FIRST-ORDER APPROXIMATION OF LARGE EIGENVALUES OF THE TWO-PHOTON ASYMMETRIC QUANTUM RABI MODEL

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ANNE BOUTET DE MONVEL[1], MIRNA CHARIF[2], AND LECH ZIELINSKI[3]

Abstract. We investigate the asymptotic distribution of large eigenvalues of the two-photon quantum Rabi model with a bias. The asymptotic formula for the m-th eigenvalue is obtained with the remainder estimate $O(m^{-1}\ln m)$ when m tends to infinity, which corresponds to the first-order approximation of large eigenvalues for this model.

Keywords: quantum Rabi model, unbounded self-adjoint operators, discrete spectrum, asymptotic distribution of eigenvalues

Mathematics Subject Classification: Primary 47A75; Secondary 47B25, 81Q10, 81V80

1. General presentation

1.1. **Introduction.** The quantum Rabi model (QRM) describes the simplest interaction between a two-level atom and a quantized single-mode radiation. We refer to [50], [51], [37], [15], for the history of the model and to [65] for a survey of theoretical and experimental results. The basic version of the model was widely used to study real atoms in quantum optics, e.g. to test experimentally the field energy quantization of the cavity electrodynamics (see [16]). However, new realizations of engineered quantum devices with important technological applications lead to various generalizations of the initial model. In particular, the superconducting circuits in the microwave regime, cooled to the ground state in cryogenic temperatures, play the role of artificial atoms and can be described by the asymmetric QRM (see [65], [32], [29], [38], [66], [67]). This model (see Definition 1.2(c)) contains an additional parameter ε (the bias of the model), which can be experimentally adjusted by the application of magnetic flux through a circuit loop.

Another type of the QRM is used in the situation when the change of level is associated with the absorption/emission of two photons instead of one photon. The corresponding two-photon QRM (see Definition 1.2(d)) was applied to describe a two-level atom interacting with squeezed light (see [2], [30]), quantum dots inserted in a cavity ([19]), trapped ions experiments (see [24]), and superconducting circuits (see [25], [26]). Both models, the one-photon and the two-photon QRM, have been subject of intensive research in connection with the quantum thermalization and integrability questions (see [15], [13], [12], [39], [40], [55], [60]). We note that the integrability of the considered models depends on the bias and is closely related to the existence of hidden symmetries and double eigenvalues (see [1], [14], [41], [44], [46], [47], [48], [53], [54], [64]). Moreover, a number of research works concern the so-called spectral collapse problem, i.e., the study of the transition from discrete to continuous spectrum of the

two-photon quantum Rabi model, which occurs when the coupling constant takes the critical value $g = 1/2$ in (1.23) (see [12], [17], [43]).

The purpose of this paper is to investigate large eigenvalues of the two-photon QRMl under the assumption that $g \neq 0$ and $-1/2 < g < 1/2$ (note that the assumption $|g| < 1/2$ is essential to ensure the fact that the spectrum is discrete). The main result of the paper is stated in Theorem 1.5. We note that the asymptotic formulas of Theorem 1.5 depend on the value of $\varepsilon/\sqrt{1-4g^2}$ in a similar manner as in the integrability problem of the model. In the next section we give an overview of results related to the behavior of large eigenvalues of the one-photon and two-photon QRM.

1.2. **Overview of related results.** We refer to [58] and [27], for the earliest investigations of large eigenvalues for the one-photon QRM in the case $\varepsilon = 0$. It is well known (see [61], [7]) that the assumption $\varepsilon = 0$ allows one to express the one-photon QRM as a direct sum of two Jacobi operators (i.e. operators defined by infinite tridiagonal matrices). Similarly, the two-photon QRM can be expressed as a direct sum of four Jacobi operators if $\varepsilon = 0$ (see [9]). A mathematical study of large eigenvalues of Jacobi operators was initiated by J. Janas and S. Naboko in the paper [36], which contains fundamental ideas of the method of approximate diagonalizations.

The question of the behavior of large eigenvalues of Jacobi operators corresponding to the one-photon QRM, was first posed by E. A. Tur [61]-[62]. This question was also mentioned by A. Boutet de Monvel, S. Naboko and L. O. Silva in [5]. Due to the difficulty of the problem, the paper [5] gives the asymptotic estimates for a simpler class of operators ("modified Jaynes-Cummings models"). However, using the ideas of [36], E. A. Tur [63] proved the two-term asymptotic formula for the m-th eigenvalue of the one-photon QRM with the remainder estimate $O(m^{-1/16})$ as $m \to \infty$ (see also [62]).

The three-term asymptotic formula for the one-photon QRM in the case $\varepsilon = 0$ was proved in the papers A. Boutet de Monvel, L. Zielinski [6]-[7]. We note that the three-term asymptotic formula allows one to recover the values of parameters of the model from its spectrum (see [8]) and was used by Z. Rudnick [57] to consider a Braak's conjecture (see [12]). Moreover, this formula coincides with the approximation proposed by I. D. Feranchuk, L. I. Komarov, A. P. Ulyanenkov [27] (see the formula (25) in [27]). The same approximation was described by E. K. Irish [34], [35], and it is well known under the name of the generalized rotating-wave approximation (GRWA). The quality of GRWA was 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 [49].

The three-term asymptotic formula for large eigenvalues of the two-photon QRM in the case $\varepsilon = 0$ was proved by A. Boutet de Monvel, L. Zielinski in [9], [11] (see also [10]) and E. A. Ianovich [33]. The asymptotic behavior of large eigenvalues for the asymmetric one-photon QRM, was investigated in the papers M. Charif, A. Fino, L. Zielinski [18] and A. Boutet de Monvel, M. Charif, L. Zielinski [4]. The two-term asymptotic formula for large eigenvalues of the asymmetric two-photon QRM was proved in the paper A. Boutet de Monvel, M. Charif, L. Zielinski [3]. The results of [3] are described in Section 2 and are used in the proof of Theorem 1.5. Other types of results in the asymptotic analysis of the QRM were considered in [42], [45], [59], [56].

1.3. **Definitions and statements.**

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 $x : \mathbb{N} \to \mathbb{C}$ equipped with the scalar product

$$\langle x, y\rangle_{\ell^2(\mathbb{N})} = \sum_{m=0}^{\infty} \overline{x(m)}y(m) \tag{1.1}$$

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

$$\ell^{2,s}(\mathbb{N}) := \{x \in \ell^2(\mathbb{N}) : \sum_{m=0}^{\infty}(1+m^2)^s\,|x(m)|^2 < \infty\} \tag{1.2}$$

(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

$$\hat{a}^\dagger\, e_n = \sqrt{n+1}\, e_{n+1} \ \text{ for } n \in \mathbb{N} \tag{1.3}$$

$$\hat{a}\, e_0 = 0 \quad \text{and} \quad \hat{a}\, e_n = \sqrt{n}\, e_{n-1} \ \text{ for } n \in \mathbb{N}\setminus\{0\}. \tag{1.4}$$

(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

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad I_2 := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \tag{1.5}$$

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

$$H_{\mathrm{TLS}} = \frac{1}{2}\begin{pmatrix} \Delta & \varepsilon \\ \varepsilon & -\Delta \end{pmatrix} = \frac{\Delta}{2}\sigma_z + \frac{\varepsilon}{2}\sigma_x \tag{1.6}$$

where Δ and ε are real parameters.

(b) The Hamiltonian of the single-mode radiation is the linear map $H_{\mathrm{rad}} : \ell^{2,1}(\mathbb{N}) \to \ell^2(\mathbb{N})$ defined by the formula

$$H_{\mathrm{rad}} e_n = \hat{a}^\dagger \hat{a}\, e_n = n e_n \text{ for } n \in \mathbb{N}. \tag{1.7}$$

(c) Let $g \in \mathbb{R}$. Then the *one-photon quantum Rabi Hamiltonian* is defined as the linear map $\mathbf{H}^{(1)}_{\mathrm{Rabi}} : \mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \to \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$ given by

$$\mathbf{H}^{(1)}_{\mathrm{Rabi}} = I_2 \otimes H_{\mathrm{rad}} + H_{\mathrm{TLS}} \otimes I_{\ell^2(\mathbb{N})} + g\sigma_x \otimes \left(\hat{a} + \hat{a}^\dagger\right). \tag{1.8}$$

(d) If $-1/2 < g < 1/2$, then the *two-photon quantum Rabi Hamiltonian* is defined as the linear map $\mathbf{H}^{(2)}_{\mathrm{Rabi}} : \mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \to \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$ given by

$$\mathbf{H}^{(2)}_{\mathrm{Rabi}} = I_2 \otimes H_{\mathrm{rad}} + H_{\mathrm{TLS}} \otimes I_{\ell^2(\mathbb{N})} + g\sigma_x \otimes \left(\hat{a}^2 + (\hat{a}^\dagger)^2\right) \tag{1.9}$$

and we let $\mathbf{H}^{(2)}_{0,\mathrm{Rabi}}$ denote the operator given by (1.9) with $\Delta = 0$, i.e.

$$\mathbf{H}^{(2)}_{0,\mathrm{Rabi}} = I_2 \otimes H_{\mathrm{rad}} + \sigma_x \otimes \left(g\left(\hat{a}^2 + (\hat{a}^\dagger)^2\right) + \frac{\varepsilon}{2}\right). \tag{1.10}$$

The following result is well-known (see [22], [23]):

Theorem 1.3 (the case $\Delta = 0$)**.** *Assume that $-\frac{1}{2} < g < \frac{1}{2}$ and denote*

$$\beta := \sqrt{1-4g^2}, \tag{1.11}$$

$$\beta_\nu = \frac{1}{2}(\beta - 1 + \nu\varepsilon), \quad \nu = \pm 1. \tag{1.12}$$

If $\mathbf{H}^{(2)}_{0,\mathrm{Rabi}}$ is given by (1.10)*, then there is an orthonormal basis $\{\mathbf{u}^0_{\nu,m}\}_{(\nu,m)\in\{-1,1\}\times\mathbb{N}}$ such that*

$$\mathbf{H}^{(2)}_{0,\mathrm{Rabi}}\mathbf{u}^0_{\nu,m} = (\beta m + \beta_\nu)\mathbf{u}^0_{\nu,m}, \ \ \nu = \pm 1 \tag{1.13}$$

The following result was proved in [3]:

Theorem 1.4. *Assume that $-\frac{1}{2} < g < \frac{1}{2}$ and $g \neq 0$. If $\mathbf{H}^{(2)}_{\mathrm{Rabi}}$ is given by* (1.9)*, then there is an orthonormal basis $\{\mathbf{u}_{\nu,m}\}_{(\nu,m)\in\{-1,1\}\times\mathbb{N}}$ such that*

$$\mathbf{H}^{(2)}_{\mathrm{Rabi}}\mathbf{u}_{\pm 1,m} = E^\pm_m \mathbf{u}_{\pm 1,m} \tag{1.14}$$

and the eigenvalue sequences $\{E^-_m\}_{m\in\mathbb{N}}$, $\{E^+_m\}_{m\in\mathbb{N}}$, satisfy the asymptotic estimate

$$E^\pm_m = \beta m + \beta_{\pm 1} + O(m^{-1/2}\ln m) \ \text{as}\ m \to \infty \tag{1.15}$$

with β, $\beta_{\pm 1}$ given by (1.11)-(1.12)*.*

The purpose of this paper is to improve the remainder estimate $O(m^{-1/2}\ln m)$ from Theorem 1.4. We will prove

Theorem 1.5. *Assume that $-\frac{1}{2} < g < \frac{1}{2}$ and $g \neq 0$. Let $\mathbf{H}^{(2)}_{\mathrm{Rabi}}$ be given by* (1.9)
(a) If $\varepsilon/\beta \notin \mathbb{Z}$, then there is an orthonormal basis $\{\mathbf{u}_{\nu,m}\}_{(\nu,m)\in\{-1,1\}\times\mathbb{N}}$ such that (1.14) *holds and*

$$E^\pm_m = \beta m + \beta_{\pm 1} + O(m^{-1}\ln m) \ \text{as}\ m \to \infty \tag{1.16}$$

(b) If $l := |\varepsilon|/\beta$ is an odd integer, then there is an orthonormal basis $\{\mathbf{u}_{\nu,m}\}_{(\nu,m)\in\{-1,1\}\times\mathbb{N}}$ such that (1.14) *holds and one has*

$$E^+_i = \beta i + \beta_1 + O(i^{-1}\ln i) \ \text{as}\ i \to \infty \tag{1.17}$$

$$E^-_{i+l} = E^+_i + O(i^{-1}\ln i) \ \text{as}\ i \to \infty \tag{1.18}$$

(c) If $l := |\varepsilon|/\beta$ is an even integer, then there is an orthonormal basis $\{\mathbf{u}_{\nu,m}\}_{(\nu,m)\in\{-1,1\}\times\mathbb{N}}$ such that (1.14) *holds and one has*

$$E^+_i = \beta i + \beta_1 + |\mathfrak{r}_i| + O(i^{-1}\ln i) \ \text{as}\ i \to \infty \tag{1.19}$$

$$E^-_{i+l} = \beta i + \beta_1 - |\mathfrak{r}_i| + O(i^{-1}\ln i)) \ \text{as}\ i \to \infty \tag{1.20}$$

with

$$\mathfrak{r}_i := i^{-1/2}\,\frac{\Delta}{2}\sqrt{\frac{\beta}{\pi|g|}}\,\cos\Big((2i+1+l)\alpha - i\frac{\pi}{2}\Big), \tag{1.21}$$

where

$$\alpha := \arctan\left(\sqrt{\frac{1-2|g|}{1+2|g|}}\right). \tag{1.22}$$

Proof. See Section 8. □

1.4. **Outline of the proof of Theorem 1.5.** The proof of Theorem 1.5 follows the same idea as the proof of Theorem 1.4 given in [3]. We first remark that the operator

$$\mathbf{H}^{(2)}_{\mathrm{Rabi}} = I_2 \otimes \hat{a}^\dagger \hat{a} + \sigma_x \otimes \Big(g\big(\hat{a}^2 + (\hat{a}^\dagger)^2\big) + \frac{\varepsilon}{2} \Big) + \frac{\Delta}{2}\, \sigma_z \otimes I_{\ell^2(\mathbb{N})} \tag{1.23}$$

is unitarily similar to the operator

$$\mathbf{H} := I_2 \otimes \hat{a}^\dagger \hat{a} - \sigma_z \otimes \Big(g\big(\hat{a}^2 + (\hat{a}^\dagger)^2\big) + \frac{\varepsilon}{2} \Big) + \frac{\Delta}{2}\, \sigma_x \otimes I_{\ell^2(\mathbb{N})}, \tag{1.24}$$

due to the fact that

$$U_{\pi/4} \sigma_x U_{\pi/4}^{-1} = -\sigma_z, \qquad U_{\pi/4} \sigma_z U_{\pi/4}^{-1} = \sigma_x$$

hold with $U_{\pi/4} = \frac{1}{\sqrt{2}} \left(\begin{smallmatrix} 1 & -1 \\ 1 & 1 \end{smallmatrix}\right)$. If $\Delta = 0$, then the operator

$$\mathbf{H}_0 := I_2 \otimes \hat{a}^\dagger \hat{a} - \sigma_z \otimes \Big(g\big(\hat{a}^2 + (\hat{a}^\dagger)^2\big) + \frac{\varepsilon}{2} \Big) \tag{1.25}$$

is similar to $H_{-1} \oplus H_1$, the direct sum of two self-adjoint operators in $\ell^2(\mathbb{N})$ whose eigenvalues are explicitly known (see Lemma 2.1).

We start our approach by moving from $\ell^2(\mathbb{N})$ to $\ell^2(\mathbb{Z})$ and replacing $H_{-1} \oplus H_1$ by $J_{-1} \oplus J_1$ where J_{-1} and J_1 are two appropriate self-adjoint operators in $\ell^2(\mathbb{Z})$. These operators were considered by Edward [21] and, one can express explicitly their eigenvalues and eigenvectors by means of Fourier series (see Proposition 2.4). The operators $J_{\pm 1}$ are not semi-bounded, but one can choose two sequences of eigenvalues $\{\lambda_j(J_{\pm 1})\}_{j \in \mathbb{Z}}$ such that $\lambda_j(J_{\pm 1}) = \lambda_j(H_{\pm 1})$ when $j \in \mathbb{N}$. Moreover, Proposition 2.10 ensures the fact that large eigenvalues of

$$\mathbf{H} := \mathbf{H}_0 + \frac{\Delta}{2}\, \sigma_x \otimes I_{\ell^2(\mathbb{N})} \tag{1.26}$$

are close to suitable eigenvalues of

$$\mathbf{J} = \mathbf{J}_0 + \frac{\Delta}{2} \sigma_x \otimes I_{\ell^2(\mathbb{Z})}$$

(where $\mathbf{J}_0$ is similar to $J_{-1} \oplus J_1$). Thanks to this result, the asymptotic estimates of Theorem 1.5 follow from analogical estimates for large eigenvalues of the operator $\mathbf{J}$.

In Section 3 we introduce the operator J acting in $\ell^2(\mathbb{Z})$ and similar to $\mathbf{J}$. In Theorem 3.2 and 3.4 we state the results corresponding to the first order approximation of large eigenvalues of J. The proof of Theorem 3.2 and 3.4 is based on similarity transformations described in Sections 4 and 5. The proof of Theorem 3.4 is completed in Section 6 and the proof of Theorem 3.2 is completed in Section 7. In Section 8 we deduce the assertion of Theorem 1.5(a) from Theorem 3.2 and the assertions of Theorem 1.5(b)-(c) from Theorem 3.4.

2. Earlier results

2.1. **Preliminaries.** In what follows, we identify $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$ with $\ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})$, writing

$$(1,0) \otimes e_j = (e_j, 0) \in \ell^2(\mathbb{N}) \times \ell^2(\mathbb{N}), \qquad (0,1) \otimes e_j = (0, e_j) \in \ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})$$

and we investigate the operator $\mathbf{H}$ given by (1.24), which is similar to $\mathbf{H}^{(2)}_{\mathrm{Rabi}}$. Then $\mathbf{H}$ can be considered as the linear map $\ell^{2,1}(\mathbb{N}) \times \ell^{2,1}(\mathbb{N}) \to \ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})$ of the form

$$\mathbf{H} = \begin{pmatrix} H_{-1} & \frac{\Delta}{2} I_{\ell^2(\mathbb{N})} \\ \frac{\Delta}{2} I_{\ell^2(\mathbb{N})} & H_1 \end{pmatrix} \tag{2.1}$$

where the operators $H_{\pm 1} : \ell^{2,1}(\mathbb{N}) \to \ell^2(\mathbb{N})$ are given by

$$H_{\pm 1} := \hat{a}^\dagger \hat{a} \pm g\left(\hat{a}^2 + (\hat{a}^\dagger)^2\right) \pm \frac{\varepsilon}{2}. \tag{2.2}$$

If $\Delta = 0$, then $\mathbf{H}^{(2)}_{0,\mathrm{Rabi}}$ is similar to

$$\mathbf{H}_0 = \begin{pmatrix} H_{-1} & 0_{\ell^2(\mathbb{N})} \\ 0_{\ell^2(\mathbb{N})} & H_1 \end{pmatrix} = H_{-1} \oplus H_1. \tag{2.3}$$

The direct computation gives the expression

$$H_\nu e_m = \left(m + \nu\frac{\varepsilon}{2}\right) e_m + \nu g\, b(m) e_{m+2} + \nu g\, b(m-2) e_{m-2} \text{ for } m \in \mathbb{N}, \tag{2.4}$$

with

$$b(m) := \sqrt{(m+1)(m+2)} \text{ for } m \in \mathbb{N} \tag{2.5}$$

and by convention $b(m-2)e_{m-2} = 0$ when $m \in \{0, 1\}$. It is well known (see [22], [23], [3]) that $H_{\pm 1}$ are lower semi-bounded self-adjoint operators in $\ell^2(\mathbb{N})$, their eigenvalues are simple and are given by the formula

$$\lambda_n(H_\nu) = \beta n + \beta_\nu, \tag{2.6}$$

where β and β_ν are given by (1.11) and (1.12). Consequently, $\mathbf{H}_0 = H_{-1} \oplus H_1$ is a lower semi-bounded self-adjoint operator in $\ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})$ and one has

Lemma 2.1. *Assume $\varepsilon \geq 0$ and denote*

$$l := \lfloor \varepsilon/\beta \rfloor = \max\{n \in \mathbb{N} : n \leq \varepsilon/\beta\}. \tag{2.7}$$

Let $\{\lambda_n(\mathbf{H}_0)\}_{n\in\mathbb{N}}$ be the non-decreasing sequence of eigenvalues of $\mathbf{H}_0 = H_{-1} \oplus H_1$, counting the multiplicities. Then

$$\begin{cases} \lambda_n(\mathbf{H}_0) = \beta n + \beta_{-1} \text{ when } n < l \\ \lambda_{l+2i}(\mathbf{H}_0) = \beta(l+i) + \beta_{-1} \text{ for } i \in \mathbb{N} \\ \lambda_{l+2i+1}(\mathbf{H}_0) = \beta i + \beta_1 \text{ for } i \in \mathbb{N} \end{cases} \tag{2.8}$$

Proof. We remark that the sequence $\{\lambda_n(\mathbf{H}_0)\}_{n\in\mathbb{N}}$ defined in (2.8) is non-decreasing and composed of the union of eigenvalues of H_{-1} and H_1 (see Corollary 2.3 in [3]). □

2.2. **Auxiliary operators $J_{\pm 1}$.** The purpose of this section, is to approximate the operators $H_{\pm 1}$ acting in $\ell^2(\mathbb{N})$ by operators $J_{\pm 1}$ acting in $\ell^2(\mathbb{Z})$.

Notation 2.2. (a) We denote by $\ell^2(\mathbb{Z})$ the complex Hilbert space of square-summable sequences $x : \mathbb{Z} \to \mathbb{C}$ equipped with the scalar product

$$\langle x, y\rangle = \sum_{k\in\mathbb{Z}} \overline{x(k)} y(k) \tag{2.9}$$

and the norm $||x|| := \langle x, x\rangle^{1/2}$.

(b) For $s > 0$ we denote

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

where

$$||x||_{\ell^{2,s}(\mathbb{Z})} := \Big(\sum_{k\in\mathbb{Z}} (1+k^2)^s \, |x(k)|^2\Big)^{1/2} \tag{2.10}$$

(c) The canonical basis of $\ell^2(\mathbb{Z})$ is denoted $\{\tilde{e}_j\}_{j\in\mathbb{Z}}$ (i.e. $\tilde{e}_j(k) = \delta_{j,k}$ for j, $k \in \mathbb{Z}$).

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

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

and we denote

$$\Lambda := \mathrm{diag}(j)_{j\in\mathbb{Z}}. \tag{2.11}$$

(e) We denote by S the shift defined in $\ell^2(\mathbb{Z})$ by $(Sx)(j) = x(j-1)$, i.e. $S\tilde{e}_j = \tilde{e}_{j+1}$.

We observe that the expression of $H_\nu e_m$ given in (2.4), contains the term $b(m)$ satisfying

$$b(m) = \sqrt{(m+1)(m+2)} = m + \tfrac{3}{2} + O(m^{-1}) \text{ as } m \to \infty \tag{2.12}$$

We define J_ν, replacing (2.4) by a similar formula acting on the canonical basis of $\ell^2(\mathbb{Z})$ by means of $m + \frac{3}{2}$ instead of $b(m) = \sqrt{(m+1)(m+2)}$.

Notation 2.3. For $\nu = \pm 1$ we define the linear maps $J_\nu : \ell^{2,1}(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ by

$$J_\nu\tilde{e}_j = \left(j + \nu\frac{\varepsilon}{2}\right)\tilde{e}_j + \nu g\,\left(j+\frac{3}{2}\right)\tilde{e}_{j+2} + \nu g\,\left(j-\frac{1}{2}\right)\tilde{e}_{j-2} \text{ for } j \in \mathbb{Z}. \tag{2.13}$$

Using Notation 2.2 we can express J_ν in the form

$$\begin{aligned} J_\nu &= \Lambda + \nu\frac{\varepsilon}{2} + \nu g\left(S^2\left(\Lambda+\frac{3}{2}\right) + \left(\Lambda+\frac{3}{2}\right)S^{-2}\right) \\ &= \Lambda + \nu\frac{\varepsilon}{2} + \nu g\left(S^2\left(\Lambda+\frac{3}{2}\right) + \text{ h.c.}\right) \end{aligned} \tag{2.14}$$

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

$$\langle f, g\rangle_{\mathrm{L}^2(\mathbb{T})} := \int_{-\pi}^{\pi} \overline{f(\theta)}\,g(\theta)\,\frac{\mathrm{d}\theta}{2\pi} \tag{2.15}$$

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

$$(\mathcal{F}_\mathbb{T} f)(j) = \int_{-\pi}^{\pi} f(\theta)\,\mathrm{e}^{-\mathrm{i}j\theta}\,\frac{\mathrm{d}\theta}{2\pi} \tag{2.16}$$

and, for $\mu = \pm 1$ we consider the operator

$$L_\nu := \mathcal{F}_\mathbb{T}^{-1} J_\nu \mathcal{F}_\mathbb{T} = -\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\theta} + \nu\frac{\varepsilon}{2} + \nu g\left(\mathrm{e}^{2\mathrm{i}\theta}\left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\theta}+\frac{3}{2}\right) + \text{ h.c.}\right)$$

Similarly as in [21] and [3], we observe that the assumption $|g| < 1/2$ ensures the fact that L_ν is the first order linear elliptic differential operator,

$$L_\nu = \frac{1}{2}\left(\left(1 + 2\nu g\cos(2\theta)\right)\left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\theta}\right) + \text{ h.c.}\right) + \nu\left(g\cos(2\theta) + \frac{\epsilon}{2}\right).$$

In what follows, we assume that $\beta = \sqrt{1-4g^2}$ is as in (1.11), and for $\nu = \pm 1$ we define

$$\Phi_\nu(\theta) := \int_0^\theta \frac{\beta\,\mathrm{d}\theta'}{1 + 2\nu g\cos(2\theta')}. \tag{2.17}$$

Then the direct computation by means of the standard change of variable $t = \tan(\theta)$ gives

$$\Phi_\nu(\theta) = \arctan\left(\sqrt{\frac{1-2\nu g}{1+2\nu g}}\tan(\theta)\right) \text{ if } -\frac{\pi}{2} < \theta < \frac{\pi}{2}, \tag{2.18}$$

hence $\Phi_\nu(\pi/2) = \pi/2$. Since the function $\theta' \to \beta/(1+2\nu g\cos(2\theta'))$ is π-periodic, one has

$$\int_{\pi/2}^{\theta} \frac{\beta\,\mathrm{d}\theta'}{1+2\nu g\cos(2\theta')} = \int_{-\pi/2}^{\theta-\pi} \frac{\beta\,\mathrm{d}\theta'}{1+2\nu g\cos(2\theta')}$$

and the above equality gives

$$\Phi_\nu(\theta) - \Phi_\nu(\pi/2) = \Phi_\nu(\theta-\pi) - \Phi_\nu(-\pi/2). \tag{2.19}$$

Moreover, Φ_ν is odd (i.e. $\Phi_\nu(-\theta) = -\Phi_\nu(\theta)$) and $\Phi_\nu(\pi/2) = \pi/2$, hence (2.19) gives

$$\Phi_\nu(\theta) = 2\Phi_\nu(\pi/2) + \Phi_\nu(\theta-\pi) = \pi - \Phi_\nu(\pi-\theta). \tag{2.20}$$

Therefore $\Phi_\nu(\pm\pi) = \pm\pi$ and we can use Φ_ν to define a diffeomorphism $\mathbb{T} \to \mathbb{T}$ and the unitary operator acting in $\mathrm{L}^2(\mathbb{T})$ by means of the change of variable $\eta = \Phi_\nu(\theta)$, given by the formula

$$(U_\nu f)(\theta) = \Phi_\nu'(\theta)^{1/2} f(\Phi_\nu(\theta)). \tag{2.21}$$

Proposition 2.4. *(a) Let us introduce*

$$q_\nu(\theta) = \nu\beta^{-1}\left(g\cos(2\Phi_\nu^{-1}(\theta)) + \frac{\varepsilon}{2}\right) \tag{2.22}$$

and

$$\widetilde{q}_\nu(\eta) := \int_0^\eta q_\nu(\eta')\,\mathrm{d}\eta'. \tag{2.23}$$

Then

$$\widetilde{q}_\nu(\Phi_\nu(\theta)) = \frac{1}{2}\left(\theta + \frac{\nu\varepsilon - 1}{\beta}\,\Phi_\nu(\theta)\right) \tag{2.24}$$

(b) Let $(f_{q_\nu,m})_{m\in\mathbb{Z}}$, be the orthonormal basis in $\mathrm{L}^2(\mathbb{T})$ given by

$$f_{q_\nu,m}(\eta) = \mathrm{e}^{\mathrm{i}m\eta}\,\mathrm{e}^{\mathrm{i}(\langle q_\nu\rangle\eta - \tilde{q}_\nu(\eta))} \tag{2.25}$$

where $\tilde{q}_\nu$ is given by (2.23) *and*

$$\langle q_\nu\rangle := \int_{-\pi}^{\pi} q_\nu(\theta)\,\frac{\mathrm{d}\theta}{2\pi} = \frac{\tilde{q}_\nu(\pi) - \tilde{q}_\nu(-\pi)}{2\pi}. \tag{2.26}$$

If U_ν is given by (2.21)*, then $(U_\nu f_{q_\nu,m})_{m\in\mathbb{Z}}$ is an orthonormal basis of eigenvectors of L_ν and*

$$L_\nu U_\nu f_{q_\nu,m} = (\beta m + \beta_\nu) U_\nu f_{q_\nu,m}, \tag{2.27}$$

where β_ν is given by (1.11)*.*

Proof. (a) We can express $\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\tilde{q}_\nu(\Phi_\nu(\theta))\right)$ in the form

$$q_\nu(\Phi_\nu(\theta))\Phi_\nu'(\theta) = \frac{\nu g\cos(2\theta)}{\beta}\,\frac{\beta}{1+2\nu g\cos(2\theta)} + \frac{\nu\varepsilon}{2\beta}\Phi_\nu'(\theta) \tag{2.28}$$

and the right-hand side of (2.28) gives the derivative of the right-hand side of (2.24),

$$\frac{1}{2}\left(1 - \frac{1}{1+2g\nu\cos(2\theta)} + \frac{\nu\varepsilon}{\beta}\Phi_\nu'(\theta)\right) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\theta - \frac{1}{\beta}\Phi_\nu(\theta) + \frac{\nu\varepsilon}{\beta}\Phi_\nu(\theta)\right).$$

This complete the proof of (2.24) due to $\Phi_\nu(0) = 0 = \widetilde{q}_\nu(0)$.

(b) If $\langle q_\nu \rangle$ is given by (2.26), then $\eta \to \langle q_\nu \rangle \eta - \tilde{q}_\nu(\eta)$ is a smooth 2π-periodic function and (see [21] or Section 3.3 in [3]) for every $m \in \mathbb{Z}$, we get

$$\beta \left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\eta} + q_\nu \right) f_{q_\nu,m} = \beta(m + \langle q_\nu \rangle) f_{q_\nu,m}. \tag{2.29}$$

Moreover, using $\Phi_\nu(\pm\pi) = \pm\pi$ and (2.24), we find

$$\langle q_\nu \rangle = \frac{\widetilde{q}_\nu(\Phi_\nu(\pi)) - \widetilde{q}_\nu(\Phi_\nu(\pi))}{2\pi} = \frac{1}{2} + \frac{\nu\varepsilon - 1}{2\beta}, \tag{2.30}$$

hence

$$\beta(m + \langle q_\nu \rangle) = \beta m + \frac{1}{2}(\beta - 1 + \nu\varepsilon) = \beta m + \beta_\nu,$$

where β_ν is given by (1.11). To complete the proof, it remains to use the identity

$$U_\nu^{-1} L_\nu U_\nu = \beta \left(-\mathrm{i}\frac{\mathrm{d}}{\mathrm{d}\eta} + q_\nu(\eta) \right), \tag{2.31}$$

which follows by a direct computation (see Lemma 3.2 in [3]). □

Combining (2.29) with (2.31), we obtain

Corollary 2.5. *For $m \in \mathbb{Z}$ we define $v_{\nu,m} := \mathcal{F}_{\mathbb{T}} U_\nu f_{q_\nu,m}$. Then $\{v_{\nu,m}\}_{m\in\mathbb{Z}}$ is an orthonormal basis of eigenvectors of J_ν and*

$$J_\nu v_{\nu,m} = (\beta m + \beta_\nu) v_{\nu,m}. \tag{2.32}$$

2.3. Operators $\mathbf{J}_0$ and $\mathbf{J}$.

Notation 2.6. We define $\mathbf{J}$ as the linear map $\ell^{2,1}(\mathbb{Z}) \times \ell^{2,1}(\mathbb{Z}) \to \ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})$ given by

$$\mathbf{J} := \begin{pmatrix} J_{-1} & \frac{\Delta}{2} I_{\ell^2(\mathbb{Z})} \\ \frac{\Delta}{2} I_{\ell^2(\mathbb{Z})} & J_1 \end{pmatrix} \tag{2.33}$$

(b) We denote $\mathbf{J}_0 := J_{-1} \oplus J_1$ and observe that we can express

$$\mathbf{J} = \mathbf{J}_0 + \mathbf{V} \text{ with } \mathbf{V} := \frac{\Delta}{2} \begin{pmatrix} 0_{\ell^2(\mathbb{Z})} & I_{\ell^2(\mathbb{Z})} \\ I_{\ell^2(\mathbb{Z})} & 0_{\ell^2(\mathbb{Z})} \end{pmatrix}, \tag{2.34}$$

where $0_{\ell^2(\mathbb{Z})}$ is the null map on $\ell^2(\mathbb{Z})$.

Due to Corollary 2.5, $\mathbf{J}_0 = J_{-1} \oplus J_1$ is a self-adjoint operator in $\ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})$ and its spectrum is composed of the union of eigenvalues of J_{-1} and J_1. More precisely, one has

Lemma 2.7. *Let $\{\mathbf{v}_m^0\}_{m\in\mathbb{Z}}$ be the orthonormal basis of $\ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})$ defined by*

$$\mathbf{v}_{2j}^0 = (v_{-1,j}, 0), \quad \mathbf{v}_{2j+1}^0 = (0, v_{1,j-l}) \text{ for } j \in \mathbb{Z}, \tag{2.35}$$

where $l := \lfloor \epsilon/\beta \rfloor$ is as in (2.7) and $\{v_{\nu,m}\}_{m\in\mathbb{Z}}$ as in Corollary 2.5. Then one has

$$\mathbf{J}_0 \mathbf{v}_m^0 = d_j \mathbf{v}_m^0 \text{ for } m \in \mathbb{Z}, \tag{2.36}$$

where the sequence $\{d_m\}_{m\in\mathbb{Z}}$ is given by the formula

$$d_{2j} := \beta j + \beta_{-1}, \quad d_{2j+1} = \beta(j - l) + \beta_1 \text{ for } j \in \mathbb{Z}. \tag{2.37}$$

Moreover, $d_m \le d_{m+1}$ holds for every $m \in \mathbb{Z}$.

Proof. It is clear that the sequence $\{d_m\}_{m\in\mathbb{Z}}$ defined in (2.37) is composed of the union of eigenvalues of J_{-1} and J_1. Moreover

$$\begin{cases} \mathbf{J}_0\mathbf{v}^0_{2j} = (J_{-1}v_{-1,j}, 0) = d_{2j}\mathbf{v}^0_{2j}, \\ \mathbf{J}_0\mathbf{v}^0_{2j+1} = (0, J_1 v_{1,j-l}) = d_{2j+1}\mathbf{v}^0_{2j+1} \end{cases} \tag{2.38}$$

and $d_m \leq d_{m+1}$ follows from the definition of l. □

Remark 2.8. The sequence $\{d_m\}_{m\in\mathbb{Z}}$ defined by (2.37) satisfies

$$d_{n+l} = \lambda_n(\mathbf{H}_0) \text{ for } n > l \tag{2.39}$$

The following auxiliary result is the crucial ingredient of our approach:

Proposition 2.9. *Assume that* $\mathbf{V}$ *is as in* (2.34) *and* $\{\mathbf{v}^0_m\}_{m\in\mathbb{Z}}$ *is the orthogonal basis introduced in Lemma 2.7. Then there exist constants* $\hat{C}$ *and* $\hat{c} > 0$ *such that one has*

$$\sup_{\{k\in\mathbb{Z}:\, |k-j|\leq \hat{c}j\}} |\langle \mathbf{v}^0_k, \mathbf{V}\mathbf{v}^0_j\rangle_{\ell^2(\mathbb{Z})\times\ell^2(\mathbb{Z})}| \leq \hat{C}(1+|j|)^{-1/2} \text{ for } j \in \mathbb{Z}. \tag{2.40}$$

Proof. See Lemma 3.4 in [3]. □

2.4. **Relation between eigenvalues of H and J.**

Proposition 2.10. *(a) We can find* $\{\lambda_j(\mathbf{J})\}_{j\in\mathbb{Z}}$*, a non-decreasing eigenvalue sequence of* $\mathbf{J}$*, counting the multiplicities, such that*

$$\lambda_j(\mathbf{J}) = d_j + O(|j|^{-1/2}) \text{ as } |j| \to \infty \tag{2.41}$$

(b) If $\{\lambda_j(\mathbf{J})\}_{j\in\mathbb{Z}}$ *is as in (a) and* $\{\lambda_n(\mathbf{H})\}_{n\in\mathbb{N}}$ *is the non-decreasing eigenvalue sequence of* $\mathbf{H}$*, counting the multiplicities, then*

$$\lambda_n(\mathbf{H}) - \lambda_{n+l}(\mathbf{J}) = O(n^{-1}) \text{ as } n \to \infty \tag{2.42}$$

Proof. (a) See Proposition 4.1 in [3].

(b) Since $\lambda_n(\mathbf{H}) = \lambda_n(\mathbf{H}_0) + O(n^{-1/2})$ as $n \to \infty$ holds due to Theorem 1.3 and 1.4, we get

$$\lambda_n(\mathbf{H}) = d_{n+l} + O(n^{-1/2}) \text{ as } n \to \infty \tag{2.43}$$

due to (2.39). Moreover, due to Lemma 5.1 in [3], there exists $\kappa \in \mathbb{Z}$ such that

$$\lambda_n(\mathbf{H}) = \lambda_{n+\kappa}(\mathbf{J}) + O(n^{-1}) \text{ as } n \to \infty \tag{2.44}$$

and, using (2.41) in (2.44), we find

$$\lambda_n(\mathbf{H}) = d_{n+\kappa} + O(n^{-1/2}) \text{ as } n \to \infty \tag{2.45}$$

Combining (2.43) with (2.45), we get $d_{n+l} - d_{n+\kappa} = O(n^{-1/2})$, which implies $\kappa = l$. □

3. First-order approximation of large eigenvalues of J

3.1. **Preliminaries.** Instead of the operator $\mathbf{J} : \ell^{2,1}(\mathbb{Z}) \times \ell^{2,1}(\mathbb{Z}) \to \ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})$, we will investigate the operator $J : \ell^{2,1}(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ given by the formula

$$J := \tilde{U}^{-1}\mathbf{J}\,\tilde{U}, \tag{3.1}$$

where $\tilde{U}$ is the isometric bijection $\ell^2(\mathbb{N}) \to \ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})$ defined by the relation $\tilde{U}\tilde{e}_m = \mathbf{v}^0_m$ for every $m \in \mathbb{Z}$ and $\{\mathbf{v}^0_m\}_{m\in\mathbb{Z}}$ is the basis of eigenvectors of $\mathbf{J}_0$ introduced in Lemma 2.7. Then we obtain the expression

$$J = D + V, \tag{3.2}$$

where

$$D = \mathrm{diag}(d_m)_{m\in\mathbb{Z}} \tag{3.3}$$

with $\{d_m\}_{m\in\mathbb{Z}}$ given by (2.37) and

$$V = \tilde{U}^{-1}\mathbf{V}\,\tilde{U}. \tag{3.4}$$

Notation 3.1. (a) If $\mathcal{V}$ is a Banach space, then $\mathcal{B}(\mathcal{V})$ denotes the Banach algebra of bounded linear operators on $\mathcal{V}$, equipped with the operator norm $||\cdot||_{\mathcal{B}(\mathcal{V})}$ and $||\cdot||$ denotes the norm of $\mathcal{B}(\ell^2(\mathbb{Z}))$.

(b) We let $\ell^2_{\mathrm{fin}}(\mathbb{Z})$ denote the subspace of $\ell^2(\mathbb{Z})$ composed of finite linear combinations of vectors from the canonical basis $\{\tilde{e}_k\}_{k\in\mathbb{N}}$.

(c) If T is a linear map $\mathrm{Dom}(T) \to \ell^2(\mathbb{Z})$ such that $\ell^2_{\mathrm{fin}}(\mathbb{Z}) \subset \mathrm{Dom}(T)$, then we write

$$T(j,k) := (T\tilde{e}_k)(j) = \langle \tilde{e}_j, T\tilde{e}_k\rangle. \tag{3.5}$$

If V is given by (3.4), then

$$V(j,k) = \langle \tilde{e}_j, V\tilde{e}_k\rangle = \langle \mathbf{v}^0_j, \mathbf{V}\mathbf{v}^0_k\rangle_{\ell^2(\mathbb{Z})\times\ell^2(\mathbb{Z})} \tag{3.6}$$

and the estimate (2.40) takes the form

$$\sup_{\{k\in\mathbb{Z}:\,|k-j|\le\hat{c}|j|\}} |V(k,j)| \le \hat{C}(1+|j|)^{-1/2} \text{ for } j\in\mathbb{Z}. \tag{3.7}$$

Moreover, for $i,j\in\mathbb{Z}$ we have

$$V(2i,2j) = \langle (v_{-1,i},0), \mathbf{V}(v_{-1,j},0)\rangle_{\ell^2(\mathbb{Z})\times\ell^2(\mathbb{Z})}$$

$$V(2i+1,2j+1) = \langle (0,v_{1,i+l}), \mathbf{V}(0,v_{1,j+l})\rangle_{\ell^2(\mathbb{Z})\times\ell^2(\mathbb{Z})}$$

$$V(2i,2j+1) = \langle (v_{-1,i},0), \mathbf{V}(0,v_{1,j+l})\rangle_{\ell^2(\mathbb{Z})\times\ell^2(\mathbb{Z})}$$

and, using the definition of $\mathbf{V}$, we find that

$$V(2i,2j) = \frac{\Delta}{2}\,\langle (v_{-1,i},0),(0,v_{-1,j})\rangle_{\ell^2(\mathbb{Z})\times\ell^2(\mathbb{Z})} = 0 \tag{3.8}$$

$$V(2i+1,2j+1) = \frac{\Delta}{2}\,\langle (0,v_{1,i+l}),(v_{1,j+l},0)\rangle_{\ell^2(\mathbb{Z})\times\ell^2(\mathbb{Z})} = 0 \tag{3.9}$$

$$V(2i,2j+1) = \frac{\Delta}{2}\,\langle (v_{-1,i},0),(v_{1,j+l},0)\rangle_{\ell^2(\mathbb{Z})\times\ell^2(\mathbb{Z})} = \frac{\Delta}{2}\,\langle v_{-1,i}, v_{1,j+l}\rangle, \tag{3.10}$$

$$V(2i+1,2j) = \overline{V(2j,2i+1)}. \tag{3.11}$$

3.2. **The case $\varepsilon/\beta \notin \mathbb{Z}$.** The assumption $\varepsilon/\beta\notin\mathbb{Z}$ ensures that all eigenvalues of J are simple and there exist constants C_0 and c_0 such that one has

$$0 < c_0 \le d_{m+1} - d_m \le C_0 \text{ for } m\in\mathbb{Z}. \tag{3.12}$$

Similarly as in [27], [34], the assumption (3.12) allows us to hope that large eigenvalues of J can be approximated by the diagonal entries $J(m,m) = d_m + V(m,m)$. Indeed, we will prove

Theorem 3.2. *Let $\{d_m\}_{m\in\mathbb{Z}}$ be a real sequence satisfying* (3.12) *and let J be the map $\ell^{2,1}(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ given by*

$$J = D + V, \tag{3.13}$$

where $D = \mathrm{diag}(d_m)_{m\in\mathbb{Z}}$ and V is a bounded self-adjoint operator in $\ell^2(\mathbb{Z})$, satisfying the estimate (3.7)*. Assume that $\{\lambda_n(J)\}_{n\in\mathbb{Z}}$ is a non-decreasing sequence of eigenvalues of J, counting the multiplicities, such that*

$$\lambda_n(J) = d_n + o(1) \text{ as } n \to \infty. \tag{3.14}$$

Then one has

$$\lambda_n(J) = d_n + V(n,n) + O(n^{-1}\ln n) \text{ as } n \to \infty. \tag{3.15}$$

Proof. See Section 7. □

Remark 3.3. If J is given by (3.1), then (3.8)-(3.9) imply

$$V(m,m) = 0 \text{ for every } m \in \mathbb{Z}. \tag{3.16}$$

3.3. **The case $\varepsilon/\beta \in \mathbb{N}$.** The assumption $\varepsilon/\beta = l \in \mathbb{N}$ implies that all eigenvalues of $\mathbf{J}$ are double and are expressed by the formula

$$d_{2j} = d_{2j+1} = \beta j + \beta_{-1} = \beta(j-l) + \beta_1, \quad j \in \mathbb{Z}. \tag{3.17}$$

Let us denote

$$\widehat{\mathcal{H}}_{2j} := \mathrm{span}\{\tilde{e}_{2j}, \tilde{e}_{2j+1}\} \tag{3.18}$$

and let $\widehat{\Pi}_n \in \mathcal{B}(\ell^2(\mathbb{N}))$ denote the orthogonal projection on $\widehat{\mathcal{H}}_n$. We consider an approximation of J by the operator J_{appr} defined as the linear map $\ell^{2,1}(\mathbb{Z}) \to \ell^2(\mathbb{Z})$ of the form

$$J_{\mathrm{appr}} := \bigoplus_{j\in\mathbb{Z}} \widehat{J}_{2j}, \tag{3.19}$$

where

$$\widehat{J}_{2j} := \widehat{\Pi}_{2j} V|_{\widehat{\mathcal{H}}_{2j}} \in \mathcal{B}(\widehat{\mathcal{H}}_{2j}). \tag{3.20}$$

We note that the matrix of $\widehat{J}_{2j}$ in the basis $\{\tilde{e}_{2j}, \tilde{e}_{2j+1}\}$ is

$$\begin{pmatrix} d_{2j} & V(2j,2j+1) \\ V(2j+1,2j) & d_{2j} \end{pmatrix}.$$

The spectrum of $\widehat{J}_{2j}$ consists of two eigenvalues $d_{2j} \pm |V(2j,2j+1)|$ and the spectrum of J_{appr} has the form

$$\{d_{2j} + \nu|V(2j,2j+1)| \colon j \in \mathbb{Z},\, \nu = \pm 1\}.$$

Our proof of Theorem 1.4 is based on the following :

Theorem 3.4. *Assume that $D = \mathrm{diag}(d_m)_{m\in\mathbb{Z}}$ with $\{d_m\}_{m\in\mathbb{Z}}$ given by* (3.17) *and assume that V is a bounded self-adjoint operator in $\ell^2(\mathbb{Z})$, satisfying* (3.7) *and* (3.16)*. Assume that $\{\lambda_n(J)\}_{n\in\mathbb{Z}}$ is a non-decreasing sequence of eigenvalues of J, counting the multiplicities, such that*

$$\lambda_n(J) = d_n + o(1) \text{ as } n \to \infty. \tag{3.21}$$

Then one has

$$\lambda_{2j}(J) = d_{2j} - |V(2j,2j+1)| + O(j^{-1}\ln j) \text{ as } j \to \infty, \tag{3.22}$$

$$\lambda_{2j+1}(H) = d_{2j} + |V(2j,2j+1)| + O(j^{-1}\ln j) \text{ as } j \to \infty. \tag{3.23}$$

Proof. See Section 6. □

3.4. **Taylor's expansion formula.** In this section we describe the Taylors's expansion formula, which is the principal tool of our approach. Assume that B and $Q \in \mathcal{B}(\ell^2(\mathbb{Z}))$ and denote

$$F_{tQ}(B) := \mathrm{e}^{-\mathrm{i}tQ}\, B\, \mathrm{e}^{\mathrm{i}tQ} \text{ for } t \in \mathbb{R}, \tag{3.24}$$

$$\mathrm{ad}^0_{\mathrm{i}Q}(B) := B,$$

$$\mathrm{ad}^1_{\mathrm{i}Q}(B) := [B, \mathrm{i}Q] = \mathrm{i}(BQ - QB)$$

and

$$\mathrm{ad}^{m+1}_{\mathrm{i}Q}(B) := [\mathrm{ad}^m_{\mathrm{i}Q}(B), \mathrm{i}Q] \text{ for } m \in \mathbb{N} \setminus \{0\}.$$

Then

$$\frac{\mathrm{d}^m}{\mathrm{d}t^m} F_{tQ}(B) = \mathrm{e}^{-\mathrm{i}tQ}\, \mathrm{ad}^m_{\mathrm{i}Q}(B)\, \mathrm{e}^{\mathrm{i}tQ} = F_{tQ}(\mathrm{ad}^m_{\mathrm{i}Q}(B)) \tag{3.25}$$

and the Taylor's expansion formula gives

$$F_{tQ}(B) = \sum_{m=0}^{N-1} \frac{t^m}{m!} \mathrm{ad}^m_{\mathrm{i}Q}(B) + \mathcal{R}^{t,N}_Q(B) \tag{3.26}$$

with

$$\mathcal{R}^{t,N}_Q(B) := \frac{t^N}{(N-1)!} \int_0^1 F_{stQ}(\mathrm{ad}^N_{\mathrm{i}Q}(B))\, (1-s)^{N-1}\, \mathrm{d}s. \tag{3.27}$$

We can also consider the case when B is an unbounded symmetric operator in $\ell^2(\mathbb{Z})$, defined on a dense domain $\mathcal{D}(B)$. Suppose that $\mathcal{D}(B)$ 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 of class $C^1(\mathbb{R}, \ell^2(\mathbb{N}))$ for every $x \in \mathcal{D}(B)$, then

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

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

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

hence (3.26)-(3.27) still hold for every $N \in \mathbb{N} \setminus \{0\}$.

4. Beginning of the proof of Theorem 3.4

4.1. **Outline of the proof.** In what follows, $J = D + V$ satisfies the assumptions of Theorem 3.4. Moreover, we assume that n is large enough and $n \in 2\mathbb{Z}$, which implies

$$d_{n-1} + \beta = d_n = d_{n+1} = d_{n+2} - \beta. \tag{4.1}$$

We let $\widetilde{\Pi}_n := I - \widehat{\Pi}_n$ denote the orthogonal projection on $\widetilde{\mathcal{H}}_n := \widehat{\mathcal{H}}_n^{\perp}$ and decompose

$$V = \widehat{\Pi}_n V \widehat{\Pi}_n + \widetilde{\Pi}_n V \widetilde{\Pi}_n + \widetilde{\Pi}_n V \widehat{\Pi}_n + \widehat{\Pi}_n V \widetilde{\Pi}_n. \tag{4.2}$$

In what follows, we denote

$$V_n^+ := \widehat{\Pi}_n V \widetilde{\Pi}_n, \tag{4.3}$$

$$V_n^- := (V_n^+)^* = \widetilde{\Pi}_n V \widehat{\Pi}_n. \tag{4.4}$$

We remark that the rows n and $n+1$ are the only non-zero rows of the matrix $(V_n^+(j,k))_{(j,k)\in\mathbb{Z}^2}$. Similarly, the columns n and $n+1$ are the only non-zero columns of the matrix $(V_n^-(j,k))_{(j,k)\in\mathbb{Z}^2}$. The first step of our approach is based on the possibility

of finding a self-adjoint bounded operator Q_n such that $\widehat{\Pi}_n \mathrm{e}^{-\mathrm{i}Q_n} J \mathrm{e}^{\mathrm{i}Q_n} \widetilde{\Pi}_n$ (and its adjoint) has the norm $O(n^{-1/2})$. More precisely, we use the orthogonal decomposition

$$\ell^2(\mathbb{Z}) = \widehat{\mathcal{H}}_n \oplus \widetilde{\mathcal{H}}_n \tag{4.5}$$

and write (4.2) in the form of 2×2 block matrix

$$V = \begin{pmatrix} \widehat{V}_n & V_n^+|_{\widetilde{\mathcal{H}}_n} \\ V_n^-|_{\widehat{\mathcal{H}}_n} & \widetilde{V}_n \end{pmatrix} = \widehat{V}_n \oplus \widetilde{V}_n + V_n^- + V_n^+, \tag{4.6}$$

where

$$\widehat{V}_n := \widehat{\Pi}_n V|_{\widehat{\mathcal{H}}_n} \in \mathcal{B}(\widehat{\mathcal{H}}_n), \tag{4.7}$$

$$\widetilde{V}_n := \widetilde{\Pi}_n V|_{\widetilde{\mathcal{H}}_n} \in \mathcal{B}(\widetilde{\mathcal{H}}_n). \tag{4.8}$$

In Section 4.3 we introduce the operators $Q_n^\pm \in \mathcal{B}(\ell^2(\mathbb{Z}))$ satisfying

$$[D, \mathrm{i}Q_n^\pm] = -V_n^\pm \text{ with } D = \mathrm{diag}(d_m)_{m\in\mathbb{Z}}, \tag{4.9}$$

where $\{d_m\}_{m\in\mathbb{Z}}$ is given by (3.17) and (4.9) is understood as the equality

$$\mathrm{i}(DQ_n^\pm - Q_n^\pm D)x = -V_n^\pm x \text{ for } x \in \ell^{2,1}(\mathbb{Z}), \tag{4.10}$$

well defined because $\ell^{2,1}(\mathbb{Z})$ is an invariant subspace of $Q_n^\pm$ (see Lemma 4.1(a)). Moreover, we will prove the estimate

$$||Q_n^\pm|| = O(n^{-1/2}) \tag{4.11}$$

and the fact that

$$\mathrm{e}^{-\mathrm{i}Q_n} J \mathrm{e}^{\mathrm{i}Q_n} = D + \widehat{V}_n \oplus \widetilde{V}_n + R_n'$$

holds with $||R_n'|| = O(n^{-1/2})$ and

$$Q_n = Q_n^+ + Q_n^-. \tag{4.12}$$

However, the error $O(n^{-1/2})$ is too rough to deduce the asymptotic formula of Theorem 3.4 and we will have to consider a second similarity transformation in Sections 5–6. Besides the operator Q_n, we introduce auxiliary cut-offs $\check{Q}_n^\pm$, which satisfy

$$||Q_n^\pm - \check{Q}_n^\pm|| = O(n^{-1}) \tag{4.13}$$

and are used to prove some estimates in Section 5.

4.2. **Operators $\check{Q}_n^-$ and $\check{Q}_n^+$.** Let Z_n^-, $Z_n^+ \subset \mathbb{Z}^2$ be defined as follows

$$Z_n^- = (\mathbb{Z} \setminus \{n, n+1\}) \times \{n, n+1\} \tag{4.14}$$

$$Z_n^+ = \{n, n+1\} \times (\mathbb{Z} \setminus \{n, n+1\}). \tag{4.15}$$

We observe that

$$(j,k) \in Z_n^- \Rightarrow d_j \neq d_n = d_{n+1} = d_k, \tag{4.16}$$

$$(j,k) \in Z_n^+ \Rightarrow d_k \neq d_n = d_{n+1} = d_j \tag{4.17}$$

and there exists $c_0 > 0$ such that

$$(j,k) \in Z_n^- \cup Z_n^+ \Rightarrow |d_j - d_k| \geq c_0 |j-k|. \tag{4.18}$$

In what follows, $c_0 > 0$ is fixed so that (4.18) holds, $\hat{C}$, $\hat{c} > 0$, are fixed so that the estimate (3.7) holds and c is fixed so that $0 < c \leq \min\{\frac{1}{2}\hat{c}, \frac{1}{2}\}$. We introduce the matrices $(\check{Q}_n^-(j,k))_{(j,k)\in\mathbb{Z}^2}$, $(\check{Q}_n^+(j,k))_{(j,k)\in\mathbb{Z}^2}$ by

$$\check{Q}_n^{\pm}(j,k) := \begin{cases} \mathrm{i}\,\dfrac{V(j,k)}{d_j - d_k} & \text{if } (j,k) \in Z_n^{\pm} \text{ and } |j-k| < cn \\ 0 & \text{otherwise} \end{cases} \tag{4.19}$$

We observe that $\check{Q}_n^-(j,k) \neq 0$ implies $j \neq k$, $k \in \{n, n+1\}$ and $|j-k| < cn \leq ck < \hat{c}k$, hence

$$|\check{Q}_n^-(j,k)| \leq \frac{\hat{C}k^{-1/2}}{|d_j - d_k|} \leq \frac{\hat{C}k^{-1/2}}{c_0|j-k|} \leq \frac{\hat{C}n^{-1/2}}{c_0|j-k|} \tag{4.20}$$

follows from (3.7), (4.18) and $k \geq n$. Since $(j,k) \in Z_n^+ \Leftrightarrow (k,j) \in Z_n^-$ and $V(k,j) = \overline{V(j,k)}$, it is clear that

$$\check{Q}_n^+(j,k) = \overline{\check{Q}_n^-(k,j)} \tag{4.21}$$

and

$$|\check{Q}_n^+(j,k)| \leq \frac{\hat{C}n^{-1/2}}{c_0|j-k|}. \tag{4.22}$$

Then the relation $(\check{Q}_n^{\pm}\tilde{e}_k)(j) = \check{Q}_n^{\pm}(j,k)$ for $j,k \in \mathbb{Z}$ defines the operators $\check{Q}_n^{\pm} \in \mathcal{B}(\ell^2(\mathbb{Z}))$ satisfying the norm estimate

$$||\check{Q}_n^{\pm}|| = O(n^{-1/2}). \tag{4.23}$$

Indeed, by definition $\check{Q}_n^- x = 0$ if $x \in \widetilde{\mathcal{H}}_n$ and for $k \in \{n, n+1\}$ we can estimate

$$||\check{Q}_n^-\tilde{e}_k||^2 = \sum_{j\in\mathbb{N}} |\check{Q}_n^-(j,k)|^2 \leq \sum_{\{j\in\mathbb{Z}:\, 0<|j-k|<cn\}} \left(\frac{\hat{C}n^{-1/2}}{c_0|j-k|}\right)^2$$

$$\leq \hat{C}^2 c_0^{-2} n^{-1} \sum_{j\in\mathbb{Z}\setminus\{k\}} |j-k|^{-2} \leq Cn^{-1},$$

i.e. $||\check{Q}_n^-|| = O(n^{-1/2})$ and (4.21) ensures $\check{Q}_n^+ = (\check{Q}_n^-)^*$, hence $||\check{Q}_n^+|| = ||\check{Q}_n^-||$.

4.3. **Operators Q_n^- and Q_n^+.** We define the matrices $(Q_n^-(j,k))_{(j,k)\in\mathbb{Z}^2}$, $(Q_n^+(j,k))_{(j,k)\in\mathbb{Z}^2}$ by

$$Q_n^{\pm}(j,k) := \begin{cases} \mathrm{i}\,\dfrac{V(j,k)}{d_j - d_k} & \text{if } (j,k) \in Z_n^{\pm} \\ 0 & \text{otherwise} \end{cases} \tag{4.24}$$

where $Z_n^{\pm}$ are given by (4.14)-(4.15). We claim that the relation $(Q_n^{\pm}\tilde{e}_k)(j) = Q_n^{\pm}(j,k)$ (for all $j,k \in \mathbb{Z}$) defines $Q_n^{\pm} \in \mathcal{B}(\ell^2(\mathbb{Z}))$ satisfying (4.13), i.e. $||Q_n^{\pm} - \check{Q}_n^{\pm}|| = O(n^{-1})$. Then, combining (4.23) with (4.13), we get $||Q_n^{\pm}|| = O(n^{-1/2})$.

In order to prove (4.13), we remark that $(Q_n^- - \check{Q}_n^-)x = 0$ if $x \in \widetilde{\mathcal{H}}_n$ and for $k \in \{n, n+1\}$ we can estimate

$$||(Q_n^- - \check{Q}_n^-)\tilde{e}_k||^2 = \sum_{\{j\in\mathbb{Z}:\, |j-k|\geq cn\}} |Q_n^-(j,k)|^2$$

$$\leq \sum_{\{j\in\mathbb{Z}:\, |j-k|\geq cn\}} \frac{|V(j,k)|^2}{c_0^2|j-k|^2} \leq \sum_{j\in\mathbb{Z}} \frac{|V(j,k)|^2}{c_0^2c^2n^2} = \frac{||V\tilde{e}_k||^2}{c_0^2c^2n^2} \leq \frac{||V||^2}{c_0^2c^2n^2},$$

i.e. $Q_n^- - \check{Q}_n^- = (Q_n^- - \check{Q}_n^-)\widehat{\Pi}_n \in \mathcal{B}(\ell^2(\mathbb{Z}))$ and

$$||Q_n^- - \check{Q}_n^-|| = O(n^{-1}).$$

Moreover, $Q_n^+ - \check{Q}_n^+ = (Q_n^- - \check{Q}_n^-)^*$ ensures

$$||Q_n^+ - \check{Q}_n^+|| = ||Q_n^- - \check{Q}_n^-|| = O(n^{-1}).$$

In what follows, $Q_n^\pm$, $\check{Q}_n^\pm$ are as before and we denote

$$Q_n := Q_n^- + Q_n^+, \qquad \check{Q}_n := \check{Q}_n^- + \check{Q}_n^+. \tag{4.25}$$

Lemma 4.1. *(a) $\ell^{2,1}(\mathbb{Z})$ is an invariant subspace of $Q_n^\pm$ and one has*

$$[D, \mathrm{i}Q_n^\pm]x = \mathrm{i}(DQ_n^\pm - Q_n^\pm D)x = -V_n^\pm x \text{ for } x \in \ell^{2,1}(\mathbb{Z}), \tag{4.26}$$

where $D = \mathrm{diag}(d_j)_{j\in\mathbb{N}}$ and $V_n^\pm$ is given by (4.4)-(4.3).
(b) $\ell^{2,1}(\mathbb{Z})$ is an invariant subspace of $\mathrm{e}^{\mathrm{i}tQ_n}$ and $t \to \mathrm{e}^{\mathrm{i}tQ_n}x$ is of class $\mathrm{C}^\infty(\mathbb{R}; \ell^{2,1}(\mathbb{N}))$ if $x \in \ell^{2,1}(\mathbb{N})$.

Proof. Similar to the proof of Lemma 4.4 in [11]. □

4.4. **The first similarity transformation.** If L_n, L_n' are linear maps defined on a dense subspace of $\ell^2(\mathbb{Z})$ such that $L_n - L_n'$ can be extended to a bounded operator on $\ell^2(\mathbb{Z})$, then we still use the notation $||L_n - L_n'||$ to denote the norm of this extension and the notation $L_n = L_n' + O(\eta_n)$ means that choosing $n_0 \in \mathbb{N}$ and $C > 0$ large enough, we ensure $||L_n - L_n'|| \leq C\eta_n$ for all $n \geq n_0$. We will prove the following

Lemma 4.2. *We assume that $J = D + V$ is as in Theorem 3.4, $n \in 2\mathbb{Z}$ and $\widehat{V}_n$, $\widetilde{V}_n$ are given by* (4.7), (4.8). *If $Q_n = Q_n^- + Q_n^+$, then the estimate*

$$\mathrm{e}^{-\mathrm{i}Q_n} J \mathrm{e}^{\mathrm{i}Q_n} = D + \widehat{V}_n \oplus \widetilde{V}_n + R_n + O(n^{-1}) \text{ as } n \to \infty \tag{4.27}$$

holds with

$$R_n := \frac{1}{2}[V, \mathrm{i}Q_n] + \frac{1}{2}[\widehat{V}_n \oplus \widetilde{V}_n, \mathrm{i}Q_n]. \tag{4.28}$$

Proof. Using (3.26)-(3.27) with $N = 2$, $t = 1$, we obtain

$$\mathrm{e}^{-\mathrm{i}Q_n} V \mathrm{e}^{\mathrm{i}Q_n} = V + [V, \mathrm{i}Q_n] + \mathcal{R}_{Q_n}^{1,2}(V), \tag{4.29}$$

$$||\mathcal{R}_{Q_n}^{1,2}(V)|| \leq ||\mathrm{ad}_{\mathrm{i}Q_n}^2(V)|| \leq C||Q_n||^2 \tag{4.30}$$

and using (3.26)-(3.27) with $N = 3$, $t = 1$, we obtain

$$\mathrm{e}^{-\mathrm{i}Q_n} D \mathrm{e}^{\mathrm{i}Q_n} = D + [D, \mathrm{i}Q_n] + \frac{1}{2}[[D, \mathrm{i}Q_n], \mathrm{i}Q_n] + \mathcal{R}_{Q_n}^{1,3}(D). \tag{4.31}$$

Since $[D, \mathrm{i}Q_n] = -V_n^- - V_n^+$ (see Lemma 4.1(a)) in (4.31), we obtain

$$\mathrm{e}^{-\mathrm{i}Q_n} D \mathrm{e}^{\mathrm{i}Q_n} = D - V_n^- - V_n^+ - \frac{1}{2}[V_n^- + V_n^+, \mathrm{i}Q_n] + \mathcal{R}_{Q_n}^{1,3}(D), \tag{4.32}$$

$$||\mathcal{R}_{Q_n}^{1,3}(D)|| \leq ||\mathrm{ad}_{\mathrm{i}Q_n}^3(D)|| = ||\mathrm{ad}_{\mathrm{i}Q_n}^2(V_n^- + V_n^+)|| \leq C||Q_n||^2 \tag{4.33}$$

and summing up (4.32), (4.29), we obtain

$$\mathrm{e}^{-\mathrm{i}Q_n} J \mathrm{e}^{\mathrm{i}Q_n} = D + V - V_n^- - V_n^+ + [V, \mathrm{i}Q_n] - \frac{1}{2}[V_n^- + V_n^+, \mathrm{i}Q_n] + O(||Q_n||^2). \tag{4.34}$$

Since $Q_n = Q_n^- + Q_n^+$, (4.11) ensures

$$||Q_n|| = O(n^{-1/2}) \tag{4.35}$$

and $||Q_n||^2 = O(n^{-1})$, we complete the proof, using $V_n^- + V_n^+ = V - \widehat{V}_n \oplus \widetilde{V}_n$ to write

$$[V, \mathrm{i}Q_n] - \frac{1}{2}[V_n^- + V_n^+, \mathrm{i}Q_n] = [V, \mathrm{i}Q_n] + \frac{1}{2}[\widehat{V}_n \oplus \widetilde{V}_n - V, \mathrm{i}Q_n] = R_n,$$

with R_n given by (4.28). □

5. The second similarity transformation

5.1. **The idea of the second similarity transformation.** Due to Lemma 4.2, the operator $J = D + V$ is similar to

$$\mathrm{e}^{-\mathrm{i}Q_n} J \mathrm{e}^{\mathrm{i}Q_n} = D + \widehat{V}_n \oplus \widetilde{V}_n + R_n + O(n^{-1}) \tag{5.1}$$

with R_n given by (4.28). Similarly as before, we can decompose

$$R_n = \begin{pmatrix} \widehat{R}_n & R_n^+|_{\widetilde{\mathcal{H}}_n} \\ R_n^-|_{\widehat{\mathcal{H}}_n} & \widetilde{R}_n \end{pmatrix} = \widehat{R}_n \oplus \widetilde{R}_n + R_n^- + R_n^+, \tag{5.2}$$

where

$$\widehat{R}_n := \widehat{\Pi}_n R_n|_{\widehat{\mathcal{H}}_n} \in \mathcal{B}(\widehat{\mathcal{H}}_n), \tag{5.3}$$

$$\widetilde{R}_n := \widetilde{\Pi}_n R_n|_{\widetilde{\mathcal{H}}_n} \in \mathcal{B}(\widetilde{\mathcal{H}}_n), \tag{5.4}$$

$$R_n^- := \widetilde{\Pi}_n R_n \widehat{\Pi}_n, \tag{5.5}$$

$$R_n^+ := \widehat{\Pi}_n R_n \widetilde{\Pi}_n. \tag{5.6}$$

In Section 5.2 we introduce the operators $Q_n' \in \mathcal{B}(\ell^2(\mathbb{Z}))$ satisfying

$$||Q_n'|| = O(n^{-1} \ln n) \tag{5.7}$$

and

$$[D, \mathrm{i}Q_n'] = -R_n^- - R_n^+ + O(n^{-1}) \tag{5.8}$$

where $[D, \mathrm{i}Q_n']x = \mathrm{i}(DQ_n' - Q_n'D)x$ is well defined for $x \in \ell^{2,1}(\mathbb{Z})$ due to the fact that $\ell^{2,1}(\mathbb{Z})$ is an invariant subspace of Q_n' (see Lemma 5.1(b)). Moreover, $\ell^{2,1}(\mathbb{Z})$ is an invariant subspace of $\mathrm{e}^{\mathrm{i}Q_n'}$ (see Lemma 5.1(c)) and in Section 6.1 we will show that

$$\begin{aligned} \mathrm{e}^{-\mathrm{i}Q_n'} \mathrm{e}^{-\mathrm{i}Q_n} J \mathrm{e}^{\mathrm{i}Q_n} \mathrm{e}^{\mathrm{i}Q_n'} &= D + \widehat{V}_n \oplus \widetilde{V}_n + \widehat{R}_n \oplus \widetilde{R}_n + O(n^{-1} \ln n) \\ &= D + (\widehat{V}_n + \widehat{R}_n) \oplus (\widetilde{V}_n + \widetilde{R}_n) + O(n^{-1} \ln n) \end{aligned}$$

5.2. **Operators Q_n'.** In what follows

$$Q_n' := \check{Q}_n' + (\check{Q}_n')^* \tag{5.9}$$

with $\check{Q}_n' \in \mathcal{B}(\ell^2(\mathbb{Z}))$ defined by the relation $(\check{Q}_n' \tilde{e}_k)(j) = \check{Q}_n'(j,k)$, where

$$\check{Q}_n'(j,k) := \begin{cases} \dfrac{(W_n \check{Q}_n)(j,k)}{d_k - d_j} & \text{if } (j,k) \in Z_n^- \cup Z_n^+ \\ 0 & \text{otherwise} \end{cases} \tag{5.10}$$

with

$$W_n := \frac{1}{2} V + \frac{1}{2} (\widehat{V}_n \oplus \widetilde{V}_n) \tag{5.11}$$

and $\check{Q}_n$ as in Section 4.

Lemma 5.1. *(a) If $(Q'_n(j,k))_{(j,k)\in\mathbb{Z}^2}$ is given by (5.10), then the relation $(\check{Q}'_n\tilde{e}_k)(j) = \check{Q}'_n(j,k)$ for $j,k\in\mathbb{Z}$ defines the operators $\check{Q}'_n\in\mathcal{B}(\ell^2(\mathbb{Z}))$ satisfying the norm estimate*

$$||\check{Q}'_n|| = O(n^{-1}\ln n). \tag{5.12}$$

(b) $\ell^{2,1}(\mathbb{Z})$ is an invariant subspace of $Q'_n := \check{Q}'_n + (\check{Q}'_n)^*$ and

$$[D,\mathrm{i}Q'_n]x = \mathrm{i}(DQ'_n - Q'_nD)x = -(\check{R}^-_n + \check{R}^+_n)x \text{ for } x\in\ell^{2,1}(\mathbb{Z}) \tag{5.13}$$

holds with $D=\mathrm{diag}(d_m)_{m\in\mathbb{N}}$ and

$$\check{R}^-_n := \widetilde{\Pi}_n[W_n,\mathrm{i}\check{Q}_n]\widehat{\Pi}_n, \tag{5.14}$$

$$\check{R}^+_n := \widehat{\Pi}_n[W_n,\mathrm{i}\check{Q}_n]\widetilde{\Pi}_n. \tag{5.15}$$

(c) $\ell^{2,1}(\mathbb{Z})$ is an invariant subspace of $\mathrm{e}^{\mathrm{i}tQ'_n}$ and $t\to\mathrm{e}^{\mathrm{i}tQ'_n}x$ is of class $\mathrm{C}^\infty(\mathbb{R};\ell^{2,1}(\mathbb{Z}))$ if $x\in\ell^{2,1}(\mathbb{Z})$.

Proof. See Sections 5.3-5.5. □

5.3. **Step 1 of the proof of Lemma 5.1.** Since $\check{Q}_n = \check{Q}^-_n + \check{Q}^+_n$, we can decompose

$$\check{Q}'_n(j,k) = \check{Q}'^+_n(j,k) + \check{Q}'^-_n(j,k)$$

with

$$\check{Q}'^\pm_n(j,k) := \begin{cases} \dfrac{(W_n\check{Q}^\pm_n)(j,k)}{d_k-d_j} & \text{if } (j,k)\in Z^-_n\cup Z^+_n \\ 0 & \text{otherwise}\end{cases} \tag{5.16}$$

We first observe that $\check{Q}'^\pm_n(j,k)\neq 0 \Rightarrow (j,k)\in Z^-_n\cup Z^+_n \Rightarrow j\neq k$ and

$$|\check{Q}'^\pm_n(j,k)| \leq \frac{|(W_n\check{Q}^\pm_n)(j,k)|}{c_0|j-k|}. \tag{5.17}$$

It is clear that (3.7) implies $W_n(j,k)\neq 0\Rightarrow j\neq k$ and

$$|j-k|<\hat{c}k \;\Rightarrow\; |W_n(j,k)| \leq \hat{C}k^{-1/2}. \tag{5.18}$$

In the remaining part of this section, we are going to check that there is $\check{Q}'^-_n\in\mathcal{B}(\ell^2(\mathbb{Z}))$ satisfying $(\check{Q}'^-_n\tilde{e}_k)(j) = \check{Q}'^-_n(j,k)$ for all $j,k\in\mathbb{Z}$ and

$$||\check{Q}'^-_n|| = O(n^{-1}\ln n). \tag{5.19}$$

Since $\check{Q}'^-_n(j,k)=0$ if $k\in\mathbb{Z}\setminus\{n,n+1\}$, one has $||\check{Q}'^-_n||\leq||\check{Q}'^-_n\tilde{e}_n||+||\check{Q}'^-_n\tilde{e}_{n+1}||$. We assume now $k\in\{n,n+1\}$ and write

$$||\check{Q}'^-_n\tilde{e}_k||^2 = \sum_{j\in\mathbb{Z}}|\check{Q}'^-_n(j,k)|^2 \leq \mathcal{M}_n(k)+\mathcal{M}'_n(k)$$

with

$$\mathcal{M}_n(k) := \sum_{\{j\in\mathbb{Z}:\,|j-k|\geq cn\}}\frac{|(W_n\check{Q}^-_n)(j,k)|^2}{c_0^2|j-k|^2}$$

$$\mathcal{M}'_n(k) := \sum_{\{j\in\mathbb{Z}:\,0<|j-k|<cn\}}\frac{|(W_n\check{Q}^-_n)(j,k)|^2}{c_0^2|j-k|^2}.$$

It is clear that

$$\mathcal{M}_n(k)\leq\sum_{j\in\mathbb{Z}}\frac{|(W_n\check{Q}^-_n)(j,k)|^2}{c_0^2c^2n^2} = \frac{||W_n\check{Q}^-_n\tilde{e}_k||^2}{c_0^2c^2n^2}\leq C_1n^{-2}. \tag{5.20}$$

Our next claim is the estimate

$$\sup_{\{j\in\mathbb{Z}:\, 0<|j-k|<cn\}} |(W_n\check{Q}_n^-)(j,k)| \le Cn^{-1}\ln n. \tag{5.21}$$

Indeed, writing

$$(W_n\check{Q}_n^-)(j,k) = \sum_{m\in\mathbb{Z}} W_n(j,m)\check{Q}_n^-(m,k)$$

and using $\check{Q}_n^-(m,k)\neq 0 \Rightarrow 0<|m-k|<cn$ with (4.20), we get

$$|(W_n\check{Q}_n^-)(j,k)| \le \sum_{\{m\in\mathbb{Z}:\, 0<|m-k|<cn\}} |W_n(j,m)|\,\frac{\hat{C}n^{-1/2}}{c_0|m-k|}. \tag{5.22}$$

However, $|j-k|<cn$ and $|m-k|<cn$ imply

$$|j-m|\le |j-k|+|k-m|<2cn \Rightarrow |W_n(j,m)|\le \hat{C}j^{-1/2}\le 2\hat{C}n^{-1/2}, \tag{5.23}$$

due to (5.18) and $j\ge k-|k-j|>k-cn\ge n-\frac{1}{2}n=\frac{1}{2}n$ (where we used $k\in\{n,n+1\}$ and $c\le\frac{1}{2}$). Using (5.21) and (5.22), we can estimate

$$\begin{aligned}\sup_{\{j\in\mathbb{Z}:\, 0<|j-k|<cn\}} |(W_n\check{Q}_n^-)(j,k)| &\le \sum_{\{m\in\mathbb{Z}:\, 0<|m-k|<cn\}} \frac{2\hat{C}^2n^{-1}}{c_0|m-k|}\\ &\le 2\hat{C}^2c_0^{-1}n^{-1}\sum_{1\le i\le cn}\frac{2}{i}\le Cn^{-1}\ln n,\end{aligned}$$

which completes the proof of (5.21).

Using (5.21), we can estimate

$$\mathcal{M}'_n(k)\le \sup_{\{j\in\mathbb{N}:\, 0<|j-k|<cn\}} |(W_n\check{Q}_n^-)(j,k)|^2 \sum_{j\in\mathbb{Z}\setminus\{k\}}\frac{1}{c_0^2|j-k|^2}\le C_2n^{-2}(\ln n)^2.$$

We conclude that $||\check{Q}_n'^-\tilde{e}_k||^2\le \mathcal{M}_n(k)+\mathcal{M}'_n(k)\le C_1n^{-2}+C_2n^{-2}(\ln n)^2$, completing the proof of (5.19).

5.4. **Step 2 of the proof of Lemma 5.1.** In this section, we are going to check that the relation $(\check{Q}_n'^+\tilde{e}_k)(j)=\check{Q}_n'^+(j,k)$ for all $j,k\in\mathbb{Z}$ defines $\check{Q}_n'^+\in\mathcal{B}(\ell^2(\mathbb{Z}))$ satisfying the norm estimate

$$||\check{Q}_n'^+|| = O(n^{-1}\ln n). \tag{5.24}$$

Due to the Schur boundedness test, it suffices to show that there is $C>0$ such that one has

$$\mathcal{Q}_n(k):=\sum_{j\in\mathbb{Z}}|\check{Q}_n'^+(j,k)|\le Cn^{-1}\ln n \text{ for every } k\in\mathbb{Z}, \tag{5.25}$$

$$\mathcal{Q}_n^*(k):=\sum_{j\in\mathbb{Z}}|\check{Q}_n'^+(k,j)|\le Cn^{-1}\ln n \text{ for every } k\in\mathbb{Z}. \tag{5.26}$$

We recall that $\check{Q}_n'^+(j,k)\neq 0\Rightarrow j\neq k$ and we decompose $\mathcal{Q}_n=\mathcal{Q}'_n+\mathcal{Q}''_n$ with

$$\mathcal{Q}'_n(k):=\sum_{\{j\in\mathbb{Z}:\, |j-k|\ge cn\}}|\check{Q}_n'^+(j,k)|, \tag{5.27}$$

$$\mathcal{Q}''_n(k):=\sum_{\{j\in\mathbb{Z}:\, 0<|j-k|<cn\}}|\check{Q}_n'^+(j,k)|. \tag{5.28}$$

Using (4.18) and the Cauchy-Schwarz inequality, we can estimate

$$\mathcal{Q}'_n(k) \leq \sum_{\{j\in\mathbb{Z}:\, |j-k|\geq cn\}} \frac{|(W_n\check{Q}_n^+)(j,k)|}{c_0|j-k|} \leq c_0^{-1}\mathcal{M}_n(k)^{1/2}\mathcal{M}'_n(k)^{1/2} \tag{5.29}$$

with

$$\mathcal{M}_n(k) := \sum_{\{j\in\mathbb{Z}:\, |j-k|\geq cn\}} |j-k|^{-2},$$

$$\mathcal{M}'_n(k) := \sum_{j\in\mathbb{Z}} |(W_n\check{Q}_n^+)(j,k)|^2.$$

However,

$$\mathcal{M}_n(k) \leq 2\sum_{i\geq cn}\frac{1}{i^2} \leq 2\int_{cn-1}^{\infty}\frac{\mathrm{d}s}{s^2} = \frac{2}{cn-1} \leq C_1 n^{-1} \tag{5.30}$$

and

$$\mathcal{M}'_n(k) = ||W_n\check{Q}_n^+\tilde{e}_k||^2 \leq ||W_n||^2\,||\check{Q}_n^+||^2 \leq C_2 n^{-1}, \tag{5.31}$$

where the last estimate is due to (4.23). Combining (5.29) with (5.30)-(5.31), we get

$$\mathcal{Q}'_n(k) \leq C' n^{-1}. \tag{5.32}$$

In order to estimate $\mathcal{Q}''_n(k)$, we assume $0 < |j-k| < cn$ and observe that

$$(W_n\check{Q}_n^+)(j,k) = \sum_{n\leq m\leq n+1} W_n(j,m)\check{Q}_n^+(m,k) \tag{5.33}$$

due to $\check{Q}_n^+ = \widehat{\Pi}_n\check{Q}_n^+$. Using $|j-k| < cn$, $m\in\{n,n+1\}$ and $|\check{Q}_n^+(m,k)| \leq \hat{C}c_0^{-1}n^{-1/2}$ (due to (4.22) and $\check{Q}_n^+(k,k)=0$), we obtain

$$\check{Q}_n^+(m,k)\neq 0 \Rightarrow |k-m| < cn \Rightarrow |j-m| \leq |j-k|+|k-m| < 2cn \leq \hat{c}n$$

$$\Rightarrow |W_n(j,m)| \leq \hat{C}m^{-1/2} \leq \hat{C}n^{-1/2} \Rightarrow |W_n(j,m)\check{Q}_n^+(m,k)| \leq \hat{C}^2c_0^{-1}n^{-1},$$

hence $|j-k| < cn \Rightarrow |(W_n\check{Q}_n^+)(j,k)| \leq 2\hat{C}^2c_0^{-1}n^{-1}$ and

$$\mathcal{Q}''_n(k) \leq \sum_{\{j\in\mathbb{Z}:\, 0<|j-k|<cn\}} \frac{|(W_n\check{Q}_n^+)(j,k)|}{c_0|j-k|}$$

$$\leq 2\hat{C}^2c_0^{-2}n^{-1} \sum_{\{j\in\mathbb{Z}:\, 0<|j-k|<cn\}} \frac{1}{|j-k|} \leq C''n^{-1}\ln n,$$

due to $\displaystyle\sum_{1\leq i\leq cn}\frac{1}{i} = O(\ln n)$. This completes the proof of (5.25).

In order to prove (5.26), we can use a similar decomposition $\mathcal{Q}_n^* = \mathcal{Q}_n'^* + \mathcal{Q}_n''^*$ and estimate

$$\mathcal{Q}_n'^*(k) \leq \sum_{\{j\in\mathbb{Z}:\, |j-k|\geq cn\}} \frac{|(W_n\check{Q}_n^+)(k,j)|}{c_0|j-k|}, \tag{5.34}$$

$$\mathcal{Q}_n''^*(k) := \sum_{\{j\in\mathbb{Z}:\, 0<|j-k|<cn\}} \frac{|(W_n\check{Q}_n^+)(k,j)|}{c_0|j-k|}. \tag{5.35}$$

However, the right hand side of (5.34) can be estimated by $\mathcal{M}_n(k)^{1/2}\mathcal{M}_n'^*(k)^{1/2}$ with $\mathcal{M}_n(k)$ as before and

$$\mathcal{M}_n'^*(k) = \sum_{j\in\mathbb{Z}} |(W_n\check{Q}_n^+)(k,j)|^2 = ||(W_n\check{Q}_n^+)^*\tilde{e}_k||^2 \le ||W_n||^2||\check{Q}_n^+||^2 \le C'n^{-1}.$$

Finally, exchanging j and k in the previous reasoning, we get $|j-k| < cn \Rightarrow |(W_n\check{Q}_n^+)(k,j)| \le 2\hat{C}^2c_0^{-1}n^{-1}$ and we can estimate the right hand side of (5.35) by $C''n^{-1}\ln n$ similarly as before. This completes the proof of (5.26).

5.5. **End of the proof of Lemma 5.1.** By the definition of $\check{Q}_n'$ given in (5.10), we get

$$\mathrm{i}(d_j-d_k)\check{Q}_n'(j,k) = \langle\tilde{e}_j, (-\mathrm{i})(\widetilde{\Pi}_nW_n\check{Q}_n\widehat{\Pi}_n + \widehat{\Pi}_nW_n\check{Q}_n\widetilde{\Pi}_n)\tilde{e}_k\rangle \tag{5.36}$$

Since $(W_n\check{Q}_n)^* = \check{Q}_nW_n$ and $(\check{Q}_n')^*(j,k) = \overline{\check{Q}_n'(k,j)}$, we can write the adjoint matrix in both sides of (5.36) as follows

$$\mathrm{i}(d_j-d_k)(\check{Q}_n')^*(j,k) = \langle\tilde{e}_j, \mathrm{i}(\widetilde{\Pi}_n\check{Q}_nW_n\widehat{\Pi}_n + \widehat{\Pi}_n\check{Q}_nW_n\widetilde{\Pi}_n)\tilde{e}_k\rangle. \tag{5.37}$$

Summing up (5.36) and (5.37), we obtain

$$\mathrm{i}(d_j-d_k)Q_n'(j,k) = -\langle\tilde{e}_j, (\check{R}_n^- + \check{R}_n^+)\tilde{e}_k\rangle = -(\check{R}_n^- + \check{R}_n^+)(j,k) \tag{5.38}$$

by the definition of $\check{R}_n^\pm$ given in (5.14)-(5.15). It is easy to see that one can deduce the assertions of Lemma 5.1(b) and (c) from (5.38), similarly as in Lemma 4.1.

6. Proof of Theorem 3.4

6.1. **Step 1 of the proof of Theorem 3.4.** Let Q_n' as in Section 5. We claim that

$$\mathrm{e}^{-\mathrm{i}Q_n'}\mathrm{e}^{-\mathrm{i}Q_n}J\mathrm{e}^{\mathrm{i}Q_n}\mathrm{e}^{\mathrm{i}Q_n'} = D + (\widehat{V}_n + \widehat{R}_n)\oplus(\widetilde{V}_n + \widetilde{R}_n) + O(n^{-1}\ln n) \tag{6.1}$$

To begin the proof of (6.1), we observe that (3.26)-(3.27) with $N=2$, $t=1$, gives

$$\mathrm{e}^{-\mathrm{i}Q_n'}D\mathrm{e}^{\mathrm{i}Q_n'} = D + [D,\mathrm{i}Q_n'] + O(||\mathrm{ad}^2_{\mathrm{i}Q_n'}(D)||). \tag{6.2}$$

Since Lemma 5.1 ensures $[D,\mathrm{i}Q_n'] = -\check{R}_n^- - \check{R}_n^+$, we get

$$\mathrm{ad}^2_{\mathrm{i}Q_n'}(D) = [-\check{R}_n^- - \check{R}_n^+, \mathrm{i}Q_n'] = O(||Q_n'||)$$

and

$$\mathrm{e}^{-\mathrm{i}Q_n'}D\mathrm{e}^{\mathrm{i}Q_n'} = D - \check{R}_n^- - \check{R}_n^+ + O(||Q_n'||). \tag{6.3}$$

Using (3.26)-(3.27) with $N=1$, $t=1$, we get

$$\mathrm{e}^{-\mathrm{i}Q_n'}(\widehat{V}_n\oplus\widetilde{V}_n + R_n)\mathrm{e}^{\mathrm{i}Q_n'} = \widehat{V}_n\oplus\widetilde{V}_n + R_n + O(||Q_n'||). \tag{6.4}$$

Due to $||Q_n'|| = O(n^{-1}\ln n)$, summing up (6.3) and (6.4), we get

$$\mathrm{e}^{-\mathrm{i}Q_n'}\mathrm{e}^{-\mathrm{i}Q_n}J\mathrm{e}^{\mathrm{i}Q_n}\mathrm{e}^{\mathrm{i}Q_n'} = D + \widehat{V}_n\oplus\widetilde{V}_n + R_n - \check{R}_n^- - \check{R}_n^+ + O(n^{-1}\ln n). \tag{6.5}$$

Since

$$R_n^- = \widetilde{\Pi}_n[W_n,\mathrm{i}Q_n]\widehat{\Pi}_n,$$
$$R_n^+ = \widehat{\Pi}_n[W_n,\mathrm{i}Q_n)]\widetilde{\Pi}_n,$$

we obtain

$$R_n^- - \check{R}_n^- = \widetilde{\Pi}_n[W_n,\mathrm{i}(Q_n-\check{Q}_n)]\widehat{\Pi}_n = O(||Q_n-\check{Q}_n||),$$
$$R_n^+ - \check{R}_n^+ = \widehat{\Pi}_n[W_n,\mathrm{i}(Q_n-\check{Q}_n)]\widetilde{\Pi}_n = O(||Q_n-\check{Q}_n||)$$

and (4.13) ensures $Q_n - \check{Q}_n = O(n^{-1})$, hence

$$R_n^\pm - \check{R}_n^\pm = O(n^{-1}). \tag{6.6}$$

Combining (6.6) and (6.5), we get

$$\mathrm{e}^{-\mathrm{i}Q'_n}\mathrm{e}^{-\mathrm{i}Q_n}J\mathrm{e}^{\mathrm{i}Q_n}\mathrm{e}^{\mathrm{i}Q'_n} = D + \widehat{V}_n \oplus \widetilde{V}_n + R_n - R_n^- - R_n^+ + O(n^{-1}\ln n) \tag{6.7}$$

and (6.1) follows due to $R_n - R_n^- - R_n^+ = \widehat{R}_n \oplus \widetilde{R}_n$.

6.2. **Step 2 of the proof of Theorem 3.4.** We claim that

$$||\widehat{\Pi}_n R_n \widehat{\Pi}_n|| = O(n^{-1}\ln n). \tag{6.8}$$

Since $R_n = [W_n, \mathrm{i}Q_n] = [W_n, \mathrm{i}Q_n^-] + [W_n, \mathrm{i}Q_n^+]$, it is clear that it suffices to prove

$$||\widehat{\Pi}_n W_n Q_n^{\pm} \widehat{\Pi}_n|| = O(n^{-1}\ln n) \tag{6.9}$$

and due to (4.13), it remains to prove the estimate

$$||\widehat{\Pi}_n W_n \check{Q}_n^{\pm} \widehat{\Pi}_n|| = O(n^{-1}\ln n). \tag{6.10}$$

We observe that

$$||\widehat{\Pi}_n W_n \check{Q}_n^{\pm} \widehat{\Pi}_n|| \leq \sum_{n\leq j,k\leq n+1} |(W_n \check{Q}_n^{\pm})(j,k)|$$

with

$$(W_n \check{Q}_n^{\pm})(j,k) = \sum_{\{m\in\mathbb{Z}:\, 0<|m-k|<cn\}} W_n(j,m)\check{Q}_n^{\pm}(m,k).$$

Assume that $j,k \in \{n, n+1\}$. Then

$$|m-k| < cn \Rightarrow |j-m| \leq |j-k| + |k-m| < 1 + cn < \hat{c}n$$

$$\Rightarrow |W_n(j,m)| \leq \hat{C} j^{-1/2} \leq \hat{C} n^{-1/2} \Rightarrow |W_n(j,m)\check{Q}_n^{\pm}(m,k)| \leq \frac{\hat{C}^2 n^{-1}}{c_0|m-k|}$$

and consequently

$$|(W_n \check{Q}_n^{\pm})(j,k)| \leq \sum_{\{m\in\mathbb{Z}:\, 0<|m-k|<cn\}} \frac{\hat{C}^2 n^{-1}}{c_0|m-k|} = O(n^{-1}\ln n), \tag{6.11}$$

where the last estimate is due to $\displaystyle\sum_{1\leq i\leq cn} \frac{1}{i} = O(\ln n)$.

6.3. **End of the proof of Theorem 3.4.** To begin we observe that (4.1) and (3.21) ensure the fact that there is $n_1 \in \mathbb{N}$ such that

$$\lambda_{n-1}(J) < d_n - \tfrac{3\beta}{4} < d_n - \tfrac{\beta}{4} < \lambda_n(J) \leq \lambda_{n+1}(J) < d_n + \tfrac{\beta}{4} < d_n + \tfrac{3\beta}{4} < \lambda_{n+2}(J) \tag{6.12}$$

holds for $n \geq n_1$. Then (6.1) ensures

$$\mathrm{e}^{-\mathrm{i}Q'_n}\mathrm{e}^{-\mathrm{i}Q_n}J\mathrm{e}^{\mathrm{i}Q_n}\mathrm{e}^{\mathrm{i}Q'_n} = D + (\widehat{V}_n + \widehat{R}_n) \oplus (\widetilde{V}_n + \widetilde{R}_n) + O(n^{-1}\ln n). \tag{6.13}$$

Since (6.8) ensures $||\widehat{R}_n||_{\mathcal{B}(\widehat{\mathcal{H}}_n)} = O(n^{-1}\ln n)$, we can write (6.13) in the form

$$\mathrm{e}^{-\mathrm{i}Q'_n}\mathrm{e}^{-\mathrm{i}Q_n}J\mathrm{e}^{\mathrm{i}Q_n}\mathrm{e}^{\mathrm{i}Q'_n} = D + \widehat{V}_n \oplus \widetilde{V}'_n + O(n^{-1}\ln n) \text{ with } \widetilde{V}'_n := \widetilde{V}_n + \widetilde{R}_n. \tag{6.14}$$

Let us introduce

$$J_n := \mathrm{e}^{\mathrm{i}Q_n}\mathrm{e}^{\mathrm{i}Q'_n}(D + \widehat{V}_n \oplus \widetilde{V}'_n)\mathrm{e}^{-\mathrm{i}Q'_n}\mathrm{e}^{-\mathrm{i}Q_n}. \tag{6.15}$$

Then one can find $C > 0$ and $n_2 \geq n_1$ such that

$$||J - J_n|| \leq Cn^{-1}\ln n \tag{6.16}$$

holds for $n \geq n_2$. Denote $J_{n,t} := J + t(J_n - J)$ for $0 \leq t \leq 1$. Then

$$\mathrm{dist}(\mathrm{spec}(J_{n,t}), \mathrm{spec}(J)) \leq Cn^{-1}\ln n \tag{6.17}$$

holds for $n \geq n_2$. Let $n_3 \geq n_2$ be such that $Cn_3^{-1} \ln n_3 < \beta/8$. Then

$$\operatorname{spec}(J_{n,t}) \cap [d_n - \beta/2, d_n + \beta/2] \subset [d_n - 3\beta/8, d_n + 3\beta/8] \tag{6.18}$$

and the spectral projector of $J_{n,t}$ on $[d_n - \beta/2, d_n + \beta/2]$ can be written in the form

$$P_{n,t} := 1_{[d_n-\beta/2, d_n+\beta/2]}(J_{n,t}) = \frac{\mathrm{i}}{2\pi} \oint_{|z-d_n|=\beta/2} (J_{n,t} - z)^{-1} \mathrm{d}z. \tag{6.19}$$

Due to (6.19), $t \to P_{n,t}$ is continuous $[0,1] \to \mathcal{B}(\ell^2(\mathbb{Z}))$ and the trace of $P_{n,t}$ is constant, hence

$$\operatorname{tr} 1_{[d_n-\beta/2, d_n+\beta/2]}(J_n) = \operatorname{tr} 1_{[d_n-\beta/2, d_n+\beta/2]}(J) = 2. \tag{6.20}$$

Due to (6.17) and (6.20), it is clear that for $n \geq n_3$ we can label the non-decreasing sequence of eigenvalues of J_n, counting multiplicities, $\{\lambda_k(J_n)\}_{k\in\mathbb{Z}}$, so that

$$\lambda_{n-1}(J_n) < d_n - \tfrac{\beta}{2} < \lambda_n(J_n) \leq \lambda_{n+1}(J_n) < d_n + \tfrac{\beta}{2} < \lambda_{n+2}(J_n) \tag{6.21}$$

and

$$\max\{|\lambda_n(J_n) - \lambda_n(J)|, |\lambda_{n+1}(J_n) - \lambda_{n+1}(J)|\} \leq Cn^{-1} \ln n. \tag{6.22}$$

Denote $\widehat{D}_n := D|_{\widehat{\mathcal{H}}_n}$ and $\widetilde{D}_n := D|_{\widetilde{\mathcal{H}}_n}$. Then

$$\widehat{D}_n + \widehat{V}_n = \begin{pmatrix} d_n & V(n,n+1) \\ V(n+1,n) & d_n \end{pmatrix}$$

and $\operatorname{spec}(\widehat{D}_n + \widehat{V}_n) = \{\hat{\lambda}_n, \hat{\lambda}_{n+1}\}$ holds with

$$\hat{\lambda}_n := d_n - |V(n,n+1)| \text{ and } \hat{\lambda}_{n+1} := d_n + |V(n,n+1)|. \tag{6.23}$$

Since $V(n,n+1) = O(n^{-1/2})$, there is $n_4 \geq n_3$ such that for $n \geq n_4$ one has

$$d_n - \tfrac{\beta}{2} < \hat{\lambda}_n \leq \hat{\lambda}_{n+1} < d_n + \tfrac{\beta}{2}. \tag{6.24}$$

However,

$$\operatorname{spec}(J_n) = \operatorname{spec}((\widehat{D}_n + \widehat{V}_n) \oplus (\widetilde{D}_n + \widetilde{V}_n')) = \operatorname{spec}(\widehat{D}_n + \widehat{V}_n) \cup \operatorname{spec}(\widetilde{D}_n + \widetilde{V}_n')$$

implies

$$\{\hat{\lambda}_n, \hat{\lambda}_{n+1}\} \subset \operatorname{spec}(J_n). \tag{6.25}$$

Combining (6.25) with (6.21), (6.24), we get $\hat{\lambda}_n = \lambda_n(J_n)$, $\hat{\lambda}_{n+1} = \lambda_{n+1}(J_n)$ and using these equalities in (6.22), we deduce that

$$\max\{|\hat{\lambda}_n - \lambda_n(J)|, |\hat{\lambda}_{n+1} - \lambda_{n+1}(J)|\} \leq Cn^{-1} \ln n \tag{6.26}$$

holds for $n \geq n_4$, completing the proof of Theorem 3.4.

7. Proof of Theorem 3.2

7.1. **Beginning of the proof.** Reasoning similarly as in the proof of Theorem 3.4, we consider the decomposition $\ell^2(\mathbb{Z}) = \widehat{\mathcal{H}}_n \oplus \widetilde{\mathcal{H}}_n$ with $\widehat{\mathcal{H}}_n = \mathbb{C}\tilde{e}_n$ and introduce

$$J_n' := \mathrm{e}^{-\mathrm{i}Q_n} J \mathrm{e}^{\mathrm{i}Q_n}, \tag{7.1}$$

where Q_n are self-adjoint bounded operators defined by the relation $(Q_n\tilde{e}_k)(j) = Q_n(j,k)$ with

$$Q_n(j,k) = \begin{cases} \mathrm{i}\,\dfrac{V(j,n)}{d_j - d_n} \text{ when } j \neq n \text{ and } k = n \\ \mathrm{i}\,\dfrac{V(n,k)}{d_n - d_k} \text{ when } j = n \text{ and } k \neq n \\ \quad 0 \qquad \text{otherwise} \end{cases} \tag{7.2}$$

Similarly as before, we find

$$||Q_n|| = O(n^{-1/2}) \text{ as } n \to \infty, \tag{7.3}$$

$\ell^{2,1}(\mathbb{Z})$ is an invariant subspace of Q_n and of $\mathrm{e}^{\mathrm{i}tQ_n}$. As before, $\widehat{\Pi}_n$ denotes the orthogonal projection on $\widehat{\mathcal{H}}_n$, $\widetilde{\Pi}_n = I - \widehat{\Pi}_n$ denotes the orthogonal projection on $\widetilde{\mathcal{H}}_n$ and

$$[D, \mathrm{i}Q_n]x = \mathrm{i}(DQ_n - Q_nD)x = -V_nx \text{ for } x \in \ell^{2,1}(\mathbb{Z}) \tag{7.4}$$

holds with $V_n = \widetilde{\Pi}_nV\widehat{\Pi}_n + \widehat{\Pi}_nV\widetilde{\Pi}_n$. Moreover, $t \to \mathrm{e}^{\mathrm{i}tQ_n}x$ is of class $\mathrm{C}^\infty(\mathbb{R}; \ell^{2,1}(\mathbb{Z}))$ if $x \in \ell^{2,1}(\mathbb{Z})$ and we obtain (5.1) in the form

$$J_n' = D_n + \widetilde{\Pi}_nV\widetilde{\Pi}_n + R_n + O(n^{-1}) \tag{7.5}$$

with $R_n = [W_n, Q_n]$ and

$$D_n = \mathrm{diag}(d_m + V(n,n)\delta_{n,m})_{m\in\mathbb{Z}}. \tag{7.6}$$

Therefore

$$||R_n|| \leq 2||W_n||\,||Q_n|| \leq C||Q_n|| = O(n^{-1/2}) \text{ as } n \to \infty \tag{7.7}$$

and the estimate (6.8) still holds, ensuring

$$R_n(n,n) = \langle \tilde{e}_n, R_n\tilde{e}_n\rangle = O(n^{-1}\ln n) \text{ as } n \to \infty \tag{7.8}$$

In Section 7.2 we will complete the proof of Theorem 3.2, using the following result

Theorem 7.1. (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*

$$\eta - \frac{\|(L-\eta)x\|^2_{\mathcal{H}}}{\eta - d'} \leq \lambda \leq \eta + \frac{\|(L-\eta)x\|^2_{\mathcal{H}}}{d'' - \eta}. \tag{7.9}$$

Proof. See [31]. □

7.2. **End of the proof.** Let c_0 be as in (3.12) and fix $0 < \delta < \frac{1}{4}c_0$, i.e. one has $d_{n-1} + 2\delta < d_n - 2\delta$ for every $n \in \mathbb{Z}$. Due to (3.21) there is $n_0 \in \mathbb{N}$ such that one has

$$d_m + \delta < \lambda_m(J) < d_m - \delta \text{ for } m \geq n_0 - 1$$

and consequently,

$$\mathrm{spec}(J_n') \cap [d_{n-1} + \delta, d_{n+1} - \delta] = \mathrm{spec}(J) \cap [d_{n-1} + \delta, d_{n+1} - \delta] = \{\lambda_n(J)\} \tag{7.10}$$

holds for $n \geq n_0$. In what follows, we assume $n \geq n_0$ and use Theorem 7.1 with $L = J_n'$, $x = \tilde{e}_n$, $d' = d_{n-1} + \delta$, $d'' = d_{n+1} - \delta$. We introduce

$$\eta_n := \langle \tilde{e}_n, J_n'\tilde{e}_n\rangle \tag{7.11}$$

and observe that (7.5)-(7.6) give

$$\eta_n = d_n + V(n,n) + R_n(n,n) + O(n^{-1}), \tag{7.12}$$

hence

$$\eta_n = d_n + V(n,n) + O(n^{-1}\ln n) \tag{7.13}$$

due to (7.8). Therefore there is n_1 such that

$$d_{n-1} + 2\delta < \eta_n < d_{n+1} - 2\delta \text{ for } n \geq n_1 \tag{7.14}$$

and

$$||(J_n' - \eta_n)\tilde{e}_n|| \leq ||R_n|| + |R_n(n,n)| + C_0 n^{-1} \tag{7.15}$$

implies

$$||(J_n' - \eta_n)\tilde{e}_n|| \leq Cn^{-1/2}. \tag{7.16}$$

and (7.9) with (7.14) ensure

$$|\lambda_n(J) - \eta_n| \leq \delta^{-1}||(J_n' - \eta_n)\tilde{e}_n||^2 \text{ for } n \geq \max\{n_0, n_1\} \tag{7.17}$$

We complete the proof of (3.22), combining (7.17), (7.16) with (7.13).

8. Proof of Theorem 1.5

8.1. **Proof of Theorem 1.5(a).** We first claim that the assumptions $\varepsilon \geq 0$ and $\varepsilon/\beta \notin \mathbb{Z}$ imply

$$\lambda_n(\mathbf{H}) - \lambda_n(\mathbf{H}_0) = O(n^{-1}\ln n) \text{ as } n \to \infty \tag{8.1}$$

Indeed, Proposition 2.10 gives

$$\lambda_n(\mathbf{H}) - \lambda_n(\mathbf{H}_0) = \lambda_{n+l}(\mathbf{J}) - \lambda_{n+l}(\mathbf{J}_0) + O(n^{-1}) \text{ as } n \to \infty \tag{8.2}$$

and Theorem 3.2 with (2.39) give

$$\lambda_{n+l}(\mathbf{J}) - \lambda_{n+l}(\mathbf{J}_0) = \lambda_{n+l}(J) - d_{n+l} = O(n^{-1}\ln n). \tag{8.3}$$

We observe that (8.1) implies (1.16) due to

$$\{\lambda_n(\mathbf{H}_0)\}_{n\in\mathbb{N}} = \{\beta n + \beta_{-1}\}_{n\in\mathbb{N}} \cup \{\beta n + \beta_1\}_{n\in\mathbb{N}}.$$

It remains to consider the case $\varepsilon < 0$. However,

$$\mathbf{H}^{(2)}_{\text{Rabi}}(\Delta, \varepsilon, g) = I_2 \otimes \hat{a}^\dagger\hat{a} + \sigma_x \otimes \Big(g\big(\hat{a}^2 + (\hat{a}^\dagger)^2\big) + \frac{\varepsilon}{2}\Big) + \frac{\Delta}{2}\sigma_z \otimes I_{\ell^2(\mathbb{N})} \tag{8.4}$$

is unitarily similar to

$$\mathbf{H}^{(2)}_{\text{Rabi}}(\Delta, -\varepsilon, -g) = I_2 \otimes \hat{a}^\dagger\hat{a} - \sigma_x \otimes \Big(g\big(\hat{a}^2 + (\hat{a}^\dagger)^2\big) + \frac{\varepsilon}{2}\Big) + \frac{\Delta}{2}\sigma_z \otimes I_{\ell^2(\mathbb{N})} \tag{8.5}$$

due to $\sigma_z^{-1}\sigma_x\sigma_z = -\sigma_x$. Thus the statement when $\varepsilon < 0$ follows from the statement for $-\varepsilon > 0$ and $-g$ instead of g.

8.2. **Beginning of the proof of Theorem 1.5(b) and (c).** Let us assume

$$l = \varepsilon/\beta \in \mathbb{N}. \tag{8.6}$$

The sequence $\{\lambda_n(\mathbf{H})\}_{n\in\mathbb{N}}$ can be expressed as the union of sequences $\{E_m^-\}_{m\in\mathbb{N}}$ and $\{E_m^+\}_{m\in\mathbb{N}}$, defined as follows

$$\begin{cases} E_n^- = \lambda_n(\mathbf{H}) \text{ when } n < l \\ E_{i+l}^- = \lambda_{2i+l}(\mathbf{H}) \text{ for } i \in \mathbb{N} \\ E_i^+ = \lambda_{2i+l+1}(\mathbf{H}) \text{ for } i \in \mathbb{N} \end{cases} \tag{8.7}$$

Then Proposition 2.10 implies

$$E_{i+l}^- = \lambda_{2(i+l)}(\mathbf{J}) + O(i^{-1}), \tag{8.8}$$

$$E_i^+ = \lambda_{2(i+l)+1}(\mathbf{J}) + O(i^{-1}) \tag{8.9}$$

and using Theorem 3.4 in (8.8)-(8.9), we get

$$E_{i+l}^- = d_{2(i+l)} - |V(2(i+l), 2(i+l)+1)| + O(i^{-1}\ln i), \tag{8.10}$$

$$E_i^+ = d_{2(i+l)} + |V(2(i+l), 2(i+l)+1)| + O(i^{-1}\ln i), \tag{8.11}$$

where $V(j,k)$ is given by (3.6). The proof of Theorem 1.5 (b) for $\varepsilon \geq 0$ will be completed in Section 8.4, by proving the estimate

$$|V(2(i+l), 2(i+l)+1)| = O(i^{-1}) \text{ if } l \text{ is odd} \tag{8.12}$$

and the proof of Theorem 1.5 (c) for $\varepsilon \geq 0$ will be completed in Section 8.5, by proving that the estimate

$$|V(2(i+l), 2(i+l)+1)| = |\mathfrak{r}_i| + O(i^{-1}) \text{ if } l \text{ is even} \tag{8.13}$$

holds with $\mathfrak{r}_i$ given by (1.21). If $\varepsilon < 0$ then we deduce the result from the statement with $-\varepsilon$ and $-g$ instead of g similarly as at the end of Section 8.1.

8.3. **Expression of $V(2j, 2j+1)$ by means of oscillatory integrals.** Due to (3.8)-(3.11),

$$V(2j, 2j+1) = \frac{\Delta}{2}\langle v_{-1,j}, v_{1,j-l}\rangle = \frac{\Delta}{2}\langle f_{-1,j}, f_{1,j-l}\rangle_{\mathrm{L}^2(\mathbb{T})}, \tag{8.14}$$

where we have denoted

$$f_{\nu,j} := \mathcal{F}_{\mathbb{T}}^{-1} v_{\nu,j}. \tag{8.15}$$

However, due to Corollary 2.5, $f_{\nu,j} = U_\nu f_{q_\nu,j}$, where U_ν is defined by (2.21) and $f_{q_\nu,j}$ by (2.25). The quantity (8.15) has the form

$$f_{\nu,j} = \mathrm{e}^{\mathrm{i}j\Phi_\nu}\mathrm{e}^{\mathrm{i}\phi_\nu}\sqrt{\Phi_\nu'}, \tag{8.16}$$

where Φ_ν is given by (2.17) and

$$\phi_\nu(\theta) := \langle q_\nu\rangle\Phi_\nu(\theta) - \tilde{q}_\nu(\Phi_\nu(\theta)) \tag{8.17}$$

with $\tilde{q}_\nu$ given by (2.22)-(2.23) and $\langle q_\nu\rangle$ given by (2.30). Using (8.16) we can express

$$\langle f_{-1,j}, f_{1,j-l}\rangle_{\mathrm{L}^2(\mathbb{T})} = \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}j(\Phi_1-\Phi_{-1})(\theta)} h(\theta)\frac{\mathrm{d}\theta}{2\pi} \tag{8.18}$$

with

$$h := \mathrm{e}^{-\mathrm{i}l\Phi_1}\mathrm{e}^{\mathrm{i}(\phi_1-\phi_{-1})}\big(\Phi_1'\Phi_{-1}'\big)^{1/2}. \tag{8.19}$$

We claim that the phase function

$$\Psi := \Phi_1 - \Phi_{-1} \tag{8.20}$$

has four non degenerated critical points:

$$\{\theta \in (-\pi, \pi] : \Psi'(\theta) = 0\} = \{\pi/4, -\pi/4, 3\pi/4, -3\pi/4\}. \tag{8.21}$$

Indeed, the direct computation gives

$$\Psi'(\theta) = \frac{\beta}{1+2g\cos(2\theta)} - \frac{\beta}{1-2g\cos(2\theta)} = 0 \;\Leftrightarrow\; \cos(2\theta) = 0 \tag{8.22}$$

and

$$\Psi''(\theta) = \left(\frac{4g\beta}{(1+2g\cos(2\theta))^2} + \frac{4g\beta}{(1-2g\cos(2\theta))^2}\right)\sin(2\theta), \tag{8.23}$$

hence

$$\begin{cases} \Psi''(\pi/4) = \Psi''(-3\pi/4) = 8g\beta \\ \Psi''(-\pi/4) = \Psi''(3\pi/4) = -8g\beta \end{cases} \tag{8.24}$$

The stationary phase method gives

$$\langle f_{-1,j}, f_{1,j-l} \rangle_{\mathrm{L}^2(\mathbb{T})} = G_1(j) + G_{-1}(j) + O(j^{-1}) \text{ as } j \to \infty \tag{8.25}$$

with

$$G_{\pm 1}(j) = \sum_{\theta \in \{\pi/4, -3\pi/4\}} \frac{1}{4\sqrt{\pi j |g| \beta}} h(\pm\theta) \mathrm{e}^{\mathrm{i}j\Psi(\pm\theta)} \mathrm{e}^{\pm \mathrm{i}\,\mathrm{sgn}(g)\,\pi/4} \tag{8.26}$$

where $\mathrm{sgn}(g) = g/|g|$. Moreover,

$$G_{-1}(j) = \overline{G_1(j)} \tag{8.27}$$

follows from that fact the functions Φ_ν, Ψ, q_ν and ψ_ν are odd.

8.4. **End of the proof of Theorem 1.5(b).** Due to (8.14) and (8.25)-(8.27), it suffices to prove that $G_1(j) = 0$ when l is odd. In what follows, we use the notation

$$\alpha_g := \arctan\left(\sqrt{\frac{1-2g}{1+2g}}\right) \tag{8.28}$$

and we remark that

$$\alpha_{-g} := \arctan\left(\sqrt{\frac{1+2g}{1-2g}}\right) = \frac{\pi}{2} - \alpha_g. \tag{8.29}$$

Due to (2.18) and (8.29), we can express

$$\Phi_1(\pi/4) = \alpha_g, \tag{8.30}$$

$$\Phi_{-1}(\pi/4) = \alpha_{-g} = \pi/2 - \alpha_g. \tag{8.31}$$

Due to (2.20) and (8.30)-(8.31), we find

$$\Phi_1(3\pi/4) = \pi - \Phi_1(\pi/4) = \pi - \alpha_g, \tag{8.32}$$

$$\Phi_{-1}(3\pi/4) = \pi - \Phi_{-1}(\pi/4) = \pi/2 + \alpha_g. \tag{8.33}$$

Using (8.30)-(8.33) and $\Psi = \Phi_1 - \Phi_{-1}$, we get

$$\Psi(\pi/4) = \alpha_g - (\pi/2 - \alpha_g) = 2\alpha_g - \pi/2, \tag{8.34}$$

$$\Psi(3\pi/4) = \pi - \alpha_g - (\pi/2 + \alpha_g) = \pi/2 - 2\alpha_g. \tag{8.35}$$

Since Ψ is odd, we find

$$\Psi(-3\pi/4) = \Psi(\pi/4), \tag{8.36}$$

$$\Psi(-\pi/4) = \Psi(3\pi/4). \tag{8.37}$$

Using $\Psi(-3\pi/4) = \Psi(\pi/4) = 2\alpha_g - \pi/2$, we obtain

$$G_1(j) = \frac{h(\pi/4) + h(-3\pi/4)}{4\sqrt{\pi j |g| \beta}} \mathrm{e}^{\mathrm{i}j(2\alpha_g - \pi/2)} \mathrm{e}^{\mathrm{i}\,\mathrm{sgn}(g)\,\frac{\pi}{4}} \tag{8.38}$$

and the assertion of Theorem 3.4(b) will be proved if we show that $h(\pi/4)+h(-3\pi/4) = 0$ when l is odd.

In order to evaluate h, we first remark that (2.24) and (2.30) allow us to express

$$\phi_\nu(\theta) = \langle q_\nu \rangle \Phi_\nu(\theta) - \tilde{q}_\nu(\Phi_\nu(\theta)) =$$

$$= \left(\frac{1}{2} + \frac{\nu\varepsilon - 1}{2\beta}\right) \Phi_\nu(\theta) - \frac{\theta}{2} - \frac{\nu\epsilon - 1}{2\beta} - \Phi_\nu(\theta) = \frac{\Phi_\nu(\theta) - \theta}{2}$$

and the equality $\phi_\nu(\theta) = \frac{1}{2}(\Phi_\nu(\theta) - \theta)$ implies

$$\phi_1 - \phi_{-1} = \frac{1}{2}(\Phi_1 - \Phi_{-1}) = \frac{1}{2}\Psi. \tag{8.39}$$

Due to (8.39) we can rewrite (8.19) in the form

$$h = \mathrm{e}^{-\mathrm{i}l\Phi_1}\mathrm{e}^{\mathrm{i}\Psi/2}\big(\Phi_1'\Phi_{-1}'\big)^{1/2}. \tag{8.40}$$

Using

$$\big(\Phi_1'\Phi_{-1}'(\pm\pi/4)\big)^{1/2} = \big(\Phi_1'\Phi_{-1}'(\pm 3\pi/4)\big)^{1/2} = \beta \tag{8.41}$$

and $\Psi(\pi/4) = \Psi(-3\pi/4)$ in (8.40), we find

$$h(-3\pi/4) = \mathrm{e}^{\mathrm{i}l(\Phi_1(\pi/4)-\Phi_1(-3\pi/4))}h(\pi/4) = (-1)^l h(\pi/4), \tag{8.42}$$

where the last equality follows from

$$\Phi_1(\pi/4) - \Phi_1(-3\pi/4) = \Phi_1(\pi/4) + \Phi_1(3\pi/4) = \pi.$$

If l is odd, then (8.42) implies $h(3\pi/4) = -h(\pi/4)$ and completes the proof of $G_1(j) = 0$.

8.5. **End of the proof of Theorem 1.5(c).** Assume that l is even. Using (8.40)-(8.41), we get

$$h(-3\pi/4) = h(\pi/4) = \mathrm{e}^{-\mathrm{i}l\alpha_g}\mathrm{e}^{\mathrm{i}(2\alpha_g-\pi/2)/2}\beta, \tag{8.43}$$

and

$$G_1(j) = \frac{2\beta}{4\sqrt{\pi j|g|\beta}}\mathrm{e}^{-\mathrm{i}l\alpha_g+\mathrm{i}(j+1/2)(2\alpha_g-\pi/2)}\mathrm{e}^{\mathrm{i}\,\mathrm{sgn}(g)\,\pi/4}. \tag{8.44}$$

Due to (8.27),

$$G_1(j) + G_{-1}(j) = \sqrt{\frac{\beta}{\pi j|g|}}\cos\Big((2j+1-l)\alpha_g - j\frac{\pi}{2} + (\mathrm{sgn}(g)-1)\frac{\pi}{4}\Big)$$

If $g > 0$ then we obtain

$$V(2j+1,2j) = \frac{\Delta}{2}\sqrt{\frac{\beta}{\pi j|g|}}\cos\Big((2(j-l)+1+l)\alpha_g - j\frac{\pi}{2}\Big) + O(j^{-1}) \tag{8.45}$$

and $l \in 2\mathbb{N} \Rightarrow l\pi/2 \in \pi\mathbb{Z}$, hence (8.45) gives

$$|V(2j+1,2j)| = |\mathfrak{r}_{j-l}| + O(j^{-1}) \tag{8.46}$$

and (8.13) holds if $g > 0$. If $g < 0$, then $\alpha_g = \pi/2 - \alpha_{|g|}$ and

$$\Big|\cos\Big((2j+1-l)\alpha_g - j\frac{\pi}{2} - \frac{\pi}{2}\Big)\Big| = \Big|\cos\Big((2j+1-l)\Big(\frac{\pi}{2} - \alpha_{|g|}\Big) - j\frac{\pi}{2} - \frac{\pi}{2}\Big)\Big|.$$

Since $l \in 2\mathbb{N} \Rightarrow l\pi/2 \in \pi\mathbb{Z}$, the above quantity can be also written in the form

$$\Big|\cos\Big(-(2j+1-l)\alpha_{|g|} + j\frac{\pi}{2}\Big)\Big| = \Big|\cos\Big((2j+1-l)\alpha_{|g|} - j\frac{\pi}{2}\Big)\Big|.$$

Thus (8.45) implies (8.46) in the case $g < 0$ as well.

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