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Numerical Results for Some Schrödinger Difference Equations

Lynn Erbe and **Allan Peterson**
University of Nebraska–Lincoln
Department of Mathematics
237 Avery Hall, Lincoln, NE 68588-0130, U.S.A.
lerbe2@math.unl.edu and apeterso@math.unl.edu

Andreas Ruffing and **Andreas Suhrer**
Munich University of Technology
Department of Mathematics
Boltzmannstrasse 3, 85747 Garching, Germany
ruffing@ma.tum.de and andreas.suhrer@t-online.de

Abstract

We perform numerical calculations for some Schrödinger difference equations. The first results are based on the oscillatory behavior of a symmetrically perturbed x^2 potential. Then we deal with quartic potentials, making use of ladder operators. In both cases the theory is well-established. The main interest lies in the numerical visualization of the oscillations and the eigenvalues. For the treatment of more sophisticated potentials, we introduce an adaptive basic linear grid. We determine and illustrate the eigenvalues of the Schrödinger operators by considering this adaptive grid. In most cases of our obtained results, we apply Kato's theory of regular perturbations for self-adjoint linear operators.

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1 Introduction

Numerical treatments of Schrödinger's equation turn out to be quite a challenging topic all over the sciences. In particular it is not clear of how to discretize the configuration

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space in advance for a given potential. In this article, we refer to several types of discretizations including so-called basic linear grids. The numerical calculations happen on two different stages: namely first a numerical maximum minimum principle and second a diagonalization of the related matrices.

2 A Short Review of Schrödinger's Equation

The Schrödinger equation with the so-called potential $U(x, y, z)$ is the basic equation of motion in nonrelativistic quantum mechanics:

$$\left(-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} + U(x, y, z)\right) \psi(x, y, z, t) = i \, (\frac{\partial \psi}{\partial t})(x, y, z, t). \tag{2.1}$$

Using the **Schrödinger operator**, or Hamilton operator H, given by

$$H := -\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} + U(x, y, z), \tag{2.2}$$

equation (2.1) may be rewritten as

$$(H\psi)(x, y, z, t) = i \, (\frac{\partial \psi}{\partial t})(x, y, z, t). \tag{2.3}$$

The following lemma deals with the separation of variables in the Schrödinger equation:

Lemma 2.1. *Let $\psi \in C^2(\mathbb{R}^3)$. A function $\varphi \in C^2(\mathbb{R}^4)$*

$$(x, y, z, t) \mapsto \varphi(x, y, z, t) := \psi(x, y, z) \, e^{-i\lambda t} \tag{2.4}$$

is a solution of the Schrödinger equation, iff λ is an eigenvalue of

$$(H\psi)(x, y, z) = \lambda \, \psi(x, y, z) \tag{2.5}$$

for all $(x, y, z) \in \mathbb{R}^3$. This equation is called the **Stationary Schrödinger Equation***.*

Proof. Let $f : \mathbb{R} \mapsto \mathbb{C}$ be given by

$$t \mapsto f(t) := e^{-i\lambda t} \tag{2.6}$$

and insert φ into equation (2.1). Then we get

$$\left(-\frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} + U(x, y, z)\right) \psi(x, y, z, t) = i \, (\frac{\partial \psi}{\partial t})(x, y, z, t) \Leftrightarrow \tag{2.7}$$

$$fH\psi = i\psi \frac{d}{dt} f \Leftrightarrow fH\psi = \lambda f \psi \Leftrightarrow H\psi = \lambda \psi. \tag{2.8}$$

The proof is complete. □

In this way, we obtain the separation of the time variable t and reduce a solution of the Schrödinger equation to a solution of an eigenvalue/eigenvector problem. Now we decompose this three dimensional equation into three one dimensional eigenvalue equations as follows: Let us set

$$U(x,y,z) = U_1(x) + U_2(y) + U_3(z) \tag{2.9}$$

$$\psi(x,y,z) = \psi_1(x)\ \psi_2(y)\ \psi_3(z) \tag{2.10}$$

$$\lambda = \lambda_1 + \lambda_2 + \lambda_3. \tag{2.11}$$

Substituting these expressions into (2.5) leads to the three one dimensional eigenvalue equations:

$$\left(-\frac{d^2}{dx^2} + U_1(x)\right)\psi_1(x) = \lambda_1\ \psi_1(x) \tag{2.12}$$

$$\left(-\frac{d^2}{dy^2} + U_2(y)\right)\psi_2(y) = \lambda_2\ \psi_2(y) \tag{2.13}$$

$$\left(-\frac{d^2}{dz^2} + U_3(z)\right)\psi_3(z) = \lambda_3\ \psi_3(z). \tag{2.14}$$

Hence we are lead to the problem of solving one dimensional eigenvalue problems (for physical reasons we are only interested in $\mathcal{L}^2(\mathbb{R})$-solutions).

In the sequel, we will use results from regular perturbation theory, which will help us to understand the oscillation phenomena occurring in several of our numerical studies. For this purpose we briefly recall some essential facts from [1].

Definition 2.2. A (possibly unbounded) operator-valued function $T(\beta)$ from a complex domain $K \subset \mathbb{C}$ into a Hilbert space S is called an **analytic family**, or an analytic family in the sense of Kato, if and only if

1. For every $\beta \in K$, $T(\beta)$ is closed and has a non-empty resolvent set.
2. For every $\beta_0 \in K$, there is a $\lambda_0 \in \rho(T(\beta_0))$ so that $\lambda_0 \in \rho(T(\beta))$ for β near β_0 and $(T(\beta) - \lambda_0)^{-1}$ is an analytic operator-valued function of β near β_0.

Lemma 2.3. *Let $H : D(H) \subseteq S \to S$ be a closed operator with nonempty resolvent set. Define $H + \beta V$ on $D(H) \cap D(V)$. Then $H + \beta V$ is an analytic family near $\beta = 0$ if and only if:*

1. $D(H) \subset D(V)$
2. *For some $x \in \mathbb{R}^+$ and $y \in \mathbb{R}_0^+$ and for all $\psi \in D(H)$, the following holds:*

$$\|V\psi\| \leq x\ \|H\psi\| + y\ \|\psi\|.$$

We have the following existence result for perturbed spectral points:

Theorem 2.4. *Let $T(\beta)$ be an analytic family in the sense of Kato. Let E_0 be a nondegenerate discrete eigenvalue of $T(\beta_0)$. Then, for β near β_0, there is exactly one point $E(\beta)$ of the spectrum $\sigma(T(\beta))$ near E_0 and this point is isolated and nondegenerate. $E(\beta)$ is an analytic function of β for β near β_0, and there is an analytic eigenvector $v(\beta)$ for β near β_0. If $T(\beta)$ is self-adjoint for $\beta - \beta_0$ real, then $v(\beta)$ can be chosen to be normalized for $\beta - \beta_0$ real.*

The following theorem concerns the radius of convergence for regular perturbation series.

Theorem 2.5. *Suppose that under the conditions of Theorem 2.4 and Lemma 2.3, we have*

$$\|V\psi\| \leq x\,\|H\psi\| + y\,\|\psi\| \qquad \psi \in D(H) \subseteq D(V).$$

Let H be self-adjoint with an unperturbed, isolated, nondegenerate eigenvalue E_0. And let $\Delta = \frac{1}{2}$ dist$(E_0, \sigma(H) \setminus \{E_0\})$. Define the function $R(x,y)$ by

$$R : \mathbb{R}^2 \to \mathbb{R}, \quad (x,y) \mapsto R(x,y) := \left(x + \frac{y + x|E_0| + x\Delta}{\Delta}\right)^{-1}.$$

Then the eigenvalue $E(\beta)$ of $H + \beta V$ near E_0 is analytic in the circle of radius $R(x,y)$ around 0.

3 Oscillation Phenomena for Perturbed x^2-Potentials

The Hermite functions φ_n where $n \in \mathbb{N}_0$ are the only solutions of the Schrödinger equation in $\mathcal{L}^2(\mathbb{R})$ for the x^2-potential as can be verified by using Lebesgue's dominated convergence principle. These functions are eigenfunctions of the Schrödinger operator with x^2-potential, the corresponding eigenvalues being for $n \in \mathbb{N}_0$

$$\lambda_n = 2n + 1. \tag{3.1}$$

In the following we consider functions $\psi_\lambda \in \mathcal{L}^2(\mathbb{R})$ with

$$\psi_\lambda := \sum_{j=0}^{\infty} c_j(\lambda) e_j \tag{3.2}$$

$$He_n = -e_n'' + Ue_n = -e_n'' + X^2 e_n = \lambda_n e_n, \tag{3.3}$$

where for $n \in \mathbb{N}_0$, the eigenfunctions e_n are the normalized Hermite functions and λ_n are the corresponding eigenvalues.

To the x^2-potential, we add a symmetric bounded linear perturbation V with the following properties (for $n \in \mathbb{N}_0$):

$$Ve_n = \alpha_n\, e_{n+1} + \beta_n\, e_{n-1}, \qquad \beta_0 = 0 \tag{3.4}$$

$$\alpha_n = \beta_{n+1} = \frac{1}{(n+1)^2}. \tag{3.5}$$

With the perturbed Schrödinger operator $H + V$ and the normalized Hermite functions e_n we get

$$(H + V)\ e_n = (2n + 1)\ e_n + \beta_{n+1}\ e_{n+1} + \beta_n\ e_{n-1}. \tag{3.6}$$

We insert ψ_λ as defined in equation (3.2) into the stationary Schrödinger equation with the perturbed Schrödinger operator $H + V$:

$$(H + V)\ \sum_{j=0}^{\infty} c_j(\lambda)\ e_j = \lambda \sum_{j=0}^{\infty} c_j(\lambda)\ e_j.$$

Comparison of the coefficients gives a three term recurrence relation for c_n:

$$c_{n+1} = (n + 1)^2 + (\lambda - 2n - 1)\ c_n + \left(1 + \frac{2}{n} + \frac{1}{n^2}\right)\ c_{n-1}, \tag{3.7}$$

where $n \in \mathbb{N}$ and the initial values are chosen as

$$c_0 = 0, \qquad c_1 = 1, \qquad c_2 = 4\lambda - 12. \tag{3.8}$$

Thus, we obtain

$$\psi(\lambda) = \sum_{j=0}^{\infty} c_j(\lambda)\ e_j \tag{3.9}$$

$$c_{n+1} = (n + 1)^2 + (\lambda - 2n - 1)\ c_n + \left(1 + \frac{2}{n} + \frac{1}{n^2}\right)\ c_{n-1}, \qquad n \in \mathbb{N} \tag{3.10}$$

$$c_0 = 0, \qquad c_1 = 1, \qquad c_2 = 4\lambda - 12. \tag{3.11}$$

Evaluating the three term recurrence relation for the $(c_n)_{n\in\mathbb{N}_0}$ numerically, we may graph the function

$$f_\lambda = \log\left(\sum_{j=0}^{n} |c_k(\lambda)|^2\right) \tag{3.12}$$

as a function of the parameter λ (see Figure 3.1). Note in this diagram the striking dependence on the chosen parameter λ. This is due to the fact that V can be considered as a perturbation of H in the sense of the stated results from Kato's perturbation theory, see Definition 2.2, Lemma 2.3 and Theorem 2.4 (resp., Theorem 2.5). As a consequence, the eigenvalues of H are analytic continuations of the eigenvalues of $H + V$.

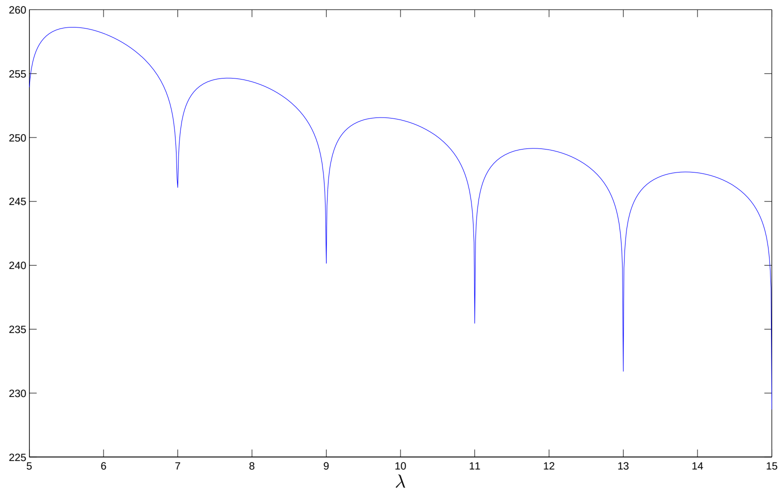

Figure 3.1: $f_\lambda = \log\left(\sum_{j=0}^{n} |c_k(\lambda)|^2\right)$, $\lambda \in [5; 15]$

4 Classical Oscillations of Power Series Solutions

Reviewing basic facts on the quadratic potential, let us consider in the sequel the power series ansatz

$$\psi_\lambda(x) = \sum_{k=0}^{\infty} c_k(\lambda) x^k \tag{4.1}$$

with $c_{2k+1} = 0$ for all $k \in \mathbb{N}_0$. Inserting ψ_λ into the stationary Schrödinger equation

$$H\psi_\lambda(x) = \lambda\psi_\lambda(x), \tag{4.2}$$

a comparison of the coefficients gives a three term recurrence relation where $k \in 2\mathbb{N}_0$:

$$c_{k+2}(\lambda) = \frac{c_{k-2}(\lambda) - \lambda c_k(\lambda)}{(k+2)(k+1)}. \tag{4.3}$$

As initial values we choose

$$c_{-2}(\lambda) = 0 \qquad c_0(\lambda) = 1 \qquad c_2(\lambda) = -\frac{\lambda}{2}. \tag{4.4}$$

Numerically evaluating the recurrence relation for the coefficients, we first plot

$$\log|\psi_\lambda(x) + 1| \tag{4.5}$$

for a constant value of λ (see Figure 4.1). In this way, we obtain the same zeros as the function ψ_λ. In a second plot (Figure 4.2) we use x as a constant and λ as variable. We

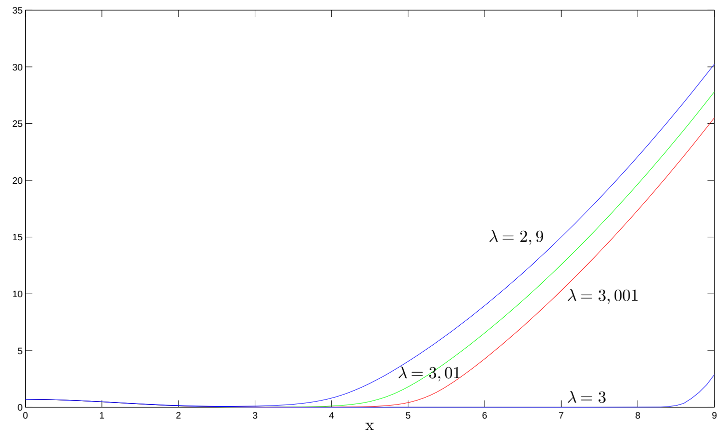

Figure 4.1: $U(x) = x^2$, $\lambda \in \{2.9, 3, 3.01, 3.001\}$, $f_\lambda(x) = \log|\psi_\lambda(x) + 1|$

plot

$$\log|\psi_\lambda(x) + 1|\,. \tag{4.6}$$

We then use x and λ as variables and plot again (see Figures 4.3 and 4.4):

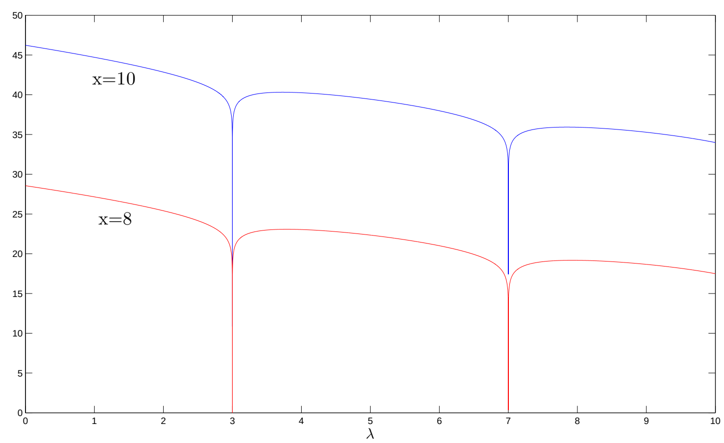

Figure 4.2: $U(x) = x^2$, $x \in \{8, 10\}$, $f_\lambda(x) = \log|\psi_\lambda(x) + 1|$

$$\log|\psi_\lambda(x) + 1|\,. \tag{4.7}$$

From standard results in quantum mechanics it is known that the energy eigenvalues of the quadratic potential are given as the odd natural numbers (for the Schrödinger operator being given by $(H\psi)(x) = -\psi''(x) + x^2\ \psi(x)$). Our numerical investigations are in agreement with this fact. We will refer to the ladder operator formalism in the next section in more detail.

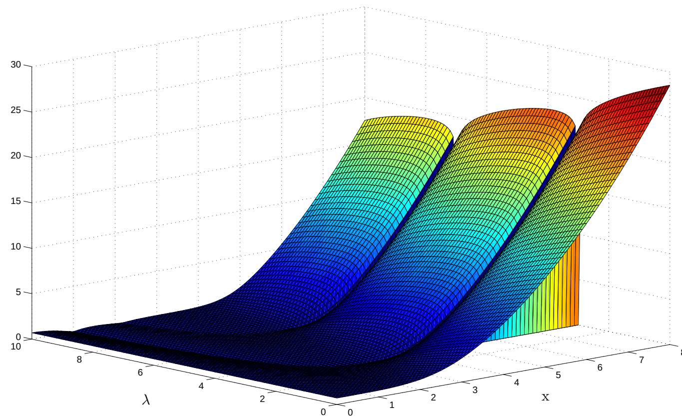

Figure 4.3: $U(x) = x^2$, $f_\lambda(x) = \log|\psi_\lambda(x) + 1|$, $x \in [0;8]$, $\lambda \in [0;10]$

5 Oscillation Behavior of Potentials of 4th Degree

For the x^2-potential (as well as at least partially for a few other simple potentials, e.g., x^6) there exists a ladder operator formalism which allows one to obtain solutions for the Schrödinger equation.

Ladder Operators. For our following purposes we use the well-known conventional ladder operators, acting on suitable common domains in $\mathcal{L}^2(\mathbb{R})$:

$$A = \frac{1}{\sqrt{2}}(D + X) \tag{5.1}$$

$$A^+ = \frac{1}{\sqrt{2}}(-D + X) \tag{5.2}$$

with the operator X

$$(Xf)(x) = xf(x) \tag{5.3}$$

and the differential operator D

$$(Df)(x) = f'(x). \tag{5.4}$$

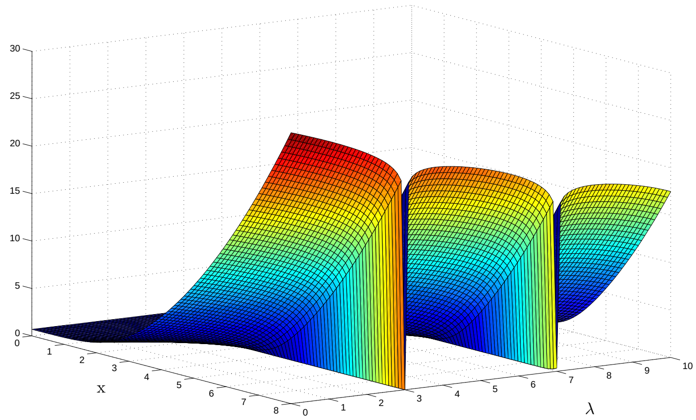

Figure 4.4: $U(x) = x^2$, $f_\lambda(x) = \log|\psi_\lambda(x)+1|$, $x \in [0;8]$, $\lambda \in [0;10]$

The ladder operators have the following **properties**:

$$A + A^+ = \sqrt{2}X \tag{5.5}$$

$$A - A^+ = \sqrt{2}D \tag{5.6}$$

$$I = AA^+ - A^+A, \tag{5.7}$$

where I is the identity operator. For $n \in \mathbb{N}_0$ and $x \in \mathbb{R}$ we define

$$H_n(x) := (-1)^n e^{x^2} D^n e^{-x^2} \tag{5.8}$$

as well as the Hermite functions e_n (non normalized) as follows

$$e_n(x) = H_n(x)e^{-\frac{1}{2}x^2}. \tag{5.9}$$

For the ladder operators and the Hermite functions the following equations hold:

$$A^+A = \frac{1}{2}(-D^2 + X^2) - \frac{1}{2}I \tag{5.10}$$

$$A^+Ae_n = ne_n, \qquad n \in \mathbb{N}_0 \tag{5.11}$$

$$AA^+ = \frac{1}{2}(-D^2 + X^2) + \frac{1}{2}I \tag{5.12}$$

$$AA^+e_n = (n+1)e_n, \qquad n \in \mathbb{N}_0. \tag{5.13}$$

The eigenvalues of the Hermite functions for the operator $(-D^2 + X^2)$ are given by the sequence $(2n+1)_{n\in\mathbb{N}_0}$. Using the properties of the ladder operators (5.5)–(5.7) and the results (5.10)–(5.13) we obtain for the operator X, as defined above:

$$X^2 = \frac{1}{2}(A + A^+)(A + A^+)$$
$$2X^2 = A^2 + A^{+^2} + A^+A + AA^+$$

$$2X^2 e_n = \alpha_n e_{n-2} + \beta_n e_{n+2} + \gamma_n e_n \qquad \text{for } n \in \mathbb{N}_0, \tag{5.14}$$

where we abbreviate for $n \in \mathbb{N}_0$

$$\alpha_n := \sqrt{n}\sqrt{n-1}, \qquad \beta_n := \sqrt{n+1}\sqrt{n+2}, \qquad \gamma_n := 2n + 1.$$

We apply $2X^2$ again in equation (5.14) to obtain a potential of degree 4:

$$\begin{aligned} 4X^4 e_n &= \alpha_n(2X^2)e_{n-2} + \beta_n(2X^2)e_{n+2} + \gamma_n(2X^2)e_n \\ &= \alpha_n\left[\alpha_{n-2}e_{n-4} + \beta_{n-2}e_n + \gamma_{n+2}e_{n+2}\right] \\ &+ \beta_n\left[\alpha_{n+2}e_n + \beta_{n+2}e_{n+4} + \gamma_{n+2}e_{n+2}\right] \\ &+ \gamma_n\left[\alpha_n e_{n-2} + \beta_n e_{n+2} + \gamma_n e_n\right], \qquad n \in \mathbb{N}_0 \end{aligned} \tag{5.15}$$

$$\begin{aligned} X^4 e_n = \alpha_n\alpha_{n-2}e_{n-4} &+ (\alpha_n\gamma_{n-2} + \gamma_n\alpha_n)e_{n-2} + (\alpha_n\beta_{n-2} + \beta_n\alpha_{n+2} + \gamma_n^2)e_n \\ &+ (\beta_n\gamma_{n+2} + \gamma_n\beta_n)e_{n+2} + \beta_n\beta_{n+2}e_{n+4}, \qquad n \in \mathbb{N}_0. \end{aligned} \tag{5.16}$$

Then we define the operator

$$H := \frac{1}{2}(-D^2 + X^2 + X^4). \tag{5.17}$$

This means we have a Schrödinger operator with the potential $U(x) = x^2 + x^4$. Using the results (5.14) and (5.16) we get for $n \in \mathbb{N}_0$:

$$He_{2n} = A_n e_{2n-4} + B_n e_{2n-2} + C_n e_{2n} + D_n e_{2n+2} + E_n e_{2n+4} \tag{5.18}$$

with

$$A_n := \frac{\alpha_{2n-2}\alpha_{2n}}{8}, \qquad B_n := \frac{\alpha_{2n}\gamma_{2n-2} + \alpha_{2n}\gamma_{2n}}{8}, \tag{5.19}$$

$$C_n := \frac{\alpha_{2n}\beta_{2n-2} + \beta_{2n}\alpha_{2n+2} + 8(2n+1)^3}{8}, \qquad D_n := \frac{\beta_{2n}\gamma_{2n+2} + \gamma_{2n}\beta_{2n}}{8}, \tag{5.20}$$

$$E_n := \frac{\beta_{2n}\beta_{2n+2}}{8}. \tag{5.21}$$

Upon substitution of

$$v_n := e_{2n} \tag{5.22}$$

equation (5.18) becomes

$$Hv_n = A_n v_{n-2} + B_n v_{n-1} + C_n v_n + D_n v_{n+1} + E_n v_{n+2}, \qquad n \in \mathbb{N}_0. \tag{5.23}$$

Now we consider functions of the form

$$\sum_{j=0}^{\infty} c_n v_n \tag{5.24}$$

and insert them into the stationary Schrödinger equation with the operator H from equation (5.17)

$$H \sum_{j=0}^{\infty} c_n v_n = \lambda \sum_{j=0}^{\infty} c_n v_n \tag{5.25}$$

to get a five term recurrence relation of type

$$c_{n+2}A_{n+2}+c_{n+1}B_{n+1}+c_n(C_n-\lambda)+c_{n-1}D_{n-1}+c_{n-2}E_{n-2}=0, \qquad n \in \mathbb{N}_0. \tag{5.26}$$

There are two paths for the initial values, which differ in the choice of c_0:

First path:

$$c_{-2} = c_{-1} = 0$$
$$c_0 = a, \qquad a \in \mathbb{R}$$
$$c_1 = 1$$

Second path:

$$c_{-2} = c_{-1} = 0$$
$$c_0 = 1$$
$$c_1 = a, \qquad a \in \mathbb{R}.$$

We evaluate the recurrence relation numerically, only considering the second path for the initial values, and plot (see Figure 5.1):

$$\log\left(\sum_{k=0}^{n} c_k^2(a)\right), \qquad c_k(a) \equiv c_k(a,\lambda). \tag{5.27}$$

The variable a results from the initial value for c_1. λ is considered to be a constant. In a second plot we choose the initial value a as a constant (see Figure 5.2) and λ from equation (5.25), (5.26) as variable. That means we plot

$$\log\left(\sum_{k=0}^{n} c_k^2(\lambda)\right), \qquad c_k(\lambda) \equiv c_k(a,\lambda) \tag{5.28}$$

for different values of a. Finally we consider both a and λ as variables and plot the three dimensional graph (see Figure 5.3) of:

$$\log\left(\sum_{k=0}^{n} c_k^2(a,\lambda)\right). \tag{5.29}$$

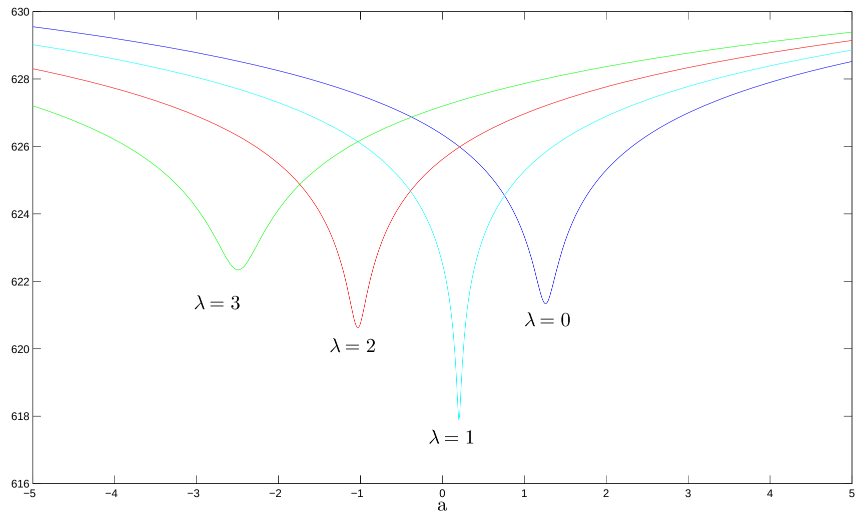

Figure 5.1: $n = 100$, $\lambda \in \{0, 1, 2, 3\}$, $f_\lambda(a) = \log\left(\sum_{k=0}^{n} c_k^2(a)\right)$

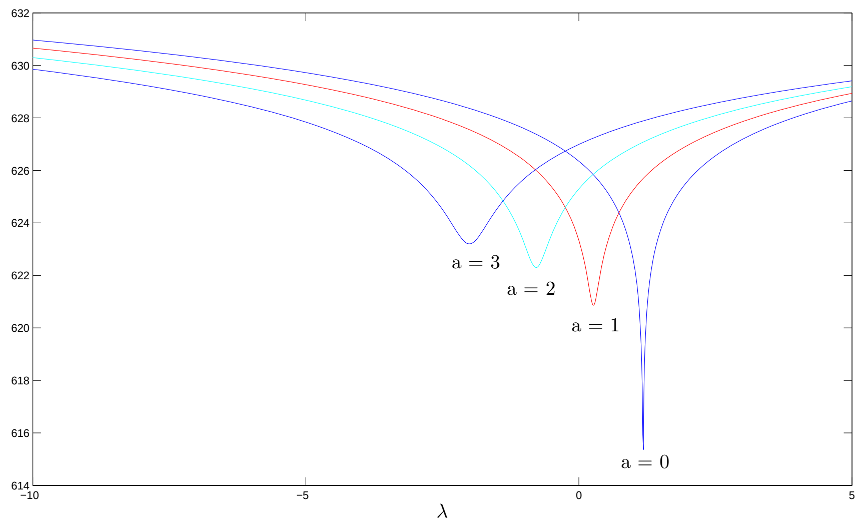

Figure 5.2: $n = 100$, $a \in \{0, 1, 2, 3\}$, $f_a(\lambda) = \log\left(\sum_{k=0}^{n} c_k^2(\lambda)\right)$

We observe that for certain values of a and λ there arise minima in the function landscape, see Figures 5.1, 5.2, and 5.3. However this already reveals that generalizing our method used so far to potentials of higher degree will cause difficulties in getting reasonable quantitative results. This is due to the fact that additional initial parameters, like a, will arise: We have to develop an alternative approach to higher degree potentials, and this will happen throughout the next section – using basic versions of Schrödinger difference equations.

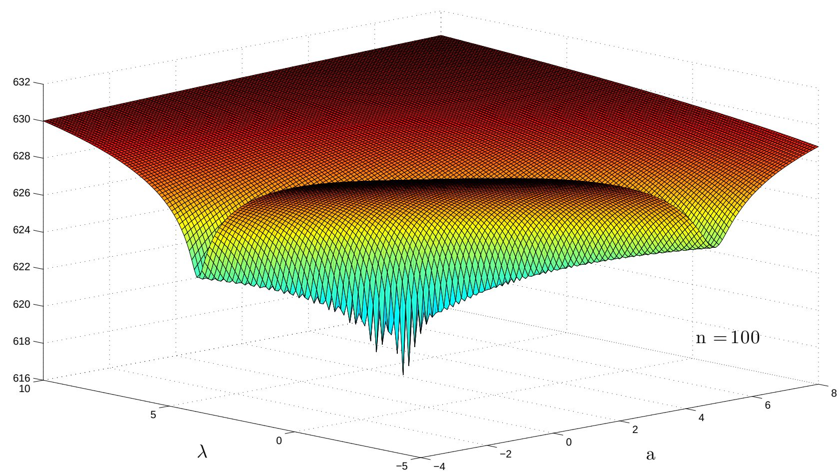

Figure 5.3: $n = 100$, $\lambda \in [-5; 10]$, $a \in [-4; 8]$, $f_a(\lambda) = \log\left(\sum_{k=0}^{n} c_k^2(a,\lambda)\right)$

6 Oscillation Behavior on q-Linear Grids

As we saw in Section 2, there exists a solution for the Schrödinger Equation with Hermite functions for the x^2-potential. For some potentials, for example the x^6 or x^2-potential, there are ladder operator formalisms to get the solution. If we want to handle any arbitrary potential, we need a relaxation of the Schrödinger operator. Therefore, we first introduce a q**-linear grid**, as an adaptive discretization, on which we search for our solutions:

$$\mathbb{R}_q = \{\pm c q^n | n \in \mathbb{Z}\}. \tag{6.1}$$

For our purposes we only consider $0 < q < 1$ and later $c = 1$. In this way, we get a grid with a very high density around zero, which allows us to scan as much information as possible close to the point zero region. On

$$l^2(\mathbb{R}_q) = \left\{ f : \mathbb{R}_q \mapsto \mathbb{R}_q | \sum_{-\infty}^{\infty} q^n (1-q) f^2(q^n) < \infty \right\}$$

we introduce the scalar product

$$(f,g) := \sum_{n=-\infty}^{\infty} q^n \left[f(q^n)g(q^n) + f(-q^n)g(-q^n) \right] (1-q) \tag{6.2}$$

and choose a **symmetric difference operator** D_q:

$$(D_q f)(x) = \frac{f(qx) - f(q^{-1}x)}{qx - q^{-1}x}. \tag{6.3}$$

With this definition we are able to provide a reasonable choice for the **discrete Schrödinger operator** on the chosen q-linear grid:

$$H_q = -D_q^2 + \alpha(R^2 + q^{-2}L^2) + V(x) \tag{6.4}$$

with an arbitrary potential V and the left-shift and right-shift operators L, R.

$$(Lf)(x) = f(q^{-1}x) \tag{6.5}$$

$$(Rf)(x) = f(qx). \tag{6.6}$$

Up to this point, we can say that the expression (6.4) provides a relaxation of the Schrödinger operator and hence ensures a numerically stable treatment. To guarantee a most efficient and at the same time simple numerical procedure, we choose α such that we are in the weighted $l^2(\mathbb{N})$-situation:

For the difference operator D_q the following equation for the "second derivative" holds:

$$(D_q^2 f)(x) = -\frac{\frac{f(q^2x)-f(x)}{q^2x-x} - \frac{f(x)-f(q^{-2}x)}{x-q^{-2}x}}{qx - q^{-1}x}. \tag{6.7}$$

The left shift part of (6.7) is

$$-\frac{\frac{f(q^2x)-f(x)}{q^2x-x}}{qx - q^{-1}x} = -\frac{f(q^2x)}{(q^2-1)(q-q^{-1})x^2}. \tag{6.8}$$

Considering the left shift part of the whole discrete Schrödinger operator we get

$$-\frac{f(q^2x)}{(q^2-1)(q-q^{-1})x^2} + \alpha f(q^2x). \tag{6.9}$$

Equation (6.9) has to be zero for $x = c = 1$ to guarantee a monolateral scenario for the related infinite Jacobi matrix, thus yielding

$$\alpha = \frac{1}{(q^2-1)(q-q^{-1})}. \tag{6.10}$$

With (6.10) we finally obtain for the **discrete Schrödinger operator**:

$$H_q = -D_q^2 + \frac{1}{(q^2-1)(q-q^{-1})}(R^2 + q^{-2}L^2) + V(x). \tag{6.11}$$

In the stationary Schrödinger equation we apply H_q on a function $f \in l^2(\mathbb{R}_q)$. Our intention is to obtain qualitative and quantitative statements about the eigenvalues of (6.11). To this end, we insert into the eigenequation

$$(H_q f)(x) = \lambda f(x) \tag{6.12}$$

the concrete form of the discrete Schrödinger operator:

$$\begin{aligned}(H_q f)(x) = &\frac{f(q^2x)}{(1-q^2)(q-q^{-1})x^2} + \frac{f(x)}{(q-q^{-1})x}\left[\frac{1}{(q^2-1)x} + \frac{1}{(1-q^{-2})x}\right] \\ &- \frac{f(q^{-2}x)}{(1-q^{-2})(q-q^{-1})x^2} + \alpha(f(q^2x) + q^{-2}f(q^{-2}x)) + V(x)f(x) \\ &= \lambda f(x).\end{aligned} \tag{6.13}$$

Note that in all these calculations, the variable x runs in $\mathbb{R}_q$. From equation (6.13) we obtain a recurrence relation for $f(q^2x)$:

$$\begin{aligned}f(q^2x)\left(\frac{1}{(1-q^2)(q-q^{-1})x^2} + \alpha\right) - f(q^{-2}x)\left(\frac{1}{(1-q^{-2})(q-q^{-1})x^2} - \alpha q^{-2}\right) \\ + f(x)\left(\frac{q+q^{-1}}{(q^2-1)(1-q^{-2})x^2} + V(x) - \lambda\right) = 0.\end{aligned} \tag{6.14}$$

Defining for $x \in \mathbb{R}_q$

$$\tilde{D}(x) := \left(\frac{q+q^{-1}}{(q^2-1)(1-q^{-2})x^2} + V(x) - \lambda\right) \tag{6.15}$$

$$D(x) := \left(\frac{q+q^{-1}}{(q^2-1)(1-q^{-2})x^2} + V(x)\right) \tag{6.16}$$

$$L(x) := \left(\frac{1}{(1-q^2)(q-q^{-1})x^2} + \alpha\right) \tag{6.17}$$

$$U(x) := \left(\frac{1}{(1-q^{-2})(q-q^{-1})x^2} - \alpha q^{-2}\right) \tag{6.18}$$

and solving equation (6.14) for $f(q^{-2}x)$ we get

$$f(q^{-2}x) = \frac{f(q^2x)L(x) + f(x)\tilde{D}(x)}{U(x)}. \tag{6.19}$$

In this way we obtain a three term recurrence relation for $f(q^{-2}x)$ for any arbitrary potential $V(x)$. In matrix-vector notation the stationary Schrödinger equation for this problem is

$$A\vec{f}(x) = \lambda\vec{f}(x) \qquad x \in \mathbb{R}_q \tag{6.20}$$

with the matrix A:

$$\begin{pmatrix} \ddots & \ddots & \ddots & 0 & & & \\ 0 & L(q^2) & D(q^2) & -U(q^2) & 0 & & \\ & 0 & L(1) & D(1) & -U(1) & 0 & \\ & & 0 & L(q^{-2}) & D(q^{-2}) & -U(q^{-2}) & 0 \\ & & & 0 & \ddots & \ddots & \ddots \end{pmatrix}$$

and the vector $\vec{f}(x)$

$$\begin{pmatrix} \vdots \\ f(q^2) \\ f(1) \\ f(q^{-2}) \\ \vdots \end{pmatrix}.$$

The upper-, sub- and diagonal entries of the matrix A satisfy (see also Figure 6.1):

$$\lim_{x\to\infty} (-U(x)) = \alpha q^{-2} \tag{6.21}$$

$$\lim_{x\to\infty} (L(x)) = \alpha \tag{6.22}$$

$$\lim_{x\to\infty} (D(x)) = V(x). \tag{6.23}$$

For a **numerical visualization** we consider $x \in \mathbb{R}_q$ $x \geq 1$ and choose as initial values

$$f(q^2) = 0 \tag{6.24}$$

$$f(1) = 1. \tag{6.25}$$

This means, the matrix A and the vector $\vec{f}$ in (6.20) reduce to

$$\begin{pmatrix} D(1) & -U(1) & 0 & & \\ L(q^{-2}) & D(q^{-2}) & -U(q^{-2}) & 0 & \\ 0 & L(q^{-4}) & D(q^{-4}) & -U(q^{-4}) & 0 \\ & 0 & \ddots & \ddots & \ddots \end{pmatrix}$$

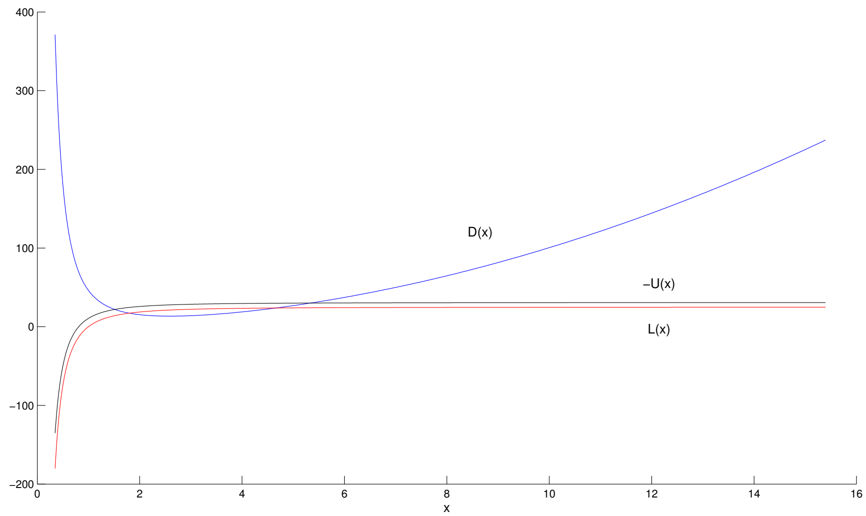

Figure 6.1: Behavior of the matrix entries, $q = 0.9$, $V(x) = x^2$, $x \in \mathbb{R}_q$

$$\begin{pmatrix} f(1) \\ f(q^{-2}) \\ \vdots \end{pmatrix}.$$

We solve the recurrence relation for $f(q^{-2}x)$ in (6.19) and plot

$$h(\lambda) = \log\left(\sum_{k=0}^{n} q^{-2k} f(cq^{-2k}, \lambda)^2\right) \tag{6.26}$$

for different potentials $V(x)$, see Figures 6.2, 6.3, 6.4, and 6.5. A numerical evaluation of the matrix A and of the eigenvalues of A with the QR-algorithm gives for $q = 0.9$ and $V(x) = x^8$:

$$\begin{pmatrix} 46.125 & 10.585 & 0 & 0 & 0 & 0 & 0 & \cdots \\ 8.5737 & 35.003 & 17.529 & 0 & 0 & 0 & 0 & \cdots \\ 0 & 14.199 & 48.548 & 22.086 & 0 & 0 & 0 & \cdots \\ 0 & 0 & 17.89 & 169.91 & 25.075 & 0 & 0 & \cdots \\ 0 & 0 & 0 & 20.311 & 856.52 & 27.037 & 0 & \cdots \\ 0 & 0 & 0 & 0 & 21.9 & 4582.7 & 28.324 & \cdots \\ \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \end{pmatrix}$$

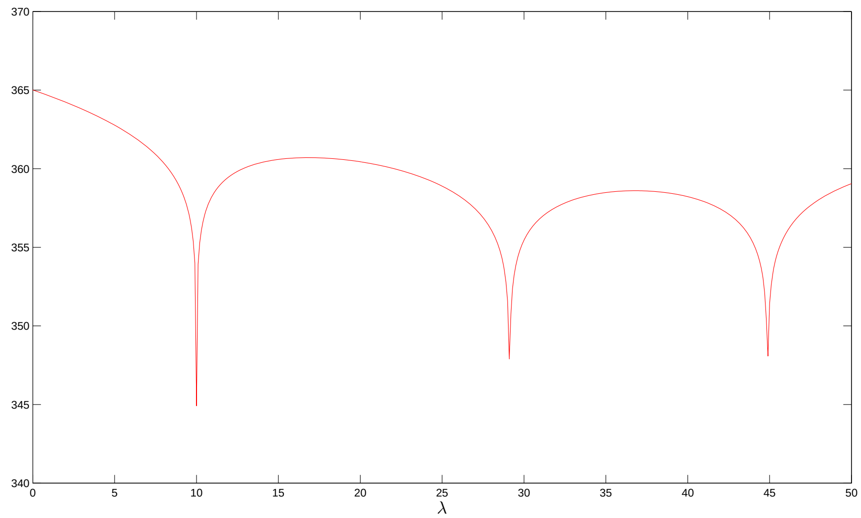

Figure 6.2: $V(x) = x^6$, $x \in \mathbb{R}_q$, $q = 0.9$, $h(\lambda) = \log\left(\sum_{k=0}^{n} q^{-2k} f(cq^{-2k}, \lambda)^2\right)$

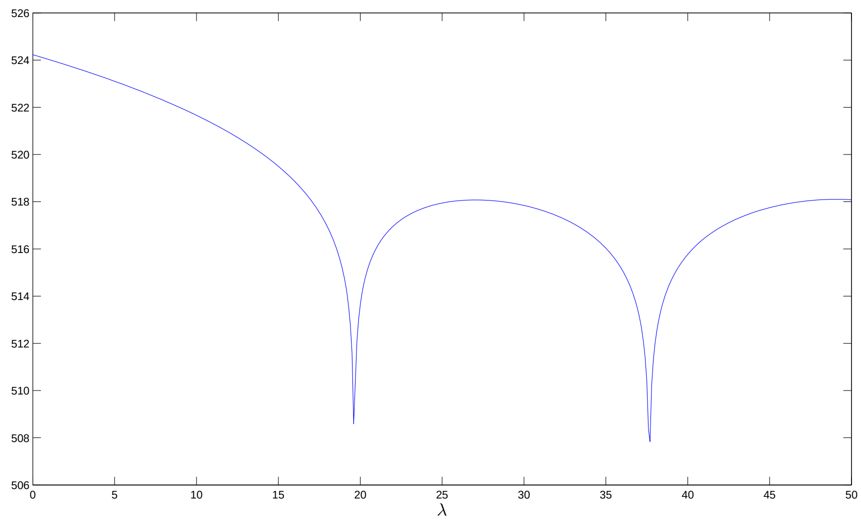

Figure 6.3: $V(x) = x^8$, $x \in \mathbb{R}_q$, $q = 0.9$, $h(\lambda) = \log\left(\sum_{k=0}^{n} q^{-2k} f(cq^{-2k}, \lambda)^2\right)$

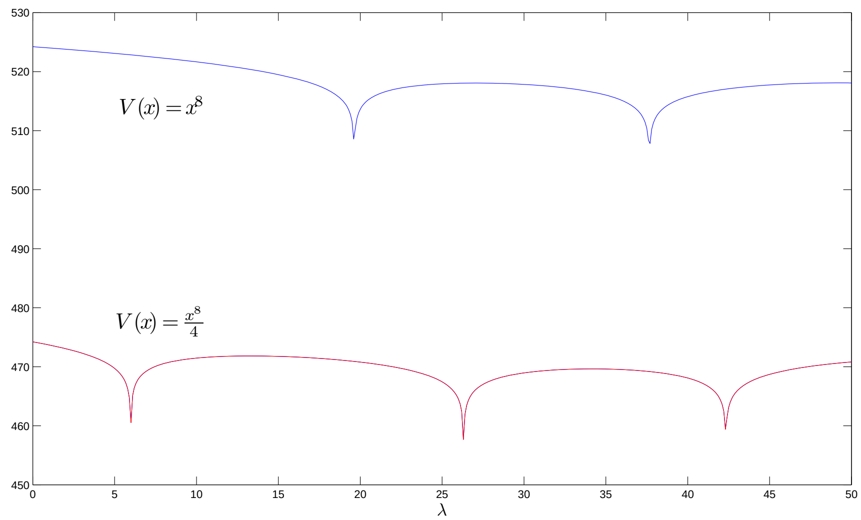

Figure 6.4: $V(x) = x^8$ and $V(x) = \dfrac{x^8}{4}$, $x \in \mathbb{R}_q$, $q = 0.9$, $h(\lambda) = \log\left(\sum_{k=0}^{n} q^{-2k} f(cq^{-2k}, \lambda)^2\right)$

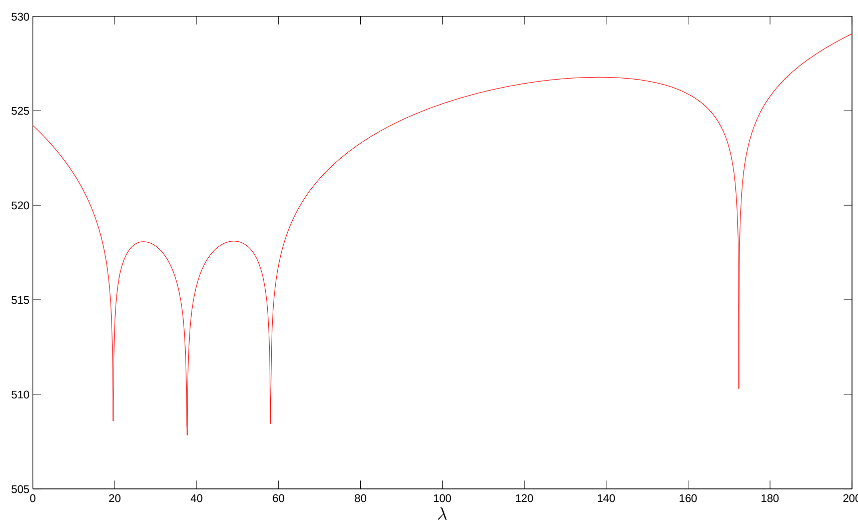

Figure 6.5: $V(x) = x^8$, $x \in \mathbb{R}_q$, $q = 0.9$, $h(\lambda) = \log\left(\sum_{k=0}^{n} q^{-2k} f(cq^{-2k}, \lambda)^2\right)$

with the vector of the eigenvalues:

$$\begin{pmatrix} 21.249 \\ 45.913 \\ 59.279 \\ 172.4 \\ 857.11 \\ 4582.8 \\ \vdots \end{pmatrix}.$$

A comparison of the numerically evaluated eigenvalues and of the minima in Figure 6.5 shows quite a good similarity, even for the first eigenvalues. We also observe, that the eigenvalues λ_n get closer to the diagonal entries of the matrix A for larger n. Note finally that the relaxation we have chosen fits well into the framework of analytic perturbation theory. See the general facts from Section 2 along with the detailed analytic investigation of the Schrödinger difference operator we used above.

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