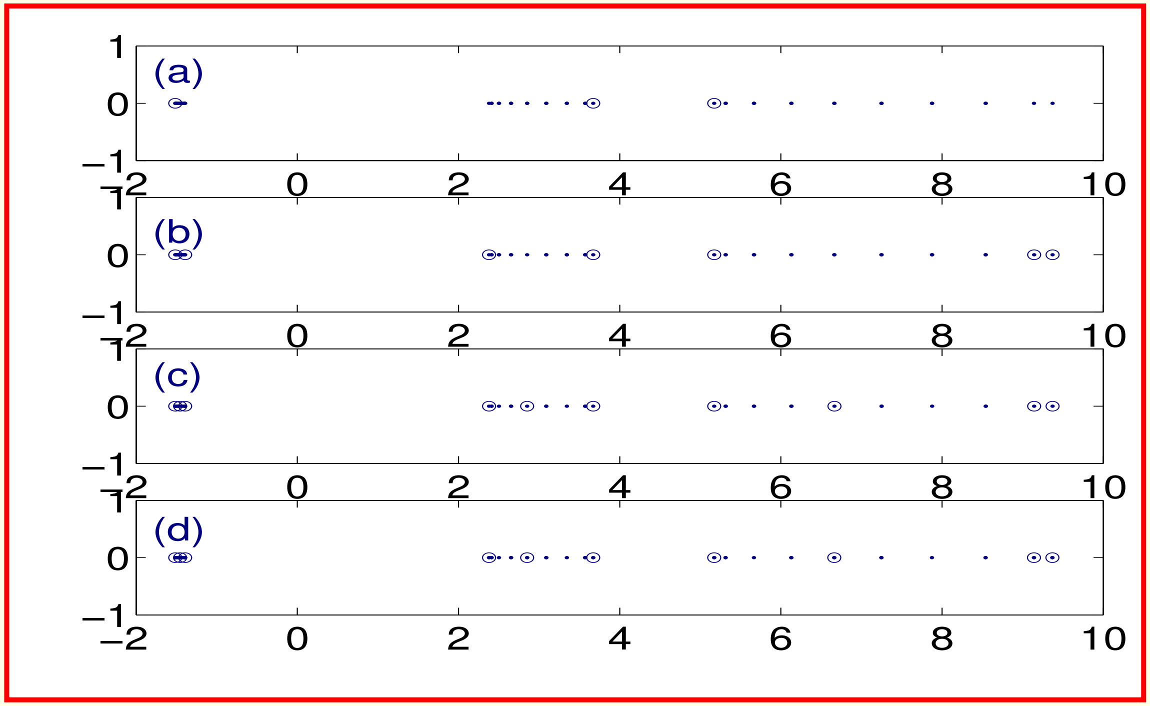
The Mathieu equation is equivalent to

$$\boxed{q\hat{\phi}_{n-P} + \left(\mu + \tfrac{2n}{P}\right)^2 \hat{\phi}_n + q\hat{\phi}_{n+P} = a\hat{\phi}_n, \quad n \in \mathbb{Z}.}$$

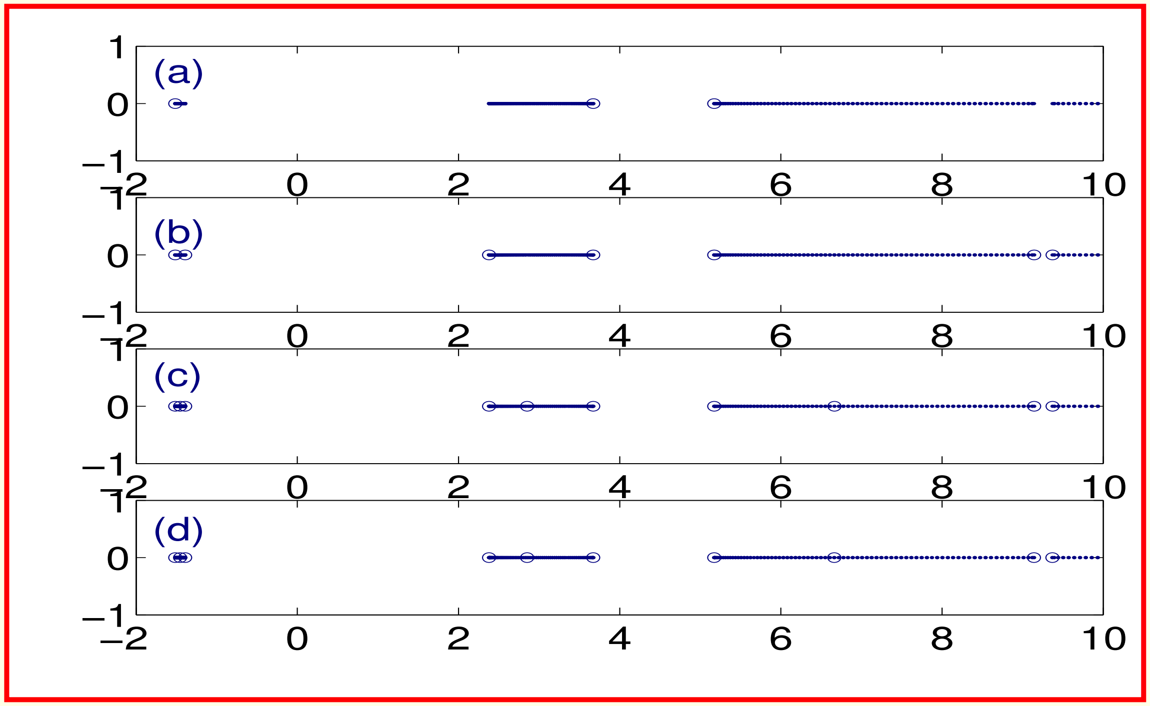
Truncation leads to the family of matrices

$$\begin{pmatrix}
(\mu - 2N/P)^2 & & q & & & & \\
& \cdots & & q & & & \\
q & & (\mu - 2/P)^2 & & \cdots & & \\
& q & & \mu^2 & & q & \\
& & \cdots & & (\mu + 2/P)^2 & & q \\
& & & q & & \cdots & \\
& & & & q & & (\mu + 2N/P)^2
\end{pmatrix},$$

of which the spectrum is computed for different μ values.



Numerical approximations of the spectrum for the Mathieu equation, using different values of the Floquet resolution.



The figures correspond to $\boldsymbol{P = 1}$, $\boldsymbol{P = 2}$, $\boldsymbol{P = 3}$, and Finite differences, 4th order

	Accuracy: 10^{-3}		Accuracy: 10^{-6}		Accuracy: 10^{-9}	
	Matrix size	CPU time	Matrix size	CPU time	Matrix size	CPU time
FFHM ($P = 1$)	5	0.5	7	0.6	9	0.5
FFHM ($P = 2$)	7	1	13	1	17	1
FFHM ($P = 4$)	9	1.5	25	2.6	33	3.3
FDM2	239	1075	8000	5.5E6	N/A	N/A
FDM4	52	25	293	1100	1630	1.5E5

Comparing the FDM (2nd and 4th order) and FFHM for computing the lowest eigenvalue $\tilde{a} \approx -1.513956885056448$ with $q = 2$. All CPU times are given relative to those of the FFHM with $P = 2$, which are $0.0004s$, $0.0007s$ and $0.0010s$, respectively.

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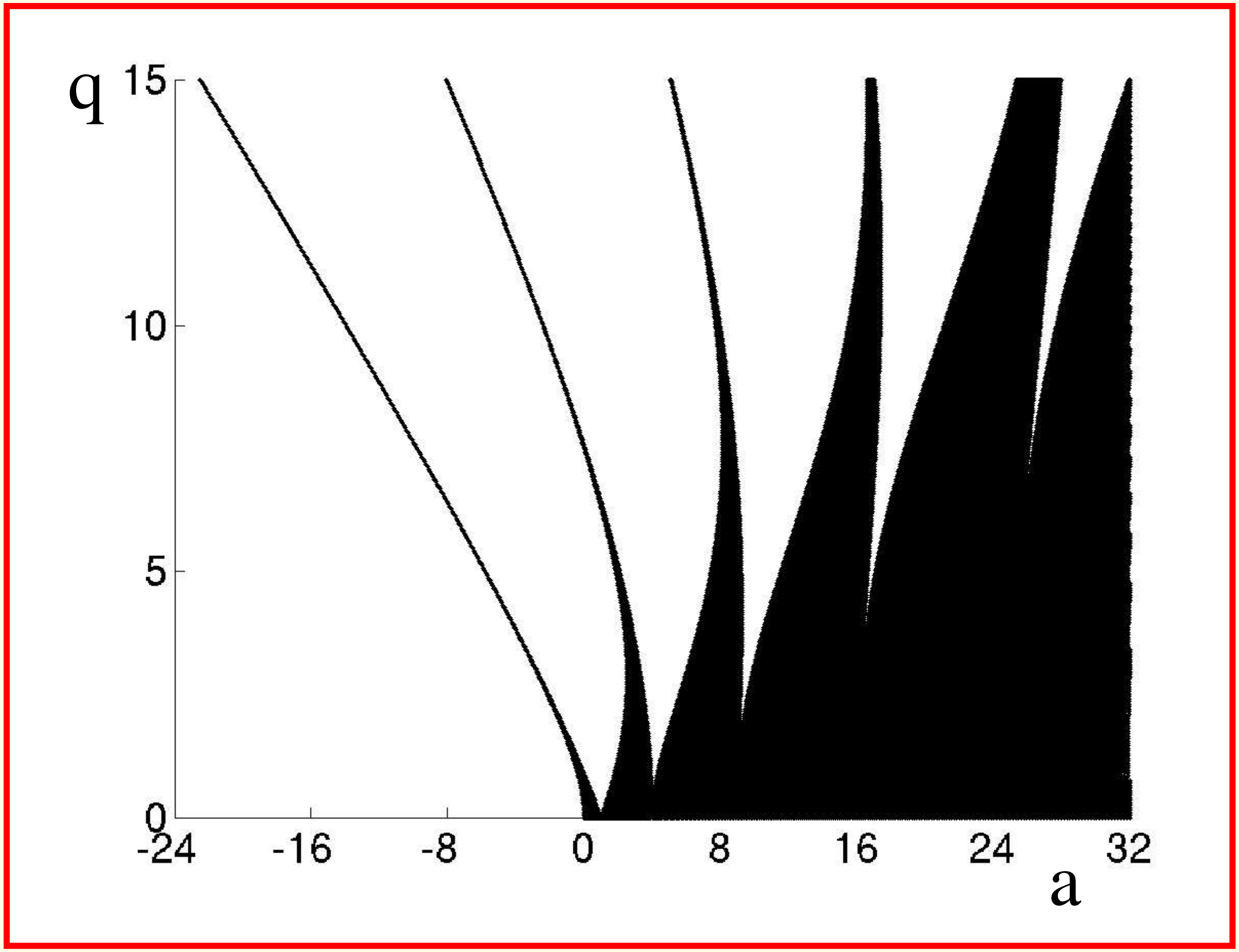
	$\delta_2 = 0.25$		$\delta_2 = 0.025$		$\delta_2 = 0.0025$	
	D	CPU time	D	CPU time	D	CPU time
FFHM ($P = 1$)	12	0.4	124	1	1190	1.3
FFHM ($P = 2$)	6	1	62	1	590	1
FFHM ($P = 4$)	3	2	31	1.3	295	1.3
FDM4 Matrix size=1172	1	5.4E5	N/A	N/A	N/A	N/A
FDM4, $D > 1$	4	8100	32	2100	310	1700

Comparing the FDM (4th order) and FFHM for computing a uniform approximation to the second spectral band with $q = 2$. All CPU times are given relative to those of the FFHM, with $P = 2$, which are $0.001s$, $0.03s$ and $0.35s$, respectively.



The spectrum of the Mathieu equation for varying values of q

5.2 Hill's equation with a finite number of gaps

Consider the two Hill equations

$$-u'' + \left(2k^2\mathrm{sn}^2(x,k) - k^2\right)u = \lambda u, \qquad \text{(a)}$$

$$-v'' + \left(6k^2\mathrm{sn}^2(x,k) - 4 - k^2\right)v = \lambda v. \qquad \text{(b)}$$

Here $\mathrm{sn}(x,k)$ is Jacobi's elliptic sine function.

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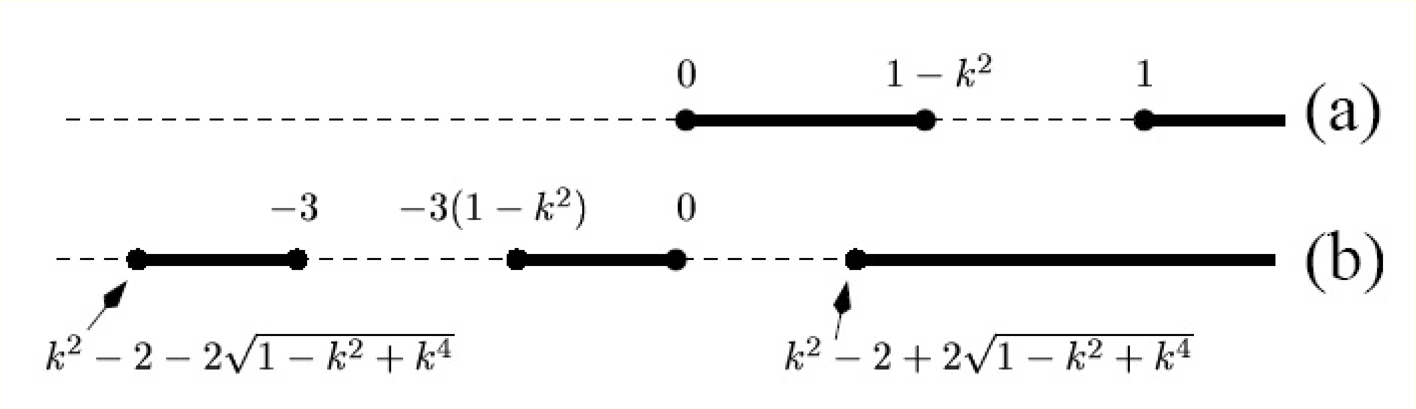
The spectra of these two equations are shown below.

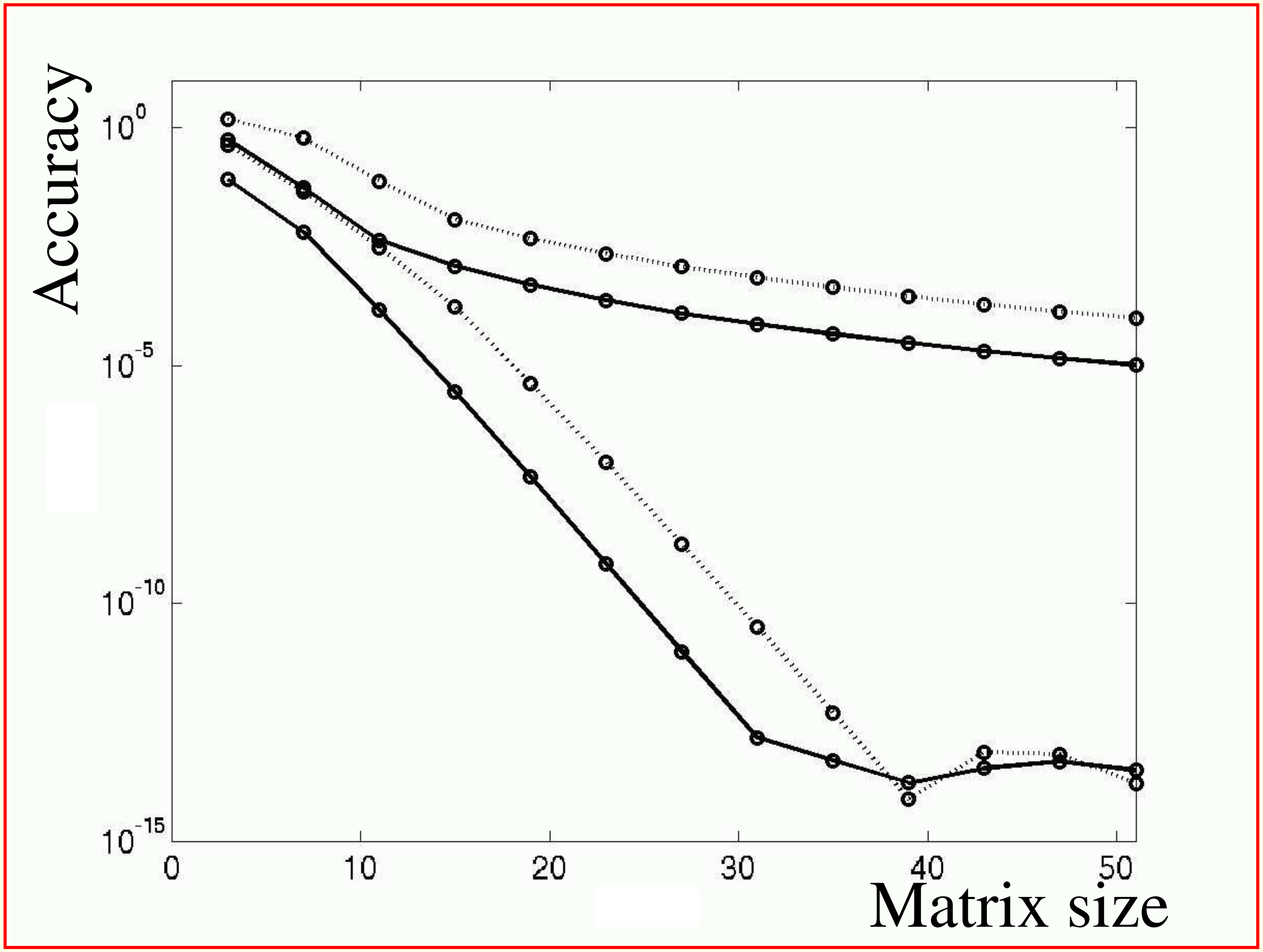


Then

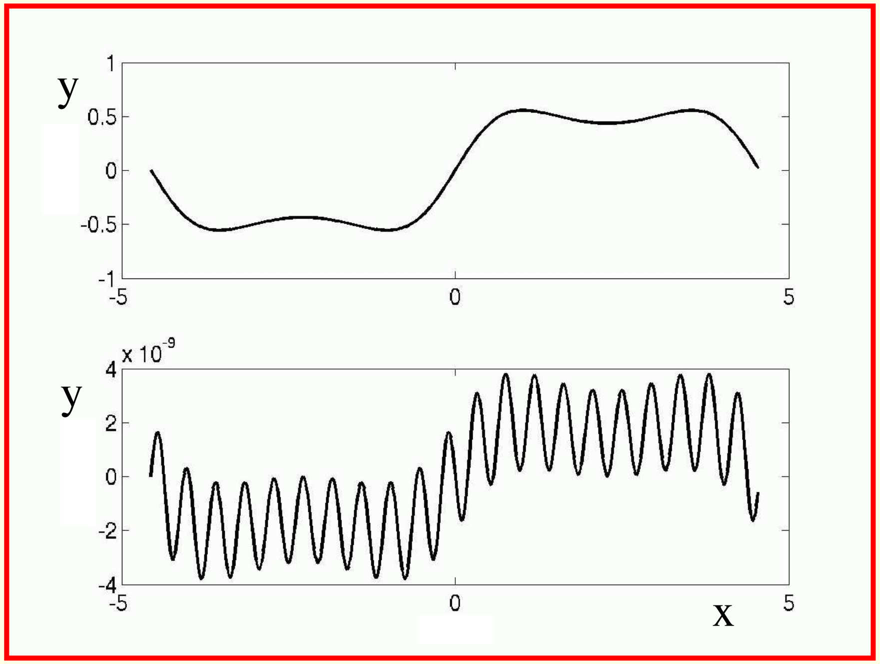
$$\begin{aligned}\mathrm{sn}^2(x,k) &= \frac{1}{k^2}\left(1-\frac{E(k)}{K(k)}\right)- \\ &\quad \frac{2\pi^2}{k^2K^2(k)}\sum_{n=1}^{\infty}\frac{nq^n}{1-q^{2n}}\cos\left(\frac{n\pi x}{K(k)}\right),\end{aligned}$$

with

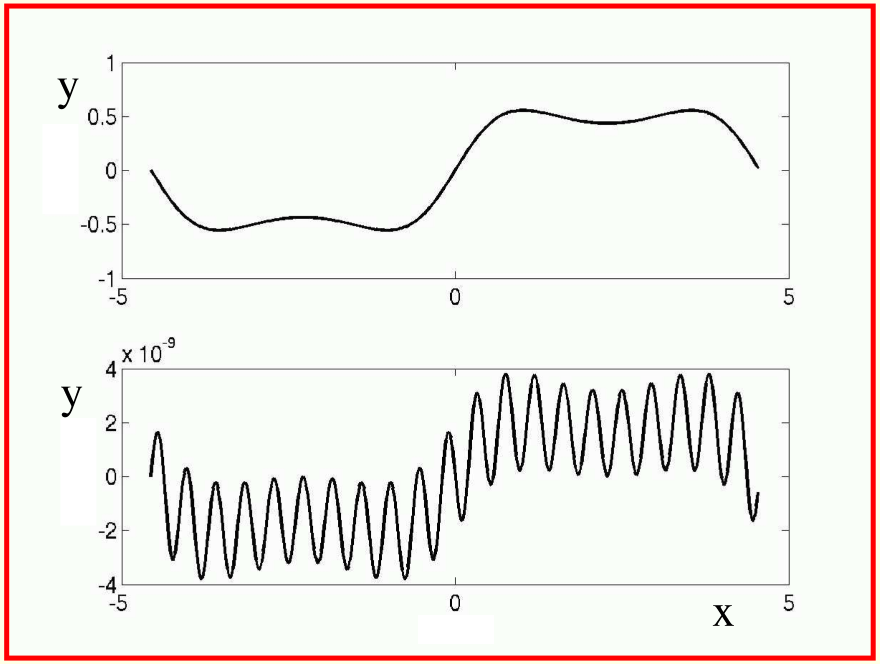
$$\left\{\begin{aligned} k' &= \sqrt{1-k^2}, \\ K(k) &= \int_0^{\pi/2}\left(1-k^2\sin^2 x\right)^{-1/2}dx, \\ E(k) &= \int_0^{\pi/2}\left(1-k^2\sin^2 x\right)^{1/2}dx, \\ q &= e^{-\pi K(k')/K(k)}. \end{aligned}\right.$$



The accuracy of Hill's method, compared to that of the 4th order finite-difference method.



The eigenfunction $\mathbf{sn}(x, k)\mathbf{dn}(x, k)$ of (b) with $k = 0.9$ and the pointwise error of its approximation.



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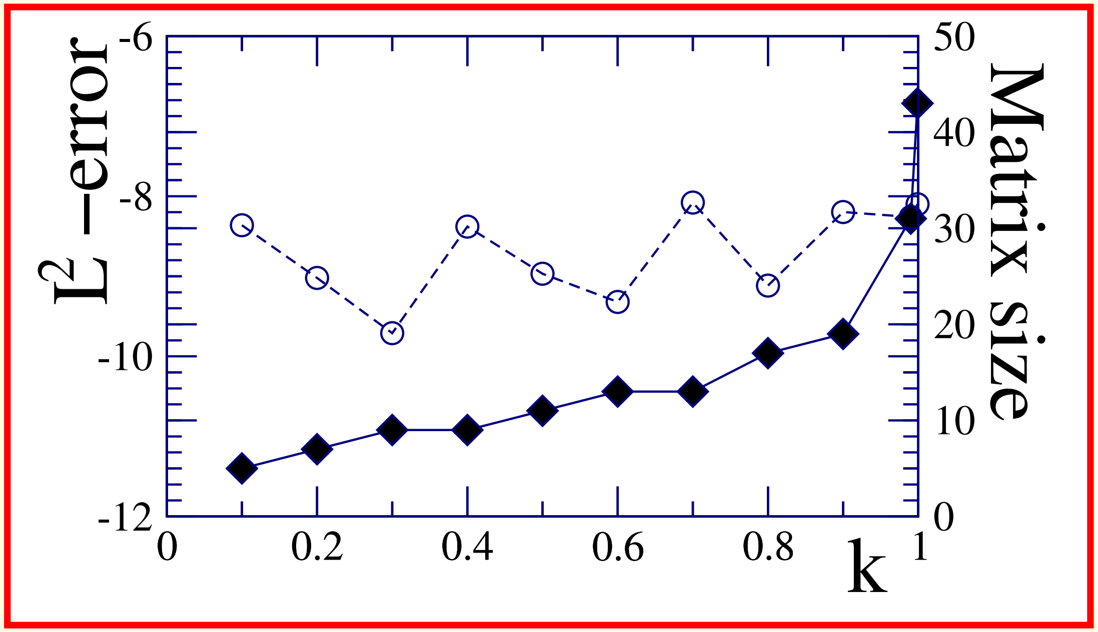


Matrix sizes required for sufficiently small L^2-error for varying k.

5.3 An example from Bose-Einstein condensates

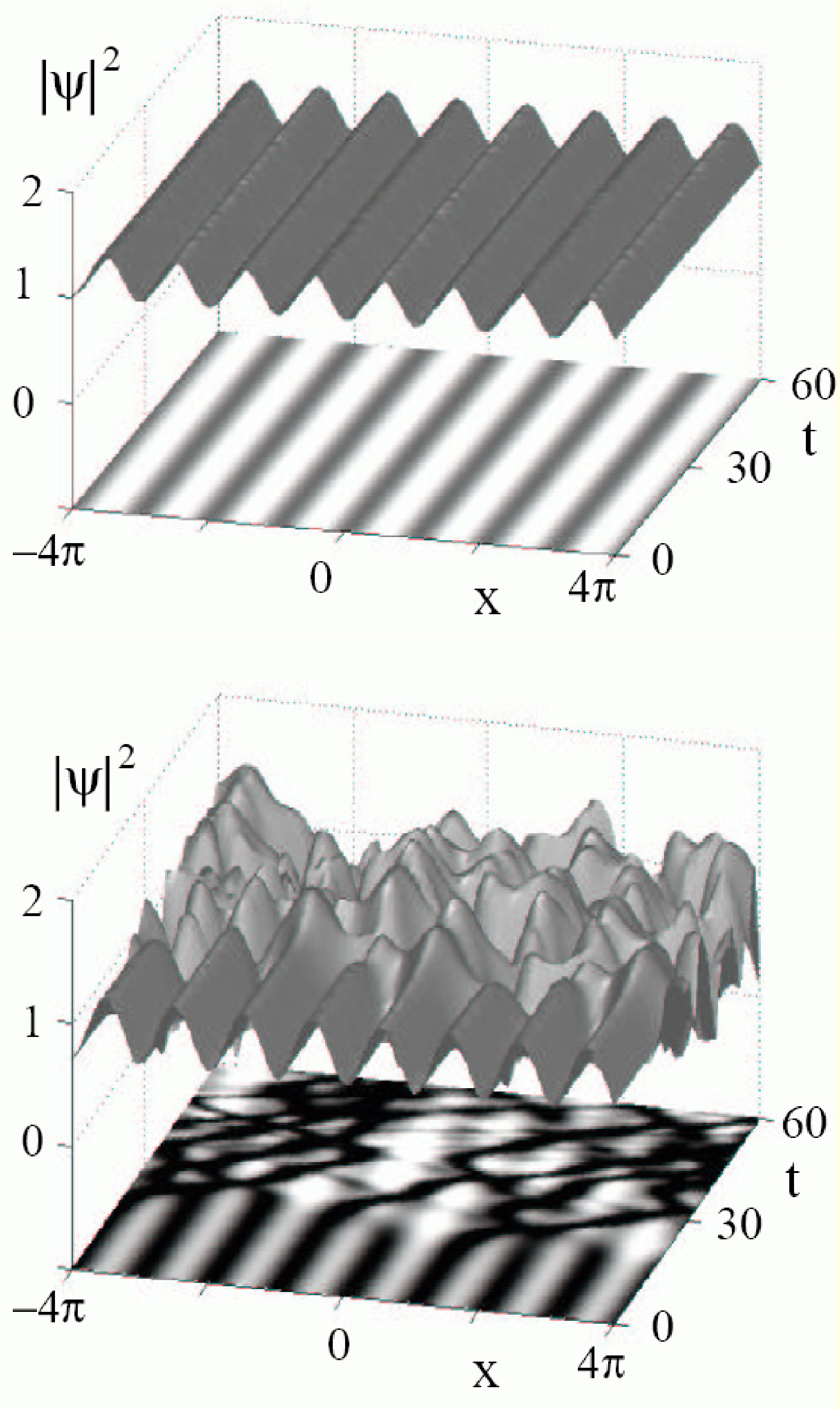
Consider

$$i\psi_t = -\tfrac{1}{2}\psi_{xx} + |\psi|^2\psi + \psi V_0 \sin^2 x.$$

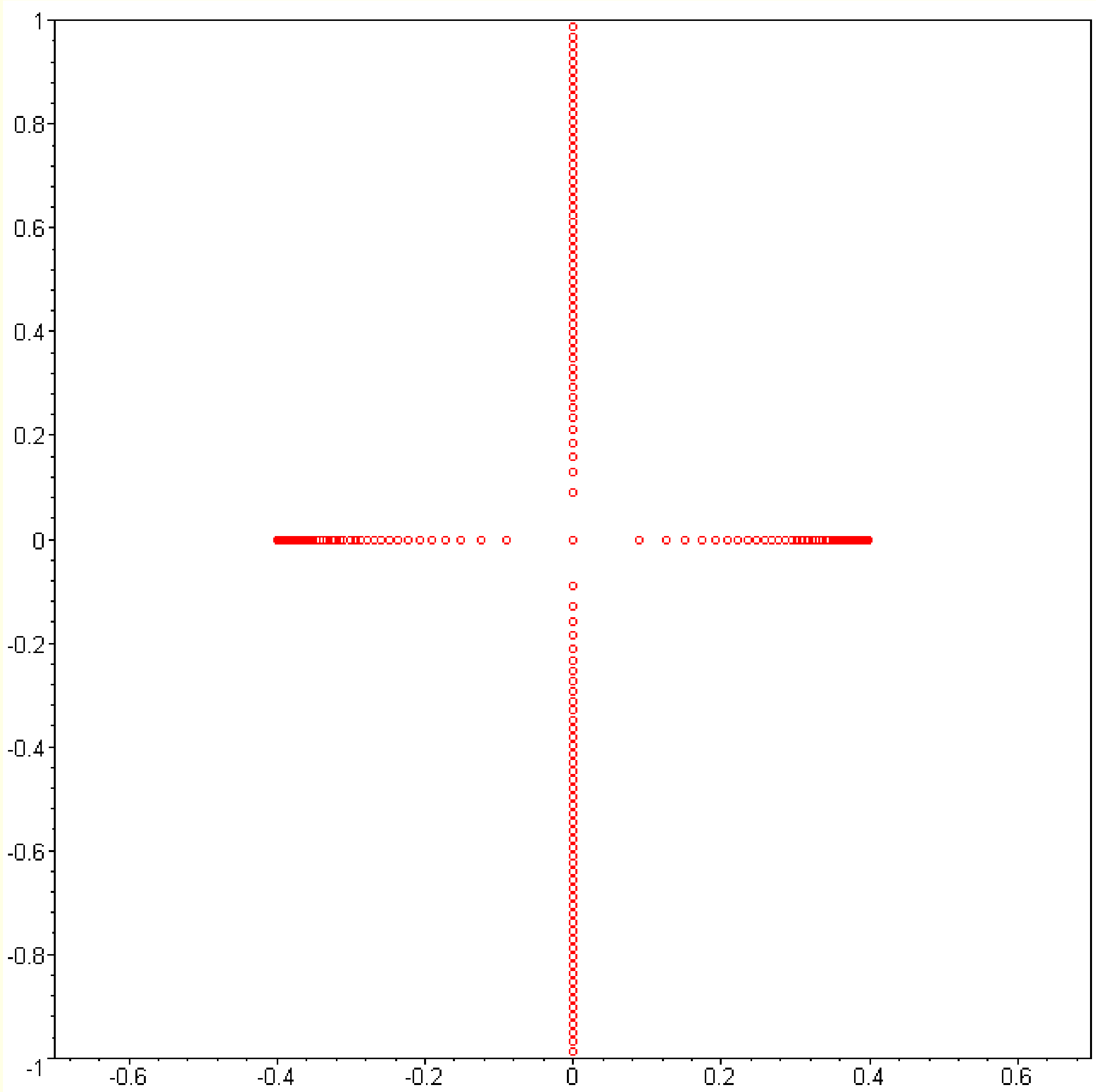
This equation has an exact solution

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

where B is a free parameter.



The dynamics of the exact solution $(*)$ with $\boldsymbol{V_0 = -1}$, $\boldsymbol{B = 1/2}$ (bottom) and $\boldsymbol{B = 1}$ (top). The top picture appears stable.



The spectra corresponding to the linear stability problem of the exact solution $(*)$ for varying $\boldsymbol{B}$ values: $\boldsymbol{B} \in [\mathbf{0}, \mathbf{1}]$.

5.4 A 2-D NLS equation periodic example

Consider

$$i\psi_t - \psi_{xx} + \psi_{yy} + 2|\psi|^2\psi = 0.$$

This equation has exact 1-D solutions of the form

$$\psi = \phi(x)e^{i\omega t} = k\,\mathrm{sn}(x, k)e^{i(1+k^2)t}.$$

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The linear stability problem is:

$$(\omega - 6\phi^2 + \rho^2 + \partial_x^2)U = \lambda V$$
$$-(\omega - 2\phi^2 + \rho^2 + \partial_x^2)V = \lambda U.$$

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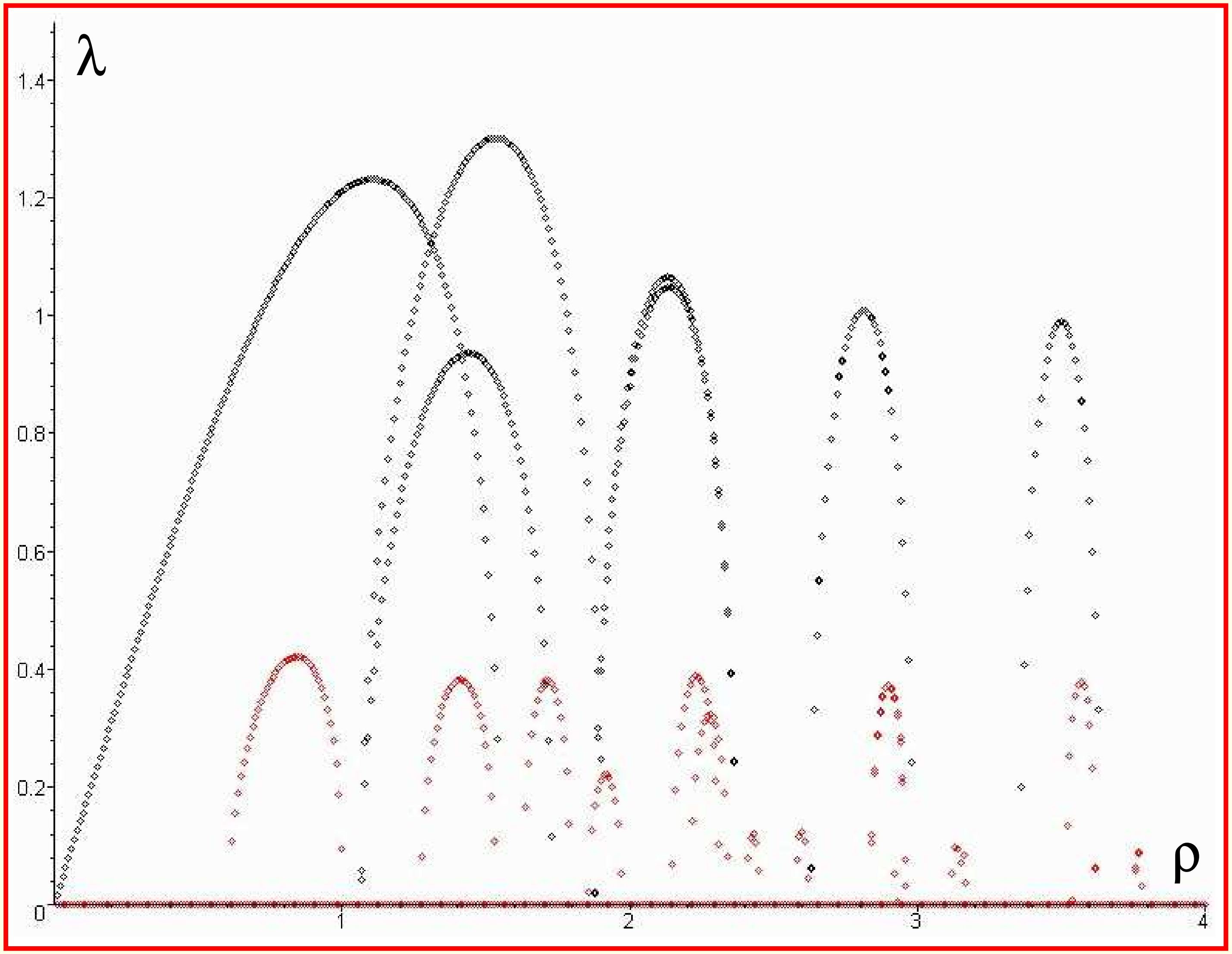
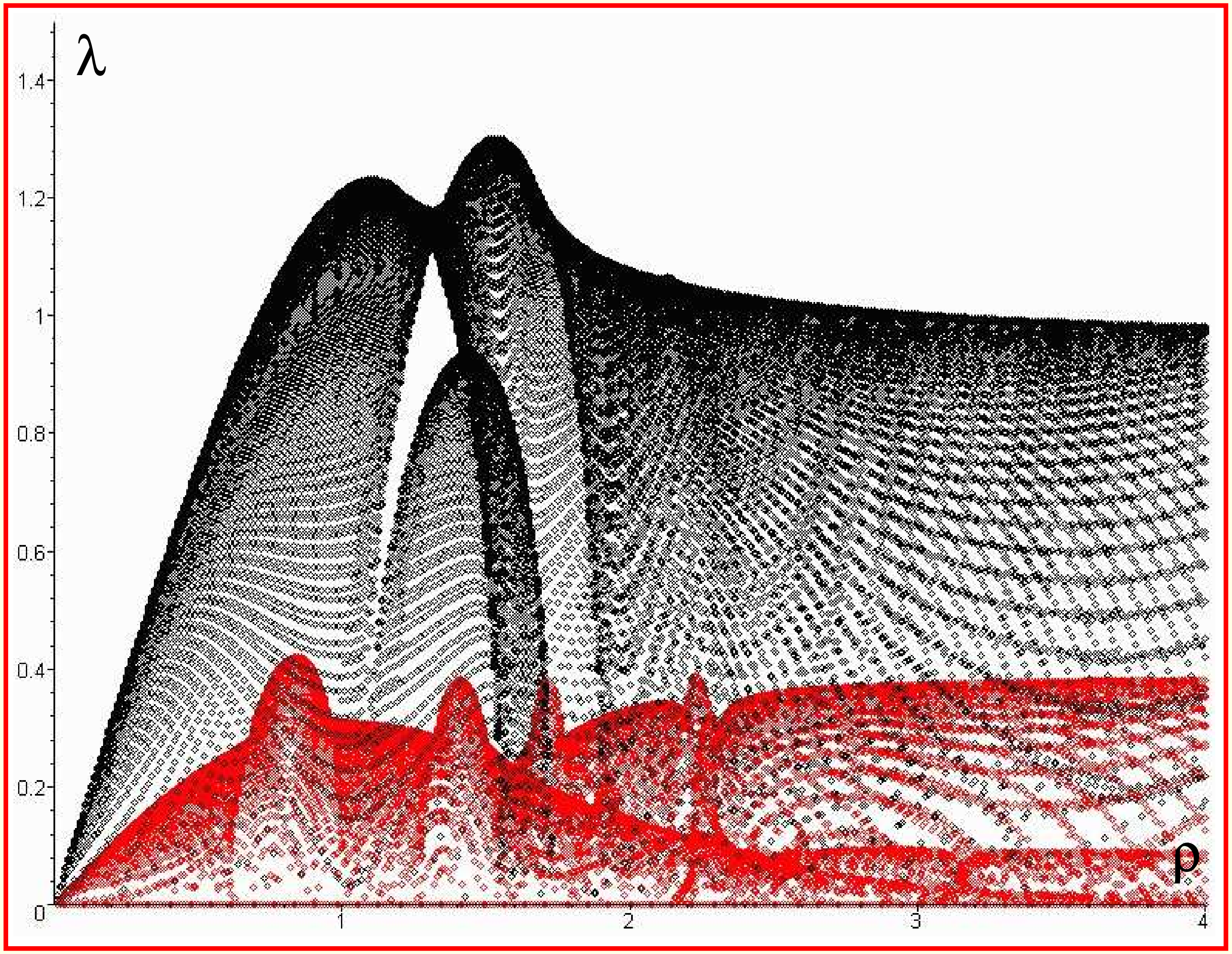
Thus: for a given value of k, compute spectra for a range of ρ values

In the literature, you may find graphs like ($\boldsymbol{k = \sqrt{0.8}}$):



Unstable eigenvalues for the linear stability problem of the $\mathbf{sn}$ solution, using periodic perturbations.

We can now compute "all" unstable modes:



Unstable eigenvalues for the linear stability problem of the **sn** solution ($\boldsymbol{k = \sqrt{0.8}}$).

5.5 A 2-D NLS equation soliton example

Consider

$$i\psi_t + \psi_{xx} - \psi_{yy} + 2|\psi|^2\psi = 0.$$

This equation has the one-dimensional soliton solution

$$\psi(x, t) = \operatorname{sech}(x) e^{it}.$$

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The associated spectral problem is

$$(\omega - 6\phi^2 - \rho^2 - \partial_x^2)U = \lambda V$$
$$-(\omega - 2\phi^2 - \rho^2 - \partial_x^2)V = \lambda U,$$

which has received lots of attention in the literature.

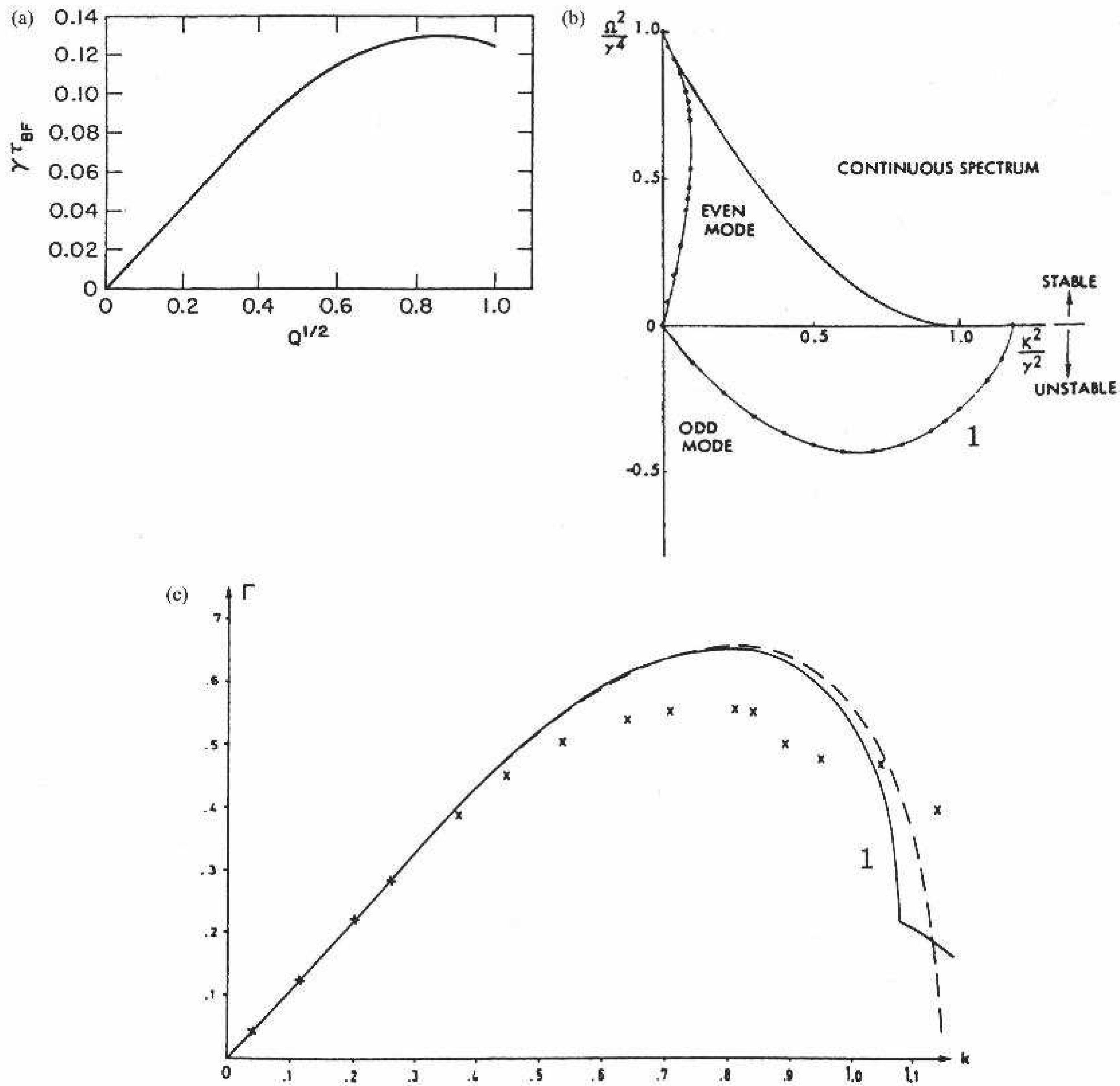
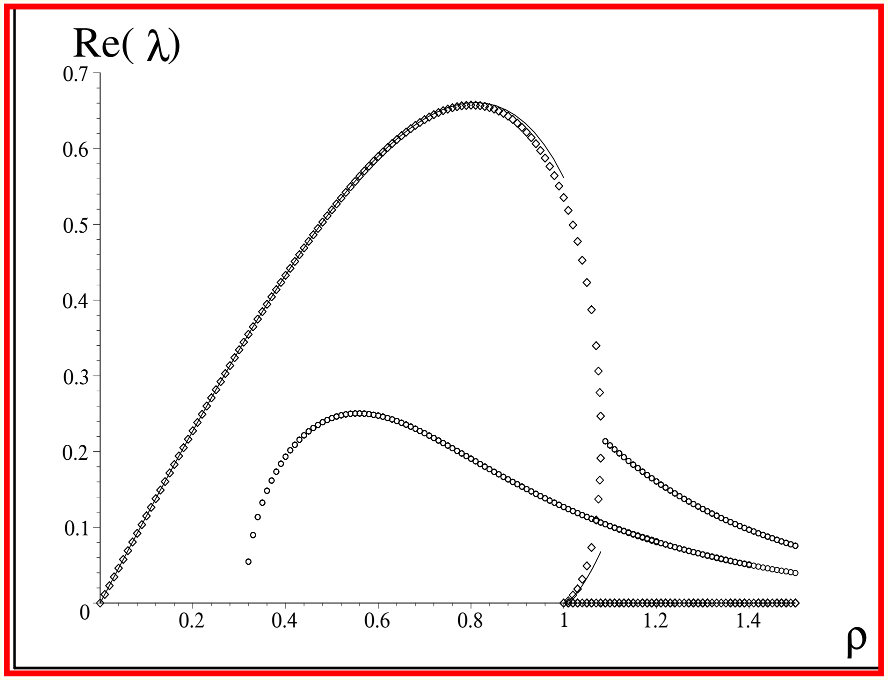
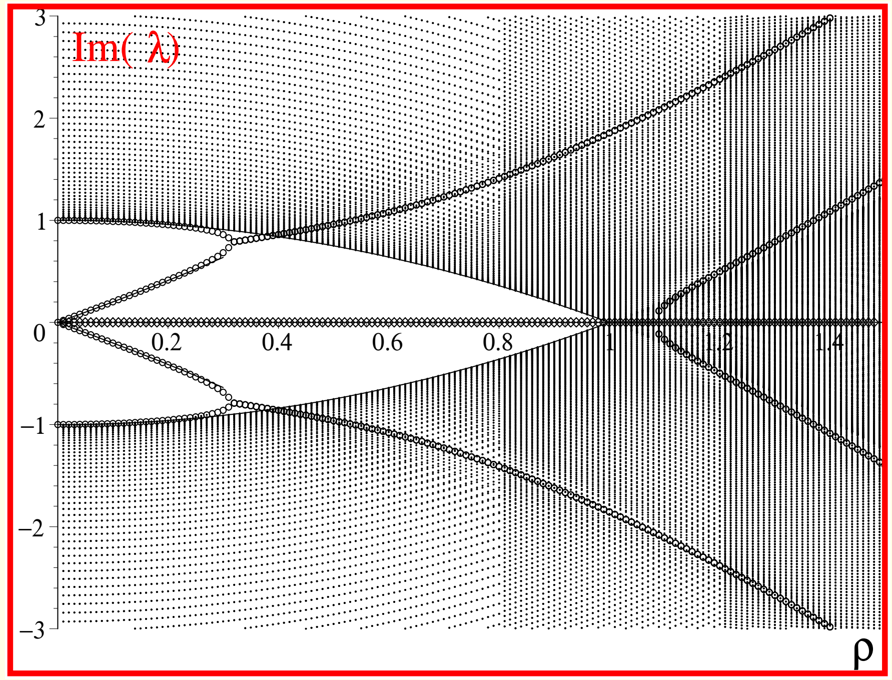


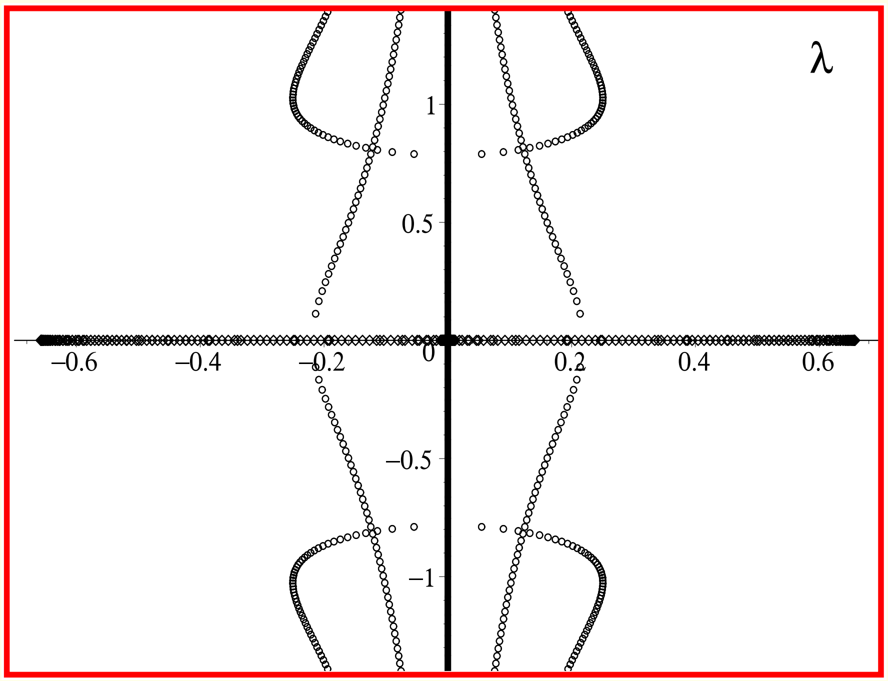
Fig. 2. The graph of the instability growth rate vs. the transverse wave number reproduced from [9] (a), [10] (b), and [12] (c). The correlation between the variables at the graphs and the variables λ and p is described in the text.



Re(λ)
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0.2
0.4
0.6
0.8
1
1.2
1.4
ρ



Im(λ)
3
2
1
0
−1
−2
−3
0.2
0.4
0.6
0.8
1
1.2
1.4
ρ



λ
1
0.5
0
−0.5
−1
−0.6
−0.4
−0.2
0.2
0.4
0.6

6 spectrUW: A black-box spectral calculator

- Hill's method constitutes a black-box algorithm $\longrightarrow$
- SpectrUW: a black-box software package for the computation of spectra of linear operators.
  - One-dimensional scalar or vector operators with parameters
  - Two-dimensional scalar or vector operators with parameters
  - Three-dimensional scalar or vector operators with parameters