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Three-term asymptotic formula for large eigenvalues of the two-photon quantum Rabi model

Anne Boutet de Monvel and Lech Zielinski

Abstract. We prove that the spectrum of the two-photon quantum Rabi Hamiltonian consists of two eigenvalue sequences $(E_m^+)_{m=0}^\infty$, $(E_m^-)_{m=0}^\infty$ satisfying a three-term asymptotic formula with the remainder estimate $O(m^{-1}\ln m)$ when m tends to infinity. Our asymptotic formula can be written so that the third term is given by an explicit oscillatory integral and an explicit remainder estimate.

1. General presentation of the paper

1.1. Introduction

In Section 1.1 we describe briefly the subject of the paper. The simplest version of our main result is stated in Section 1.2 and its refinements are described in Section 1.3. An overview of related results is presented in Section 1.4 and the organization of the paper in Section 1.5.

The simplest interaction between a two-level atom and a classical light field is described by the semi-classical Rabi model [35,36]. The quantum Rabi model (QRM) couples a two-level system (TLS) with a quantized single-mode radiation and is considered as a particularly important model in quantum electrodynamics: we refer to [11] concerning the historical aspects of the QRM and to the review paper [46] for a list of research works and experimental realizations of the QRM.

The simplest QRM is defined by the one-photon Hamiltonian $\mathbf{H}_{\text{Rabi}}^{(1)}$ given in Definition 1.2 (c). The operator $\mathbf{H}_{\text{Rabi}}^{(1)}$ is a self-adjoint operator depending on two real parameters: g (the coupling constant) and Δ (the energy separation in the TLS). Its spectrum is discrete and the fundamental question is how to find a good approximation of the corresponding eigenvalues.

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The first step in this direction, is the *rotating-wave approximation* (RWA) introduced in the famous paper of Jaynes and Cummings [29]. However, the RWA is a correct approximation only when g is close to 0 and Δ close to 1 for $\mathbf{H}^{(1)}_{\mathrm{Rabi}}$ given in Definition 1.2 (c). The most popular idea of going beyond the limitations of RWA, bears the name of the *generalized rotating-wave approximation* (GRWA) after E. K. Irish [23]. It appears (see [24]) that the same idea was considered before by I. D. Feranchuk, L. I. Komarov, and A. P. Ulyanenkov [19], under the name of the *zeroth order approximation* of the operator method (see also [18]). According to [19, (25)], the spectrum of $\mathbf{H}^{(1)}_{\mathrm{Rabi}}$ is composed of two eigenvalue sequences $(E^+_m)^\infty_{m=0}$ and $(E^-_m)^\infty_{m=0}$, satisfying

$$E^\pm_m \approx m - g^2 \pm \mathrm{r}_m \tag{1.1}$$

with

$$\mathrm{r}_m := (-1)^m \frac{\Delta}{2} \frac{\cos\left(4g\sqrt{m} - \frac{\pi}{4}\right)}{\sqrt{2\pi g\sqrt{m}}} \tag{1.2}$$

for large values of m. The quality of this approximation were investigated by numerous numerical calculations. In particular, a thorough numerical analysis of 40,000 eigenvalues was performed by L. T. H. Nguyen, C. Reyes-Bustos, D. Braak, and M. Wakayama [34]. A good approximation of large eigenvalues by (1.1)–(1.2) is explained by the estimate

$$E^\pm_m = m - g^2 \pm \mathrm{r}_m + O(m^{-1/2+\varepsilon}) \quad \text{as } m \to \infty, \tag{1.3}$$

where r_m is given by (1.2) and $\varepsilon > 0$ (see [3, 6]). We remark that the three-term asymptotic formula (1.2)–(1.3) allows one to recover the values of parameters of the model from its spectrum (see [4]).

In this paper we consider the two-photon QRM defined by the Hamiltonian $\mathbf{H}^{(2)}_{\mathrm{Rabi}}$ given in Definition 1.2 (d). This model was proposed in [20] to describe a two-level atom interacting with squeezed light (see [14, 16, 17] and Section 1.4 for more references).

In what follows, we assume that the coupling constant satisfies the condition $0 < g < \frac{1}{2}$, which ensures the fact that the spectrum of $\mathbf{H}^{(2)}_{\mathrm{Rabi}}$ is discrete (see Section 1.4 for a discussion of the case $g \geq \frac{1}{2}$). In [5] we proved that if $0 < g < \frac{1}{2}$, then the spectrum of $\mathbf{H}^{(2)}_{\mathrm{Rabi}}$ is composed of two eigenvalue sequences $(E^+_m)^\infty_{m=0}$ and $(E^-_m)^\infty_{m=0}$, satisfying

$$E^\pm_m = \left(m + \frac{1}{2}\right)\sqrt{1 - 4g^2} - \frac{1}{2} + O(m^{-1/3}) \quad \text{as } m \to \infty.$$

The purpose of this paper, is to obtain the three-term asymptotic formula

$$E^\pm_m = \left(m + \frac{1}{2}\right)\sqrt{1 - 4g^2} - \frac{1}{2} \pm \mathrm{r}_m + O(m^{-1}\ln m) \quad \text{as } m \to \infty, \tag{1.4}$$

where $\mathfrak{r}_m$ is given by (1.9). It is easy to check that the three-term asymptotic formula (1.4) allows one to recover the values of parameters of the model from its spectrum.

The idea of the proof of Theorem 1.3 was described in [7] and a similar result was obtained by E. A. Ianovich in [22]. However, in this paper, we describe a different approach, allowing one to express the third term in the form of an explicit oscillatory integral and to give explicit constants in the remainder estimates (see Section 7.5).

1.2. The three-term asymptotic formula for the two-photon QRM

Notation 1.1. (a) In what follows, $\mathbb{Z}$ is the set of integers and $\mathbb{N} := \{n \in \mathbb{Z} : n \geq 0\}$.

(b) We denote by $\ell^2(\mathbb{N})$ the complex Hilbert space of square-summable sequences $x\colon \mathbb{N} \to \mathbb{C}$ equipped with the scalar product

$$\langle x, y\rangle_{\ell^2(\mathbb{N})} = \sum_{m=0}^{\infty} \overline{x(m)}\, y(m)$$

and the norm $\|x\|_{\ell^2(\mathbb{N})} := \langle x, x\rangle_{\ell^2(\mathbb{N})}^{1/2}$. For $s > 0$, we denote

$$\ell^{2,s}(\mathbb{N}) := \Big\{x \in \ell^2(\mathbb{N})\colon \sum_{m=0}^{\infty} (1+m^2)^s |x(m)|^2 < \infty\Big\}.$$

(c) The canonical basis of $\ell^2(\mathbb{N})$ is denoted $\{e_n\}_{n\in\mathbb{N}}$ (i.e., $e_n(m) = \delta_{n,m}$ for n, $m \in \mathbb{N}$).

(d) The annihilation and creation operators, $\hat{a}$ and $\hat{a}^\dagger$, are the linear maps

$$\ell^{2,1/2}(\mathbb{N}) \to \ell^2(\mathbb{N})$$

satisfying

$$\hat{a}^\dagger e_n = \sqrt{n+1}\, e_{n+1} \qquad \text{for } n \in \mathbb{N},$$
$$\hat{a} e_0 = 0 \quad \text{and} \quad \hat{a} e_n = \sqrt{n}\, e_{n-1} \qquad \text{for } n \in \mathbb{N} \setminus \{0\}.$$

(e) Using $(1,0) \in \mathbb{C}^2$ and $(0,1) \in \mathbb{C}^2$ as the canonical basis of the Euclidean space $\mathbb{C}^2$, we denote by σ_x, σ_z, I_2, the linear operators in $\mathbb{C}^2$ defined by the matrices

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad I_2 := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Definition 1.2. (a) The two-level system (TLS) Hamiltonian is the linear map in $\mathbb{C}^2$ defined by the matrix

$$H_{\mathrm{TLS}} = \frac{1}{2}\begin{pmatrix} \Delta & 0 \\ 0 & -\Delta \end{pmatrix} = \frac{1}{2}\Delta\sigma_z$$

where Δ is a real parameter.

(b) The Hamiltonian of the single-mode radiation is the linear map

$$H_{\mathrm{rad}}\colon \ell^{2,1}(\mathbb{N}) \to \ell^2(\mathbb{N})$$

defined by the formula

$$H_{\mathrm{rad}} e_n = \hat{a}^\dagger \hat{a} e_n = n e_n \quad \text{for } n \in \mathbb{N}.$$

(c) Let $g > 0$. Then the *one-photon quantum Rabi Hamiltonian* is defined as the linear map

$$\mathbf{H}^{(1)}_{\mathrm{Rabi}}\colon \mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \to \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$$

given by

$$\mathbf{H}^{(1)}_{\mathrm{Rabi}} = I_2 \otimes H_{\mathrm{rad}} + H_{\mathrm{TLS}} \otimes I_{\ell^2(\mathbb{N})} + g\sigma_x \otimes (\hat{a} + \hat{a}^\dagger).$$

(d) If $0 < g < \frac{1}{2}$, then the *two-photon quantum Rabi Hamiltonian* is defined as the linear map

$$\mathbf{H}^{(2)}_{\mathrm{Rabi}}\colon \mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \to \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$$

given by

$$\mathbf{H}^{(2)}_{\mathrm{Rabi}} = I_2 \otimes H_{\mathrm{rad}} + H_{\mathrm{TLS}} \otimes I_{\ell^2(\mathbb{N})} + g\sigma_x \otimes (\hat{a}^2 + (\hat{a}^\dagger)^2) \tag{1.5}$$

and we let $\mathbf{H}^{(2)}_{0,\mathrm{Rabi}}$ denote the operator given by (1.5) with $\Delta = 0$, i.e.,

$$\mathbf{H}^{(2)}_{0,\mathrm{Rabi}} = I_2 \otimes H_{\mathrm{rad}} + g\sigma_x \otimes (\hat{a}^2 + (\hat{a}^\dagger)^2).$$

The case $g \geq \frac{1}{2}$ is discussed in Section 1.4.

In what follows, we assume that $0 < g < \frac{1}{2}$ and introduce

$$\beta := \sqrt{1 - 4g^2},$$

$$\alpha := \arctan\Bigl(\sqrt{\frac{1-2g}{1+2g}}\Bigr). \tag{1.6}$$

If $0 < g < \frac{1}{2}$, then the spectrum of $\mathbf{H}^{(2)}_{0,\mathrm{Rabi}}$ is explicitly known (see [16, 17]): it is composed of the sequence of eigenvalues

$$E^0_m = m\beta + \frac{\beta - 1}{2}, \quad m = 0, 1, 2, \ldots \tag{1.7}$$

and each eigenvalue E^0_m is of multiplicity 2. Thus, $0 < g < \frac{1}{2}$ ensures the fact that $\mathbf{H}^{(2)}_{0,\mathrm{Rabi}}$ is a self-adjoint operator with compact resolvent and the same can be said about $\mathbf{H}^{(2)}_{\mathrm{Rabi}}$ because $\mathbf{H}^{(2)}_{\mathrm{Rabi}} - \mathbf{H}^{(2)}_{0,\mathrm{Rabi}}$ is bounded. The explicit values of the eigenvalues of $\mathbf{H}^{(2)}_{\mathrm{Rabi}}$ are not known when $\Delta \neq 0$, but we can describe their asymptotic behavior in the following result.

Theorem 1.3. *If* $0 < g < \frac{1}{2}$ *then one can find* $\{v_m^+\}_{m\in\mathbb{N}} \cup \{v_m^-\}_{m\in\mathbb{N}}$, *an orthonormal basis of* $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$, *such that*

$$\mathbf{H}^{(2)}_{\mathrm{Rabi}} v_m^{\pm} = E_m^{\pm} v_m^{\pm}, \quad m = 0, 1, 2, \ldots,$$

and the eigenvalue sequences $(E_m^+)_{m\in\mathbb{N}}$, $(E_m^-)_{m\in\mathbb{N}}$, *satisfy the large* m *estimates*

$$E_m^{\pm} = m\beta + \frac{\beta - 1}{2} \pm \mathfrak{r}_m + O(m^{-1}\ln m) \tag{1.8}$$

with $\mathfrak{r}_m$ *given by the formula*

$$\mathfrak{r}_m = \begin{cases} \dfrac{\Delta}{2}\sqrt{\dfrac{\beta}{\pi g m}}\cos((2m+1)\alpha) & \text{if } m \text{ is even,} \\ \dfrac{\Delta}{2}\sqrt{\dfrac{\beta}{\pi g m}}\sin((2m+1)\alpha) & \text{if } m \text{ is odd,} \end{cases} \tag{1.9}$$

where $\beta = \sqrt{1 - 4g^2}$ *and* α *is given by* (1.6).

Remarks. (1) The operator $\mathbf{H}^{(2)}_{\mathrm{Rabi}}$, its eigenvalues $E_m^{\pm}$, the correction $\mathfrak{r}_m$, and the remainder term $O(m^{-1}\ln m)$ in (1.8), depend on the parameters g and Δ. For sake of simplicity, this dependence is not mentioned in the statement of Theorem 1.3, but this issue is discussed in Section 1.3.

(2) In spite of the fact that $\mathbf{H}^{(2)}_{\mathrm{Rabi}} - \mathbf{H}^{(2)}_{0,\mathrm{Rabi}}$ is not compact, the estimate (1.8) implies

$$E_m^{\pm} - E_m^{\mathbf{0}} \to 0 \quad \text{as } m \to \infty. \tag{1.10}$$

A similar property for $\mathbf{H}^{(1)}_{\mathrm{Rabi}}$ was first proved by E. A. Ianovich [45] (see also [44]).

1.3. Refinements of Theorem 1.3

In this section we assume that $0 < g < \frac{1}{2}$. It is easy to check (see [5]) that $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$ is a direct sum of four subspaces

$$\begin{aligned}
&\mathcal{H}_0^- \text{ spanned by } \mathcal{B}_0^- = \{(1,0)\otimes e_{4k} : k \in \mathbb{N}\} \cup \{(0,1)\otimes e_{4k+2} : k \in \mathbb{N}\},\\
&\mathcal{H}_0^+ \text{ spanned by } \mathcal{B}_0^+ = \{(0,1)\otimes e_{4k} : k \in \mathbb{N}\} \cup \{(1,0)\otimes e_{4k+2} : k \in \mathbb{N}\},\\
&\mathcal{H}_1^- \text{ spanned by } \mathcal{B}_1^- = \{(1,0)\otimes e_{4k+1} : k \in \mathbb{N}\} \cup \{(0,1)\otimes e_{4k+3} : k \in \mathbb{N}\},\\
&\mathcal{H}_1^+ \text{ spanned by } \mathcal{B}_1^+ = \{(0,1)\otimes e_{4k+1} : k \in \mathbb{N}\} \cup \{(1,0)\otimes e_{4k+3} : k \in \mathbb{N}\},
\end{aligned}$$

which are invariant for $\mathbf{H}_{\mathrm{Rabi}}^{(2)}$. The matrix of $\mathbf{H}_{\mathrm{Rabi}}^{(2)}$ in the basis $\mathscr{B}_{\mu}^{\pm}$ is a Jacobi (i.e., tridiagonal) matrix,

$$\begin{pmatrix} \hat{d}_{\mu}^{\pm}(0) & \hat{b}_{\mu}^{\pm}(0) & 0 & 0 & \\ \hat{b}_{\mu}^{\pm}(0) & \hat{d}_{\mu}^{\pm}(1) & \hat{b}_{\mu}^{\pm}(1) & 0 & \\ 0 & \hat{b}_{\mu}^{\pm}(1) & \hat{d}_{\mu}^{\pm}(2) & \hat{b}_{\mu}^{\pm}(2) & \\ 0 & 0 & \hat{b}_{\mu}^{\pm}(2) & \hat{d}_{\mu}^{\pm}(3) & \\ & & & & \ddots \end{pmatrix} \tag{1.11}$$

whose diagonal entries are

$$\hat{d}_{\mu}^{\pm}(m) := 2m + \mu \pm (-1)^m \frac{\Delta}{2} \tag{1.12}$$

and the off-diagonal entries are

$$\hat{b}_{\mu}(m) := g\sqrt{(2m+1+\mu)(2m+2+\mu)}, \tag{1.13}$$

Clearly, the diagonal part is a lower semi-bounded self-adjoint operator with the domain $\ell^{2,1}(\mathbb{N})$ and its spectrum is discrete. Since

$$0 < g < \frac{1}{2} \Longrightarrow \lim_{m\to\infty} \frac{\hat{d}_{\mu}^{\pm}(m)^2}{\hat{b}_{\mu}(m)^2 + \hat{b}_{\mu}(m)^2} = \frac{1}{2g^2} > 2, \tag{1.14}$$

the Janas–Naboko criterion [27, Theorem 4.1] implies that the off-diagonal part has a relative bound $c < 1$ with respect to the diagonal part, hence $\widehat{J}_{\mu}^{\pm}$ is a lower semi-bounded self-adjoint operator with the domain $\ell^{2,1}(\mathbb{N})$ and its spectrum is discrete. The fact that $\mathbf{H}_{\mathrm{Rabi}}^{(2)}$ is similar to the direct sum

$$\widehat{J}_0^- \oplus \widehat{J}_0^+ \oplus \widehat{J}_1^- \oplus \widehat{J}_1^+,$$

allows us to label the spectrum of $\mathbf{H}_{\mathrm{Rabi}}^{(2)}$, using the sequences $\{E_m^-\}_{m\in\mathbb{N}}$, $\{E_m^+\}_{m\in\mathbb{N}}$, defined by

$$E_{2n+\mu}^{\pm} = \lambda_n(\widehat{J}_{\mu}^{\pm}) \quad \text{for } n \in \mathbb{N},\ \mu = 0, 1,$$

where $\lambda_n(\widehat{J}_{\mu}^{\pm})$ denotes the n-th eigenvalue of $\widehat{J}_{\mu}^{\pm}$, i.e., $\{\lambda_n(\widehat{J}_{\mu}^{\pm})\}_{n\in\mathbb{N}}$ is the sequence of eigenvalues of $\widehat{J}_{\mu}^{\pm}$ ordered so that

$$\lambda_0(\widehat{J}_{\mu}^{\pm}) < \cdots < \lambda_n(\widehat{J}_{\mu}^{\pm}) < \lambda_{n+1}(\widehat{J}_{\mu}^{\pm}) < \cdots .$$

In Section 7.5, we prove that for every $0 < g < \frac{1}{2}$ and $\Delta \in \mathbb{R}$, the n-th eigenvalue of $\widehat{J}_{\mu}^{\pm}$ satisfies

$$\lambda_n(\widehat{J}_{\mu}^{\pm}) - (E_{2n+\mu}^{0} \pm \mathfrak{r}_{2n+\mu}) = O(n^{-1}\ln n) \quad \text{as } n \to \infty,$$

where $E^0_m = m\beta + \frac{\beta-1}{2}$, $\mathfrak{r}_m$ is given by (1.9), and the remainder estimate $O(n^{-1}\ln n)$ depends on g and Δ. More precisely, we give an explicit value $\nu_{g,\Delta}$ such that for $n > \nu_{g,\Delta}$, the interval $[E^0_{2n+\mu} - \beta, E^0_{2n+\mu} + \beta]$ contains a single eigenvalue of $\widehat{J}^{\pm}_{\mu}$, which is precisely $\lambda_n(\widehat{J}^{\pm}_{\mu})$ (i.e., precisely the n-th eigenvalue of $\widehat{J}^{\pm}_{\mu}$). Moreover, (see Section 7.5), we give explicit values of constants $\widetilde{C}_{g,\Delta}$, $C_{g,\Delta}$, such that for $n > \nu_{g,\Delta}$ one has the estimate

$$|\lambda_n(\widehat{J}^{\pm}_{\mu}) - (E^0_{2n+\mu} \pm \tilde{\mathfrak{r}}_{2n+\mu})| \leq \frac{\widetilde{C}_{g,\Delta} + C_{g,\Delta}\ln n}{n}, \tag{1.15}$$

where $\tilde{\mathfrak{r}}_{2n+\mu}$ is given by an explicit oscillatory integral (see Section 3.3) and the standard stationary phase method allows one to find a constant $C'_{g,\Delta}$ such that the estimate $|\tilde{\mathfrak{r}}_{2n+\mu} - \mathfrak{r}_{2n+\mu}| \leq C'_{g,\Delta} n^{-1}$ holds for all $n \geq 1$.

We observe that our expressions of $\nu_{g,\Delta}$, $\widetilde{C}_{g,\Delta}$, $C_{g,\Delta}$, are continuous functions of g and Δ, but they all tend to infinity as g approaches $\frac{1}{2}$ or 0, which means that the results of this paper cannot be used to investigate the issues of g approaching $\frac{1}{2}$ or 0. We discuss the issues of g approaching $\frac{1}{2}$ or 0 in Section 1.4.

We remark that the estimate (1.15) can be applied to investigate the spacing $\lambda_{n+1}(\widehat{J}^{\pm}_{\mu}) - \lambda_n(\widehat{J}^{\pm}_{\mu})$ similarly to L. T. H. Nguyen, C. Reyes-Bustos, D. Braak, and M. Wakayama investigated the one-photon QRM in [34]. Moreover, similarly to the work of Z. Rudnick [38], (1.15) can be used to investigate an analogue of Braak's G-function conjecture on the location of eigenvalues (see [9]). If $\frac{\alpha}{\pi}$ is irrational, then the sequences $\{\cos((2m+1)\alpha)\}_{m\in\mathbb{N}}$ and $\{\sin((2m+1)\alpha)\}_{m\in\mathbb{N}}$ are dense in $[-1, 1]$ and one can easily obtain a result of density 1 similarly to Z. Rudnick. If $\frac{\alpha}{\pi}$ is rational, then these sequences are periodic. If moreover $2\frac{\alpha}{\pi} = \frac{k}{l}$ with k odd and l even, then these sequences never take the value 0 and for $n \geq n_0$ one can locate $\lambda_n(\widehat{J}_{\pm 1,\mu})$ either below or above $E^0_{2n+\mu}$, hence all eigenvalues of $\mathbf{H}^{(2)}_{\text{Rabi}}$ are simple except a finite number. We remark that double eigenvalues are crucial for the question of the integrability of the model (see [8, 9]). Finally, using $E^0_{2n+1} = E^0_{2n} + \beta$ and (1.15), we get $\lambda_n(J^{\pm}_1) - \lambda_n(J^{\pm}_0) \to \beta$ as $n \to \infty$, hence large eigenvalues cannot be common for a couple of operators with different values of μ (see Maciejewski and Stachowiak [33], where the existence of this type of eigenvalue crossing was discovered).

1.4. Overview of related results and comments

1.4.1. Earlier results. We refer to [19, 40], for the earliest investigations of large eigenvalues of QRM. It is well known (see [4, 43]) that $\mathbf{H}^{(1)}_{\text{Rabi}}$ can be expressed as a direct sum $J^- \oplus J^+$ of two Jacobi operators, i.e., operators defined by infinite tridiagonal matrices acting in $\ell^2(\mathbb{N})$. A mathematical study of large eigenvalues of Jacobi matrices was initiated by J. Janas and S. Naboko in the paper [28], which contains fundamental ideas of the method of approximate diagonalizations.

The question of the behavior of large eigenvalues of Jacobi matrices $J^{\pm}$, was first posed by E. A. Tur [43,44] and it was mentioned by A. Boutet de Monvel, S. Naboko, and L. O. Silva in [1,2]. Due to the difficulty of the problem, the papers [1,2] give the asymptotic estimates for a simpler class of operators ("modified Jaynes–Cummings models"). However, using the ideas of [28], E. A. Ianovich [45] proved the two-term asymptotic formula

$$\lambda_n(J^{\pm}) = n - g^2 + O(n^{-1/16}) \quad \text{as } n \to \infty,$$

where $\{\lambda_n(J^{\pm})\}_{n\in\mathbb{N}}$ denotes the increasing sequence of eigenvalues of $J^{\pm}$ (see also [44]). In [3,6] we proved the three-term asymptotic formula

$$\lambda_n(J^{\pm}) = n - g^2 \pm \mathrm{r}_n + O(n^{-1/2+\varepsilon}) \quad \text{as } n \to \infty, \tag{1.16}$$

where r_n is given by (1.2), $\varepsilon > 0$, and [4] explains how to recover the parameters of the model from its spectrum. The estimate (1.16) was used to investigate the spacing $\lambda_{n+1}(J^{\pm}) - \lambda_n(J^{\pm})$ in [34] and to consider a Braak's conjecture in [38].

1.4.2. Problems when $g \to 0$ and $g \to \frac{1}{2}$. The key ingredient of this paper is given in Lemma 2.6, where the estimate $O((\beta g n)^{-1/2})$ is obtained by means of the stationary phase method with the large parameter $\beta g n$. In particular, no uniform control is possible when $g \to 0$. It is not a surprise, as the eigenvalues are explicit if $g = 0$ and (1.10) is not true in the case $g = 0$, $\Delta \neq 0$. If gn is small, then one should choose a quite different approach. We remark that the paper [13] gives an explicit value $c_\Delta > 0$ such that the n-th eigenvalue of $\widehat{J}^{\pm}_{\mu}$ is an analytic function of g if $0 \le gn < c_\Delta$. Moreover, [13] describes the algorithm of obtaining the correction terms and gives the remainder estimates, including the case of the eigenvalue crossing for $g = 0$.

Similarly, $g \to \frac{1}{2}$ implies $\beta \to 0$ and $\beta g n$ cannot be considered as a large parameter. In particular, our analysis cannot be used to investigate the case $g = \frac{1}{2}$. This is a natural consequence of a drastic change of spectral properties of the model when $g \ge \frac{1}{2}$ (see Section 1.4.3).

1.4.3. Remarks on the case $g \ge \frac{1}{2}$. We observe that the off-diagonal entries of the Jacobi matrix (1.11) satisfy the Carleman condition

$$\sum_{m=0}^{\infty} \frac{1}{\hat{b}^{\pm}_{\mu}(m)} = \infty$$

which ensures the existence of a self-adjoint extension for every $g > 0$ (see [42, Lemma 2.16 and condition (2.165)]). Let $\widehat{J}^{\pm}_{\mu}$ denote this self-adjoint extension and let $\mathrm{Dom}(\widehat{J}^{\pm}_{\mu})$ denote its domain equipped with the graph norm. Then $\mathrm{Dom}(\widehat{J}^{\pm}_{\mu})$ is a Banach space and it is easy to see that the map $x \to x$ is continuous $\ell^{2,1}(\mathbb{N}) \to \mathrm{Dom}(\widehat{J}^{\pm}_{\mu})$.

If $0 < g < \frac{1}{2}$, then the $\ell^{2,1}(\mathbb{N})$-norm is equivalent to the graph norm of $\widehat{J}_\mu^\pm$ and $\mathrm{Dom}(\widehat{J}_\mu^\pm) = \ell^{2,1}(\mathbb{N})$ by the Janas–Naboko criterion [27, Theorem 4.1].

It appears that the spectrum of $\widehat{J}_\mu^\pm$ is the whole $\mathbb{R}$ when $g > \frac{1}{2}$ (see [26, Theorem 6.1]) or a half-line when $g = \frac{1}{2}$ and $\Delta = 0$ (see [39]). This implies that $\mathrm{Dom}(\widehat{J}_\mu^\pm)$ is strictly larger than $\ell^{2,1}(\mathbb{N})$ when $g \geq \frac{1}{2}$. Indeed, in case of the equality $\ell^{2,1}(\mathbb{N}) = \mathrm{Dom}(\widehat{J}_\mu^\pm)$, the $\ell^{2,1}(\mathbb{N})$-norm and the graph norm of $\widehat{J}_\mu^\pm$ are equivalent by Banach isomorphism theorem, hence the map $x \to x$ is compact from $\mathrm{Dom}(\widehat{J}_\mu^\pm)$ to $\ell^2(\mathbb{N})$ and the spectrum is discrete for any value of Δ.

The most interesting case $g = \frac{1}{2}$ and $\Delta \neq 0$ corresponds to the situation called "the spectral collapse" (see [10, 12, 14]). It appears that the spectrum is a union of a discrete spectrum and a half-line (see [30]).

1.4.4. Integrability of the model. The fundamental question about the integrability of the model is related to the presence of double eigenvalues (see [8,9]). The result of this paper can be applied to prove absence of large double eigenvalues in some cases (see the end of Section 1.3), but no information about small eigenvalues is available. We refer to [10,14,31], where the integrability question was investigated by means of the spectral determinant and to [32], where a different approach was developed.

1.5. Organization of the paper

Throughout the whole paper we assume $0 < g < \frac{1}{2}$ and use the notation $\beta = \sqrt{1 - 4g^2}$. For simplicity, the parameter g is not written for objects and constants depending on g.

Our approach is based on an analysis of operators acting in $\ell^2(\mathbb{Z})$. In Theorem 2.3 (a) we consider the operators $\widetilde{J}_\gamma^0$, which are special case of operators considered by Edward [15]. In Section 2.2 we describe explicit expressions of their eigenvalues and eigenvectors by means of the discrete Fourier transform. In Theorem 2.3 (b) we give the asymptotic behavior of large eigenvalues of operators $\widetilde{J}_\gamma^\delta$, considered as perturbations of $\widetilde{J}_\gamma^0$.

In Section 3 we show that the assertion of Theorem 2.3 (b) follows from a ZOA result stated in Proposition 3.1. The proof of Proposition 3.1 begins in Section 4 and is completed in Section 6. In Section 7 we show how to deduce Theorem 1.3 from Theorem 2.3. Section 8 contains auxiliary results about oscillatory integrals and perturbations of an isolated eigenvalue for self-adjoint operators.

2. An auxiliary problem in $\ell^2(\mathbb{Z})$

2.1. Behavior of large eigenvalues for auxiliary operators $\widetilde{J}_\gamma^\delta$

Notation 2.1. (a) If $L\colon \mathrm{Dom}(L) \to \mathcal{V}$ is a linear map defined on a dense subspace of the Banach space $\mathcal{V}$, then $\mathrm{spec}(L)$ denotes the spectrum of L. We write $L \in \mathcal{B}(\mathcal{V})$ if and only if L has an extension to a bounded operator on $\mathcal{V}$ and $\|\cdot\|_{\mathcal{B}(\mathcal{V})}$ denotes the corresponding operator norm.

(b) We denote by $\ell^2(\mathbb{Z})$ the complex Hilbert space of square-summable sequences $x\colon \mathbb{Z} \to \mathbb{C}$ equipped with the scalar product

$$\langle x, y\rangle = \sum_{k\in\mathbb{Z}} \overline{x(k)}\, y(k)$$

and the norm $\|x\| := \langle x, x\rangle^{1/2}$. The norm $\|\cdot\|_{\mathcal{B}(\ell^2(\mathbb{Z}))}$ will be abbreviated $\|\cdot\|$.

(c) For $s > 0$, we denote

$$\ell^{2,s}(\mathbb{Z}) := \{x \in \ell^2(\mathbb{Z}) : \|x\|_{\ell^{2,s}(\mathbb{Z})} < \infty\}$$

where

$$\|x\|_{\ell^{2,s}(\mathbb{Z})} := \Big(\sum_{k\in\mathbb{Z}} (1 + k^2)^s |x(k)|^2\Big)^{1/2}.$$

(d) The canonical basis of $\ell^2(\mathbb{Z})$ is denoted $\{\tilde{e}_j\}_{j\in\mathbb{Z}}$ (i.e., one has $\tilde{e}_j(k) = \delta_{j,k}$ for $j, k \in \mathbb{Z}$) and $\ell^2_{\mathrm{fin}}(\mathbb{Z})$ denotes the set of finite linear combinations of vectors belonging to $\{\tilde{e}_j\}_{j\in\mathbb{Z}}$.

(e) If $L\colon \mathrm{Dom}(L) \to \ell^2(\mathbb{Z})$ is a linear map such that $\ell^2_{\mathrm{fin}}(\mathbb{Z}) \subset \mathrm{Dom}(L)$, then we use the notation

$$L(j,k) := (L\tilde{e}_k)(j) = \langle \tilde{e}_j, L\tilde{e}_k\rangle.$$

(f) If $(\tilde{d}_j)_{j\in\mathbb{Z}}$ is real valued, then $\widetilde{D} := \mathrm{diag}(\tilde{d}_j)_{j\in\mathbb{Z}}$ is the self-adjoint operator in $\ell^2(\mathbb{Z})$ satisfying

$$\widetilde{D}\tilde{e}_j = \tilde{d}_j \tilde{e}_j \quad \text{for every } j \in \mathbb{Z},$$

and we denote

$$\Lambda := \mathrm{diag}(j)_{j\in\mathbb{Z}}.$$

(g) We denote by S the shift defined in $\ell^2(\mathbb{Z})$ by the formula $(Sx)(j) = x(j-1)$.

Definition 2.2. In what follows, γ, δ and g are fixed real numbers.

(a) We define $\widetilde{J}_\gamma^0$ as the linear map $\ell^{2,1}(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ given by

$$\widetilde{J}_\gamma^0 := \Lambda + g(S(\Lambda+\gamma) + (\Lambda+\gamma)S^{-1}) = \Lambda + g(S(\Lambda+\gamma) + \text{h.c.}) \qquad (2.1)$$

(b) We define $\widetilde{J}_\gamma^\delta$ as the linear map $\ell^{2,1}(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ given by the formula

$$\widetilde{J}_\gamma^\delta := \widetilde{J}_\gamma^0 + D_\delta, \tag{2.2}$$

where

$$D_\delta := \operatorname{diag}(\delta(-1)^j)_{j\in\mathbb{Z}}. \tag{2.3}$$

Using the above definition, we find that the action of $\widetilde{J}_\gamma^\delta$ can be represented by the tridiagonal $\mathbb{Z} \times \mathbb{Z}$ matrix

$$\begin{pmatrix} \ddots & & & & & & \\ & -2+\delta & g(-2+\gamma) & 0 & 0 & 0 & \\ & g(-2+\gamma) & -1-\delta & g(-1+\gamma) & 0 & 0 & \\ & 0 & g(-1+\gamma) & \delta & g\gamma & 0 & \\ & 0 & 0 & g\gamma & 1-\delta & g(1+\gamma) & \\ & 0 & 0 & 0 & g(1+\gamma) & 2+\delta & \\ & & & & & & \ddots \end{pmatrix}$$

whose diagonal entries $\{\tilde{d}_\delta(j)\}_{j\in\mathbb{Z}}$ are given by

$$\tilde{d}_\delta(j) := j + \delta(-1)^j \tag{2.4}$$

and whose off-diagonal entries $\{\tilde{b}_\gamma(j)\}_{j\in\mathbb{Z}}$ are given by

$$\tilde{b}_\gamma(j) := g(j+\gamma).$$

Theorem 2.3. *Let $\widetilde{J}_\gamma^0$ be given by (2.1) and $\widetilde{J}_\gamma^\delta$ by (2.2)–(2.3). If $0 < g < \frac{1}{2}$ then*

(a) *the spectrum of $\widetilde{J}_\gamma^0$ is composed of a non-decreasing sequence of eigenvalues $\{E_{\gamma,j}^0\}_{j\in\mathbb{Z}}$ of the form*

$$E_{\gamma,j}^0 := \beta j + \Big(\gamma - \frac{1}{2}\Big)(\beta - 1), \tag{2.5}$$

where $\beta = \sqrt{1-4g^2}$;

(b) *the spectrum of $\widetilde{J}_\gamma^\delta$ is composed of a non-decreasing sequence of eigenvalues $\{\lambda_j(\widetilde{J}_\gamma^\delta)\}_{j\in\mathbb{Z}}$ which can be labeled so that*

$$\lambda_j(\widetilde{J}_\gamma^\delta) = E_{\gamma,j}^0 + \mathrm{r}_\gamma^\delta(j) + O(j^{-1}\ln j) \quad \textit{as } j \to \infty$$

holds with

$$\mathrm{r}_\gamma^\delta(j) = \delta\Big(\frac{\beta}{2\pi g j}\Big)^{1/2}\cos(4\alpha j + \hat{\theta}_\gamma), \tag{2.6}$$

where $E_{\gamma,j}^0$ is given by (2.5), $\beta = \sqrt{1-4g^2}$, α is given by (1.6), and

$$\hat{\theta}_\gamma = \Big(\gamma - \frac{1}{2}\Big)(4\alpha - \pi) + \frac{\pi}{4}. \tag{2.7}$$

Proof. (a) This result was proved in [15]. We describe a simplified proof in Section 2.2.

(b) See Sections 3.2–3.3. ∎

2.2. Diagonalization of $\tilde{J}^0_\gamma$

In what follows, $\mathbb{T} := \mathbb{R}/2\pi\mathbb{Z}$ is identified with $]-\pi,\pi]$ and $\mathrm{L}^2(\mathbb{T})$ denotes the Hilbert space of Lebesgue square integrable functions $]-\pi,\pi] \to \mathbb{C}$ equipped with the scalar product

$$\langle f, g\rangle_{\mathrm{L}^2(\mathbb{T})} := \int_{-\pi}^{\pi} \overline{f(\theta)} g(\theta) \frac{\mathrm{d}\,\theta}{2\pi}$$

and the norm $\|f\|_{\mathrm{L}^2(\mathbb{T})} = \langle f, f\rangle^{1/2}_{\mathrm{L}^2(\mathbb{T})}$. We let $\mathcal{F}_\mathbb{T}$ denote the isometric isomorphism $\mathrm{L}^2(\mathbb{T}) \to \ell^2(\mathbb{Z})$ given by

$$(\mathcal{F}_\mathbb{T} f)(j) = \int_{-\pi}^{\pi} f(\theta) \mathrm{e}^{-\mathrm{i}j\theta} \frac{\mathrm{d}\,\theta}{2\pi}$$

and consider the operator

$$L^0_\gamma := \mathcal{F}_\mathbb{T}^{-1} \tilde{J}^0_\gamma \mathcal{F}_\mathbb{T} = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\,\theta} + g\Big(\mathrm{e}^{\mathrm{i}\theta}\Big(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\,\theta} + \gamma\Big) + \mathrm{h.c.}\Big).$$

Similarly to [5, 15], we observe that the assumption $0 < g < \frac{1}{2}$ ensures the fact that L^0_γ is the first order linear elliptic differential operator,

$$L^0_\gamma = \frac{1}{2}\Big((1 + 2g\cos(\theta))\Big(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\,\theta}\Big) + \mathrm{h.c.}\Big) + (2\gamma - 1)g\cos(\theta)$$

and we introduce

$$\Phi(\theta) := \int_0^\theta \frac{\beta\,\mathrm{d}\,\theta'}{1 + 2g\cos(\theta')}. \tag{2.8}$$

An easy calculation allows one to express the right-hand side of (2.8),

$$\Phi(\theta) = 2\arctan\Big(\sqrt{\frac{1-2g}{1+2g}}\tan\Big(\frac{\theta}{2}\Big)\Big) \quad \text{if } -\pi < \theta < \pi. \tag{2.9}$$

Moreover, $\Phi(\pi) = \pi$ and Φ is odd, i.e., $\Phi(-\theta) = -\Phi(\theta)$. We can use Φ to define a diffeomorphism $\mathbb{T} \to \mathbb{T}$ and consider the change of variable $\eta = \Phi(\theta)$ to define the unitary operator acting in $\mathrm{L}^2(\mathbb{T})$ according to the formula

$$(U_\Phi f)(\theta) = \Phi'(\theta)^{1/2} f(\Phi(\theta)).$$

A direct computation (see [5]) gives

$$U_{\Phi}^{-1} L_{\gamma}^{0} U_{\Phi} = \beta\Big(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\,\eta} + q_{\gamma}(\eta)\Big) \tag{2.10}$$

with

$$q_{\gamma}(\eta) := \beta^{-1}(2\gamma - 1) g \cos(\Phi^{-1}(\eta)). \tag{2.11}$$

In the following, q_{γ} is given by (2.11) and

$$\tilde{q}_{\gamma}(\eta) := \int_{0}^{\eta} q_{\gamma}(\eta')\,\mathrm{d}\,\eta'.$$

We claim that

$$\tilde{q}_{\gamma}(\Phi(\theta)) = \Big(\gamma - \frac{1}{2}\Big)(\theta - \beta^{-1}\Phi(\theta)). \tag{2.12}$$

Indeed,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}\,\theta}(\tilde{q}_{\gamma}(\Phi(\theta))) &= q_{\gamma}(\Phi(\theta))\Phi'(\theta) = \frac{(2\gamma-1) g \cos(\theta)}{\beta}\,\frac{\beta}{1 + 2g\cos(\theta)} \\ &= \frac{2\gamma - 1}{2}\Big(1 - \frac{1}{1 + 2g\cos(\theta)}\Big) = \Big(\gamma - \frac{1}{2}\Big)(1 - \beta^{-1}\Phi'(\theta))\end{aligned}$$

implies $\tilde{q}_{\gamma}(\Phi(\theta)) = \big(\gamma - \frac{1}{2}\big)(\theta - \beta^{-1}\Phi(\theta)) + C_0$ and $C_0 = 0$ holds due to $\Phi(0) = 0$ and $\tilde{q}_{\gamma}(\Phi(0)) = \tilde{q}_{\gamma}(0) = 0$.

Using $\Phi(\pm\pi) = \pm\pi$ in (2.12), we compute

$$\langle q_{\gamma}\rangle := \frac{\tilde{q}_{\gamma}(\pi) - \tilde{q}_{\gamma}(-\pi)}{2\pi} = \Big(\gamma - \frac{1}{2}\Big)(1 - \beta^{-1}). \tag{2.13}$$

Further on, we are going to use the function

$$\varphi_{\gamma}(\theta) := \langle q_{\gamma}\rangle \Phi(\theta) - \tilde{q}_{\gamma}(\Phi(\theta)). \tag{2.14}$$

Using (2.13) and (2.12) in (2.14), we find the expression

$$\varphi_{\gamma}(\theta) = \Big(\gamma - \frac{1}{2}\Big)(\Phi(\theta) - \theta). \tag{2.15}$$

In what follows, we define $(f_{q_{\gamma},j})_{j\in\mathbb{Z}}$ to be the orthonormal basis in $\mathrm{L}^2(\mathbb{T})$ given by

$$f_{q_{\gamma},j}(\eta) = \mathrm{e}^{\mathrm{i}j\eta}\mathrm{e}^{\mathrm{i}(\langle q_{\gamma}\rangle\eta - \tilde{q}_{\gamma}(\eta))}$$

We remark that $\eta \to \langle q_{\gamma}\rangle\eta - \tilde{q}_{\gamma}(\eta)$ is a smooth 2π-periodic function and (see [7,15]), for every $j \in \mathbb{Z}$, we get

$$\beta\Big(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\eta} + q_\gamma\Big) f_{q_\gamma,j} = E^0_{\gamma,j} f_{q_\gamma,j}, \tag{2.16}$$

where $E^0_{\gamma,j} = \beta(j + \langle q_\gamma\rangle) = \beta j + \big(\gamma - \frac{1}{2}\big)(\beta - 1)$ is given by (2.5). Combining (2.16) with (2.10), we obtain

Corollary 2.4. *Let $\{f^0_{\gamma,j}\}_{j\in\mathbb{Z}}$ be the orthonormal basis of* $\mathrm{L}^2(\mathbb{T})$ *given by*

$$f^0_{\gamma,j}(\theta) := (U_\Phi f_{q_\gamma,j})(\theta) = \Phi'(\theta)^{1/2}\mathrm{e}^{\mathrm{i}j\Phi(\theta)}\mathrm{e}^{\mathrm{i}\varphi_\gamma(\theta)}, \tag{2.17}$$

where φ_γ is given by (2.15). *Then*

$$L^0_\gamma f^0_{\gamma,j} = E^0_{\gamma,j} f^0_{\gamma,j} \tag{2.18}$$

holds with $E^0_{\gamma,j}$ given by (2.5).

It is clear that the assertion of Theorem 2.3 (a) follows from Corollary 2.4. Indeed, using (2.18) and $\widetilde{J}^0_\gamma = \mathcal{F}_{\mathbb{T}} L^0_\gamma \mathcal{F}^{-1}_{\mathbb{T}}$, we get

$$\widetilde{J}^0_\gamma u^0_{\gamma,j} = E^0_{\gamma,j} u^0_{\gamma,j} \quad \text{with } u^0_{\gamma,j} := \mathcal{F}_{\mathbb{T}} f^0_{\gamma,j}. \tag{2.19}$$

2.3. An auxiliary estimate

Notation 2.5. (a) For $f \in \mathrm{L}^2(\mathbb{T})$, we write $T_\pi f := f \circ \tau_\pi$ with $\tau_\pi\colon \mathbb{T} \to \mathbb{T}$ given by

$$\tau_\pi(\theta + 2\pi\mathbb{Z}) := \theta + \pi + 2\pi\mathbb{Z}$$

(b) For $j, n \in \mathbb{Z}$, we denote

$$V^\delta_\gamma(j,n) := \delta\langle f^0_{\gamma,j}, T_\pi f^0_{\gamma,n}\rangle_{\mathrm{L}^2(\mathbb{T})}, \tag{2.20}$$

where $f^0_{\gamma,j}$ is given by (2.17).

Lemma 2.6. *Let*

$$\widehat{C}_\gamma := 8(g\beta\sqrt{3})^{-1/2}(2|2\gamma - 1| + 5\pi^{-1}).$$

Then the estimate

$$\sup_{\{k\in\mathbb{Z}:|k|\le gn\}} |V^\delta_\gamma(n+k,n)| \le |\delta|\widehat{C}_\gamma n^{-1/2}$$

holds for every $n \in \mathbb{N}$ such that $n \ge (g\beta)^{-1}$.

Proof. We proeceed in four steps.

Step 1. By definition (2.20),

$$V_\gamma^\delta(n,n+k) = \frac{\delta}{2\pi}\int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}n\Phi-\mathrm{i}(n+k)T_\pi\Phi}\mathrm{e}^{\mathrm{i}(\varphi_\gamma-T_\pi\varphi_\gamma)}(\Phi')^{1/2}(T_\pi\Phi')^{1/2}. \tag{2.21}$$

In what follows, $\mathcal{I}$ denotes a real interval and, for $h,\Psi \in C^1(\mathcal{I})$, we denote

$$\Gamma_{\mathcal{I}}^h(\Psi) := \int_{\mathcal{I}} \mathrm{e}^{\mathrm{i}\Psi(\theta)}h(\theta)\,\mathrm{d}\theta.$$

The equality (2.21) can be written in the form

$$V_\gamma^\delta(n,n+k) = \frac{\delta}{2\pi}\Gamma_{[-\pi,\pi]}^{h_\gamma}(n\beta\Psi_{k/n})$$

with

$$\begin{cases} \Psi_{k/n} := \beta^{-1}\Big(\Phi - \Big(1+\dfrac{k}{n}\Big)T_\pi\Phi\Big), \\ h_\gamma(\theta) := \tilde{h}_\gamma(\theta)\mathrm{e}^{\mathrm{i}\psi_\gamma(\theta)}, \end{cases} \tag{2.22}$$

where

$$\begin{cases} \tilde{h}_\gamma := (\Phi')^{1/2}(T_\pi\Phi')^{1/2}, \\ \psi_\gamma := \varphi_\gamma - T_\pi\varphi_\gamma, \end{cases}$$

and φ_γ given by (2.15). We observe that

$$|h_\gamma(\theta)| = \tilde{h}_\gamma(\theta) = \beta(1-4g^2\cos^2\theta)^{-1/2} \le 1,$$

$$\Psi'_{k/n}(\theta) = \frac{1}{1+2g\cos\theta} - \frac{1+\frac{k}{n}}{1-2g\cos\theta}, \tag{2.23}$$

$$\Psi''_{k/n}(\theta) = \Big(\frac{1}{(1+2g\cos\theta)^2} + \frac{1+\frac{k}{n}}{(1-2g\cos\theta)^2}\Big)\cdot 2g\sin\theta. \tag{2.24}$$

Step 2. We claim that if $|k| < \frac{n}{2}$ and $\mathcal{I} = \big[\frac{\pi}{3}, 2\frac{\pi}{3}\big]$, then

$$|\Gamma_{\mathcal{I}}^{h_\gamma}(n\beta\Psi_{k/n})| \le \frac{8}{(n\beta g\sqrt{3})^{1/2}}\Big(1+\int_{\mathcal{I}}|h'_\gamma|\Big). \tag{2.25}$$

Assume that $|k| < \frac{n}{2}$. If $\theta \in [0,\pi]$, then $\sin\theta \ge 0$ and using (2.24), we get

$$k \ge 0 \Rightarrow \Psi''_{k/n}(\theta) \ge \Psi''_0(\theta) \ge 4g\sin\theta, \tag{2.26}$$

due to the convexity inequality $\frac{1}{2}((1-t)^{-2}+(1+t)^{-2}) \geq 1$ for $0 < t \leq 1$. Similarly,

$$0 \geq \frac{k}{n} \geq -\frac{1}{2} \implies \Psi''_{k/n}(\theta) \geq \Big(1+\frac{k}{n}\Big)\Psi''_0(\theta) \geq \frac{1}{2}\Psi''_0(\theta) \geq 2g\sin\theta. \tag{2.27}$$

If $\theta \in \big[\frac{\pi}{3}, 2\frac{\pi}{3}\big]$, then $\sin\theta \geq \frac{\sqrt{3}}{2}$ and (2.26)–(2.27) imply $|\Psi''_{k/n}(\theta)| \geq g\sqrt{3}$. Thus, $n\beta|\Psi''_{k/n}| \geq n\beta g\sqrt{3}$ and we complete the proof of (2.25), using Lemma 8.1 (b) with $\lambda = n\beta g\sqrt{3}$ and $\Psi = \frac{\Psi_{k/n}}{\lambda}$.

Step 3. We claim that if $|k| < gn$ and $\mathcal{I} = \big[0, \frac{\pi}{3}\big]$, then

$$|\Gamma^{h_\gamma}_{\mathcal{I}}(n\beta\Psi_{k/n})| \leq \frac{6}{n\beta g}\Big(1 + \int_{\mathcal{I}} |h'_\gamma|\Big). \tag{2.28}$$

Indeed, due to (2.23),

$$-\Psi'_{k/n}(\theta) = \frac{4g\cos\theta + (1+2g\cos\theta)\frac{k}{n}}{1-4g^2\cos^2\theta} \geq 4g\cos\theta + (1+2g\cos\theta)\frac{k}{n},$$

and $\frac{|k|}{n} < g$ ensures

$$4g\cos\theta + (1+2g\cos\theta)\frac{k}{n} \geq 4g\cos\theta - (1+2g\cos\theta)g =$$

$$= (2-g)\cdot 2g\cos\theta - g \geq (2-g)g - g \geq \frac{g}{2},$$

where we used that $\cos\theta \geq \frac{1}{2}$ holds for $\theta \in \big[0, \frac{\pi}{3}\big]$ and $g < \frac{1}{2}$. Since $\Psi''_{k/n}(\theta) \geq 0$ and $n\beta|\Psi'_{k/n}(\theta)| \geq n\beta\frac{g}{2}$, we complete the proof of (2.28), using Lemma 8.1 (a) with $\lambda = n\beta\frac{g}{2}$ and $\Psi = \frac{\Psi_{k/n}}{\lambda}$.

Step 4. We first observe that (2.25) holds when $\mathcal{I} = \big[-2\frac{\pi}{3}, -\frac{\pi}{3}\big]$ as well. Similarly, (2.28) holds when $\mathcal{I} = \big[-\frac{\pi}{3}, 0\big]$ and when $\mathcal{I} = \pm\big[2\frac{\pi}{3}, \pi\big]$. Since the condition $n\beta g \geq 1$ implies $6(n\beta g)^{-1} < 8(n\beta g\sqrt{3})^{-1/2}$, we can replace the right-hand side of (2.28) by the right-hand side of (2.25) and, combining these six estimates, we get

$$|\Gamma^{h_\gamma}_{[-\pi,\pi]}(n\beta\Psi_{k/n})| \leq \frac{8}{(n\beta g\sqrt{3})^{1/2}}\Big(6 + \int_{-\pi}^{\pi} |h'_\gamma|\Big).$$

To complete the proof, it suffices to show the estimate

$$\int_{-\pi}^{\pi} |h'_\gamma| \leq 4 + 4\pi|2\gamma - 1|. \tag{2.29}$$

We first claim that

$$\int_{-\pi}^{\pi} |\tilde{h}'_\gamma| \leq 4. \tag{2.30}$$

Indeed, $\tilde{h}_\gamma$ is monotonic on $\pm\big[0, \frac{\pi}{2}\big]$ and $\pm\big[\frac{\pi}{2}, \pi\big]$, hence $0 < \tilde{h}_\gamma \leq 1$ implies

$$\int_{\pm[0,\pi/2]} |\tilde{h}'_\gamma| \leq 1 \quad \text{and} \quad \int_{\pm[\pi/2,\pi]} |\tilde{h}'_\gamma| \leq 1.$$

We next observe that $\psi'_\gamma = \varphi'_\gamma - T_\pi \varphi'_\gamma$ holds with $\varphi'_\gamma(\theta) = \big(\gamma - \frac{1}{2}\big)(\Phi' - 1)$ and

$$\int_{-\pi}^{\pi} |\psi'_\gamma| \leq 2 \int_{-\pi}^{\pi} |\varphi'_\gamma| \leq \int_{-\pi}^{\pi} 2\Big|\gamma - \frac{1}{2}\Big|(\Phi' + 1) = 4\pi|2\gamma - 1|. \tag{2.31}$$

The estimate (2.29) follows from $|h'_\gamma| \leq |\tilde{h}'_\gamma| + |\psi'_\gamma|$, (2.30) and (2.31). ■

3. A ZOA remainder estimate with explicit constants

3.1. Statement of the result

The assertion of Theorem 2.3 is a variant of the ZOA (zeroth order approximation) method considered in [18]. Its idea consists in using the diagonal entries of a perturbation as the first correction for eigenvalues of a perturbed diagonal matrix. In Section 3.2 and 3.3 we will show that Theorem 2.3 follows from.

Proposition 3.1. *Let $J : \ell^{2,1}(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ be given by the formula*

$$J = \Lambda + V,$$

where $\Lambda = \operatorname{diag}(j)_{j\in\mathbb{Z}}$ and $V \in \mathcal{B}(\ell^2(\mathbb{Z}))$ is a self-adjoint operator satisfying the estimate

$$\sup_{\{k\in\mathbb{Z}:|k|\leq\hat{c}|n|\}} |V(n+k, n)| \leq \widehat{C}|n|^{-1/2} \quad \text{for } n \geq \hat{\nu}, \tag{3.1}$$

where $\hat{\nu} > 0$, $\widehat{C} > 0$, and $0 < \hat{c} < 1$ are some constants independent of n. Denote

$$\nu := \max\{\hat{\nu}, 64\widehat{C}^2, 8\|V\|^2(3 + 2\|V\|)^2(128\widehat{C}^2 + \hat{c}^{-1})\}. \tag{3.2}$$

Then

(a) *the spectrum of J is composed of a non-decreasing sequence of eigenvalues $\{\lambda_j(J)\}_{j\in\mathbb{Z}}$ which can be labeled so that for $n > \nu + 1 + \|V\|$ one has*

$$n - \frac{3}{8} < \lambda_n(J) < n + \frac{3}{8}; \tag{3.3}$$

(b) *if* $n > \nu + 1 + \|V\|$, *then the estimate*

$$|\lambda_n(J) - n - V(n,n)| \leq \frac{\widetilde{C} + 4\widehat{C}^2(1 + \ln n)}{n} \tag{3.4}$$

holds with

$$\widetilde{C} := (16\widehat{C}^2 + (8\hat{c})^{-1})\|V\|(1 + 128\|V\|) + 2\|V\|^2\hat{c}^{-1}. \tag{3.5}$$

Proof. (a) See Section 5.

(b) See Section 6. ∎

3.2. Proof of Theorem 2.3 (b)

In what follows, we describe how to deduce the assertion of Theorem 2.3 (b) from Proposition 3.1. We begin by introducing $\widetilde{U}_\gamma$, the unitary operator in $\ell^2(\mathbb{Z})$ satisfying $\widetilde{U}_\gamma \tilde{e}_j = u^0_{\gamma,j}$, where $\{\tilde{e}_j\}_{j\in\mathbb{Z}}$ is the canonical basis of $\ell^2(\mathbb{Z})$ and $\{u^0_{\gamma,j}\}_{j\in\mathbb{Z}}$ is the basis introduced in (2.19). We claim that the hypotheses of Proposition 3.1 are satisfied if

$$J = \widetilde{U}_\gamma^{-1} \widetilde{J}^\delta_\gamma \widetilde{U}_\gamma,$$

where $\widetilde{J}^\delta_\gamma$ is as in Definition 2.2. Indeed, if $\beta = \sqrt{1 - 4g^2}$ and

$$\beta_\gamma = \Big(\gamma - \frac{1}{2}\Big)(\beta - 1),$$

then $E^0_j = \beta j + \beta_\gamma$, hence (2.19) gives

$$\widetilde{U}_\gamma^{-1} \widetilde{J}^0_\gamma \widetilde{U}_\gamma = \beta\Lambda + \beta_\gamma$$

and

$$\widetilde{U}_\gamma^{-1} \widetilde{J}^\delta_\gamma \widetilde{U}_\gamma = \beta\Lambda + \beta_\gamma + V^\delta_\gamma$$

holds with

$$V^\delta_\gamma := \widetilde{U}_\gamma^{-1} D_\delta \widetilde{U}_\gamma,$$

where $D_\delta = \mathrm{diag}(\delta(-1)^j)_{j\in\mathbb{Z}}$ (see (2.3)). Therefore,

$$\langle \tilde{e}_j, V^\delta_\gamma \tilde{e}_k\rangle = \langle u^0_{j,\gamma}, D_\delta u^0_{j,\gamma}\rangle = \langle f^0_{j,\gamma}, \mathcal{F}_{\mathbb{T}}^{-1} D_\delta \mathcal{F}_{\mathbb{T}} f^0_{j,\gamma}\rangle_{\mathrm{L}^2(\mathbb{T})}, \tag{3.6}$$

where we used $u^0_{j,\gamma} = \mathcal{F}_{\mathbb{T}} f^0_{j,\gamma}$ and the isometry $\mathcal{F}_{\mathbb{T}}$. Since $\mathcal{F}_{\mathbb{T}}^{-1} D_\delta \mathcal{F}_{\mathbb{T}} = \delta T_\pi$ holds with T_π introduced in Notation 2.5, (3.6) gives

$$\langle \tilde{e}_j, V^\delta_\gamma \tilde{e}_k\rangle = V^\delta_\gamma(j,k)$$

with $V_\gamma^\delta(\cdot,\cdot)$ expressed by (2.20). We observe that Proposition 3.1 can be applied to $V = \beta^{-1}V_\gamma^\delta = V_\gamma^{\delta/\beta}$ and

$$J := \widetilde{U}_\gamma^{-1}\beta^{-1}(\widetilde{J}_\gamma^\delta - \beta_\gamma)\widetilde{U}_\gamma = \Lambda + \beta^{-1}V_\gamma^\delta.$$

Indeed, Lemma 2.6 ensures that $V = V_\gamma^{\delta/\beta}$ satisfies the estimate (3.1) with $\hat{c} = g$ and $\widehat{C} = \widehat{C}_{\delta,\gamma}$ given by

$$\widehat{C}_{\delta,\gamma} = \beta^{-1}|\delta|\widehat{C}_\gamma = 8|\delta|(g\sqrt{3})^{-1/2}\beta^{-3/2}(2|2\gamma-1| + 5\pi^{-1}). \tag{3.7}$$

Taking

$$\lambda_j(\widetilde{J}_\gamma^\delta) = \beta\lambda_j(J) + \beta_\gamma, \tag{3.8}$$

we get the non-decreasing sequence of eigenvalues of $\widetilde{J}_\gamma^\delta$ satisfying

$$|\lambda_n(\widetilde{J}_\gamma^\delta) - E_{\gamma,n}^0 - V_\gamma^\delta(n,n)| = \beta|\lambda_n(J) - n - V_\gamma^{\delta/\beta}(n,n)|. \tag{3.9}$$

Due to Proposition 3.1, the quantity (3.9) is $O(n^{-1}\ln n)$ as $n \to \infty$ and, to complete the proof of Theorem 2.3 (b), it remains to prove the estimate

$$V_\gamma^\delta(n,n) = \mathrm{r}_\gamma^\delta(n) + O(n^{-1}) \quad \text{as } n \to \infty, \tag{3.10}$$

where r_γ^δ is given by (2.6)–(2.7). The proof of (3.10) is given in Section 3.3.

Moreover, combining (3.9) with the assertions of Proposition 3.1 we obtain

Corollary 3.2. *Let $\widetilde{J}_\gamma^\delta$ and $E_{\gamma,n}^0$ be as in Theorem 2.3.*

(a) *If $\widehat{C}_{\delta,\gamma}$ is given by (3.7) and*

$$\nu_{\delta,\gamma} := \max\{(g\beta)^{-1}, 64\widehat{C}_{\delta,\gamma}^2, 8\delta^2\beta^{-2}(3+2|\delta|\beta^{-1})(128\widehat{C}_{\delta,\gamma}^2 + g^{-1})\}, \tag{3.11}$$

then the spectrum of $\widetilde{J}_\gamma^\delta$ is composed of a non-decreasing sequence of eigenvalues $\{\lambda_j(\widetilde{J}_\gamma^\delta)\}_{j\in\mathbb{Z}}$ which can be labeled so that

$$E_{\gamma,n}^0 - \frac{3}{8}\beta < \lambda_n(\widetilde{J}_\gamma^\delta) < E_{\gamma,n}^0 + \frac{3}{8}\beta \tag{3.12}$$

holds for $n > \nu_{\delta,\gamma} + 1 + \left|\frac{\delta}{\beta}\right|$.

(b) *If $n > \nu_{\delta,\gamma} + 1 + \left|\frac{\delta}{\beta}\right|$, then the estimate*

$$|\lambda_n(\widetilde{J}_\gamma^\delta) - E_{\gamma,n}^0 - V_\gamma^\delta(n,n)| \le \frac{\widetilde{C}_{\delta,\gamma} + 4\beta\widehat{C}_{\delta,\gamma}^2(1+\ln n)}{n} \tag{3.13}$$

holds with

$$\widetilde{C}_{\delta,\gamma} := (16\widehat{C}_{\delta,\gamma}^2 + (8g)^{-1})(|\delta| + 128\delta^2\beta^{-1}) + 2\delta^2\beta^{-1}g^{-1}. \tag{3.14}$$

Proof. We observe that $\nu_{\delta,\gamma}$ is obtained from ν expressed by (3.2) with $\widehat{C} = \widehat{C}_{\delta,\gamma}$ given by (3.7) and

$$\|V\| = \|V_\gamma^{\delta/\beta}\| = \|D_{\delta/\beta}\| = \left|\frac{\delta}{\beta}\right|.$$

Therefore, (3.8) and (3.3) imply (3.12) for $n > \nu_{\delta,\gamma} + 1 + \left|\frac{\delta}{\beta}\right|$.

Similarly, (3.4) allows us to estimate the quantity (3.9) by the right-hand side of (3.13) with $\widetilde{C}_{\delta,\gamma} = \beta\widetilde{C}$ where $\widetilde{C}$ is given by (3.5) with $\widehat{C} = \widehat{C}_{\delta,\gamma}$ and $\|V\| = \left|\frac{\delta}{\beta}\right|$. ∎

3.3. Proof of (3.10)

We can express

$$V_\gamma^\delta(n,n) = \delta \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}n\Psi(\theta)} h_\gamma(\theta)\frac{\mathrm{d}\theta}{2\pi}, \tag{3.15}$$

where $\Psi := \Phi - T_\pi\Phi$ with Φ given by (2.8), $h_\gamma = \sqrt{\Phi' T_\pi \Phi'}\mathrm{e}^{\mathrm{i}\varphi_\gamma - \mathrm{i}T_\pi\varphi_\gamma}$ with φ_γ given by (2.15), and T_π is the translation defined in Notation 2.5.

Using $k = 0$ in (2.22) and (2.23)–(2.24), we find that $\Psi = \beta\Psi_0$ has two non-degenerated critical points $\pm\frac{\pi}{2}$. Applying the stationary phase formula, we obtain

$$V_\gamma^\delta(n,n) = \delta \sum_{\nu=\pm 1} \frac{h_\gamma\left(\nu\frac{\pi}{2}\right)\mathrm{e}^{\mathrm{i}n\Psi(\nu\pi/2)+\mathrm{i}\nu\pi/4}}{\sqrt{2\pi n\left|\Psi''\left(\nu\frac{\pi}{2}\right)\right|}} + O(n^{-1}). \tag{3.16}$$

Since Φ is odd, we get

$$\Psi\left(\pm\frac{\pi}{2}\right) = \Phi\left(\pm\frac{\pi}{2}\right) - \Phi\left(\mp\frac{\pi}{2}\right) = 2\Phi\left(\pm\frac{\pi}{2}\right) = \pm 2\Phi\left(\frac{\pi}{2}\right) = \pm 4\alpha \tag{3.17}$$

where (2.9) was used to write $\Phi\left(\frac{\pi}{2}\right) = 2\alpha$ with α given by (1.6). Denote

$$\tilde{\theta}_\gamma := \varphi_\gamma\left(\frac{\pi}{2}\right) = \left(\gamma - \frac{1}{2}\right)\left(2\alpha - \frac{\pi}{2}\right)$$

(see (2.15)). Then

$$\psi_\gamma\left(\pm\frac{\pi}{2}\right) = \pm 2\varphi_\gamma\left(\frac{\pi}{2}\right) = \pm 2\tilde{\theta}_\gamma$$

and

$$h_\gamma\left(\pm\frac{\pi}{2}\right) = \beta\mathrm{e}^{\pm 2\mathrm{i}\tilde{\theta}_\gamma}, \tag{3.18}$$

hence we get two conjugated terms corresponding to $\nu = \pm 1$ in (3.16). Therefore, using (3.18), (3.17), and $\left|\Psi''\left(\pm\frac{\pi}{2}\right)\right| = 4g\beta$ in (3.16), we get

$$\begin{aligned} V_\gamma^\delta(n,n) &= \delta\frac{2\mathrm{Re}\left(\beta\mathrm{e}^{2\mathrm{i}\tilde{\theta}_\gamma}\mathrm{e}^{\mathrm{i}4n\alpha+\mathrm{i}\pi/4}\right)}{\sqrt{2\pi n\cdot 4g\beta}} + O(n^{-1}) \\ &= \delta\frac{\sqrt{\beta}\cos\left(4n\alpha + 2\tilde{\theta}_\gamma + \frac{\pi}{4}\right)}{\sqrt{2\pi n g}} + O(n^{-1}). \end{aligned}$$

To complete the proof of (3.10), we observe that

$$\hat{\theta}_\gamma = 2\tilde{\theta}_\gamma + \frac{\pi}{4} = \Big(\gamma - \frac{1}{2}\Big)(4\alpha - \pi) + \frac{\pi}{4}$$

as claimed in (2.7).

4. Auxiliary operators Q_n and $Q_{n,\rho}$

4.1. Definitions

In what follows, we introduce auxiliary self-adjoint bounded operators $\{Q_n\}_{n\in\mathbb{Z}}$ (see Definition 4.2 and Lemma 4.3) and for $\rho \geq 0$, we define

$$Q_{n,\rho} := \sum_{i\in\mathbb{Z}\cap[-\rho,\rho]} Q_{n+i}. \tag{4.1}$$

In Section 5, the spectrum of J will be investigated via an analysis of operators

$$J'_{n,\rho} := \mathrm{e}^{-\mathrm{i}Q_{n,\rho}} J \mathrm{e}^{\mathrm{i}Q_{n,\rho}}.$$

Notation 4.1. For $n \in \mathbb{Z}$ and $\rho \geq 0$, we consider the orthogonal decomposition

$$\ell^2(\mathbb{Z}) = \widehat{\mathcal{H}}_{n,\rho} \oplus \widetilde{\mathcal{H}}_{n,\rho}$$

where

$$\widehat{\mathcal{H}}_{n,\rho} = \operatorname{span}\{\tilde{e}_{n+i}\}_{i\in\mathbb{Z}\cap[-\rho,\rho]}, \quad \widetilde{\mathcal{H}}_{n,\rho} = (\widehat{\mathcal{H}}_{n,\rho})^\perp.$$

We define $\widehat{\Pi}_{n,\rho} \in \mathcal{B}(\ell^2(\mathbb{Z}))$ (respectively $\widetilde{\Pi}_{n,\rho} \in \mathcal{B}(\ell^2(\mathbb{Z}))$) as the orthogonal projection on $\widehat{\mathcal{H}}_{n,\rho}$ (respectively on $\widetilde{\mathcal{H}}_{n,\rho}$). If $\rho = 0$, then we abbreviate

$$\widehat{\mathcal{H}}_{n,0} = \widehat{\mathcal{H}}_n, \quad \widetilde{\mathcal{H}}_{n,0} = \widetilde{\mathcal{H}}_n, \quad \widehat{\Pi}_{n,0} = \widehat{\Pi}_n, \quad \widetilde{\Pi}_{n,0} = \widetilde{\Pi}_n.$$

Definition 4.2. Let $V \in \mathcal{B}(\ell^2(\mathbb{Z}))$ be a self-adjoint operator satisfying the assumptions of Proposition 3.1. For $n \in \mathbb{Z}$ we define the matrix $(Q_n(j,k))_{(j,k)\in\mathbb{Z}^2}$ by

$$Q_n(j,k) = \begin{cases} \mathrm{i}\dfrac{V(j,n)}{j-n} & \text{when } j \neq n \text{ and } k = n, \\ \mathrm{i}\dfrac{V(n,k)}{n-k} & \text{when } j = n \text{ and } k \neq n, \\ 0 & \text{otherwise.} \end{cases} \tag{4.2}$$

Then $Q_n(k,j) = \overline{Q_n(j,k)}$ and

$$Q_n(j,k) \neq 0 \implies (\text{either } (j \neq n \text{ and } k = n) \text{ or } (j = n \text{ and } k \neq n)). \tag{4.3}$$

Lemma 4.3. *Under the assumptions of Proposition 3.1, we can define a self-adjoint operator $Q_n \in \mathcal{B}(\ell^2(\mathbb{Z}))$ such that $(Q_n \tilde{e}_k)(j) = Q_n(j,k)$ holds with $(Q_n(j,k))_{j,k\in\mathbb{Z}}$ given by Notation 4.1 and*

$$\|Q_n\|^2 \leq 4\widehat{C}^2 n^{-1} + \hat{c}^{-2}\|V\|^2 n^{-2}$$

holds for $n \geq \hat{\nu}$.

Proof. We first observe that

$$\|Q_n \widehat{\Pi}_n\|^2 = \|Q_n e_n\|^2 = \sum_{j\in\mathbb{Z}} |Q_n(j,n)|^2 \leq \sum_{j\in\mathbb{Z}\setminus\{n\}} \frac{|V(j,n)|^2}{(j-n)^2} \leq \mathcal{M}_n + \mathcal{M}'_n$$

holds with

$$\mathcal{M}_n := \sum_{\{j\in\mathbb{Z}:0<|j-n|\leq\hat{c}n\}} \frac{|V(j,n)|^2}{(j-n)^2} \leq \sum_{m\in\mathbb{Z}\setminus\{0\}} \frac{\widehat{C}^2 n^{-1}}{m^2} = \frac{\pi^2\widehat{C}^2}{3n} < \frac{4\widehat{C}^2}{n}$$

due to (3.1) and

$$\mathcal{M}'_n := \sum_{\{j\in\mathbb{Z}:|j-n|>\hat{c}n\}} \frac{|V(j,n)|^2}{(j-n)^2} \leq \sum_{j\in\mathbb{Z}} \frac{|V(j,n)|^2}{\hat{c}^2 n^2} = \frac{\|V\tilde{e}_n\|^2}{\hat{c}^2 n^2} \leq \frac{\|V\|^2}{\hat{c}^2 n^2}.$$

We observe that (4.3) implies

$$\widehat{\Pi}_n Q_n \widehat{\Pi}_n = 0 = \widetilde{\Pi}_n Q_n \widetilde{\Pi}_n$$

and

$$Q_n = \widetilde{\Pi}_n Q_n \widehat{\Pi}_n + \widehat{\Pi}_n Q_n \widetilde{\Pi}_n.$$

Therefore,

$$\langle x, Q_n y\rangle = \langle \widetilde{\Pi}_n x, Q_n \widehat{\Pi}_n y\rangle + \langle Q_n \widehat{\Pi}_n x, \widetilde{\Pi}_n y\rangle$$

and

$$\begin{aligned}|\langle x, Q_n y\rangle| &\leq \|Q_n \widehat{\Pi}_n\|(\|\widetilde{\Pi}_n x\|\|\widehat{\Pi}_n y\| + \|\widehat{\Pi}_n x\|\|\widetilde{\Pi}_n y\|)\\ &\leq \|Q_n \widehat{\Pi}_n\|\|x\|\|y\|,\end{aligned}$$

i.e., $\|Q_n\|^2 = \|Q_n \widehat{\Pi}_n\|^2 \leq \mathcal{M}_n + \mathcal{M}'_n$. ∎

4.2. Properties of Q_n and $Q_{n,\rho}$

Lemma 4.4. *Let $Q_n \in \mathcal{B}(\ell^2(\mathbb{Z}))$ be as in Lemma 4.3 and $Q_{n,\rho}$ given by (4.1). Then*

(a) *the subspace $\ell^{2,1}(\mathbb{Z})$ is invariant for Q_n and for every $x \in \ell^{2,1}(\mathbb{Z})$,*

$$\mathrm{i}[Q_n, \Lambda]x = \mathrm{i}(Q_n\Lambda - \Lambda Q_n)x = V_n x \tag{4.4}$$

holds with

$$V_n := \widetilde{\Pi}_n V \widehat{\Pi}_n + \widehat{\Pi}_n V \widetilde{\Pi}_n; \tag{4.5}$$

(b) *if $Q_{n,\rho}$ is given by (4.1), then the subspace $\ell^{2,1}(\mathbb{Z})$ is invariant for $\mathrm{e}^{\mathrm{i}tQ_{n,\rho}}$ and $t \to \mathrm{e}^{\mathrm{i}tQ_{n,\rho}}x$ is of class $\mathrm{C}^\infty(\mathbb{R};\ell^{2,1}(\mathbb{Z}))$ if $x \in \ell^{2,1}(\mathbb{Z})$.*

Proof. (a) Let V_n be given by (4.5). Then one has

$$V_n(j,k) = (V_n\tilde{e}_k)(j) = \begin{cases} V(j,n) & \text{when } j \neq n \text{ and } k = n, \\ V(n,k) & \text{when } j = n \text{ and } k \neq n, \\ 0 & \text{otherwise,} \end{cases} \tag{4.6}$$

and combining (4.6) with (4.2) we obtain

$$\mathrm{i}(j-k)Q_n(j,k) = -V_n(j,k) \quad \text{for every } j,k \in \mathbb{Z}. \tag{4.7}$$

However, (4.7) implies

$$\mathrm{i}\Big(j + \frac{1}{2}\Big)(Q_n\tilde{e}_k)(j) = \mathrm{i}\Big(Q_n\Big(k + \frac{1}{2}\Big)\tilde{e}_k\Big)(j) - (V_n\tilde{e}_k)(j) \tag{4.8}$$

and ensures $Q_n\tilde{e}_k \in \ell^{2,1}(\mathbb{Z})$. Moreover, (4.8) ensures the equality

$$\mathrm{i}\Big(\Lambda + \frac{1}{2}\Big)Q_n x = \mathrm{i}Q_n\Big(\Lambda + \frac{1}{2}\Big)x - V_n x \tag{4.9}$$

for $x \in \ell^2_{\mathrm{fin}}(\mathbb{Z})$. If $y \in \ell^2_{\mathrm{fin}}(\mathbb{Z})$, then using (4.9) with $x = \big(\Lambda + \frac{1}{2}\big)^{-1} y$, we obtain

$$\mathrm{i}\Big(\Lambda + \frac{1}{2}\Big)Q_n\Big(\Lambda + \frac{1}{2}\Big)^{-1} y = \mathrm{i}Q_n' y \tag{4.10}$$

with $Q_n' \in \mathcal{B}(\ell^2(\mathbb{Z}))$ given by

$$Q_n' := Q_n + \mathrm{i}V_n\Big(\Lambda + \frac{1}{2}\Big)^{-1}.$$

Due to (4.10), for every $y \in \ell^2_{\mathrm{fin}}(\mathbb{Z})$ one has

$$\mathrm{i}Q_n\Big(\Lambda + \frac{1}{2}\Big)^{-1} y = \mathrm{i}\Big(\Lambda + \frac{1}{2}\Big)^{-1} Q_n' y \tag{4.11}$$

and by continuity, (4.11) holds for every $y \in \ell^2(\mathbb{Z})$. Consider now $x \in \ell^{2,1}(\mathbb{Z})$ and take $y = \big(\Lambda + \frac{1}{2}\big)x$ in (4.11). This gives

$$\mathrm{i}Q_n x = \mathrm{i}\Big(\Lambda + \frac{1}{2}\Big)^{-1} Q'_n \Big(\Lambda + \frac{1}{2}\Big)x \in \ell^{2,1}(\mathbb{Z})$$

and

$$\mathrm{i}\Big(\Lambda + \frac{1}{2}\Big)Q_n x = \mathrm{i}Q'_n\Big(\Lambda + \frac{1}{2}\Big)x = \mathrm{i}Q_n\Big(\Lambda + \frac{1}{2}\Big)x - V_n x,$$

implying (4.4) for every $x \in \ell^{2,1}(\mathbb{Z})$.

(c) We observe that (4.11) holds for every $y \in \ell^2(\mathbb{Z})$ and implies (4.10) for every $y \in \ell^2(\mathbb{Z})$. If $Q'_{n,\rho} := \sum_{i \in \mathbb{Z} \cap [-\rho,\rho]} Q'_{n+i}$, then (4.10) implies

$$(Q'_{n,\rho})^m y = \Big(\Lambda + \frac{1}{2}\Big)(Q_{n,\rho})^m \Big(\Lambda + \frac{1}{2}\Big)^{-1} y$$

for every $m \in \mathbb{N}$ and $y \in \ell^2(\mathbb{Z})$. Therefore,

$$\begin{aligned}
\mathrm{e}^{\mathrm{i}tQ_{n,\rho}}\Big(\Lambda + \frac{1}{2}\Big)^{-1} y &= \lim_{N\to\infty} \sum_{m=0}^{N} \frac{(\mathrm{i}t)^m}{m!}(Q_{n,\rho})^m\Big(\Lambda + \frac{1}{2}\Big)^{-1} y = \\
&= \lim_{N\to\infty} \sum_{m=0}^{N} \frac{(\mathrm{i}t)^m}{m!}\Big(\Lambda + \frac{1}{2}\Big)^{-1}(Q'_{n,\rho})^m y \\
&= \Big(\Lambda + \frac{1}{2}\Big)^{-1} \mathrm{e}^{\mathrm{i}tQ'_{n,\rho}} y \in \ell^{2,1}(\mathbb{Z})
\end{aligned}$$

if $y \in \ell^2(\mathbb{Z})$ and setting $x = \big(\Lambda + \frac{1}{2}\big)^{-1} y$, we find that $t \to \big(\Lambda + \frac{1}{2}\big)\mathrm{e}^{\mathrm{i}tQ_{n,\rho}} x = \mathrm{e}^{\mathrm{i}tQ'_{n,\rho}} y$ is $\mathrm{C}^\infty(\mathbb{R}; \ell^2(\mathbb{Z}))$ for every $x \in \ell^{2,1}(\mathbb{Z})$. ■

5. Proof of Proposition 3.1 (a)

5.1. Taylor's expansion formula

Assume that B and $Q \in \mathcal{B}(\ell^2(\mathbb{Z}))$ and denote

$$\begin{aligned}
F_{tQ}(B) &:= \mathrm{e}^{-\mathrm{i}tQ} B \mathrm{e}^{\mathrm{i}tQ} \quad \text{for } t \in \mathbb{R},\\
\mathrm{ad}^0_{\mathrm{i}Q}(B) &:= B,\\
\mathrm{ad}^1_{\mathrm{i}Q}(B) &:= [B, \mathrm{i}Q] = \mathrm{i}(BQ - QB),
\end{aligned}$$

and

$$\mathrm{ad}^{m+1}_{\mathrm{i}Q}(B) := [\mathrm{ad}^m_{\mathrm{i}Q}(B), \mathrm{i}Q] \quad \text{for } m \in \mathbb{N}^*.$$

Then

$$\frac{\mathrm{d}^m}{\mathrm{d}t^m}F_{tQ}(B) = \mathrm{e}^{-\mathrm{i}tQ}\mathrm{ad}^m_{\mathrm{i}Q}(B)\mathrm{e}^{\mathrm{i}tQ} = F_{tQ}(\mathrm{ad}^m_{\mathrm{i}Q}(B))$$

and the Taylor formula gives

$$F_{tQ}(B) = \sum_{m=0}^{N-1}\frac{t^m}{m!}\mathrm{ad}^m_{\mathrm{i}Q}(B) + \mathscr{R}^{t,N}_Q(B) \tag{5.1}$$

with

$$\mathscr{R}^{t,N}_Q(B) := \frac{t^N}{(N-1)!}\int_0^1 F_{stQ}(\mathrm{ad}^N_{\mathrm{i}Q}(B))(1-s)^{N-1}\,\mathrm{d}s. \tag{5.2}$$

We can also consider the case when B is an unbounded symmetric operator in $\ell^2(\mathbb{Z})$, defined on a dense domain $\mathrm{Dom}(B)$. Suppose that $\mathrm{Dom}(B)$ is an invariant subspace for Q and $\mathrm{e}^{\mathrm{i}tQ}$ for every $t \in \mathbb{R}$. If $t \to B\mathrm{e}^{\mathrm{i}tQ}x$ is $C^1(\mathbb{R}, \ell^2(\mathbb{Z}))$ for every $x \in \mathrm{Dom}(B)$, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \mathrm{e}^{\mathrm{i}tQ}x, B\mathrm{e}^{\mathrm{i}tQ}y\rangle = \langle B\mathrm{e}^{\mathrm{i}tQ}x, \mathrm{i}Q\mathrm{e}^{\mathrm{i}tQ}y\rangle + \langle \mathrm{i}Q\mathrm{e}^{\mathrm{i}tQ}x, B\mathrm{e}^{\mathrm{i}tQ}y\rangle$$

holds for every $x, y \in \mathrm{Dom}(B)$. If the form $(x, y) \to \langle Bx, \mathrm{i}Qy\rangle + \langle \mathrm{i}Qx, By\rangle$ can be extended from $\mathrm{Dom}(B) \times \mathrm{Dom}(B)$ to a bounded form on $\ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})$, then we can introduce $[B, \mathrm{i}Q] \in \mathscr{B}(\ell^2(\mathbb{Z}))$ defined by this form and we can write

$$\frac{\mathrm{d}}{\mathrm{d}t}F_{tQ}(B) = \mathrm{e}^{-\mathrm{i}tQ}[B, \mathrm{i}Q]\mathrm{e}^{\mathrm{i}tQ} = F_{tQ}([B, \mathrm{i}Q])$$

and (5.1)–(5.2) still hold for every $N \in \mathbb{N} \setminus \{0\}$.

5.2. A similarity transformation

In what follows, V_n are as in Lemma 4.4 (a) and

$$V_{n,\rho} := -[\Lambda, \mathrm{i}Q_{n,\rho}] = \sum_{i\in\mathbb{Z}\cap[-\rho,\rho]} V_{n+i}. \tag{5.3}$$

Then

$$V - V_{n,\rho} = \widehat{V}_{n,\rho} \oplus \widetilde{V}_{n,\rho} \tag{5.4}$$

holds with

$$\widehat{V}_{n,\rho} := \sum_{i\in\mathbb{Z}\cap[-\rho,\rho]} V(n+i, n+i)\widehat{\Pi}_{n+i} \tag{5.5}$$

and

$$\widetilde{V}_{n,\rho} := \widetilde{\Pi}_{n,\rho}V_{n,\rho}|_{\widetilde{\mathscr{H}}_{n,\rho}}. \tag{5.6}$$

We claim that the operator

$$J'_{n,\rho} := \mathrm{e}^{-\mathrm{i}Q_{n,\rho}}(\Lambda + V)\mathrm{e}^{\mathrm{i}Q_{n,\rho}} \tag{5.7}$$

can written in the form

$$J'_{n,\rho} = \Lambda + (\widehat{V}_{n,\rho} \oplus \widetilde{V}_{n,\rho}) + R_{n,\rho} \tag{5.8}$$

with

$$\|R_{n,\rho}\| \leq 4\|V\|\|Q_{n,\rho}\|. \tag{5.9}$$

To prove this claim, we first observe that (5.1)–(5.2) with $N = 1$ and $N = 2$ respectively, imply

$$\mathrm{e}^{-\mathrm{i}Q_{n,\rho}} V \mathrm{e}^{\mathrm{i}Q_{n,\rho}} = V + \mathcal{R}^{1,1}_{Q_{n,\rho}}(V), \tag{5.10}$$

$$\mathrm{e}^{-\mathrm{i}Q_{n,\rho}} \Lambda \mathrm{e}^{\mathrm{i}Q_{n,\rho}} = \Lambda + [\Lambda, \mathrm{i}Q_{n,\rho}] + \mathcal{R}^{1,2}_{Q_{n,\rho}}(\Lambda), \tag{5.11}$$

and, combining (5.10)–(5.11) with (5.3), we get

$$J'_{n,\rho} = \Lambda + V - V_{n,\rho} + \mathcal{R}^{1,1}_{Q_{n,\rho}}(V) + \mathcal{R}^{1,2}_{Q_{n,\rho}}(\Lambda).$$

Due to (5.4), we get (5.8) with $R_{n,\rho} = \mathcal{R}^{1,1}_{Q_{n,\rho}}(V) + \mathcal{R}^{1,2}_{Q_{n,\rho}}(\Lambda)$ and (5.9) follows from

$$\|\mathcal{R}^{1,1}_{Q_{n,\rho}}(V)\| \leq \|[V, Q_{n,\rho}]\| \leq 2\|V\|\|Q_{n,\rho}\|$$

$$\|\mathcal{R}^{1,2}_{Q_{n,\rho}}(\Lambda)\| \leq \frac{1}{2}\|[V_{n,\rho}, Q_{n,\rho}]\| \leq \|V_{n,\rho}\|\|Q_{n,\rho}\|$$

and $\|V_{n,\rho}\| \leq \|V - V_{n,\rho}\| + \|V\| \leq 2\|V\|$.

5.3. A condition for $\|R_{n,\rho}\| < \frac{1}{4}$

Let $R_{n,\rho}$ be as is Section 5.2 and

$$C_0 := 4\widehat{C}^2 + (32\hat{c})^{-1}. \tag{5.12}$$

We claim that $\|R_{n,\rho}\| < \frac{1}{4}$ holds if $\rho \geq \frac{1}{2}$ and

$$n - \rho > \max\{\hat{\nu}, 256(2\rho + 1)^2 C_0\|V\|^2\}. \tag{5.13}$$

In order to prove this claim, we first observe that, using $C_0 \geq (32\hat{c})^{-1}$ in (5.13) and $\rho \geq \frac{1}{2} \Rightarrow (2\rho + 1)^2 \geq 4$, we can estimate

$$n - \rho > 256(2\rho + 1)^2 C_0\|V\|^2 \geq 1024(32\hat{c})^{-1}\|V\|^2 = 32\hat{c}^{-1}\|V\|^2,$$

hence

$$\frac{\hat{c}^{-1}\|V\|^2}{n - \rho} < \frac{1}{32}. \tag{5.14}$$

Moreover,

$$\|Q_{n,\rho}\| \le \sum_{i\in\mathbb{Z}\cap[-\rho,\rho]} \|Q_{n+i}\| \le (1+2\rho)\Big(\frac{4\widehat{C}^2}{n-\rho} + \frac{\hat{c}^{-2}\|V\|^2}{(n-\rho)^2}\Big)^{1/2} \tag{5.15}$$

where the last estimate is due to Lemma 4.3. However, using (5.14) to estimate the last term of (5.15), we get

$$\|Q_{n,\rho}\|^2 \le (1+2\rho)^2 C_0 (n-\rho)^{-1}. \tag{5.16}$$

Combining (5.9) with (5.16), we find

$$\|R_{n,\rho}\|^2 \le 16\|Q_{n,\rho}\|^2\|V\|^2 \le \frac{16(1+2\rho)^2 C_0\|V\|^2}{n-\rho} \tag{5.17}$$

and the assumption (5.13) allows us to estimate the right-hand side of (5.17) by $\frac{1}{16}$, i.e., we obtain $\|R_{n,\rho}\|^2 < \frac{1}{16}$.

5.4. End of the proof of Proposition 3.1 (a)

Let $\widehat{V}_{n,\rho}$ and $\widetilde{V}_{n,\rho}$ be as in (5.5)–(5.6). Then

$$\Lambda + V - V_{n,\rho} = \widehat{J}_{n,\rho} \oplus \widetilde{J}_{n,\rho}$$

holds with

$$\widehat{J}_{n,\rho} = \Lambda|_{\widehat{\mathcal{H}}_{n,\rho}} + \widehat{V}_{n,\rho} \quad \text{and} \quad \widetilde{J}_{n,\rho} = \Lambda|_{\widetilde{\mathcal{H}}_{n,\rho}} + \widetilde{V}_{n,\rho}.$$

In what follows, we assume $\rho = \|V\| + 1$. Thus, the assumption $n > \nu + 1 + \|V\| = \nu + \rho$ implies $n - \rho > \nu \ge \max\{\hat{\nu}, 64\widehat{C}^2\}$ and this inequality ensures that

$$|i| \le \rho \Rightarrow |V(n+i,n+i)| \le \widehat{C}(n-i)^{-1/2} \le \widehat{C}(n-\rho)^{-1/2} \le \frac{1}{8}. \tag{5.18}$$

However, $\widehat{J}_{n,\rho}$ is similar to $\mathrm{diag}(n+i+V(n+i,n+i))_{i\in\mathbb{Z}\cap[-\rho,\rho]}$ and (5.18) ensures

$$\mathrm{spec}(\widehat{J}_{n,\rho}) \cap \Big[n - \frac{5}{8}, n + \frac{5}{8}\Big] = \{n + V(n,n)\} \subset \Big[n - \frac{1}{8}, n + \frac{1}{8}\Big].$$

Moreover, $\|\widetilde{V}_{n,\rho}\| \le \|V\|$ implies

$$\mathrm{spec}(\widetilde{J}_{n,\rho}) \subset \bigcup_{i\in\mathbb{Z}\setminus[-\rho,\rho]} [n+i-\|V\|, n+i+\|V\|]$$

and the choice $\rho = \|V\| + 1$ ensures

$$\mathrm{spec}(\widetilde{J}_{n,\rho}) \cap \Big[n - \frac{5}{8}, n + \frac{5}{8}\Big] = \emptyset.$$

Using $\operatorname{spec}(\widehat{J}_{n,\rho} \oplus \widetilde{J}_{n,\rho}) = \operatorname{spec}(\widehat{J}_{n,\rho}) \cup \operatorname{spec}(\widetilde{J}_{n,\rho})$, we get

$$\operatorname{spec}(\widehat{J}_{n,\rho} \oplus \widetilde{J}_{n,\rho}) \cap \left[n - \frac{5}{8}, n + \frac{5}{8}\right] = \{n + V(n,n)\}.$$

Let ν be given by (3.2). Then

$$\nu \geq 8\|V\|^2(3 + 2\|V\|)^2(128\widehat{C}^2 + \hat{c}^{-1}) = 256 C_0 (2\rho + 1)^2 \|V\|^2$$

if $\rho = \|V\| + 1$ and C_0 is given by (5.12). Thus, $n > \nu + 1 + \|V\|$ ensures that the condition (5.13) is satisfied, hence $\|R_{n,\rho}\| < \frac{1}{4}$ holds. We can write

$$J'_{n,\rho} = \widehat{J}_{n,\rho} \oplus \widetilde{J}_{n,\rho} + R_{n,\rho},$$

and apply Lemma 8.2 (a) to the operators $L = \widehat{J}_{n,\rho} \oplus \widetilde{J}_{n,\rho}$, $R = R_{n,\rho}$, taking $\lambda = n + V(n,n)$, $d' = n - \frac{5}{8}$, $d'' = n + \frac{5}{8}$ and $\tau = \frac{1}{4}$. We obtain

$$\operatorname{spec}(J'_{n,\rho}) \cap \left[n - \frac{1}{2}, n + \frac{1}{2}\right] = \{\lambda'\}$$

and

$$n - \frac{3}{8} < n + V(n,n) - \|R_{n,\rho}\| \leq \lambda' \leq n + V(n,n) + \|R_{n,\rho}\| < n + \frac{3}{8}.$$

Since $\operatorname{spec}(J'_{n,\rho}) = \operatorname{spec}(J)$, we can identify $\lambda' = \lambda_n(J)$ if $n > \nu + 1 + \|V\|$.

6. Proof of Proposition 3.1 (b)

6.1. Use of the Kato–Temple estimate

We continue our investigation of the operator J satisfying the assumptions of Proposition 3.1. In Section 5 we proved the assertion (a) that allows us to label the eigenvalue sequence $\{\lambda_j(J)\}_{j\in\mathbb{Z}}$ so that (3.3) holds for $n > \nu + 1 + \|V\|$. In what follows, we use (5.7) with $\rho = 0$ and consider

$$J'_n := \mathrm{e}^{-\mathrm{i}Q_n}(\Lambda + V)\mathrm{e}^{\mathrm{i}Q_n},$$

where $Q_n = Q_{n,0}$ and $J'_n = J'_{n,0}$. We also abbreviate $\widehat{V}_n = \widehat{V}_{n,0}$, $\widetilde{V}_n = \widetilde{V}_{n,0}$, $R_n = R_{n,0}$ and write

$$J'_n = \Lambda + \widehat{V}_n \oplus \widetilde{V}_n + R_n. \tag{6.1}$$

We recall that $n > \nu + 1 + \|V\|$ ensures $|V(n,n)| < \frac{1}{8}$ and we get $\|R_n\| < \frac{1}{4}$ similarly to the estimate $\|R_{n,\rho}\| < \frac{1}{4}$ proved in Section 5. We introduce

$$\eta_n := J'_n(n,n) = \langle \tilde{e}_n, J'_n \tilde{e}_n \rangle$$

and claim that

$$|\lambda_n(J) - \eta_n| \leq 32\|R_n\|^2. \tag{6.2}$$

In order to prove (6.2), we observe that (6.1) implies

$$J_n' \tilde{e}_n = (n + V(n,n))\tilde{e}_n + R_n \tilde{e}_n,$$

hence

$$\eta_n = n + V(n,n) + R_n(n,n) \in \left[n - \frac{3}{8}, n + \frac{3}{8}\right] \tag{6.3}$$

due to $|V(n,n)| \leq \frac{1}{8}$ and $\|R_n\| < \frac{1}{4}$. Writing

$$(J_n' - \eta_n)\tilde{e}_n = (n + V(n,n) - \eta_n)\tilde{e}_n + R_n \tilde{e}_n,$$

we get

$$\|(J_n' - \eta_n)\tilde{e}_n\| \leq |n + V(n,n) - \eta_n| + \|R_n\| = |R_n(n,n)| + \|R_n\| \leq 2\|R_n\|. \tag{6.4}$$

We will complete the proof, using the Kato–Temple estimate stated in Theorem 8.3. More precisely, writing (8.10) with $d' = n - \frac{1}{2}$, $d'' = n + \frac{1}{2}$, $\lambda = \lambda_n(J_n')$ and $\eta = \eta_n$, we get

$$|\lambda_n(J_n') - \eta_n| \leq 8\|(J_n' - \eta_n)e_n\|^2 \tag{6.5}$$

due to (6.3), which ensures $\min\{\eta - d', d'' - \eta\} \leq \frac{1}{8}$. It remains to observe that (6.4) allows us to estimate the right-hand side of (6.5) by $32\|R_n\|^2$ and $\lambda_n(J_n') = \lambda_n(J)$.

6.2. An analysis of R_n

We will refine the estimate $\|R_n\| \leq 4\|V\|\|Q_n\|$ from Section 5. We claim that

$$R_n = \left[V - \frac{1}{2}V_n, \mathrm{i}Q_n\right] + R_n'$$

holds with

$$\|R_n'\| \leq 4\|Q_n\|^2\|V\|. \tag{6.6}$$

In order to prove (6.6), we observe that (5.1)–(5.2) with $N = 2$ gives

$$\mathrm{e}^{-\mathrm{i}Q_n} V \mathrm{e}^{\mathrm{i}Q_n} = V + [V, \mathrm{i}Q_n] + \mathcal{R}^{1,2}_{Q_n}(V) \tag{6.7}$$

and (5.1)–(5.2) with $N = 3$ gives

$$\mathrm{e}^{-\mathrm{i}Q_n} \Lambda \mathrm{e}^{\mathrm{i}Q_n} = \Lambda + [\Lambda, \mathrm{i}Q_n] + \frac{1}{2}[[\Lambda, \mathrm{i}Q_n], \mathrm{i}Q_n] + \mathcal{R}^{1,3}_{Q_n}(\Lambda). \tag{6.8}$$

Using $[\Lambda, \mathrm{i}Q_n] = -V_n$ and summing up (6.7) and (6.8), we obtain

$$\mathrm{e}^{-\mathrm{i}Q_n} J \mathrm{e}^{\mathrm{i}Q_n} = \Lambda + V - V_n + \left[V - \frac{1}{2}V_n, \mathrm{i}Q_n\right] + R_n'$$

with

$$R'_n = \mathcal{R}^{1,2}_{Q_n}(V) + \mathcal{R}^{1,3}_{Q_n}(\Lambda). \tag{6.9}$$

However,

$$\begin{aligned} \|\mathcal{R}^{1,2}_{Q_n}(V)\| &\leq \frac{1}{2}\|\mathrm{ad}^2_{\mathrm{i}Q_n}(V)\| \leq 2\|Q_n\|^2\|V\|, \\ \|\mathcal{R}^{1,3}_{Q_n}(\Lambda)\| &\leq \frac{1}{6}\|\mathrm{ad}^3_{\mathrm{i}Q_n}(\Lambda)\| = \frac{1}{6}\|\mathrm{ad}^2_{\mathrm{i}Q_n}(V_n)\| \leq \frac{2}{3}\|Q_n\|^2\|V_n\| \end{aligned} \tag{6.10}$$

and combining (6.9)–(6.10), we get

$$\|R'_n\| \leq \|Q_n\|^2\Big(2\|V\| + \frac{2}{3}\|V_n\|\Big).$$

It remains to observe that $\|V_n\| \leq \|V - V_n\| + \|V\| \leq 2\|V\|$.

6.3. An estimate of $W_n = \big[V - \frac{1}{2}V_n, \mathrm{i}Q_n\big]$

We introduce

$$W_n := \Big[V - \frac{1}{2}V_n, \mathrm{i}Q_n\Big]$$

and consider $W_n(n,n) = (W_n\tilde{e}_n)(n)$. We claim that

$$n > \nu + 1 + \|V\| \Rightarrow |W_n(n,n)| \leq \frac{2\|V\|^2\hat{c}^{-1} + 4\widehat{C}^2(1 + \ln n)}{n}. \tag{6.11}$$

In order to prove (6.11), we denote $V'_n := V - \frac{1}{2}V_n$ and observe that

$$|V'_n(j,k)| \leq |V(j,k)|$$

holds for every $j, k \in \mathbb{Z}$. Thus, we can estimate

$$|(V'_nQ_n)(n,n)| \leq \sum_{j\in\mathbb{Z}} |V(n,j)Q_n(j,n)| \leq \sum_{j\in\mathbb{Z}\setminus\{n\}} \frac{|V(j,n)|^2}{|j-n|} \leq \mathcal{M}_n + \mathcal{M}'_n$$

with

$$\begin{aligned} \mathcal{M}_n &:= \sum_{\{j\in\mathbb{Z}:|j-n|>\hat{c}n\}} \frac{|V(j,n)|^2}{|j-n|} \leq \sum_{j\in\mathbb{Z}} \frac{|V(j,n)|^2}{\hat{c}n} = \frac{\|V\tilde{e}_n\|^2}{\hat{c}n} \leq \frac{\|V\|^2}{\hat{c}n}, \\ \mathcal{M}'_n &:= \sum_{\{j\in\mathbb{Z}:0<|j-n|\leq\hat{c}n\}} \frac{|V(j,n)|^2}{|j-n|} \leq \sum_{\{m\in\mathbb{Z}:0<|m|\leq\hat{c}n\}} \frac{\widehat{C}^2n^{-1}}{|m|} \leq 2(1+\ln n)\frac{\widehat{C}^2}{n} \end{aligned}$$

where we used (3.1).

6.4. End of the proof of Proposition 3.1 (b)

We first write

$$|\lambda_n(J) - n - V(n,n)| \le |\lambda_n(J) - \eta_n| + |\eta_n - n - V(n,n)|. \tag{6.12}$$

Using (6.12), (6.2), and $\eta_n - n - V(n,n) = R_n(n,n) = W_n(n,n) + R'_n(n,n)$, we get

$$|\lambda_n(J) - n - V(n,n)| \le 32\|R_n\|^2 + \|R'_n\| + |W_n(n,n)|. \tag{6.13}$$

Due to (5.9) and (6.6),

$$32\|R_n\|^2 + \|R'_n\| \le 32(4\|Q_n\|\|V\|)^2 + 4\|Q_n\|^2\|V\| \tag{6.14}$$

Since the assumptions of Proposition 3.1 imply that (5.14) holds with $\rho = 0$, hence the estimate (5.16) holds with $\rho = 0$, i.e., one has

$$\|Q_n\|^2 \le C_0 n^{-1} \quad \text{for } n > \nu + 1 + \|V\|. \tag{6.15}$$

Using (6.15) in (6.14), we obtain

$$32\|R_n\|^2 + \|R'_n\| \le 4C_0\|V\|(1 + 128\|V\|)n^{-1}. \tag{6.16}$$

Using (6.16) and (6.11), we find that the right-hand side of (6.13) can be estimated by the right-hand side of (3.4), which completes the proof of Proposition 3.1.

7. Proof of Theorem 1.3

7.1. Step 1 of the proof of Theorem 1.3

Notation 7.1. (a) We let $\widehat{S} \in \mathcal{B}(\ell^2(\mathbb{N}))$ denote the shift given by $\widehat{S}e_j = e_{j+1}$ and $\widehat{S}^*$ denotes the adjoint of $\widehat{S}$.

(b) We introduce $\widehat{\Lambda} = \operatorname{diag}(j)_{j\in\mathbb{N}}$ defined as the linear map $\ell^{2,1}(\mathbb{N}) \to \ell^2(\mathbb{N})$ satisfying $\widehat{\Lambda}e_j = je_j$ for every $j \in \mathbb{N}$.

(c) If $b\colon \mathbb{N} \to \mathbb{R}$, then $b(\widehat{\Lambda}) := \operatorname{diag}(b(j))_{j\in\mathbb{N}}$ is the self-adjoint operator in $\ell^2(\mathbb{N})$ satisfying $b(\widehat{\Lambda})e_j = b(j)e_j$ for every $j \in \mathbb{N}$.

Definition 7.2. For $\mu = 0, 1$, we define $\widehat{J}^{\pm}_{\mu}\colon \ell^{2,1}(\mathbb{N}) \to \ell^2(\mathbb{N})$ by the formula

$$\widehat{J}^{\pm}_{\mu} = \hat{d}^{\pm}_{\mu}(\widehat{\Lambda}) + \widehat{S}\hat{b}_{\mu}(\widehat{\Lambda}) + \hat{b}_{\mu}(\widehat{\Lambda})\widehat{S}^*,$$

with $\{\hat{d}^{\pm}_{\mu}(m)\}_{m\in\mathbb{N}}$, $\{\hat{b}^{\pm}_{\mu}(m)\}_{m\in\mathbb{N}}$ given by equations (1.12) and (1.13), respectively. The matrix $(\langle e_j, \widehat{J}^{\pm}_{\mu}e_k\rangle)_{(j,k)\in\mathbb{N}^2}$ is given by (1.11) and (1.14) ensures that $\widehat{J}^{\pm}_{\mu}$ is a lower semi-bounded self-adjoint operator with discrete spectrum due to the Janas–Naboko criterion [27, Theorem 4.1].

Lemma 7.3. *The operator* $\mathbf{H}^{(2)}_{\mathrm{Rabi}}$ *is similar to the direct sum*

$$\hat{J}_0^+ \oplus \hat{J}_0^- \oplus \hat{J}_1^+ \oplus \hat{J}_1^-$$

Proof. See [5, Section 2.2]. ■

Notation 7.4. (a) If $\mathcal{J} \subset \mathbb{Z}$, then $\ell^2(\mathcal{J})$ is identified with the closed subspace of $\ell^2(\mathbb{Z})$ generated by $\{\tilde{e}_j\}_{j\in\mathcal{J}}$, i.e., with $\{x \in \ell^2(\mathbb{Z}) : x(k) = 0 \text{ for } k \in \mathbb{Z} \setminus \mathcal{J}\}$. Thus, we can write

$$\ell^2(\mathbb{Z}) = \ell^2(\mathbb{Z} \setminus \mathbb{N}) \oplus \ell^2(\mathbb{N}).$$

(b) If $\mathcal{J} \subset \mathbb{Z}$, then $\Pi_{\mathcal{J}}$ denotes the orthogonal projection $\ell^2(\mathbb{Z}) \to \ell^2(\mathcal{J})$.
(c) We identify $\tilde{e}_j$ and e_j for $j \geq 0$.

Definition 7.5. We define $\hat{J}^\delta_\gamma : \ell^{2,1}(\mathbb{N}) \to \ell^2(\mathbb{N})$ by the formula

$$\hat{J}^\delta_\gamma := \Pi_{\mathbb{N}} \tilde{J}^\delta_\gamma|_{\ell^2(\mathbb{N})},$$

where $\tilde{J}^\delta_\gamma$ is given by Definition 2.2. The matrix $(\langle e_j, \hat{J}^\delta_\gamma e_k\rangle)_{(j,k)\in\mathbb{N}^2}$ has the form

$$\begin{pmatrix} \delta & g\gamma & 0 & 0 & \\ g\gamma & 1-\delta & g(1+\gamma) & 0 & \\ 0 & g(1+\gamma) & 2+\delta & g(2+\gamma) & \\ 0 & 0 & g(2+\ g) & 3+\delta & \\ & & & & \ddots \end{pmatrix}$$

Its diagonal entries, $\tilde{d}_\delta(j) = j + (-1)^j\delta$ are given by (2.4) and Notation 7.4 gives

$$\hat{J}^\delta_\gamma = \tilde{d}_\delta(\hat{\Lambda}) + g\hat{S}(\hat{\Lambda} + \gamma) + g(\hat{\Lambda} + \gamma)\hat{S}^*.$$

In what follows, we are interested in $\hat{J}^\delta_\gamma$ with $\delta = \pm\frac{\Delta}{4}$ and either $\gamma = \frac{3}{4}$ or $\gamma = \frac{5}{4}$. More precisely, we denote

$$\gamma(\mu) := \frac{3}{4} + \frac{\mu}{2} \quad \text{for } \mu \in \{0, 1\} \tag{7.1}$$

and we investigate the approximation of $\hat{J}^\pm_\mu$ by $2\hat{J}^{\pm\Delta/4}_{\gamma(\mu)} + \mu$. Indeed, if $\hat{d}^\pm_\mu$ is as in (1.12), then

$$\hat{d}^\pm_\mu(m) = 2\tilde{d}_{\pm\Delta/4}(m) + \mu$$

and

$$2\hat{J}^{\pm\Delta/4}_{\gamma(\mu)} + \mu - \hat{J}^\pm_\mu = \hat{S}r_\mu(\hat{\Lambda}) + r_\mu(\hat{\Lambda})\hat{S}^*$$

holds with

$$r_\mu(m) := 2g(m + \gamma(\mu)) - \hat{b}_\mu(m) \tag{7.2}$$

(where $\hat{b}_\mu$ is as in (1.13)). We claim that $r_\mu(m) = O(m^{-1})$ as $m \to \infty$. Indeed,

$$r_\mu(m) = g\sqrt{\Big(2m+\mu+\frac{3}{2}\Big)^2} - g\sqrt{(2m+\mu+1)(2m+\mu+2)} \tag{7.3}$$

and, using $\big(2m+\mu+\frac{3}{2}\big)^2 - \big(\frac{1}{2}\big)^2 = (2m+\mu+1)(2m+\mu+2)$, we can rewrite (7.3) as

$$r_\mu(m) = \frac{\frac{g}{4}}{2m+\mu+\frac{3}{2}+\sqrt{(2m+\mu+1)(2m+\mu+2)}}. \tag{7.4}$$

7.2. Step 2 of the proof of Theorem 1.3

Lemma 7.6. *Assume that $\{\lambda_n(\widehat{J}^\delta_\gamma)\}_{n\in\mathbb{N}}$ is the non-decreasing sequence of eigenvalues of the operator $\widehat{J}^\delta_\gamma$ introduced in Definition 7.5, $\{\lambda_j(\widetilde{J}^\delta_\gamma)\}_{j\in\mathbb{Z}}$ is as in Theorem 2.3 and either $\gamma = \frac{3}{4}$ or $\gamma = \frac{5}{4}$. We denote*

$$\nu_\delta := 2 + \Big|\frac{\delta}{\beta}\Big| + \max\{\nu_{\delta,5/4}, \beta^{-1} + 4\beta^{-2}(3+|\delta|)\}, \tag{7.5}$$

where $\nu_{\delta,\gamma}$ is given by (3.11). Then there exists $\kappa(\delta) \in \mathbb{Z}$ which is independent of n and such that for $n > \nu_\delta$ one has

$$|\lambda_{n+\kappa(\delta)}(\widehat{J}^\delta_\gamma) - \lambda_n(\widetilde{J}^\delta_\gamma)| \le \frac{3+|\delta|}{4(\beta n - 1)} < \frac{\beta}{16}, \tag{7.6}$$

$$E^0_{\gamma,n} - \frac{7}{16}\beta < \lambda_{n+\kappa(\delta)}(\widehat{J}^\delta_\gamma) < E^0_{\gamma,n} + \frac{7}{16}\beta, \tag{7.7}$$

where $E^0_{\gamma,n} = \beta n + \beta_\gamma$ is given by (2.5).

Proof. We introduce $\check{J}^\delta_\gamma : \ell^{2,1}(\mathbb{Z}\setminus\mathbb{N}) \to \ell^2(\mathbb{Z}\setminus\mathbb{N})$ by the formula

$$\check{J}^\delta_\gamma := \Pi_{\mathbb{Z}\setminus\mathbb{N}} \widetilde{J}^\delta_\gamma|_{\ell^2(\mathbb{Z}\setminus\mathbb{N})}.$$

We observe that the matrix $(\langle e_j, \check{J}^\delta_\gamma e_k\rangle)_{(j,k)\in(\mathbb{Z}\setminus\mathbb{N})^2}$ has the form

$$\begin{pmatrix} \ddots & & & \\ & -3-\delta & g(-3+\gamma) & 0 \\ & g(-3+\gamma) & -2+\delta & g(-2+\gamma) \\ & 0 & g(-2+\gamma) & -1-\delta \end{pmatrix}$$

We first claim that

$$\operatorname{spec}(\check{J}^\delta_\gamma \oplus \widehat{J}^\delta_\gamma) \cap \Big[|\delta| + \frac{5}{8}, \infty\Big) = \operatorname{spec}(\widehat{J}^\delta_\gamma) \cap \Big[|\delta| + \frac{5}{8}, \infty\Big). \tag{7.8}$$

Indeed, (7.8) follows from the inclusion

$$\operatorname{spec}(\check{J}_\gamma^\delta) \cap \Big[|\delta| + \frac{5}{8}, \infty\Big) = \emptyset,$$

which is an easy consequence of the estimate

$$\sup \operatorname{spec}(\check{J}_\gamma^\delta) \le \sup\{-j + (-1)^j \delta + \rho_j : j \in \mathbb{N} \setminus \{0\}\}, \tag{7.9}$$

where $\rho_j = g(|\gamma - j| + |\gamma - j - 1|)$ for $j \ge 2$ and $\rho_1 = g|\gamma - 2| < \frac{5}{8}$ due to the assumption that $\gamma = \frac{3}{4}$ or $\frac{5}{4}$. The estimate (7.9) is well known, see, e.g., [42, Lemma 1.8].

It remains to compare the eigenvalues of $\tilde{J}_\gamma^\delta$ and $\check{J}_\gamma^\delta \oplus \hat{J}_\gamma^\delta$. For this purpose we consider $\tilde{J}_\gamma^\delta - \hat{J}_\gamma^\delta \oplus \hat{J}_\gamma^\delta = \tilde{J}_\gamma^0 - \hat{J}_\gamma^0 \oplus \hat{J}_\gamma^0$ and observe that

$$R_\gamma = \tilde{J}_\gamma^0 - \hat{J}_\gamma^0 \oplus \hat{J}_\gamma^0 = g(\gamma - 1)(S\Pi_{-1} + S^{-1}\Pi_0), \tag{7.10}$$

hence

$$\|R_\gamma\| = 2g|\gamma - 1| = \frac{1}{2}g < \frac{1}{4}. \tag{7.11}$$

Our next claim is that

$$\|R_\gamma \tilde{J}_\gamma^0\| \le \frac{9}{16}. \tag{7.12}$$

Indeed, (7.10)–(7.11) imply $\|\tilde{J}_\gamma^0 R_\gamma\| \le \frac{1}{4}(\|\tilde{J}_\gamma^0 \tilde{e}_{-1}\| + \|\tilde{J}_\gamma^0 \tilde{e}_0\|)$ and (7.12) follows from

$$\|\tilde{J}_\gamma^0 \tilde{e}_{-1}\| + \|\tilde{J}_\gamma^0 \tilde{e}_0\| \le 1 + g(2-\gamma) + 2g|\gamma - 1| + g\gamma < \frac{9}{4}.$$

We will deduce (7.6) from Lemma 8.2 applied to $L = \tilde{J}_\gamma^\delta$. Indeed, if $n > \nu_\delta$ then Corollary 3.2 ensures

$$E_{\gamma,n}^0 - \frac{3}{8}\beta < \lambda_n(\tilde{J}_\gamma^\delta) < E_{\gamma,n}^0 + \frac{3}{8}\beta, \tag{7.13}$$

$$d'' := E_{\gamma,n}^0 + \frac{1}{2}\beta + \frac{1}{16}\beta < \lambda_{n+1}(\tilde{J}_\gamma^\delta),$$

$$d' := E_{\gamma,n}^0 - \frac{1}{2}\beta - \frac{1}{16}\beta > \lambda_{n-1}(\tilde{J}_\gamma^\delta),$$

i.e., (8.1) holds with $\tau := \frac{\beta}{16}$ and we claim that the condition (8.2) holds for $n > \nu_\delta$. Indeed, we observe that, using $\|R_\gamma\| < \frac{1}{4}$, (7.12), $\beta < 1$, we get

$$\Big\|R_\gamma\Big(\tilde{J}_\gamma^\delta + \mathrm{i}\frac{\beta}{16}\Big)\Big\| \le \|R_\gamma \tilde{J}_\gamma^0\| + \Big(|\delta| + \frac{1}{16}\Big)\|R_\gamma\| < \frac{1}{4}(3 + |\delta|)$$

and it is easy to check that

$$n > \nu_\delta \implies \frac{1}{4}(3 + |\delta|) < \frac{1}{16}\beta(\beta n - 1) < \frac{1}{16}\beta d', \tag{7.14}$$

where the last estimate follows from

$$d' = E^0_{\gamma,n} - \frac{1}{2}\beta - \frac{1}{16}\beta > \beta n - 1.$$

Thus, $n > \nu_\delta$ implies $d' \geq 1 + |\delta|$ and $\|R_\gamma(\widetilde{J}^\delta_\gamma + \mathrm{i}\frac{\beta}{16})\| < \frac{\beta}{16}d'$, i.e., (8.2) holds for with $\tau = \frac{\beta}{16}$ and Lemma 8.2 ensures that

$$|\lambda_{n+\kappa(\delta)}(\widehat{J}^\delta_\gamma) - \lambda_n(\widetilde{J}^\delta_\gamma)| \leq \frac{\|R_\gamma(\widetilde{J}^\delta_\gamma + \mathrm{i}\frac{\beta}{16})\|}{\lambda_n(\widetilde{J}^\delta_\gamma)} < \frac{3+|\delta|}{4d'} < \frac{3+|\delta|}{4(\beta n - 1)} \tag{7.15}$$

holds with a certain $\kappa(\delta) \in \mathbb{Z}$ independent of $n > \nu_\delta$. The right-hand side of (7.15) can be estimated by $\frac{\beta}{16}$ due to (7.14), implying the last inequality of (7.6). Finally, (7.7) follows from (7.6) and (7.13) . ■

7.3. Step 3 of the proof of Theorem 1.3

Lemma 7.7. *The assertion of Lemma 7.6 holds with $\kappa(\delta) = 0$.*

Proof. Due to Lemma 7.6, there is a constant C_δ independent of n such that

$$|\lambda_n(\widehat{J}^\delta_\gamma) - \lambda_{n-\kappa(\delta)}(\widetilde{J}^\delta_\gamma)| \leq C_\delta n^{-1} \tag{7.16}$$

holds for $n \geq 1$. Due to Theorem 2.3, there is a constant C'_δ independent of n such that

$$|\lambda_{n-\kappa(\delta)}(\widetilde{J}^\delta_\gamma) - E^0_{\gamma,n-\kappa(\delta)}| \leq C'_\delta n^{-1/2} \tag{7.17}$$

holds for $n \geq 1$. Combining (7.16) and (7.17), we get

$$|\lambda_n(\widehat{J}^\delta_\gamma) - E^0_{\gamma,n-\kappa(\delta)}| \leq C''_\delta n^{-1/2} \tag{7.18}$$

with $C''_\delta := C_\delta + C'_\delta$. Consider $\delta' \in \mathbb{R}$. Then the min-max principle ensures

$$\sup_{j\in\mathbb{N}} |\lambda_j(\widehat{J}^\delta_\gamma) - \lambda_j(\widehat{J}^{\delta'}_\gamma)| \leq |\delta - \delta'|. \tag{7.19}$$

Using (7.19), (7.18), and an analogical estimate for δ', we obtain

$$|E^0_{\gamma,n-\kappa(\delta)} - E^0_{\gamma,n-\kappa(\delta')}| \leq (C''_\delta + C''_{\delta'})n^{-1/2} + |\delta - \delta'|$$

for $n \geq 1$ and consequently

$$\limsup_{n\to\infty} |E^0_{\gamma,n-\kappa(\delta)} - E^0_{\gamma,n-\kappa(\delta')}| \leq |\delta - \delta'|. \tag{7.20}$$

However, combining (7.20) with

$$\lim_{n\to\infty} |E^0_{\gamma,n-\kappa(\delta)} - E^0_{\gamma,n-\kappa(\delta')}| = |\kappa(\delta) - \kappa(\delta')|\beta,$$

we find $|\kappa(\delta) - \kappa(\delta')| \le \beta^{-1}|\delta - \delta'|$. Thus, $\kappa: \mathbb{R} \to \mathbb{Z}$ is locally constant, hence $\kappa(\delta) = \kappa(0)$ and it remains to prove that $\kappa(0) = 0$. However, the result of Janas and Malejki [25, Theorem 3.4] says that for every $N \in \mathbb{N}$ one has

$$\lambda_n(\widehat{J}^0_\gamma) = E^0_{\gamma,n} + O(n^{-N}) \quad \text{as } n \to \infty. \tag{7.21}$$

Therefore, using (7.21) and (7.18) with $\delta = 0$, we get

$$|E^0_{\gamma,n-\kappa(0)} - E^0_{\gamma,n}| \le \widetilde{C}_{\delta'} n^{-1/2} \tag{7.22}$$

and $\kappa(0) = 0$ follows from (7.22). ∎

7.4. Step 4 of the proof of Theorem 1.3

Lemma 7.8. *Let $\{\lambda_n(\widehat{J}^\delta_\gamma)\}_{n\in\mathbb{N}}$ and ν_δ be as in Lemma 7.6. Let $\{\lambda_n(\widehat{J}^\pm_\mu)\}_{n\in\mathbb{N}}$ be the non-decreasing sequence of eigenvalues of $\widehat{J}^\pm_\mu$. If $\gamma(\mu)$ is given by (7.1), then*

$$|2\lambda_n(\widehat{J}^{\pm\Delta/4}_{\gamma(\mu)}) + \mu - \lambda_n(\widehat{J}^\pm_\mu)| \le \frac{2 + \left|\frac{\Delta}{20}\right|}{4(\beta n - 1)} \tag{7.23}$$

holds for $n > \nu_{\Delta/4}$.

Proof. We will deduce the assertion of Lemma 7.8 from Lemma 8.2 applied to

$$L^\pm_\mu := 2\widehat{J}^{\pm\Delta/4}_{\gamma(\mu)} + \mu.$$

We observe that $2\lambda_n(\widehat{J}^{\pm\Delta/4}_{\gamma(\mu)}) + \mu = \lambda_n(L^\pm_\mu)$ and

$$2E^0_{\gamma(\mu),n} + \mu = E^0_{2n+\mu}, \tag{7.24}$$

where $E^0_m = \beta m + \frac{\beta-1}{2}$ is given by (1.7). Due to Lemma 7.7, (7.7) holds with $\kappa(\delta) = 0$ and $\delta = \pm\frac{\Delta}{4}$, hence $n > \nu_{\Delta/4} = \nu_{-\Delta/4}$ ensures

$$E^0_{2n+\mu} - \frac{7}{8}\beta < \lambda_n(L^\pm_\mu) < E^0_{2n+\mu} + \frac{7}{8}\beta,$$

$$d'' := E^0_{2n+\mu} + \beta + \frac{1}{16}\beta < \lambda_{n+1}(L^\pm_\mu),$$

$$d' := E^0_{2n+\mu} - \beta - \frac{1}{16}\beta > \lambda_{n-1}(L^\pm_\mu).$$

Thus, (8.1) holds with $\tau := \frac{\beta}{16}$ and it remains to check that the condition (8.2) holds for $n > \nu_{\Delta/4}$ with $R = R_\mu$ given by

$$R_\mu := r_\mu(\widehat{\Lambda})\widehat{S}^* + \widehat{S}r_\mu(\widehat{\Lambda}),$$

where $r_\gamma(m)$ was introduced in (7.2). However, using the expression (7.4), we find

$$\|r_{\gamma(\mu)}(\widehat{\Lambda})\| = \sup_{m\in\mathbb{N}} |r_\mu(m)| = r_\mu(0) < \frac{1}{20},$$

$$\|r_{\gamma(\mu)}(\widehat{\Lambda})\widehat{\Lambda}\| = \sup_{m\in\mathbb{N}} |r_\mu(m)m| = \lim_{m\to\infty} r_\mu(m)m = \frac{g}{16} < \frac{1}{32}.$$

Using $\widehat{S}\widehat{\Lambda} = (\widehat{\Lambda} - I)\widehat{S}$ and $\widehat{S}^*\widehat{\Lambda} = (\widehat{\Lambda} + I)\widehat{S}^*$, we find

$$\widehat{J}_\gamma^0 = \widehat{\Lambda} + g\widehat{\Lambda}(\widehat{S} + \widehat{S}^*) + g(\gamma - 1)\widehat{S} + g\gamma\widehat{S}^*,$$

$$\widehat{S}^*\widehat{J}_\gamma^0 = \widehat{\Lambda}\widehat{S}^* + g\Lambda\widehat{S}^*(\widehat{S} + \widehat{S}^*) + \widehat{S}^* + g\widehat{S}^*(\widehat{S} + \widehat{S}^*) + g(\gamma - 1) + g\gamma(S^*)^2,$$

and $\|R_\mu\widehat{J}_\gamma^0\| \le \|r_\mu(\widehat{\Lambda})\widehat{J}_\gamma^0\| + \|r_\mu(\widehat{\Lambda})\widehat{S}^*\widehat{J}_\gamma^0\|$ can be estimated by

$$\|r_\mu(\widehat{\Lambda})\widehat{\Lambda}\|(2 + 4g) + \|r_\mu(\widehat{\Lambda})\|(1 + 4g + 4g\gamma) < \frac{1}{3},$$

hence

$$\left\|R_\mu\left(L_\mu^\pm + \mathrm{i}\frac{\beta}{16}\right)\right\| \le 2\|R_\mu\widehat{J}_\gamma^0\| + \|R_\mu\|\left(\mu + \frac{1}{16} + \left|\frac{\Delta}{4}\right|\right) < 1 + \left|\frac{\Delta}{40}\right|$$

and

$$\frac{1}{16}\beta d' > \frac{1}{8}\beta(\beta n - 1) > \frac{1}{2}\left(3 + \left|\frac{\Delta}{4}\right|\right), \tag{7.25}$$

where the last inequality is ensured by $n > \nu_{\Delta/4}$ (see (7.14) with $\delta = \pm\frac{\Delta}{4}$). Since the right-hand side of (7.25) is greater than $1 + \left|\frac{\Delta}{4}\right|$, the condition (8.2) holds if $n > \nu_{\Delta/4}$ and $\tau = \frac{\beta}{16}$. Therefore, Lemma 8.2 ensures that

$$|\lambda_n(L_\mu^\pm) - \lambda_{n+\kappa(\Delta)}(\widehat{J}_\mu^\pm)| \le \frac{\left\|R_\mu\left(L_\mu^\pm + \mathrm{i}\frac{\beta}{16}\right)\right\|}{2\lambda_n(\widehat{J}_{\gamma(\mu)}^{\pm\Delta/4}) + \mu} < \frac{1 + \left|\frac{\Delta}{40}\right|}{2(\beta n - 1)} \tag{7.26}$$

holds for $n > \nu_{\Delta/4}$ with a certain $\kappa(\Delta) \in \mathbb{Z}$ independent of n. In order to complete the proof of (7.23), it remains to show that $\kappa(\Delta) = 0$. However, Lemma 8.2 (c) ensures

$$\lambda_n(\widehat{J}_\mu^\pm) = \lambda_n(L_\mu^\pm) + O(n^{-1}) \quad \text{as } n \to \infty \tag{7.27}$$

and, combining (7.27) with (7.26), we get

$$\lambda_n(\widehat{J}_\mu^\pm) - \lambda_{n+\kappa(\Delta)}(\widehat{J}_\mu^\pm) = O(n^{-1}) \quad \text{as } n \to \infty,$$

hence $\kappa(\Delta) = 0$. ∎

7.5. End of the proof of Theorem 1.3

Combining Lemma 7.6 and 7.8, we get the estimate

$$|2\lambda_n(\widetilde{J}^{\pm\Delta/4}_{\gamma(\mu)}) + \mu - \lambda_n(\widehat{J}^{\pm}_{\mu})| \le \frac{2\big(3+|\frac{\Delta}{4}|\big)+2+|\frac{\Delta}{20}|}{4(\beta n-1)} \quad \text{for } n > \nu_{\Delta/4}, \tag{7.28}$$

where ν_δ is given by (7.5). Using (7.28), (7.24), and the approximation of $\lambda_n(\widetilde{J}^{\delta}_{\gamma})$ given in (3.13)–(3.14) in the case $\delta = \pm\frac{\Delta}{4}$, $\gamma(0) = \frac{3}{4}$, $\gamma(1) = \frac{5}{4}$, we obtain the estimate

$$|\lambda_n(\widehat{J}^{\pm}_{\mu}) - E^0_{2n+\mu} - 2V^{\pm\Delta/4}_{\gamma(\mu)}(n,n)| \le \mathcal{R}^{\Delta}_{\mu}(n) \quad \text{for } n > \nu_{\Delta/4},$$

where ν_δ is given by (7.5), $V^{\delta}_{\gamma}(n,n)$ is given by the explicit integral (3.15) and

$$\mathcal{R}^{\Delta}_{\mu}(n) := \frac{8+0.55|\Delta|}{4(\beta n-1)} + 2\frac{\widetilde{C}_{\Delta/4,\gamma(\mu)} + 4\beta\widehat{C}^2_{\Delta/4,\gamma(\mu)}(1+\ln n)}{n},$$

where $\gamma(0) = \frac{3}{4}$, $\gamma(1) = \frac{5}{4}$, $\widehat{C}_{\delta,\gamma}$ is given by (3.7), and $\widetilde{C}_{\delta,\gamma}$ by (3.14).

Due to (3.10), the correction term $2V^{\pm\Delta/4}_{\gamma(\mu)}(n,n) = V^{\pm\Delta/2}_{\gamma(\mu)}(n,n)$ can be investigated by a standard stationary phase method as indicated in Section 3.3. In particular, one can find a constant $C > 0$ such that

$$|V^{\pm\Delta/2}_{\gamma(\mu)}(n,n) - \mathrm{r}^{\pm\Delta/2}_{\gamma(\mu)}(n)| \le Cn^{-1}$$

and (2.7) gives

$$\hat{\theta}_{\gamma(0)} = \hat{\theta}_{3/4} = \frac{1}{4}(4\alpha-\pi) + \frac{\pi}{4} = \alpha,$$

$$\hat{\theta}_{\gamma(1)} = \hat{\theta}_{5/4} = \frac{3}{4}(4\alpha-\pi) + \frac{\pi}{4} = 3\alpha - \frac{\pi}{2},$$

hence

$$\mathrm{r}^{\pm\Delta/2}_{\gamma(0)}(n) = \mathrm{r}^{\pm\Delta/2}_{3/4}(n) = \pm\frac{\Delta}{2}\Big(\frac{\beta}{2\pi g n}\Big)^{1/2}\cos((4n+1)\alpha) + O(n^{-1}),$$

$$\mathrm{r}^{\pm\Delta/2}_{\gamma(1)}(n) = \mathrm{r}^{\pm\Delta/2}_{5/4}(n) = \pm\frac{\Delta}{2}\Big(\frac{\beta}{2\pi g n}\Big)^{1/2}\sin((4n+3)\alpha) + O(n^{-1}). \tag{7.29}$$

Due to Lemma 7.3,

$$\mathrm{spec}(\mathbf{H}^{(2)}_{\mathrm{Rabi}}) = \mathrm{spec}(\widehat{J}^{-}_{0}) \cup \mathrm{spec}(\widehat{J}^{+}_{0}) \cup \mathrm{spec}(\widehat{J}^{-}_{1}) \cup \mathrm{spec}(\widehat{J}^{-}_{1})$$

and we complete the proof of Theorem 1.3, combining (7.24)–(7.29) with the notation

$$\begin{cases} E^{\pm}_m = \lambda_n(\widehat{J}^{\pm}_0) & \text{if } m = 2n, \\ E^{\pm}_m = \lambda_n(\widehat{J}^{\pm}_1) & \text{if } m = 2n+1. \end{cases}$$

8. Appendix

8.1. Estimates of oscillatory integrals

Lemma 8.1. *Assume that* $h \in C^1([\theta_0, \theta_1])$ *and that* $\Psi \in C^2([\theta_0, \theta_1])$ *is real-valued.*

(i) *If the derivative* $\theta \to \Psi'(\theta)$ *is monotonic and* $|\Psi'(\theta)| \geq 1$ *for all* $\theta \in [\theta_0, \theta_1]$, *then one has*

$$\left| \int_{\theta_0}^{\theta_1} \mathrm{e}^{\mathrm{i}\lambda\Psi(\theta)} h(\theta)\,\mathrm{d}\theta \right| \leq \frac{3}{\lambda}\Big(|h(\theta_0)| + \int_{\theta_0}^{\theta_1} |h'(\theta)|\,\mathrm{d}\theta\Big) \quad \textit{for } \lambda > 0.$$

(ii) *If* $|\Psi''(\theta)| \geq 1$ *for all* $\theta \in [\theta_0, \theta_1]$, *then one has*

$$\left| \int_{\theta_0}^{\theta_1} \mathrm{e}^{\mathrm{i}\lambda\Psi(\theta)} h(\theta)\,\mathrm{d}\theta \right| \leq \frac{8}{\lambda^{1/2}}\Big(|h(\theta_0)| + \int_{\theta_0}^{\theta_1} |h'(\theta)|\,\mathrm{d}\theta\Big) \quad \textit{for } \lambda > 0.$$

Proof. See [41, Section VIII.1.2]. ■

8.2. General estimates of perturbed eigenvalues

In this section L is a self-adjoint operator in the Hilbert space $\mathcal{H}$ and $\|\cdot\|$ denotes the norm of $\mathcal{B}(\mathcal{H})$. We assume that λ is an isolated simple eigenvalue of a self-adjoint operator L and consider the spectrum of $L + R$ near λ, assuming that R is self-adjoint and bounded.

Lemma 8.2. *Let* L *be a self-adjoint operator in the Hilbert space* $\mathcal{H}$. *Assume that* $0 < d' < d''$ *and* $\tau > 0$ *are such that*

$$\operatorname{spec}(L) \cap [d', d''] = \{\lambda\} \subset [d' + 2\tau, d'' - 2\tau], \tag{8.1}$$

where λ *is a simple eigenvalue of* L. *Let* R *be bounded and self-adjoint in* $\mathcal{H}$.

(a) *If* $\|R\| < \tau$, *then*

$$\operatorname{spec}(L + R) \cap [d' + \tau, d'' - \tau] = \{\lambda'\} \subset [\lambda - \|R\|, \lambda + \|R\|],$$

where λ' *is a simple eigenvalue of* $L + R$.

(b) *If* RL *is bounded and*

$$\|R(L + \mathrm{i}\tau)\| < \tau d', \tag{8.2}$$

then

$$\operatorname{spec}(L + R) \cap [d' + \tau, d'' - \tau] = \{\lambda'\} \subset [\lambda - \tau_\lambda, \lambda + \tau_\lambda]$$

holds with

$$\tau_\lambda := \lambda^{-1} \| R(L + \mathrm{i}\tau) \| \tag{8.3}$$

and λ' is a simple eigenvalue of $L + R$.

(c) *If RL is bounded, L has a discrete spectrum and is bounded below, then one has*

$$\lambda_n(L + R) = \lambda_n(L) + O(\lambda_n(L)^{-1}) \quad \text{as } n \to \infty,$$

where $\{\lambda_n(L)\}_{n\in\mathbb{N}}$ (respectively $\{\lambda_n(L + R)\}_{n\in\mathbb{N}}$) is the non-decreasing sequence of eigenvalues of L (respectively $L + R$), counting multiplicities.

Proof. (a) Assume that $z \in \mathbb{C} \setminus \{\lambda\}$ is such that $d' + \tau \le |z| \le d'' - \tau$. Since

$$\|(L - z)^{-1}\| = \frac{1}{\operatorname{dist}(\operatorname{spec}(L), z)} \le \frac{1}{\min\{|z - \lambda|, \tau\}},$$

the estimate

$$\|R(L - z)^{-1}\| \le \|R\| \|(L - z)^{-1}\| \le \max\left\{\frac{\|R\|}{|\lambda - z|}, \mu_\tau\right\} \tag{8.4}$$

holds with $\mu_\tau = \frac{\|R\|}{\tau} < 1$. If $z \in [d' + \tau, d'' - \tau] \setminus [\lambda - \|R\|, \lambda + \|R\|]$, then $|z - \lambda| > \|R\|$ and (8.4) ensures $\|R(L - z)^{-1}\| < 1$, hence

$$(L + R - z)^{-1} = (L - z)^{-1}(I + R(L - z)^{-1})^{-1}$$

is well defined, i.e.,

$$\operatorname{spec}(L + R) \cap [d' + \tau, d'' - \tau] \subset [\lambda - \|R\|, \lambda + \|R\|].$$

To end the proof, consider $z \in \mathbb{C}$ satisfying $|z - \lambda| = \tau$. Then

$$|z| \in [\lambda - \tau, \lambda + \tau] \subset [d' + \tau, d'' - \tau] \tag{8.5}$$

and for $t \in [0, 1]$ we can define $(L - z)^{-1}(I + tR(L - z)^{-1})^{-1} = (L_t - z)^{-1}$ where $L_t = L + tR$. The spectral projector of L_t associated to $[\lambda - \tau, \lambda + \tau]$ has the form

$$P_t = \mathbf{1}_{[\lambda-\tau,\lambda+\tau]}(L_t) = \frac{\mathrm{i}}{2\pi} \int_{|z-\lambda|=\tau} (L_t - z)^{-1} dz \tag{8.6}$$

and $t \to P_t$ is continuous $[0, 1] \to \mathcal{B}(\mathcal{H})$, hence $\operatorname{rank}(P_t) = \operatorname{rank}(P_0) = 1$.

(b) We proceed in three steps.

Step 1. We assume that $z \in \mathbb{C} \setminus \{\lambda\}$ satisfies $d' + \tau \leq |z| \leq d'' - \tau$ and we claim that

$$\|(L + \mathrm{i}\tau)^{-1}(L - z)^{-1}\| \leq \frac{1}{\min\{\lambda|\lambda - z|, \tau d'\}}. \tag{8.7}$$

In order to show (8.7), we observe that

$$\|(L + \mathrm{i}\tau)^{-1}(L - z)^{-1}\| = \sup_{s \in \mathrm{spec}(L)} \left| \frac{1}{(s + \mathrm{i}\tau)(s - z)} \right| = \sup_{s \in \mathrm{spec}(L)} \frac{1}{\nu_{\tau,z}(s)},$$

where $\nu_{\tau,z}(s) := \sqrt{\tau^2 + s^2}|s - z|$.

If $d' + \tau \leq |z| \leq d'' - \tau$ and $s \in \mathrm{spec}(L)$, then we can consider four cases:

(i) if $s \geq d''$, then $\nu_{\tau,z}(s) \geq s(s - |z|) \geq d''(d'' - |z|) > d''\tau$;

(ii) if $s = \lambda$, then $\nu_{\tau,z}(\lambda) \geq \lambda|\lambda - z|$;

(iii) if $\tau \leq s \leq d'$, then $\nu_{\tau,z}(s) \geq s(|z| - s) \geq s(d' + \tau - s) \geq \tau d'$;

(iv) if $s < \tau$, then $\nu_{\tau,z}(s) \geq \tau(|z| - s) \geq \tau(|z| - \tau) \geq \tau d'$.

Thus, $\nu_{\tau,z}(s) \geq \min\{\lambda|\lambda - z|, \tau d'\}$ holds in all cases.

Step 2. Let τ_λ be given by (8.3). We claim that

$$\mathrm{spec}(L + R) \cap [d' + \tau, d'' - \tau] \subset [\lambda - \tau_\lambda, \lambda + \tau_\lambda]. \tag{8.8}$$

Consider $z \in \mathbb{C}$ such that $d' + \tau \leq |z| \leq d'' - \tau$. Due to (8.7),

$$\begin{aligned} \|R(L - z)^{-1}\| &\leq \|R(L + \mathrm{i}\tau)\| \|(L + \mathrm{i}\tau)^{-1}(L - z)^{-1}\| \\ &\leq \max\left\{\frac{\|R(L + \mathrm{i}\tau)\|}{\lambda|\lambda - z|}, \mu_\tau\right\}, \end{aligned} \tag{8.9}$$

where

$$\mu_\tau := \frac{\|R(L + \mathrm{i}\tau)\|}{d'\tau} < 1$$

due to (8.2). If $|z - \lambda| > \tau_\lambda$, then the right-hand side of (8.9) is strictly less than 1, hence $\|R(L - z)^{-1}\| < 1$ and $(L + R - z)^{-1} = (L - z)^{-1}(I + R(L - z)^{-1})^{-1}$ is well defined, i.e., (8.8) holds.

Step 3. To end the proof, consider $z \in \mathbb{C}$ satisfying $|z - \lambda| = \tau$. Then (8.5) holds and (8.2) implies $\tau_\lambda < \tau d' \lambda^{-1} < \tau$, hence $\frac{\|R(L+\mathrm{i}\tau)\|}{\lambda\tau} = \frac{\tau_\lambda}{\tau} < 1$. Therefore, the right-hand side of (8.9) is strictly less than 1 and, for $t \in [0, 1]$, we can define $(L_t - z)^{-1}$ with $L_t = L + tR$ similarly to (b) and its spectral projector is given by (8.6), hence $\mathrm{rank}(P_t) = \mathrm{rank}(P_0) = 1$.

(c) See Rozenblum [37, Theorem 1.1]. ∎

8.3. Kato–Temple estimate

Theorem 8.3 (Kato–Temple). *Assume that the operator L is self-adjoint in the Hilbert space $\mathcal{H}$ and has exactly one eigenvalue λ in the interval $[d', d'']$. If x is an element of the domain of L such that $\|x\|_{\mathcal{H}} = 1$ and $\eta := \langle x, Lx\rangle_{\mathcal{H}}$ belongs to $]d', d''[$, then*

$$\eta - \frac{\|(L-\eta)x\|^2}{\eta - d'} \le \lambda \le \eta + \frac{\|(L-\eta)x\|^2}{d'' - \eta}. \tag{8.10}$$

Proof. See [21]. ∎

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Anne Boutet de Monvel
UFR de Mathématiques et Informatique, Université Paris Cité, Boîte courrier 7012, 75205 Paris Cedex 13, France; anne.boutet-de-monvel@imj-prg.fr

Lech Zielinski
Laboratoire de Mathématiques Pures et Appliquées Joseph Liouville UR 2597, Université du Littoral Côte d'Opale, 50 rue Ferdinand Buisson, 62228 Calais, France; lech.zielinski@univ-littoral.fr