

Research Article

A Note on the Asymptotic and Threshold Behaviour of Discrete Eigenvalues inside the Spectral Gaps of the Difference Operator with a Periodic Potential

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Received 1 August 2017; Revised 10 January 2018; Accepted 28 January 2018; Published 22 February 2018

Academic Editor: Antonio Scarfone

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The asymptotic and threshold behaviour of the eigenvalues of a perturbed difference operator inside a spectral gap is investigated. In particular, applications of the Titchmarsh-Weyl m -function theory as well as the Birman-Schwinger principle is performed to investigate the existence and behaviour of the eigenvalues of the operator $H_0 + \lambda W_n$ inside the spectral gap of H_0 in the limits $\lambda \uparrow \infty$ and $\lambda \downarrow 0$.

1. Introduction

We consider the Schrödinger difference equation

$$H_\lambda u = (H_0 + \lambda W_n) u_n = E u_n, \quad n \in [0, \infty), \quad (1)$$

in the Hilbert space $l^2(\mathbb{Z})$ of all square summable sequences $\{x_n\}_1^\infty$ such that $\sum_1^\infty |x_n|^2 < \infty$. Here, $H_0 = -\Delta + V_n$, the Laplacian $-\Delta$ is a second-order finite difference operator given by $(-\Delta u)(n) := -u_{n+1} + 2u_n - u_{n-1}$. The operator H_0 describes a well-understood system with V_n being the background periodic or quasi-periodic potential. The parameter λ , called the coupling constant, is real and positive and E is a complex parameter. The sequences $\{V_n\}_0^\infty$ are real and are such that $V_{a+n} = V_a$, for some $a \in \mathbb{Z}^+$. The perturbing term W_n satisfies the scattering condition

$$\sum_{n=0}^{\infty} n |W_n| < \infty. \quad (2)$$

The domain D_{H_λ} of H_λ consists of all $x \in l^2(\mathbb{Z})$ such that $H_\lambda x \in l^2(\mathbb{Z})$. The operators H_λ and H_0 are known to be self-adjoint [1, 2].

Operators of the form $H_\lambda = H_0 + \lambda W$, either in the difference or in the continuum form, occur frequently in

quantum mechanics as mathematical models of Schrödinger type that models semiconductors with impurities [1, 3]. The impurity levels in solids reduce the width of the gap where they are situated, and this feature has important consequences from the point of view of conductivity properties of the solids. Furthermore, such impurity levels lead to a selective absorption of certain photon energies which is an important element in the theory of crystal colours. Perhaps the most appealing example in nature is the Al_2O_3 crystal, which has a large gap between the first and the second bands: it is transparent and colourless. By replacing the Al^+ -ion by Cr^{3+} , one obtains a familiar complementary colour red, and this is due to the fact that the impurity levels lead to the absorption of green light [4, 5]. Recent and relevant results on the application of the solutions of Schrödinger equations with physical potential models in the field of thermal physics, for example, can be found in the work of Jia et al. [6–9].

The spectrum $\rho(H_0)$ of the self-adjoint operator H_0 is real and consists of two absolutely continuous bands separated by a gap. By a spectral gap of H_0 , we mean an interval (a, b) such that $a < b$, $a, b \in \rho(H_0)$, and $(a, b) \cap \rho(H_0) = \emptyset$. We choose our V_n 's such that the gaps are empty when $\lambda = 0$. For $\lambda > 0$, the spectrum of H_λ is made up of the continuous part which coincides with that of $\rho(H_0)$ together with at most a finite number of eigenvalues inside the gap of $\rho(H_0)$

[3, 10–12]. Of interest to this work are the conditions on W_n guaranteeing the existence of such eigenvalues and their asymptotic behaviour as λ varies.

The case where V_n is not periodic but decays fast enough to zero as $n \rightarrow 0$ was studied in [13], and a formula of the type known as Levinson's theorem was derived which counts the number of eigenvalues or bound states outside the continuous band $[0, 4]$. We would like to obtain the corresponding results when V_n is periodic and determine how those eigenvalues vary as the coupling constant becomes large and small. Some results do exist for the Schrödinger case; however, in the discrete case this has not been looked at (see, e.g., [3]).

Since there are no eigenvalues when $\lambda = 0$, by general results of perturbation theory, eigenvalues of H_λ can appear in a gap only by emerging from one of its end points as λ is varied. Likewise, eigenvalues can disappear from the gap only by converging to an end point [14–18]. We call λ_0 a *coupling constant threshold* of the family of the operators H_λ at the gap end points a and b if there exists an eigenvalue branch $E(\lambda)$ of H_λ such that $E(\lambda) \downarrow a$ or $E(\lambda) \uparrow b$, as either $\lambda \uparrow \lambda_0$ or $\lambda \downarrow \lambda_0$, respectively, or both. In particular, the case where $E(\lambda) \downarrow a$ as $\lambda \downarrow \lambda_0$ corresponds to the situation where an eigenvalue appears at a as $\lambda \downarrow \lambda_0 + \epsilon$. For more results in connection with the Schrödinger case, see, for example, [3].

The purpose of this work is to (1) study the analytic behaviour of the eigenvalue $E(\lambda)$ near the coupling constant threshold and (2) study the asymptotic behaviour of the discrete spectrum in the gaps of the spectrum of H_0 as the coupling constant grows to infinity. Our main tool will be the Birman-Schwinger operator and the Titchmarsh-Weyl m -function theory.

2. The Birman-Schwinger Principle

The spectrum $\rho(H_0)$ of H_0 is real and consists of two absolutely continuous bands covering the closed intervals $[E_0, E_1] \cup [E_2, E_3]$, where $0 < E_0 < E_1 < E_2 < E_3$. Since W_n is assumed to be relatively H_0 -compact, we also have that $\rho_{\text{ess}}(H_0 + \lambda W_n) = \rho_{\text{ess}}(H_0)$.

If we let $E(\lambda) \in (E_1, E_2)$, then the *Birman-Schwinger kernel* is defined by [19, 20]

$$K_E = |W_n|^{1/2} (H_0 - E) W_n^{1/2}. \quad (3)$$

The Birman-Schwinger principle implies the following.

Let H_0 be a self-adjoint operator and $E \in \rho(H_0)$, and suppose that $W_n \geq 0$ is a bounded operator with $W_n(H_0 - E)^{-1}$ compact. Then the Birman-Schwinger kernel K_E is compact and the following are equivalent:

- (1) E is an eigenvalue of H_λ with multiplicity m .
- (2) λ^{-1} is an eigenvalue of K_E with multiplicity m .

The following results are well known, we state them without proof, and the proofs for the continuous case can be found in [3], for example.

Proposition 1. *Suppose that $W_n \leq 0$ ($W_n \geq 0$), and then the nonzero eigenvalues of K_E are strictly monotone increasing (or decreasing) respectively.*

Proposition 2. *There exists a $\lambda \in \mathbb{R}$ such that $H_0 + \lambda W_n$ has an eigenvalue in (E_1, E_2) .*

The following lemma summarizes all the information concerning the operator K_E and the behaviour of the eigenvalues inside the spectral gap, and its proof can be found in [3].

Lemma 3. *Let $W_n \leq 0$ ($W_n \neq 0$). Then*

- (1) *if $\lambda = 0$ is a coupling constant threshold of $H_0 + \lambda W_n$ then $\|K_E\|$ is unbounded as $E \uparrow E_2$,*
- (2) *if $\|K_E\|$ stays bounded as $E \uparrow E_2$, then $\lim_{E \uparrow E_2} K_E = K_{E_2}$ exists,*
- (3) *K_{E_2} is compact iff $K_E \rightarrow K_{E_2}$ in norm,*
- (4) *if $\dim E_{(E_1, E_2)}(H_0 + \lambda W_n) = \infty$ for some $\lambda = \lambda_1 > 0$ then $\dim E_{(E_1, E_2)}(H_0 + \lambda W_n) = \infty$ for all $\lambda > \lambda_1$,*
- (5) *K_{E_2} is compact iff $\dim E_{(E_1, E_2)}(H_0 + \lambda W_n) < \infty$ for all $\lambda > 0$,*
- (6) *suppose that $\lambda = 0$ is not a coupling constant threshold and $\dim E_{(E_1, E_2)}(H_0 + \lambda W_n) < \infty$ for all $\lambda > 0$. Then K_{E_2} is compact,*
- (7) *K_{E_2} exists and is not compact iff $\lambda = 0$ is not a coupling constant threshold and there exists $\lambda^* > 0$ such that $\dim E_{(E_1, E_2)}(H_0 + \lambda W_n) = \infty$ for $\lambda > \lambda^*$ and $\dim E_{(E_1, E_2)}(H_0 + \lambda W_n) < \infty$ for $\lambda < \lambda^*$.*

The threshold behaviour is described in the following lemma.

Lemma 4. *Suppose that $W_n \leq 0$ ($W_n \neq 0$) and suppose $\lambda = 0$ is not a threshold. Then E_2 is not an eigenvalue of H_0 iff all eigenvalues $E_i(\lambda)$ which are absorbed at $\lambda = 0$ obey $(E_i(\lambda) - E_2)\lambda^{-1} \rightarrow 0$.*

3. The $m(E)$ -Function Theory

Let $\theta_n(E, \lambda)$ and $\phi_n(E, \lambda)$ be the two linearly independent solutions of (1) satisfying the following initial conditions for all $E \in \mathbb{C}$:

$$\begin{aligned} \theta_0(E, \lambda) &= \phi_1(E, \lambda) = 1, \\ \theta_1(E, \lambda) &= \phi_0(E, \lambda) = 1, \end{aligned} \quad (4)$$

and then there exists a solution $\psi_n(E, \lambda) = \theta_n(E, \lambda) + m(E, \lambda)\phi_n(E, \lambda)$, which is in $L^2(0, \infty)$. The function $m(E, \lambda)$ is defined by

$$m(E, \lambda) = -\lim_{n \rightarrow \infty} \frac{\theta_n(E, \lambda)}{\phi_n(E, \lambda)}. \quad (5)$$

The general proof for the existence of the limit in (5) may be found in [1, 21]. The $m(E)$ -function is analytic for $\text{Im}(E) \neq 0$, and it has a nonreal limit as $\text{Im}(E) \rightarrow 0$ in the bands and is real in the gaps except for the poles of $m(E)$ at the eigenvalues of H_λ . Of interest is the behaviour of $m(E)$ at the end points of the gaps, if the endpoints are either half-bound states or otherwise. $E(\lambda) = E_1$ is a half-bound state

(HBS) provided that $\{\phi_n(E)\}$ is abounded sequence but not in $l^2(0, \infty)$ and a non-half-bound state (non-HBS) otherwise. A similar definition may be given at the other end point of the spectral gap. In [13], there are the results of a version of Levinson's Theorem for the system

$$-u_{n+1} + 2u_n - u_{n-1} + V_n u_n = E u_n, \quad n \in [0, \infty), \quad (6)$$

with $\sum_0^\infty n|V_n| < \infty$.

Imposing the boundary conditions $u_0 + \alpha u_1 = 0$, the spectrum of (6) is $[0, 4]$, with a finite number of eigenvalues in the intervals $(-\infty, 0) \cup (4, \infty)$. At an eigenvalue $E_0 \in (-\infty, 0) \cup (4, \infty)$, we have that

$$(E - E_0) m(E) \longrightarrow k_1 \neq 0 \quad \text{as } E \longrightarrow E_0. \quad (7)$$

At the points $E = 0, 4$ it turns out that

$$(E - E_i)^{1/2} m(E) \longrightarrow \begin{cases} k_2 \neq 0, & \text{if } E_i = 0 \text{ or } 4 \text{ is HBS} \\ 0, & \text{else.} \end{cases} \quad (8)$$

It is natural to ask whether the theory of [13] carries over to the periodic version (1) in the presents of a gap and possible half-bound states at the ends of each gap.

4. The Bound States of $H_0 + \lambda W_n$

We consider the following system:

$$(H_0 + \lambda W_n) u_n = -u_{n+1} + 2u_n - u_{n-1} + (V_n + \lambda W_n) u_n = E u_n, \quad u_n \in l^2(\mathbb{Z}), \quad (9)$$

where $V_{n+a} = V_n$, for some $a \in \mathbb{Z}$, and $\sum |n|W_n < \infty$. Let θ_n, ϕ_n be the solutions of $H_0 u_n = E u_n$ satisfying the following initial conditions: $\theta_0 = 1, \theta_1 = 0$, and $\phi_0 = 0, \phi_1 = 1$

Let

$$\psi(n) = \begin{pmatrix} \theta_n & \phi_n \\ \theta_{n+1} & \phi_{n+1} \end{pmatrix}, \quad \text{i.e. } \psi(0) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (10)$$

and this defines the fundamental matrix for $(H_0 - E)u = 0$, and moreover $\psi(n+a) = \psi(n)\psi(a)$ and $\det \psi(a) = \det \psi(0) = 1$. The eigenvalues of $\psi(a)$ are

$$\mu_\pm = \frac{D \pm \sqrt{D^2 - 4}}{2}, \quad D = \theta_a + \phi_{a+1}. \quad (11)$$

The gaps and bounds are given by $|D(E)| > 2$ and $|D(E)| < 2$, respectively. Let us just look at the specific situation where E is near E_1 . We set

$$\alpha = \ln \mu_+ = \ln \frac{D + \sqrt{D^2 - 4}}{2}, \quad (12)$$

and notice that we can view E as an even function of α in the vicinity of E_1 ; that is, for α small

$$\begin{aligned} \sqrt{D^2 - 4} &= \sqrt{[2 + c(E - E_1) + \dots]^2 - 4} \\ &= \sqrt{2|c|} \sqrt{E_1 - E (1 + \text{powers of } (E - E_1))}, \end{aligned} \quad (13)$$

so that E goes around $E_1, \sqrt{D^2 - 4} \rightarrow -\sqrt{D^2 - 4}$, and $\mu_+ \rightarrow -\mu_-$, that is, $\alpha \rightarrow -\alpha$. Denoting the eigenfunctions corresponding to μ_\pm by q_\pm where

$$q_\pm = \left(1, \frac{\mu_\pm - \theta_a}{\phi_a} \right), \quad (14)$$

provided $\phi_a \neq 0$ (if $\phi_a = 0$, we shift the origin), we now define the periodic vector functions

$$\widetilde{q}_\pm(n) = \psi(n) q_\pm, \quad 0 \leq n \leq a-1, \quad (15)$$

with $\widetilde{q}_\pm(n) = \widetilde{q}_\pm(n+a)$. Let

$$f_n = \begin{cases} 0, & 0 \leq n \leq a-1 \\ f_{n+a} = f_n + 1, & \text{elsewhere,} \end{cases} \quad (16)$$

$$\widetilde{p}_\pm(n) = e^{\pm f(n) \mp n/a \alpha} \widetilde{q}_\pm(n),$$

and it follows that $\widetilde{p}_\pm(n+a) = \widetilde{p}_\pm(n)$. Let

$$\Psi^\pm = \phi(n) q_\pm(n) = e^{\pm(n/a)\alpha} \widetilde{p}_\pm(n). \quad (17)$$

These are the exponential solutions which behave in the following way:

$$\Psi^\pm \longrightarrow 0 \quad \text{as } n \longrightarrow \mp\infty, \quad (18)$$

As for the Wronskian $\widetilde{W} = W(\Psi^+, \Psi^-)$, we have

$$\widetilde{W} = \frac{\mu_- - \mu_+}{\phi_a} = -\frac{\sqrt{D^2 - 4}}{\phi_a}. \quad (19)$$

We have that $\phi_a < 0$ (at the right endpoint of a gap where $D(E) > 2$). This follows from general principles below since when $W_n < 0$, the eigenvalues in the gap must appear at the right endpoint if E increases. It follows directly in this way: if we write $\Psi^- = \theta + m\phi$, where $m = (\mu_- - \theta_a)/\phi_a$, then $m(E)$ is the Titchmarsh-Weyl function. In the Schrödinger case $\text{Im } m(E)$ is positive for $\text{Im } E > 0$. Let us see what it is here: from

$$\begin{aligned} u_{n+1} - 2u_n + u_{n-1} + V_n u_n &= E u_n, \\ \bar{u}_{n+1} - 2\bar{u}_n + \bar{u}_{n-1} + V_n \bar{u}_n &= \bar{E} \bar{u}_n, \end{aligned} \quad (20)$$

summing from 1 to ∞ gives

$$u_0 \bar{u}_1 - \bar{u}_0 u_1 = (E - \bar{E}) \sum_1^\infty u_n \bar{u}_n, \quad (21)$$

where $u_0 \bar{u}_1 - \bar{u}_0 u_1 = \bar{m}(E) - m(E)$ so that $\text{Im } m(E) < 0$ when $\text{Im } (E) > 0$. If E is close to E_1 in the upper half plane, then $\text{Im } \mu_- > 0$ and hence $\psi_a < 0$.

Now let us consider the Birman-Schwinger kernel:

$$K_E = |W_n|^{1/2} (H_0 - E) W_n^{1/2}, \quad (22)$$

and, assuming $W_n \leq 0$, K_E has eigenvalue 1 iff $E \in \rho(H)$. The resolvent $(H_0 - E)^{-1}$ is given by

$$\begin{aligned} ((H_0 - E)^{-1} u)_n &= \frac{1}{W} \Psi_n^- \sum_{-\infty}^{n-1} \Psi_m^+ u_m + \frac{1}{W} \Psi_n^+ \sum_n^{\infty} \Psi_m^- u_m \\ &= \sum R_{nm} u_m, \end{aligned} \quad (23)$$

with

$$R_{mn} = \frac{1}{W} \Psi_n^- \Psi_m^+ \chi_{n \geq m+1} + \frac{1}{W} \Psi_n^+ \Psi_m^- \chi_{m \geq n}. \quad (24)$$

Using (17), we get (using α as a variable)

$$\begin{aligned} R_{mn} &= \frac{1}{W} e^{-\alpha|n-m|} p_-(n, \alpha) p_+(m, \alpha) \chi_{n \geq m+1} \\ &\quad + \frac{1}{W} e^{-\alpha|n-m|} p_+(n, \alpha) p_-(m, \alpha) \chi_{m \geq n}, \end{aligned} \quad (25)$$

where $p_{\pm}(n, \alpha)$ is the first component of $\widetilde{p}_{\pm}(n)$. $p_+(n, \alpha)$ is analytic in α with $p_+(n, \alpha) = p_+(n, -\alpha)$. We note that

$$\widetilde{W} = -\frac{2 \sinh \alpha}{\psi_a} > 0, \quad (E < E_1). \quad (26)$$

We aim to determine the limit as $\alpha \rightarrow 0$ of R_{mn} . There is a diverging rank one piece which we can isolate.

$$\begin{aligned} R_{mn} &= \frac{1}{W} e^{-\alpha|n|} p_-(n, 0) e^{-\alpha|m|} p_+(m, 0) \\ &\quad + \frac{1}{W} [e^{-\alpha|n-m|} - e^{-\alpha|n|} e^{-\alpha|m|}] p_+(n, 0) p_+(m, 0) \\ &\quad + M_{mn} + N_{mn}, \end{aligned} \quad (27)$$

where

$$\begin{aligned} M_{mn} &= \frac{1}{W} e^{-\alpha|n-m|} [p_-(n, \alpha) p_+(m, \alpha) \\ &\quad - p_-(n, 0) p_+(m, 0)] \chi_{n \geq m+1}, \\ N_{mn} &= \frac{1}{W} e^{-\alpha|n-m|} [p_+(n, \alpha) p_-(m, \alpha) \\ &\quad - p_+(n, 0) p_-(m, 0)] \chi_{m \geq n}. \end{aligned} \quad (28)$$

The first term gives a rank one contribution to K_E and it diverges as $E \uparrow E_1$, with $\lambda \uparrow \infty$. The other terms when sandwiched between $|W|^{1/2}$ go to finite limits in Hilbert Schmidt norm. The rank one piece gives rise to a bound state near E_1 in the weak coupling limit (if $\sum W_n e^{-2\alpha|n|} p_+(n, 0)^2 \leq 0$, even if W_n changes sign). If $\sum W_n e^{-2\alpha|n|} p_+(n, 0)^2 \geq 0$, then the eigenvalue gets absorbed at $E = E_2$ as $\lambda \downarrow 0$.

5. Conclusion

By using the standard results derived for the continuous Schrödinger operator case, some insights into the asymptotic

behaviour of eigenvalues of the difference Schrödinger operator in the limit of the large and small coupling constant have been derived. This forms the basis for future work on the investigation of the asymptotic behaviour of the number of the eigenvalues inside the spectral gap for a large coupling constant which are not covered in this note.

Conflicts of Interest

The authors declare that there are no conflicts of interest regarding the publication of this paper.

Acknowledgments

The authors would like to thank Professor Martin Klaus (Virginia Tech) for several useful discussions at the time when this paper was conceived of. Gift Muchatibaya and Josiah Mushanyu would like to acknowledge the support of the University of Zimbabwe when this project was underway.

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