# A FIRST-ORDER PHASE TRANSITION IN A CLASS OF UNBOUNDED JACOBI MATRICES: CRITICAL COUPLING

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Abstract. We consider a class of Jacobi matrices with unbounded coefficients. This class is known to exhibit a first-order phase transition in the sense that, as a parameter is varied, one has purely discrete spectrum below the transition point and purely absolutely continuous spectrum above the transition point. We determine the spectral type and solution asymptotics at the transition point.

## 1. Introduction

In this paper we analyze spectral properties of Jacobi matrices,

$$J = \begin{pmatrix} b_1 & a_1 & 0 & 0 & \cdots \\ a_1 & b_2 & a_2 & 0 & \cdots \\ 0 & a_2 & b_3 & a_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{1}$$

acting in $\ell^2(\mathbb{Z}_+)$, and asymptotic properties of solutions to the associated difference equation

$$a_n u_{n+1} + b_n u_n + a_{n-1} u_{n-1} = E u_n. \tag{2}$$

Recently, there has been interest in the case of unbounded coefficients $a_n, b_n$; see, for example, [1, 2, 3, 8, 9, 10, 11, 12, 18].

Motivated in particular by [4, 15, 16, 17], Janas and Naboko [10] studied a large class of Jacobi matrices with unbounded and periodically modulated entries. To be specific, they considered the case $a_n = c_n \mu_n$, $b_n = d_n r_n$, where $\{c_n\}$ is strictly positive and $N$-periodic and $\{d_n\}$ is $M$-periodic. The sequences $\{\mu_n\}$, $\{r_n\}$ are unbounded and satisfy a number of conditions. The main example one should have

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in mind is $\mu_n = r_n = n^\alpha$, where $0 < \alpha \le 1$. Let us consider this special case, that is,

$$a_n = c_n n^\alpha, \quad b_n = d_n n^\alpha. \tag{3}$$

Since the Carleman condition holds, that is,

$$\sum_{n=1}^{\infty} a_n^{-1} = \infty,$$

$J$ defines a self-adjoint operator in $\ell^2(\mathbb{Z}_+)$. The spectral type of $J$ is closely related to the location of zero relative to the spectrum of the associated periodic Jacobi matrix $J_{\mathrm{per}}$ which is given by

$$J_{\mathrm{per}} = \begin{pmatrix} d_1 & c_1 & 0 & 0 & \cdots \\ c_1 & d_2 & c_2 & 0 & \cdots \\ 0 & c_2 & d_3 & c_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$

Clearly, $J_{\mathrm{per}}$ is $K$-periodic, where $K$ is the least common multiple of $M$ and $N$. Its characteristic polynomial, $d(E)$, is given by

$$d(E) = \mathrm{Tr}\left[ \prod_{n=1}^{K} \begin{pmatrix} 0 & 1 \\ -c_{n-1}c_n^{-1} & (E-d_n)c_n^{-1} \end{pmatrix} \right].$$

It is well known that the spectrum of $J_{\mathrm{per}}$ is given by

$$\sigma(J_{\mathrm{per}}) = \{E \in \mathbb{R} : |d(E)| \le 2\}.$$

This set is the union of $K$ bands (non-degenerate closed intervals) whose interiors are mutually disjoint. The following was shown in [10]:

**Theorem 1** (Janas-Naboko)**.** (a) *If $|d(0)| < 2$, then the spectrum of $J$ is purely absolutely continuous and $\sigma(J) = \mathbb{R}$.*
(b) *If $|d(0)| > 2$, then the spectrum of $J$ is purely discrete.*

In other words, if zero is not one of the band edges of $\sigma(J_{\mathrm{per}})$, one has a complete understanding of the spectral type of $J$. Moreover, Janas and Naboko also described the asymptotic behavior of the solutions of (2); compare [10, Theorems 3.1 and 4.2].

The question of what happens at transition points, corresponding to $d(0) = \pm 2$, was left open in [10]. It was pointed out that new methods and ideas would be necessary to understand these critical cases. It is our goal here to study this scenario in a simple special case. We shall see that even in this simple situation, the analysis is already quite involved. Moreover, in this way the main new ideas are more transparent.

We will study the case where the $a_n$'s and $b_n$'s are given by (3) and both periods, $M$ and $N$, are small. Specifically, let us consider the case

$$M = 2, \quad N = 1, \quad c_n \equiv 1, \quad b_{2n-1} \equiv b, \quad b_{2n} \equiv \tilde{b}.$$

We find

$$d(0) = -2 + b\tilde{b}.$$

Fix $b > 0$. Then, by Theorem 1, $J$ has purely absolutely continuous spectrum for (not too large) $\tilde{b} > 0$ and purely discrete spectrum for $\tilde{b} < 0$. Similarly, for $b < 0$, $J$ has purely absolutely continuous spectrum for $\tilde{b} < 0$ (again, the absolutely value should not be too large) and purely discrete spectrum for $\tilde{b} > 0$. Thus, if we fix some non-zero value for $b$, the case $\tilde{b} = 0$ is the critical case for which Theorem 1 does not apply.

It is our goal to study this particular case, that is, we want to determine the spectral type and solution asymptotics for

$$a_n = n^\alpha, \quad b_n = \begin{cases} bn^\alpha & \text{if } n \text{ is odd,} \\ 0 & \text{if } n \text{ is even,} \end{cases}$$

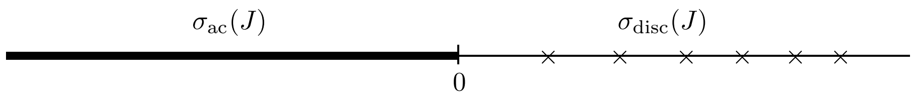
where $b \neq 0$ and $0 < \alpha \leq 1$. Our main results in the case $b > 0$ (when $b < 0$, one has to reflect the energy about zero) are as follows:

- If $2/3 < \alpha \leq 1$, the spectrum of $J$ is purely absolutely continuous on $(-\infty, 0)$. Moreover, explicit solution asymptotics are given. These results are stated in more detail and proven in Section 3.
- If $0 < \alpha \leq 1$, zero is not an eigenvalue of $J$. See Section 4.
- If $0 < \alpha \leq 1$, the spectrum of $J$ is purely discrete in $(0, \infty)$. The eigenvalues are simple and the $n$-th eigenvalue, $E_n$, obeys the bounds

  $$C_1(b) n^\alpha \leq E_n \leq C_2(b) n^\alpha.$$

  We also provide explicit expressions for the (positive and finite) constants $C_1(b), C_2(b)$. These results and their proofs can be found in Section 5.

This determines the spectral type completely when $2/3 < \alpha \leq 1$. In this case, the spectrum looks essentially like




We expect this picture also when $0 < \alpha \leq 2/3$. Thus, we leave the question of proving purely absolutely continuous spectrum on the negative energy axis for these values of $\alpha$ as an open problem. This and other open problems suggested by our work will be discussed in Section 6.

## 2. Preliminaries

We will study the Jacobi matrix

$$J = \begin{pmatrix} b_1 & a_1 & 0 & 0 & \cdots \\ a_1 & b_2 & a_2 & 0 & \cdots \\ 0 & a_2 & b_3 & a_3 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}, \tag{4}$$

acting in $\ell^2(\mathbb{Z}_+)$, where the parameters $a_n, b_n$ are given by

$$a_n = n^\alpha, \quad b_n = \begin{cases} bn^\alpha & \text{if } n \text{ is odd,} \\ 0 & \text{if } n \text{ is even.} \end{cases} \tag{5}$$

Here, $b \neq 0$. Note that if $J_{\{a_n\},\{b_n\}}$ denotes the Jacobi matrix corresponding to the sequences $\{a_n\}$ and $\{b_n\}$, and $U$ denotes the unitary transformation of $\ell^2$, given by $(U\psi)_n = (-1)^n \psi_n$, then

$$U J_{\{a_n\},\{b_n\}} U = -J_{\{a_n\},\{-b_n\}}.$$

We will therefore restrict our attention in what follows to the case $b > 0$. Consider solutions of the difference equation

$$a_n u_{n+1} + b_n u_n + a_{n-1} u_{n-1} = E u_n. \tag{6}$$

Defining

$$U_n = \begin{pmatrix} u_{n-1} \\ u_n \end{pmatrix},$$

the recursion (6) is equivalent to

$$U_{n+1} = T_n U_n,$$

where

$$T_n = \begin{pmatrix} 0 & 1 \\ -\frac{a_{n-1}}{a_n} & \frac{E-b_n}{a_n} \end{pmatrix}.$$

Let

$$B_n = T_{2n} T_{2n-1},$$

so that

$$U_{2n+1} = (B_n \times \cdots \times B_1) U_1. \tag{7}$$

We have

$$\begin{aligned} B_n &= \begin{pmatrix} 0 & 1 \\ -(1-\frac{1}{2n})^\alpha & \frac{E}{(2n)^\alpha} \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -(1-\frac{1}{2n-1})^\alpha & \frac{E-b(2n-1)^\alpha}{(2n-1)^\alpha} \end{pmatrix} \\ &= \begin{pmatrix} -1 & -b \\ 0 & -1 \end{pmatrix} + \frac{1}{(2n)^\alpha} \begin{pmatrix} 0 & E \\ -E & -bE \end{pmatrix} + \frac{1}{2n} \begin{pmatrix} \alpha & 0 \\ 0 & \alpha \end{pmatrix} + O(n^{-2\alpha}). \end{aligned}$$

We see from (7) that we should study the product of the form $B_n \times \cdots \times B_1$. However, we shall study a slightly different sequence of products whose usefulness will become clearer below. To define this auxiliary problem, we have to introduce a few matrices. Let

$$C_n = \begin{pmatrix} 1 & -b \\ 1 & 0 \end{pmatrix} + \frac{1}{(2n)^\alpha} \begin{pmatrix} bE + E/(2b) & 0 \\ E/(2b) & -E/2 \end{pmatrix} + \frac{1}{2n} \begin{pmatrix} 0 & 0 \\ -\alpha & \alpha b \end{pmatrix}$$

and

$$\tilde{B}_n = \begin{pmatrix} 0 & 1 \\ -1 & 2 \end{pmatrix} + \frac{1}{(2n)^\alpha} \begin{pmatrix} 0 & 0 \\ 0 & bE \end{pmatrix} + \frac{1}{n} \begin{pmatrix} 0 & 0 \\ \alpha & -\alpha \end{pmatrix}.$$

**Lemma 2.1.** *We have*

$$C_n B_n C_n^{-1} = -\tilde{B}_n + O(n^{-2\alpha}).$$

*Proof.* This is tedious but straightforward. □

## 3. The Absolutely Continuous Spectrum and Solution Asymptotics at Negative Energies

Motivated by (7) and Lemma 2.1, we will study asymptotics for the auxiliary problem

$$V_{n+1} = (\tilde{B}_n \times \cdots \times \tilde{B}_1) V_1. \tag{8}$$

This problem is a more general version of the one studied in [9, Section 3]. There, products of matrices of the form

$$\hat{B}_n = \begin{pmatrix} 0 & 1 \\ -1 & 2 \end{pmatrix} + \frac{1}{n} \begin{pmatrix} 0 & 0 \\ 1 & \lambda \end{pmatrix}$$

were studied. We will employ a similar strategy to find solution asymtotics for the more general problem at hand. This explains why we introduced the matrices $\tilde{B}_n$ and derived Lemma 2.1 in the previous section.

**Theorem 2.** *Suppose that $2/3 < \alpha \le 1$ and $b > 0$. Then, for every $E < 0$, (8) has two linearly independent solutions*

$$V_n^{\pm} = \begin{pmatrix} v_{n-1}^{\pm} \\ v_n^{\pm} \end{pmatrix} \tag{9}$$

*with asymptotics given by*

$$v_n^{\pm} = n^{-\alpha/4} \exp\left( \pm i \frac{\sqrt{-bE}}{2^{\alpha/2}} \cdot \frac{n^{1-\frac{\alpha}{2}}}{1-\frac{\alpha}{2}} \right) (1 + o(1)) \text{ as } n \to \infty. \tag{10}$$

*Proof.* We make the ansatz

$$z_n = n^{\gamma} \exp\left(A n^{\delta}\right)$$

and define the matrix

$$S_n = \begin{pmatrix} \overline{z_{n-1}} & z_{n-1} \\ \overline{z_n} & z_n \end{pmatrix}.$$

Our goal is to choose $\gamma, A, \delta$ such that

$$S_{n+1}^{-1} \tilde{B}_n S_n = I + R_n,\ \{\|R_n\|\} \in \ell^1. \tag{11}$$

Consequently, an arbitrary non-trivial solution of (8) has the form $V_n = S_n W_n$, where $W_n$ is a sequence of vectors which tends to a non-zero vector $W$. Since (11) will be shown to hold if we let

$$\gamma = -\frac{\alpha}{4},\ A = \frac{\sqrt{bE}}{2^{\alpha/2}(1-\frac{\alpha}{2})},\ \delta = 1 - \frac{\alpha}{2}, \tag{12}$$

the assertion of the theorem then follows immediately.

Let us consider the matrix $S_{n+1}^{-1} \tilde{B}_n S_n$. It is readily checked that

$$S_{n+1}^{-1} \begin{pmatrix} 0 & 1 \\ -1 & 2 \end{pmatrix} S_n = (\det S_{n+1})^{-1} \begin{pmatrix} x_n & y_n \\ -\overline{y_n} & -\overline{x_n} \end{pmatrix},$$

where

$$x_n = z_n \overline{z_{n-1}} + \overline{z_n} z_{n+1} - 2|z_n|^2,$$
$$y_n = z_n z_{n-1} + z_n z_{n+1} - 2 z_n^2,$$

and

$$S_{n+1}^{-1} \begin{pmatrix} 0 & 0 \\ a & b \end{pmatrix} S_n = (\det S_{n+1})^{-1} \begin{pmatrix} s_n & t_n \\ -\overline{t_n} & -\overline{s_n} \end{pmatrix},$$

where

$$s_n = -a z_n \overline{z_{n-1}} - b|z_n|^2,$$
$$t_n = -a z_n z_{n-1} - b z_n^2.$$

Putting this together, we obtain

$$S_{n+1}^{-1} \tilde{B}_n S_n = (\det S_{n+1})^{-1} \begin{pmatrix} a_n & b_n \\ -\overline{b_n} & -\overline{a_n} \end{pmatrix},$$

where

$$a_n = z_n\overline{z_{n-1}} + \overline{z_n}z_{n+1} - 2|z_n|^2 + \tfrac{1}{(2n)^\alpha}\left[-bE|z_n|^2\right] + \tfrac{1}{n}\left[-\alpha z_n\overline{z_{n-1}} + \alpha|z_n|^2\right],$$
$$b_n = z_n z_{n-1} + z_n z_{n+1} - 2z_n^2 + \tfrac{1}{(2n)^\alpha}\left[-bE z_n^2\right] + \tfrac{1}{n}\left[-\alpha z_n z_{n-1} + \alpha z_n^2\right].$$

We consider first the off-diagonal elements of $S_{n+1}^{-1}\tilde{B}_n S_n$:

$$(\det S_{n+1})^{-1} b_n = \frac{z_n z_{n-1} + z_n z_{n+1} - 2z_n^2 - \frac{bE}{(2n)^\alpha} z_n^2 + \frac{\alpha}{n}\left[z_n^2 - z_n z_{n-1}\right]}{z_{n+1}\overline{z_n} - \overline{z_{n+1}} z_n}$$
$$= \frac{z_n^{-1} z_{n-1} + z_n^{-1} z_{n+1} - 2 - \frac{bE}{(2n)^\alpha} + \frac{\alpha}{n}\left[1 - z_n^{-1} z_{n-1}\right]}{z_{n+1}\overline{z_n} z_n^{-2} - \overline{z_{n+1}} z_n^{-1}}.$$

For the denominator in the last expression, we find

$$z_{n+1}\overline{z_n} z_n^{-2} - \overline{z_{n+1}} z_n^{-1} = 2A\delta n^{\delta-1}(1 + o(1)),$$

provided we choose $\delta$ as in (12) (which implies $1/2 \le \delta \le 2/3$).

For the numerator, we find after lengthy but straightforward calculations,

$$z_n^{-1} z_{n-1} + z_n^{-1} z_{n+1} - 2 - \tfrac{bE}{(2n)^\alpha} + \tfrac{\alpha}{n} - \tfrac{\alpha}{n} z_n^{-1} z_{n-1} = X n^{\delta-2} + Y n^{2\delta-2} + O(n^{4\delta-4}),$$

where

$$X = A\delta(\delta - 1) + 2\gamma A\delta + \alpha A\delta, \quad Y = (A\delta)^2 - \frac{bE}{2^\alpha}.$$

If $\gamma, A, \delta$ are chosen as in (12), then $X = Y = 0$ and hence

$$(\det S_{n+1})^{-1} b_n = O\left(n^{3\delta-3}\right) = O\left(n^{-\frac{3}{2}\alpha}\right),$$

which is summable by our assumption on $\alpha$.

Next, we consider the diagonal elements of $S_{n+1}^{-1}\tilde{B}_n S_n$:

$$|a_n - \det S_{n+1}| = \left| z_n\overline{z_{n-1}} + \overline{z_{n+1}} z_n - 2|z_n|^2 - \tfrac{bE|z_n|^2}{(2n)^\alpha} + \tfrac{\alpha}{n}\left[-z_n\overline{z_{n-1}} + |z_n|^2\right]\right|$$
$$= \left|\overline{z_n} z_{n-1} + z_{n+1}\overline{z_n} - 2|z_n|^2 - \tfrac{bE|z_n|^2}{(2n)^\alpha} + \tfrac{\alpha}{n}\left[-\overline{z_n} z_{n-1} + |z_n|^2\right]\right|$$
$$= \left| z_n z_{n-1} + z_n z_{n+1} - 2z_n^2 - \tfrac{bE z_n^2}{(2n)^\alpha} + \tfrac{\alpha}{n}\left[-z_n z_{n-1} + z_n^2\right]\right|$$
$$= |b_n|,$$

and hence $\left|(\det S_{n+1})^{-1} a_n - 1\right| = \left|(\det S_{n+1})^{-1} b_n\right|$. This shows that (11) holds, concluding the proof. $\square$

The special case $\alpha = 1$ deserves an additional remark. Theorem 2 above gives the asymptotics

$$n^{-1/4} \exp\left(\pm i\sqrt{-2bEn}\right)(1 + o(1)) \text{ as } n \to \infty \tag{13}$$

for a pair of linearly independent solutions of the auxiliary problem (8). This can also be shown by an application of the Birkhoff-Adams Theorem; see [5, Theorem 8.36]. The latter result concerns second-order difference equations of the form

$$x(n+2) + p_1(n)x(n+1) + p_2(n)x(n) = 0, \tag{14}$$

where $p_1(n)$ and $p_2(n)$ have asymptotic expansions

$$p_1(n) = \sum_{j=0}^{\infty} \frac{c_j}{n^j}, \quad p_2(n) = \sum_{j=0}^{\infty} \frac{d_j}{n^j}$$

with $d_0 \neq 0$. In our situation, we have

$$c_0 = -2, \quad c_1 = 1 - \frac{bE}{2}, \quad d_0 = 1, \quad d_1 = -1.$$

We have to compute the roots $\lambda_1, \lambda_2$ of the characteristic equation $\lambda^2 + c_0\lambda + d_0 = 0$ and find $\lambda_1 = \lambda_2 = 1$. Moreover, if $E \neq 0$, we have $2d_1 \neq c_0 c_1$. Thus, part (b) of [5, Theorem 8.36] tells us that there are two linearly independent solutions $x_1(n)$, $x_2(n)$ of (14) whose asymptotics are given by (13). (Note, however, that there is a misprint in formula (8.6.7) of [5]: $n^{\gamma_i}$ should be replaced by $n^{\alpha}$.)

**Theorem 3.** *Suppose that $2/3 < \alpha \leq 1$ and $b > 0$. Then, for every $E < 0$, (7) has two linearly independent solutions*

$$U^{\pm}_{2n+1} = \begin{pmatrix} u^{\pm}_{2n} \\ u^{\pm}_{2n+1} \end{pmatrix}$$

*with asymptotics given by*

$$U^{\pm}_{2n+1} = (-1)^n T V^{\pm}_n (1 + o(1)),$$

*where*

$$T = \frac{1}{b} \begin{pmatrix} 0 & b \\ -1 & 1 \end{pmatrix}$$

*and $V^{\pm}_n$ are given by (9) and (10). Moreover, the spectrum of $J$ is purely absolutely continuous on $(-\infty, 0)$.*

*Proof.* By standard results of asymptotic analysis (centered around Levinson's Theorem; compare [5, Section 8.3] and [6]), Lemma 2.1 implies that the solutions of (7) behave asymptotically like the solutions of the system

$$\tilde{U}_{2n+1} = \left[ (-C_n^{-1} \tilde{B}_n C_n) \times \cdots \times (-C_1^{-1} \tilde{B}_1 C_1) \right] \tilde{U}_1.$$

Since $C_m C_{m-1}^{-1} = I + O(m^{-2})$, we may as well consider the system

$$\hat{U}_{2n+1} = (-1)^n C_n^{-1} \left[ \tilde{B}_n \times \cdots \times \tilde{B}_1 \right] \hat{U}_1.$$

Now the first assertion is an immediate consequence of Theorem 2.

To prove that the spectrum of $J$ is purely absolutely continuous on $(-\infty, 0)$, it suffices to show that for every $E < 0$, there does not exist a subordinate solution of (6) in the sense of Gilbert-Pearson (cf. [7]; see also [13, 14]). Thus, we claim that for every pair of non-trivial solutions $u^{(1)}$, $u^{(2)}$ of (6), we have

$$\limsup_{N \to \infty} \left[ \frac{\sum_{n=1}^{N} \left| u_n^{(1)} \right|^2}{\sum_{n=1}^{N} \left| u_n^{(2)} \right|^2} \right] > 0. \tag{15}$$

Since every solution $u$ of (6) is given by a linear combination of the two solutions whose asymptotic behavior is given by $(-1)^n T V^{\pm}_n (1 + o(1))$, there are ($u$-dependent) positive constants $C_1, C_2$ such that

$$C_1 N^{1-\frac{\alpha}{2}} \leq \sum_{n=1}^{N} |u_n|^2 \leq C_2 N^{1-\frac{\alpha}{2}}.$$

From this, (15) follows immediately. $\square$

## 4. Solution Asymptotics at Zero Energy

In this section we study the asymptotics of the matrix product $B_n \times \cdots \times B_1$, and hence the asymptotics of solutions, for $E = 0$. We show in particular that there are no non-trivial solutions in $\ell^2$.

**Theorem 4.** *For zero energy, $E = 0$, the difference equation* (6) *has two linearly independent solutions $u_n^{(j)}$, $j = 1, 2$, with asymptotics given by*

$$\begin{pmatrix} u_{2n}^{(1)} \\ u_{2n+1}^{(1)} \end{pmatrix} = \begin{pmatrix} (-1)^n n^{-\frac{\alpha}{2}}(1 + o(1)) \\ 0 \end{pmatrix}$$

*and*

$$\begin{pmatrix} u_{2n}^{(2)} \\ u_{2n+1}^{(2)} \end{pmatrix} = \begin{pmatrix} (-1)^n \left[ bn^{1-\frac{\alpha}{2}} + O(n^{-\frac{\alpha}{2}} \log n) \right] (1 + o(1)) \\ (-1)^n n^{-\frac{\alpha}{2}}(1 + o(1)) \end{pmatrix}.$$

*In particular, zero is not an eigenvalue of $J$.*

*Proof.* We have

$$\begin{aligned} B_n &= \begin{pmatrix} 0 & 1 \\ -(1 - \frac{1}{2n})^\alpha & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ -(1 - \frac{1}{2n-1})^\alpha & -b \end{pmatrix} \\ &= \begin{pmatrix} -1 & -b \\ 0 & -1 \end{pmatrix} + \begin{pmatrix} \frac{\alpha}{2n} & 0 \\ 0 & \frac{\alpha}{2n} \end{pmatrix} + O(n^{-2}) \begin{pmatrix} r_n & 0 \\ 0 & s_n \end{pmatrix} \end{aligned}$$

with bounded sequences $\{r_n\}$, $\{s_n\}$.

That is,

$$B_n = -M_b + \frac{\alpha}{2n} I + \begin{pmatrix} O(n^{-2}) & 0 \\ 0 & O(n^{-2}) \end{pmatrix}, \text{ where } M_b = \begin{pmatrix} 1 & b \\ 0 & 1 \end{pmatrix}.$$

Therefore,

$$B_n \times \cdots \times B_1 = (-1)^n M_b^n \left( M_b^{-n}(-B_n) M_b^{n-1} \right) \times \cdots \times \left( M_b^{-1}(-B_1) M_b^0 \right).$$

Since

$$M_b^{-j}(-B_j) M_b^{j-1} = I - \frac{\alpha}{2j} \begin{pmatrix} 1 & -b \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} O(j^{-2}) & O(j^{-1}) \\ 0 & O(j^{-2}) \end{pmatrix},$$

we obtain

$$B_n \times \cdots \times B_1 = (-1)^n \begin{pmatrix} 1 & bn \\ 0 & 1 \end{pmatrix} \left[ \prod_{j=1}^n \left( 1 - \frac{\alpha}{2j} \right) \right] U_n,$$

where

$$\begin{aligned} U_n &= \prod_{j=1}^n \left[ \begin{pmatrix} 1 + O(j^{-2}) & 0 \\ 0 & 1 + O(j^{-2}) \end{pmatrix} + \begin{pmatrix} 0 & O(j^{-1}) \\ 0 & 0 \end{pmatrix} \right] \\ &= \begin{pmatrix} C_1 + o(1) & O(\log n) \\ 0 & C_2 + o(1) \end{pmatrix}. \end{aligned}$$

Here, $C_1, C_2$ are suitable non-zero constants.

On the other hand,

$$\prod_{j=1}^n \left( 1 - \frac{\alpha}{2j} \right) = n^{-\frac{\alpha}{2}} (C_3 + o(1))$$

with a suitable constant $C_3 \neq 0$.

Putting everything together, we find that

$$B_n \times \cdots \times B_1 = (-1)^n n^{-\frac{\alpha}{2}} \begin{pmatrix} C_1C_3 + o(1) & C_2C_3bn + O(\log n) \\ 0 & C_2C_3 + o(1) \end{pmatrix}.$$

The assertion follows. □

## 5. The Discrete Spectrum

In this section we study positive energies and prove that the spectrum in $(0, \infty)$ is purely discrete and accumulates only at $\infty$. Moreover, we provide upper and lower bounds for eigenvalues.

Fix the parameters $b > 0$ and $0 < \alpha \leq 1$. For $a > 0$, we define

$$\mathcal{H}_a^{(1)} = \operatorname{span}\left\{\delta_{2n-1} : 1 \leq n \leq \frac{1}{2}\left(\frac{2a}{b}\right)^{1/\alpha}\right\}, \quad \mathcal{H}_a^{(2)} = \left(\mathcal{H}_a^{(1)}\right)^{\perp}.$$

**Lemma 5.1.** *For $a > 0$ and $\psi \in \mathcal{H}_a^{(2)} \cap D(J)$, we have $\|(J - aI)\psi\| \geq a\|\psi\|$.*

*Proof.* Consider the even and odd subspaces of $\ell^2$,

$$\ell^2_{\mathrm{e}} = \{f \in \ell^2 : f_{2n-1} = 0 \ \forall n \in \mathbb{Z}_+\}, \quad \ell^2_{\mathrm{o}} = \{f \in \ell^2 : f_{2n} = 0 \ \forall n \in \mathbb{Z}_+\}$$

and the respective orthogonal projections, $P_{\mathrm{e}}$ and $P_{\mathrm{o}}$. We write a vector $\psi \in \ell^2$ as $\psi = \psi_{\mathrm{e}} + \psi_{\mathrm{o}} = P_{\mathrm{e}}\psi + P_{\mathrm{o}}\psi$.

Let $S$ be the shift, given by $(S\psi)_n = \psi_{n+1}$, and let $A$ and $B$ be diagonal matrices with $A_{n,n} = a_n$ and $B_{n,n} = b_n$, respectively. Then we can write the Jacobi matrix $J$ in the form

$$J = SA + AS^* + B.$$

If we write

$$J - aI = \left(\begin{array}{c|c} P_{\mathrm{o}}(J - aI)P_{\mathrm{o}} & P_{\mathrm{o}}(J - aI)P_{\mathrm{e}} \\ \hline P_{\mathrm{e}}(J - aI)P_{\mathrm{o}} & P_{\mathrm{e}}(J - aI)P_{\mathrm{e}} \end{array}\right)$$

and use

$$BP_{\mathrm{e}} = 0, \ P_{\mathrm{o}}(SA + AS^*)P_{\mathrm{o}} = 0, \ P_{\mathrm{e}}(SA + AS^*)P_{\mathrm{e}} = 0,$$

we obtain

$$J - aI = \left(\begin{array}{c|c} (B - aI)P_{\mathrm{o}} & P_{\mathrm{o}}J_AP_{\mathrm{e}} \\ \hline P_{\mathrm{e}}J_AP_{\mathrm{o}} & -aP_{\mathrm{e}} \end{array}\right).$$

Here, $J_A$ denotes the matrix $SA + AS^*$. This yields

$$(J-aI)^2 - a^2I = \left(\begin{array}{c|c} (B^2 - 2aB)P_{\mathrm{o}} + (P_{\mathrm{e}}\ J_AP_{\mathrm{o}})^*(P_{\mathrm{e}}J_AP_{\mathrm{o}}) & (B - aI)P_{\mathrm{o}}J_AP_{\mathrm{e}} - aP_{\mathrm{o}}J_AP_{\mathrm{e}} \\ \hline P_{\mathrm{e}}J_AP_{\mathrm{o}}(B - aI)P_{\mathrm{o}} - aP_{\mathrm{e}}J_AP_{\mathrm{o}} & (P_{\mathrm{o}}J_AP_{\mathrm{e}})^*(P_{\mathrm{o}}J_AP_{\mathrm{e}}) \end{array}\right)$$

We want to show that

$$\langle[(J - aI)^2 - a^2I]\psi, \psi\rangle \geq 0 \text{ for } \psi \in \mathcal{H}_a^{(2)}. \tag{16}$$

Observe first that

$$(B^2 - 2aB)P_{\mathrm{o}} \geq 0 \text{ on } \mathcal{H}_a^{(2)}, \tag{17}$$

since

$$(b(2n - 1)^{\alpha})^2 - 2ab(2n - 1)^{\alpha} \geq 0 \Leftrightarrow 2n - 1 \geq \left(\frac{2a}{b}\right)^{1/\alpha}.$$

Now, let $\psi \in \mathcal{H}_a^{(2)} \cap D(J)$ be given and write

$$\psi_{\mathrm{e}} = P_{\mathrm{e}}\psi, \ \psi_{\mathrm{o}} = P_{\mathrm{o}}\psi, \ \phi_{\mathrm{e}} = P_{\mathrm{e}}J_A\psi_{\mathrm{o}}, \ \phi_{\mathrm{o}} = P_{\mathrm{o}}J_A\psi_{\mathrm{e}}.$$

Then
$\langle [(J-aI)^2 - a^2 I]\psi, \psi\rangle = \langle (B^2 - 2aB)\psi_{\mathrm{o}}, \psi_{\mathrm{o}}\rangle + \|\phi_{\mathrm{e}}\|^2 + \|\phi_{\mathrm{o}}\|^2 + 2\mathrm{Re}\langle (B-2a)\phi_{\mathrm{o}}, \psi_{\mathrm{o}}\rangle.$
In view of (17), (16) follows from this once we show that

$$|\langle (B-2a)\phi_{\mathrm{o}}, \psi_{\mathrm{o}}\rangle| \le \frac{1}{2}\left[\langle (B^2 - 2aB)\psi_{\mathrm{o}}, \psi_{\mathrm{o}}\rangle + \|\phi_{\mathrm{e}}\|^2 + \|\phi_{\mathrm{o}}\|^2\right]. \tag{18}$$

Since

$$|\langle (B-2a)\phi_{\mathrm{o}}, \psi_{\mathrm{o}}\rangle| \le \|\phi_{\mathrm{o}}\| \cdot \|(B-2a)\psi_{\mathrm{o}}\| \le \frac{1}{2}\|\phi_{\mathrm{o}}\|^2 + \frac{1}{2} \cdot \|(B-2a)\psi_{\mathrm{o}}\|^2,$$

(18) follows from

$$\frac{1}{2} \cdot \|(B-2a)\psi_{\mathrm{o}}\|^2 \le \langle (B^2 - 2aB)\psi_{\mathrm{o}}, \psi_{\mathrm{o}}\rangle. \tag{19}$$

But (19) is a consequence of

$$0 \le \langle (B^2 - 4a^2)\psi_{\mathrm{o}}, \psi_{\mathrm{o}}\rangle$$

which in turn follows immediately from the assumption $\psi \in \mathcal{H}_a^{(2)}$. □

The following theorem describes the positive spectrum of $J$, which turns out to be discrete in $[0, \infty)$. It is therefore interesting to study the distribution of eigenvalues

$$0 < E_1(b) < E_2(b) < \cdots$$

Note that all eigenvalues must be simple. Let $N(E)$ denote the number of eigenvalues of $J$ in the interval $(0, E)$.

**Theorem 5.** *Let $0 < \alpha \le 1$ and $b > 0$.*
(a) *$\sigma(J) \cap (0, \infty)$ is discrete and can accumulate only at $\infty$, not at 0.*
(b) *The eigenvalue counting function $N$ obeys the estimate*

$$N(E) \le \frac{1}{2}\left(\frac{E}{b}\right)^{\frac{1}{\alpha}}.$$

(c) *The $n$-th eigenvalue, $E_n(b)$, obeys the lower bound*

$$E_n(b) \ge 2^\alpha b n^\alpha.$$

(d) *If $b \ge \sqrt{6}$, then*

$$E_n(b) \le \frac{2^{2+\alpha}}{(3^{1/\alpha} - 1)^\alpha} b n^\alpha.$$

(e) *If $b < \sqrt{6}$, then*

$$E_n(b) \le C b^{1-2\alpha} n^\alpha$$

*for some constant $C > 0$.*

*Proof.* (a) and (b) are immediate consequences of Lemma 5.1: On $\mathcal{H}_a^{(2)}$, we have $(J-aI)^2 \ge a^2$, and hence the dimension of the range of the spectral projection of $J$ onto the interval $(0, 2a)$ is bounded by

$$\dim \mathcal{H}_a^{(1)} = \frac{1}{2}\left(\frac{2a}{b}\right)^{1/\alpha}.$$

(c) follows from (b): For $\varepsilon > 0$, we have

$$n = N(E_n(b) + \varepsilon) \le \frac{1}{2}\left(\frac{E_n(b) + \varepsilon}{b}\right)^{1/\alpha},$$

and hence

$$E_n(b) + \varepsilon \geq 2^\alpha b n^\alpha.$$

Now let $\varepsilon$ go to zero. This yields the claimed lower bound for $E_n(b)$.

In order to prove the upper bounds in (d) and (e), we note the following. If, for $n \geq 1$ and $a > 0$, we can find test functions $f^{(1)}, \dots, f^{(n)}$ with disjoint supports obeying the estimate

$$\|(J - aI)f^{(k)}\|^2 \leq a^2 \|f^{(k)}\|^2 \tag{20}$$

for $1 \leq k \leq n$, then $E_n(b) \leq 2a$.

We first prove the estimate in (d). Our test functions will be of the form $\delta_{2m-1}$, where $m$ is chosen such that

$$|b(2m-1)^\alpha - a| < \frac{a}{2}.$$

Equivalently,

$$\left(\frac{a}{2b}\right)^{1/\alpha} < 2m - 1 < \left(\frac{3a}{2b}\right)^{1/\alpha}. \tag{21}$$

For these test functions, we have

$$\begin{aligned}\|(J - aI)\delta_{2m-1}\|^2 - a^2\|\delta_{2m-1}\|^2 &\leq 2(2m-1)^{2\alpha} + |b(2m-1)^\alpha - a|^2 - a^2 \\ &< \frac{9a^2}{2b^2} + \frac{a^2}{4} - a^2.\end{aligned}$$

If $b \geq \sqrt{6}$, this shows that $\|(J - aI)\delta_{2m-1}\|^2 - a^2\|\delta_{2m-1}\|^2$ is negative. Note that the number of test functions we obtain this way, $n$, is restricted by the condition

$$n \leq \frac{1}{2}\left[\left(\frac{3a}{2b}\right)^{1/\alpha} - \left(\frac{a}{2b}\right)^{1/\alpha}\right].$$

Thus, if we choose

$$a \geq 2b\left(\frac{2n}{3^{1/\alpha} - 1}\right)^\alpha,$$

we can find $n$ test functions with disjoint supports obeying (20). This yields the estimate in (d).

Let us turn to part (e). Again, our test functions will be supported on odd sites $2m - 1$, subject to (21). We partition the interval in (21) into $n$ subintervals $J_1, \dots, J_n$ of equal size, roughly given by

$$\Delta_n = \frac{1}{n}\left[\left(\frac{3a}{2b}\right)^{1/\alpha} - \left(\frac{a}{2b}\right)^{1/\alpha}\right].$$

Since we need this to be at least 2, we get a first condition for $a$:

$$\Delta_n \geq 2. \tag{22}$$

We will return to this condition below.

The function $f^{(k)}$ will be supported on the odd sites within $J_k$ and on these sites, it alternates between the values 1 and $-1$. Our goal is to prove the estimate (20). By definition of $f^{(k)}$, we have that

$$\|f^{(k)}\|^2 \approx \frac{\Delta_n}{2}.$$

Using the fact that $J_k$ lies within the interval (21), we obtain

$$\begin{aligned}\|(J-aI)f^{(k)}\|^2 &\le \Delta_n \cdot \sup_{2m-1\in J_k} |b(2m-1)^\alpha - a|^2 + \text{const} \cdot \sup_{2m-1\in J_k} (2m)^{2\alpha} + \\ &\quad + \sum_{2m-1\in J_k} |(2m+1)^\alpha - (2m-1)^\alpha|^2 \\ &\le \Delta_n \frac{a^2}{4} + \text{const} \cdot \left[\left(\frac{3a}{2b}\right)^{1/\alpha}\right]^{2\alpha} + \text{const} \cdot \Delta_n \sup_{2m-1\in J_k} (2m-1)^{2(\alpha-1)}\end{aligned}$$

with suitable uniform constants. Thus, in order to satisfy (20), we need

$$\text{const} \cdot \left[\left(\frac{3a}{2b}\right)^2 + \Delta_n \sup_{2m-1\in J_k} (2m-1)^{2(\alpha-1)}\right] \le \Delta_n \frac{a^2}{4}. \tag{23}$$

Let us first prove

$$\text{const} \cdot \left(\frac{3a}{2b}\right)^2 \le \Delta_n \frac{a^2}{8}. \tag{24}$$

This inequality is equivalent to

$$\left(\frac{18 \cdot \text{const}}{\left(\frac{3}{2}\right)^{1/\alpha} - \left(\frac{1}{2}\right)^{1/\alpha}}\right)^\alpha b^{1-2\alpha} n^\alpha \le a. \tag{25}$$

Note that the factor in front of $b^{1-2\alpha}$ is uniformly bounded from above by some $C > 0$ for all $\alpha \in (0,1]$.

Since, by (21), $2m-1 \ge \left(\frac{a}{2b}\right)^{1/\alpha}$ on $J_k$, we have

$$\Delta_n \sup_{2m-1\in J_k} (2m-1)^{2(\alpha-1)} \le \Delta_n \left[\left(\frac{a}{2b}\right)^{1/\alpha}\right]^{2(\alpha-1)}$$

Thus, to complement (24), it suffices to show

$$\text{const} \cdot \Delta_n \left(\frac{a}{2b}\right)^{\frac{2(\alpha-1)}{\alpha}} \le \Delta_n \frac{a^2}{8} \tag{26}$$

This inequality is equivalent to

$$(8 \cdot \text{const})^{\alpha/2} (2b)^{1-\alpha} \le a. \tag{27}$$

Since we already have the condition $a \ge C \cdot b^{1-2\alpha}$ from (25), (27) is automatically satisfied if $C$ obeys, in addition to the property above,

$$C \ge \max_{0<\alpha\le 1} 8 \cdot \text{const}^{\alpha/2} 2^{1-\alpha} (\sqrt{6})^\alpha.$$

(Here we used $b \le \sqrt{6}$.)

Finally, we need to satisfy (22). Using $a \ge C b^{1-2\alpha} n^\alpha$, one checks that $\Delta_n \ge 2$ holds as long as

$$\frac{C\left[\left(\frac{3}{2}\right)^{1/\alpha} - \left(\frac{1}{2}\right)^{1/\alpha}\right]^\alpha}{2^\alpha (\sqrt{6})^{2\alpha}} \ge 1.$$

(Here we used again that $b \le \sqrt{6}$.) This can again be satisfied uniformly in $\alpha \in (0,1]$ by choosing $C$ large enough.

Putting everything together, if $C$ is so large that it satisfies the three properties found above, then for

$$a \geq C b^{1-2\alpha} n^{\alpha},$$

we can find $n$ test functions $f^{(1)}, \ldots, f^{(n)}$ obeying (20). $\square$

## 6. Open Problems

In this section we list a number of questions and directions for future research that are suggested by our and previous work.

(1) More general entries: We expect that one can relax the assumption $\mu_n = r_n = n^{\alpha}$ and perform a similar analysis, akin to [10], for more general unbounded sequences.
(2) The $n$-dependence of $E_n(b)$: In fact, a stronger statement on the behavior of $E_n(b)$ for large $n$ would be desirable. Is it possible to find a function $F(b)$ such that $E_n(b) \sim F(b)n^{\alpha}$ (in the sense that $E_n(b)F(b)^{-1}n^{-\alpha} \to 1$ as $n \to \infty$)?
(3) The $b$-dependence of $E_n(b)$: Some improved estimates on the dependence of $E_n(b)$ on $b$ would be of interest; especially in the case $\alpha \in (1/2, 1)$ for which the statement in Theorem 5.(e) does not appear to be optimal.
(4) Eigenfunction asymptotics for positive energies: We established explicit asymptotics of the solutions to the associated difference equation for all energies in $(-\infty, 0]$. Is it possible to prove similar results for energies in $(0, \infty)$? We would expect the formula from Theorem 2 to hold also for positive energies.
(5) More detailed questions as $\tilde{b}$ crosses zero: Combining the results of [10] and the present paper, we obtain a rather detailed picture of the spectrum and the spectral type as $\tilde{b}$ makes a transition through the critical value $\tilde{b} = 0$ (cf. the discussion at the end of Section 1). This suggests that even more detailed questions could be addressed. For example, what happens to the spectral function as $\tilde{b}$ passes through zero? Do we see some concentration at the eventual eigenvalues?

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