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THREE-TERM ASYMPTOTIC FORMULA FOR LARGE EIGENVALUES OF THE QUANTUM RABI MODEL WITH A RESONANT BIAS

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

Abstract. We investigate the asymptotic distribution of large eigenvalues of the asymmetric quantum Rabi model with an integer static bias. For this model, we consider a variant of the generalized rotating-wave approximation, corresponding to perturbations of double eigenvalues. Using this idea, we obtain a three-term asymptotic formula for the m-th eigenvalue with the remainder estimate $O(m^{-1/2}\ln m)$ when m tends to infinity.

1. General presentation of the paper

1.1. **Introduction.** In Section 1.1 we briefly present the subject of the paper. In Section 1.2 we give an overview of related works. The main result is stated in Section 1.3, and Section 1.4 gives an outline of its proof.

Our purpose is to investigate the behaviour of large eigenvalues of the Rabi model (QRM). The QRM describes the simplest interaction between a two-level atom and a quantized single-mode radiation. It has been widely used to study various problems of quantum optics, condensed matter physics, and quantum information; we refer to [22], [23], [15], [7], for the history of the model, and to the survey [36] for a list of theoretical and experimental results.

The simplest QRM (see Definition 1.1(b)) is given by the Hamiltonian $\mathbf{H}_{\mathrm{Rabi}}^{\Delta,g}$, depending on the coupling constant $g \in \mathbb{R}$ and the energy separation of the two-level system $\Delta \in \mathbb{R}$. Its spectrum is discrete, and the fundamental question is how to find a good approximation of the corresponding eigenvalues. One of the most popular approximations, bears the name of the *generalized rotating-wave approximation* (GRWA) after E. K. Irish [13]. The same idea was considered before by I. D. Feranchuk, L. I. Komarov, A. P. Ulyanenkov [10], under the name of the *zeroth order approximation of the operator method* (see also [11]). It appears that the GRWA is closely related to the three-term asymptotic formula obtained in [4]. A high quality of this approximation for large eigenvalues, was confirmed by the results of numerical computations of D. Braak, L. T. H. Nguyen, C. Reyes-Bustos, M. Wakayama [8].

The authors of [8] give also conjectures on the behaviour of large eigenvalues for the generalization of the QRM, called *the asymmetric quantum Rabi model* (AQRM), see Definition 1.1(c). Its Hamiltonian, $\mathbf{H}_{\mathrm{Rabi}}^{\Delta,g,l}$ contains an additional parameter l, called the static bias of the model. The AQRM is a particularly important model in the quantum electrodynamics of superconducting circuits, where the additional term appears due to the tunneling between two current states (see [12], [36], [24], [16]). See also recent experimental realizations of this model in [38], [39].

In this paper, we investigate the AQRM under the assumption that the static basis $l \in \mathbb{Z}$. In what follows, the integer static basis is called resonant, and we propose a variant of GRWA for perturbations of double eigenvalues. Moreover, we prove that, for $l \in \mathbb{Z}$, the large eigenvalues of AQRM satisfy a three-term asymptotic formula, which is similar to the formula for the QRM. We refer to [19], [31], [28], for other results in the asymptotic analysis of the AQRM.

We observe that the AQRM with an integer bias, is the subject of numerous research works. One of the most intensely studied aspects of this model, is the question of its integrability (see [6], [17], [27], [32]), related to the existence of hidden symmetries and double eigenvalues: the AQRM is expected to be integrable when the static basis l is integer (see [1], [18], [20], [21], [25], [26], [35]).

1.2. **Overview of results related to approximations of eigenvalues of QRM.** We refer to [30] and [10], for the earliest investigations of large eigenvalues of QRM. It is well known (see [33], [4]) that $\mathbf{H}^{\Delta,g}_{\mathrm{Rabi}}$ can be expressed as a direct sum $J_- \oplus J_+$ of two Jacobi operators (i.e. operators defined by infinite tridiagonal matrices), hence the spectrum of the QRM is composed of two eigenvalue sequences $\{E^+_m\}_{m\in\mathbb{N}}$, $\{E^-_m\}_{m\in\mathbb{N}}$ (corresponding to the spectrum of J_+ and J_- respectively). A mathematical study of large eigenvalues of Jacobi matrices, was initiated by J. Janas and S. Naboko in the paper [14], which contains fundamental ideas of the method of approximate diagonalizations.

The question of the behaviour of large eigenvalues of Jacobi matrices $J_\pm$ which correspond to the QRM, was first posed by E. A. Tur [33]-[34] and it was mentioned by A. Boutet de Monvel, S. Naboko and L. O. Silva in [2]. Due to the difficulty of the problem, the paper [2] gives the asymptotic estimates for a simpler class of operators ("modified Jaynes-Cummings models"). However, using the ideas of [14], E. A. Ianovich [37] proved the two-term asymptotic formula

$$E^\pm_m = m - g^2 + O(m^{-1/16}) \text{ as } m \to \infty,$$

(see also [34]). However, the GRWA claims $E^\pm_m \approx E^\pm_{m,\mathrm{GRWA}}$, and according to the formula (25) in the paper I. D. Feranchuk, L. I. Komarov, A. P. Ulyanenkov [10]),

$$E^\pm_{m,\mathrm{GRWA}} \approx m - g^2 \pm \mathfrak{r}_m \text{ as } m \to \infty$$

holds with

$$\mathfrak{r}_m := (-1)^m \frac{\Delta}{2} \frac{\cos\big(4g\sqrt{m} - \frac{\pi}{4}\big)}{\sqrt{2\pi g\sqrt{m}}}. \tag{1.1}$$

It appears that the three-term asymptotic formula

$$E^\pm_m = m - g^2 \pm \mathfrak{r}_m + O(m^{-1/2+\varepsilon}) \text{ as } m \to \infty, \tag{1.2}$$

holds with $\varepsilon > 0$ and $\mathfrak{r}_m$ given by (1.1) (see A. Boutet de Monvel, L. Zielinski [3]-[4]). The estimate (1.2) was used by Z. Rudnick [29] to consider a Braak's conjecture (see [6]), and to check that the parameters of QRM are determined by its spectrum (see [5]).

If $l \neq 0$, then $\mathbf{H}^{\Delta,g,l}_{\mathrm{Rabi}}$ cannot be written as a direct sum of Jacobi matrices, but a two-term asymptotic formula for large eigenvalues was obtained for this model in the paper M. Charif, A. Fino, L. Zielinski [9] (see Section 2).

1.3. **Statement of the result.** In what follows, we denote by $\mathbb{Z}$ the set of integers, $\mathbb{N} := \{j \in \mathbb{Z} : j \geq 0\}$ and $\ell^2(\mathbb{N})$ is the complex Hilbert space of square-summable sequences $x : \mathbb{N} \to \mathbb{C}$ equipped with the scalar product

$$\langle x, y\rangle = \sum_{m=0}^{\infty} \overline{x(m)} y(m)$$

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

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

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, $m \in \mathbb{N}$). 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

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

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

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

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

The quantum Rabi model is described in

Definition 1.1. (a) The Hamiltonian of the single-mode radiation, is the linear map $H_{\text{rad}} : \ell^{2,1}(\mathbb{N}) \to \ell^2(\mathbb{N})$ defined by the formula

$$H_{\text{rad}} e_n = \hat{a}^\dagger \hat{a} \, e_n = n e_n \text{ for } n \in \mathbb{N}. \tag{1.3}$$

(b) The *quantum Rabi Hamiltonian* is defined as the linear map $\mathbf{H}^{\Delta,g}_{\text{Rabi}} : \mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \to \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$ given by

$$\mathbf{H}^{\Delta,g}_{\text{Rabi}} = I_2 \otimes H_{\text{rad}} + \frac{\Delta}{2} \sigma_z \otimes I_{\ell^2(\mathbb{N})} + g\sigma_x \otimes \big(\hat{a} + \hat{a}^\dagger\big), \tag{1.4}$$

where $g \in \mathbb{R}$ and $\Delta \in \mathbb{R}$ are fixed parameters.

(c) The *asymmetric quantum Rabi Hamiltonian* is defined as the linear map $\mathbf{H}^{\Delta,g,l}_{\text{Rabi}} : \mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \to \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$ given by

$$\mathbf{H}^{\Delta,g,l}_{\text{Rabi}} = I_2 \otimes H_{\text{rad}} + \left(\frac{l}{2} \, \sigma_x + \frac{\Delta}{2} \, \sigma_z\right) \otimes I_{\ell^2(\mathbb{N})} + g\sigma_x \otimes \big(\hat{a} + \hat{a}^\dagger\big), \tag{1.5}$$

where $g \in \mathbb{R}$, $\Delta \in \mathbb{R}$ and $l \in \mathbb{R} \setminus \{0\}$ are fixed parameters.

Our main result is

Theorem 1.2. *Assume that $g \neq 0$ and $l \in \mathbb{Z}$. 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*

$$\mathbf{H}^{\Delta,g,l}_{\text{Rabi}} v^\pm_m = E^\pm_m v^\pm_m, \quad m = 0, 1, 2, \ldots$$

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

$$E^-_{i+|l|} = i + \tfrac{|l|}{2} - g^2 - |\mathfrak{r}_i| + O(i^{-1/2} \ln i) \ \textit{as } i \to \infty, \tag{1.6}$$

$$E^+_i = i + \tfrac{|l|}{2} - g^2 + |\mathfrak{r}_i| + O(i^{-1/2} \ln i) \ \textit{as } i \to \infty, \tag{1.7}$$

where

$$\begin{cases} \mathfrak{r}_i := \dfrac{\Delta}{2}\dfrac{\cos\big(4|g|\sqrt{i}-\frac{\pi}{4}\big)}{\sqrt{2\pi|g|\sqrt{i}}} & \textit{if } l \textit{ is even} \\[2ex] \mathfrak{r}_i := \dfrac{\Delta}{2}\dfrac{\sin\big(4|g|\sqrt{i}-\frac{\pi}{4}\big)}{\sqrt{2\pi|g|\sqrt{i}}} & \textit{if } l \textit{ is odd} \end{cases} \tag{1.8}$$

1.4. **Outline of the proof of Theorem 1.2.** In Section 2 we recall some results from [9]. We first introduce the operator $\mathbf{H}$, which is similar to $\mathbf{H}_{\text{Rabi}}^{\Delta,g,l}$ and the operator $\mathbf{H}_0$, which is similar to $\mathbf{H}_{\text{Rabi}}^{0,g,l}$ (i.e. with $\Delta = 0$). It appears that the operator $\mathbf{H}_0$ can be written as the direct sum $H_{-1} \oplus H_1$ and Proposition 2.1 gives information on eigenvalues and eigenvectors of $H_{\pm 1}$. Proposition 2.2 gives a special property of eigenvectors of $\mathbf{H}_0$ and Proposition 2.3 gives the two-term asymptotic formula for large eigenvalues of $\mathbf{H}$.

Throughout the paper, $\{d_n\}_{n\in\mathbb{N}}$ denotes the non-decreasing sequence of eigenvalues of $\mathbf{H}_0$, counting the multiplicities. The sequence $\{d_n\}_{n\in\mathbb{N}}$ can be easily expressed by means of the eigenvalues of $H_{\pm 1}$, which are explicitly known. It appears that the assumption $l \in \mathbb{Z}$ implies the fact that the eigenvalues d_n are simple if $n < |l|$ and the eigenvalues $d_{|l|+2i} = d_{|l|+2i+1}$ are double for any $i \in \mathbb{N}$.

In Section 3 we consider $\mathbf{H}$ as a perturbation of $\mathbf{H}_0$. More precisely, we consider the matrix of $\mathbf{H}$ in the basis $\{\mathbf{v}_n^0\}_{n\in\mathbb{N}}$ formed by eigenvectors of $\mathbf{H}_0$ and in Proposition 3.1, we formulate a variant of the generalized rotating-wave approximation. In Section 3.3 we show that Theorem 1.2 can be deduced by combining the assertion of Proposition 3.1 with the results of Section 2, i.e. we prove the implication

$$\text{Propositions 2.1, 2.2, 2.3, 3.1} \implies \text{Theorem 1.2}$$

In Sections 4 - 7 we give the proof of Proposition 3.1, according to the following scheme

$$\begin{cases} \text{Lemma 4.1} \implies \text{Lemma 5.1}, \\ \text{Lemmas 5.1, 6.1} \implies \text{Proposition 3.1} \end{cases}$$

Our reasoning follows an idea similar to the successive diagonalization procedure of Janas, Naboko [14]. A suitable approximation of the n-th eigenvalue of H, is obtained in two steps. In Section 4 we introduce bounded self-adjoint operators Q_n and in Section 5 we describe the structure of $H_n' = \mathrm{e}^{-\mathrm{i}Q_n} H \mathrm{e}^{\mathrm{i}Q_n}$. In Section 6 we introduce bounded self-adjoint operators Q_n' and in Section 7 we complete the proof of Proposition 3.1, using a special structure of $H_n'' = \mathrm{e}^{-\mathrm{i}Q_n'} H_n' \mathrm{e}^{\mathrm{i}Q_n'}$.

2. Earlier results

2.1. **The initial reformulation.** Our purpose is to investigate the operator

$$\mathbf{H}_{\text{Rabi}}^{\Delta,g,l} = I_2 \otimes \hat{a}^\dagger \hat{a} + \sigma_x \otimes \big(g\big(\hat{a}+\hat{a}^\dagger\big) + \tfrac{l}{2}\big) + \tfrac{\Delta}{2}\sigma_z \otimes I_{\ell^2(\mathbb{N})}. \tag{2.1}$$

We first claim that it suffices to prove Theorem 1.2 under the assumption $l \in \mathbb{N}$. Indeed, the operator $\mathbf{H}_{\text{Rabi}}^{\Delta,g,l}$ is unitarily similar to

$$\mathbf{H}_{\text{Rabi}}^{\Delta,-g,-l} = I_2 \otimes \hat{a}^\dagger \hat{a} - \sigma_x \otimes \big(g\big(\hat{a}+\hat{a}^\dagger\big) + \tfrac{l}{2}\big) + \tfrac{\Delta}{2}\sigma_z \otimes I_{\ell^2(\mathbb{N})} \tag{2.2}$$

due to $\sigma_z^{-1}\sigma_x\sigma_z = -\sigma_x$ and the assertion of Theorem 1.2 in the case $l \in \mathbb{Z} \setminus \mathbb{N}$ follows by applying Theorem 1.2 to $\mathbf{H}_{\text{Rabi}}^{\Delta,-g,|l|}$ instead of $\mathbf{H}_{\text{Rabi}}^{\Delta,g,l}$.

In what follows, we assume $l \in \mathbb{N}$ and, similarly as in Section 2.1 of [9], instead of the operator $\mathbf{H}_{\mathrm{Rabi}}^{\Delta,g,l}$, we are going to study the operator

$$\mathbf{H} := I_2 \otimes \hat{a}^\dagger \hat{a} - \sigma_z \otimes \big(g\big(\hat{a} + \hat{a}^\dagger\big) + \tfrac{l}{2}\big) + \tfrac{\Delta}{2}\sigma_x \otimes I_{\ell^2(\mathbb{N})}, \tag{2.3}$$

which is unitarily similar to $\mathbf{H}_{\mathrm{Rabi}}^{\Delta,g,l}$ 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 $U_{\pi/4} = \frac{1}{\sqrt{2}}\left(\begin{smallmatrix} 1 & -1 \\ 1 & 1 \end{smallmatrix}\right)$. 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 consider $\mathbf{H}$ 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

$$\mathbf{H} = \begin{pmatrix} H_{-1} & \frac{\Delta}{2} I_{\ell^2(\mathbb{N})} \\ \frac{\Delta}{2} I_{\ell^2(\mathbb{N})} & H_1 \end{pmatrix} \tag{2.4}$$

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

$$H_{\pm 1} := \hat{a}^\dagger \hat{a} \pm g\big(\hat{a} + \hat{a}^\dagger\big) \pm \tfrac{l}{2}. \tag{2.5}$$

We consider the decomposition

$$\mathbf{H} := \mathbf{H}_0 + \mathbf{V} \tag{2.6}$$

with

$$\mathbf{H}_0 := \begin{pmatrix} H_{-1} & 0_{\ell^2(\mathbb{N})} \\ 0_{\ell^2(\mathbb{N})} & H_1 \end{pmatrix} = H_{-1} \oplus H_1 \tag{2.7}$$

and

$$\mathbf{V} = \begin{pmatrix} 0_{\ell^2(\mathbb{N})} & \frac{\Delta}{2} I_{\ell^2(\mathbb{N})} \\ \frac{\Delta}{2} I_{\ell^2(\mathbb{N})} & 0_{\ell^2(\mathbb{N})} \end{pmatrix} \tag{2.8}$$

2.2. **Eigenvalues and eigenvectors of $H_{\pm 1}$.** As before, $\{e_n\}_{n\in\mathbb{N}}$ is the canonical basis of $\ell^2(\mathbb{N})$ and $H_{\pm 1}$ are given by (2.5). One has

Proposition 2.1. *Let $\{v_{\pm 1,n}\}_{n\in\mathbb{N}}$ denote the orthonormal basis given by*

$$v_{\pm 1,n} := \mathrm{e}^{\pm g(\hat{a} - \hat{a}^\dagger)} e_n. \tag{2.9}$$

Then
(a) for every $n \in \mathbb{N}$ one has

$$H_{\pm 1} v_{\pm 1,n} = \big(n - g^2 \pm \tfrac{l}{2}\big) v_{\pm 1,n} \tag{2.10}$$

(b) the following large n estimate

$$||v_{\pm 1,n} - u_{\pm 1,n}|| = O(n^{-1/2}) \tag{2.11}$$

holds with $u_{\pm 1,n} \in \ell^2(\mathbb{N})$ given by the formula

$$u_{\pm 1,n}(j) := \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}(n-j)\theta \mp 2\mathrm{i}gn^{1/2}\sin\theta + \mathrm{i}g^2 \sin\theta\cos\theta} \, \frac{\mathrm{d}\theta}{2\pi}. \tag{2.12}$$

Proof. (a) See Lemma 2.3 in [9]. (b) See Proposition 2.6 in [9]. □

2.3. **Eigenvalues and eigenvectors of $\mathbf{H}_0$.** In what follows, $\{v_{\pm 1,n}\}_{n\in\mathbb{N}}$ denotes the basis introduced in (2.9) and we assume $l \in \mathbb{N}$. The basis of eigenvectors of $\mathbf{H}_0 = H_{-1} \oplus H_1$, has the form $\{(v_{-1,n}, 0) : n \in \mathbb{N}\} \cup \{(0, v_{1,n}) : n \in \mathbb{N}\}$ and we can label it as follows:

$$\mathbf{v}_n^0 = (v_{-1,n}, 0) \text{ for } n = 0, \dots, l-1, \tag{2.13}$$

$$\mathbf{v}_{l+2i}^0 = (v_{-1,l+i}, 0) \text{ for } i \in \mathbb{N}, \tag{2.14}$$

$$\mathbf{v}_{l+2i+1}^0 = (0, v_{1,i}) \text{ for } i \in \mathbb{N}. \tag{2.15}$$

Then we obtain

$$\mathbf{H}_0 \mathbf{v}_n^0 = d_n \mathbf{v}_n^0 \text{ for } n \in \mathbb{N}, \tag{2.16}$$

where $\{d_n\}_{n\in\mathbb{N}}$ is the eigenvalue sequence given by

$$d_n = n - \tfrac{l}{2} - g^2 \text{ for } n = 0, \dots, l-1, \tag{2.17}$$

$$d_{l+2i} = d_{l+2i+1} = \tfrac{l}{2} + i - g^2 \text{ for } i \in \mathbb{N} \tag{2.18}$$

and it is easy to check that $d_j \le d_{j+1}$ holds for every $j \in \mathbb{N}$.

We introduce the matrix $(V(j,k))_{j,k\in\mathbb{N}}$ whose entries are

$$V(j,k) := \langle \mathbf{v}_j^0, \mathbf{V}\mathbf{v}_k^0 \rangle_{\ell^2(\mathbb{N})\times\ell^2(\mathbb{N})}, \tag{2.19}$$

where $\mathbf{V}$ is given by (2.8) and $\{\mathbf{v}_n^0\}_{n\in\mathbb{N}}$ is given by (2.13)-(2.15).

By the definition of $\mathbf{V}$, if $i, j \in \mathbb{N}$ then

$$V(l+2i, l+2j) = \tfrac{\Delta}{2} \langle (v_{-1,l+i}, 0), (0, v_{-1,l+j}) \rangle_{\ell^2(\mathbb{N})\times\ell^2(\mathbb{N})} = 0 \tag{2.20}$$

$$V(l+2i+1, l+2j+1) = \tfrac{\Delta}{2} \langle (0, v_{1,i}), (v_{1,j}, 0) \rangle_{\ell^2(\mathbb{N})\times\ell^2(\mathbb{N})} = 0 \tag{2.21}$$

$$V(l+2i, l+2j+1) = \tfrac{\Delta}{2} \langle (v_{-1,l+i}, 0), (v_{1,j}, 0) \rangle_{\ell^2(\mathbb{N})\times\ell^2(\mathbb{N})} = \tfrac{\Delta}{2} \langle v_{-1,l+i}, v_{1,j} \rangle, \tag{2.22}$$

$$V(l+2i+1, l+2j) = \overline{V(l+2j, l+2i+1)}. \tag{2.23}$$

Our analysis will use the following

Proposition 2.2. *Let the matrix $(V(j,k))_{j,k\in\mathbb{N}}$ be given by* (2.19)*. Then*

$$V(j,j) = 0 \textit{ for every } j \in \mathbb{N} \tag{2.24}$$

and there exist constants $\hat{C}$, $\hat{c} > 0$, such that one has

$$|j-k| < \hat{c}k^{1/2} \Rightarrow |V(j,k)| \le \hat{C}k^{-1/4} \textit{ for } j,\, k \in \mathbb{N} \tag{2.25}$$

Proof. The estimate (2.25) is proved in Corollary 5.2 of [9]. □

2.4. **Two-term asymptotic formula.** One has the following

Proposition 2.3. *Let $\{d_n\}_{n\in\mathbb{N}}$ be the eigenvalue sequence of $\mathbf{H}_0$ given by* (2.17)-(2.18) *and let $\{\lambda_n(\mathbf{H})\}_{n\in\mathbb{N}}$ denote the non-decreasing eigenvalue sequence of $\mathbf{H}$, counting the multiplicities. Then one has the following*

$$\lambda_n(\mathbf{H}) = d_n + O(n^{-1/4}) \textit{ as } n \to \infty \tag{2.26}$$

Proof. See the estimate (2.17) in [9]. □

3. The generalized rotating-wave approximation

3.1. **Notations.** 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 $\mathcal{B}(\ell^2(\mathbb{N}))$. If $T \in \mathcal{B}(\ell^2(\mathbb{N}))$ and $j, k \in \mathbb{N}$, then we write

$$T(j,k) := (Te_k)(j) = \langle e_j, Te_k \rangle. \tag{3.1}$$

In what follows, $\mathbf{H} = \mathbf{H}_0 + \mathbf{V}$ with $\mathbf{H}_0$ and $\mathbf{V}$ given by (2.7)-(2.8). Let $\tilde{U}$ be the unitary operator in $\ell^2(\mathbb{N})$ satisfying $\tilde{U}e_n = \mathbf{v}_n^0$, where $\{e_n\}_{n\in\mathbb{N}}$ is the canonical basis of $\ell^2(\mathbb{N})$ and $\{\mathbf{v}_n^0\}_{n\in\mathbb{N}}$ is the basis introduced in (2.13)-(2.15). Then the operator

$$H := \tilde{U}^{-1}\mathbf{H}\,\tilde{U} \tag{3.2}$$

can be expressed in the form

$$H = D + V, \tag{3.3}$$

where $D = \mathrm{diag}(d_j)_{j\in\mathbb{N}}$ is the linear map $\ell^{2,1}(\mathbb{N}) \to \ell^2(\mathbb{N})$ satisfying

$$De_j = d_j e_j \text{ for } j \in \mathbb{N} \tag{3.4}$$

with $\{d_n\}_{n\in\mathbb{N}}$ given by (2.17)-(2.18) and

$$V := \tilde{U}^{-1}\mathbf{V}\,\tilde{U}. \tag{3.5}$$

Using the convention (3.1) to express $V(j,k)$, we get

$$V(j,k) = (Ve_k)(j) = \langle \mathbf{v}_j^0, \mathbf{V}\mathbf{v}_k^0 \rangle_{\ell^2(\mathbb{N})\times\ell^2(\mathbb{N})},$$

which corresponds to (2.19).

3.2. **Statement of the result.** The idea of GRWA consists in a simplification of the Hamiltonian H by neglecting some entries of its matrix so that the new matrix can be explicitly diagonalized. The quantum Rabi model considered in [10], [13], corresponds to the case when the QRM can be represented by a direct sum of two Jacobi matrices and the generalized rotating-wave approximation consists in neglecting the off-diagonal entries. The situation is more complicated in the case $l \in \mathbb{N} \setminus \{0\}$, when we need to consider the 2×2 blocks whose diagonal entries are double eigenvalues of H_0.

In what follows, $H = D + V$ is as in Section 3.1 and $n \in 2\mathbb{N} + l$, i.e. $n = 2i + l$ holds with a certain $i \in \mathbb{N}$. Let us denote

$$\widehat{\mathcal{H}}_n := \mathrm{span}\{e_n, e_{n+1}\} \tag{3.6}$$

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 H by the operator H_{GRWA} defined as the linear map $\ell^{2,1}(\mathbb{N}) \to \ell^2(\mathbb{N})$ of the form

$$H_{\mathrm{GRWA}} := \mathrm{diag}(d_0, \ldots, d_{l-1}) \oplus \bigoplus_{i\in\mathbb{N}} \widehat{H}_{l+2i}, \tag{3.7}$$

where

$$\widehat{H}_n := \widehat{\Pi}_n V|_{\widehat{\mathcal{H}}_n} \in \mathcal{B}(\widehat{\mathcal{H}}_n). \tag{3.8}$$

We remark that the matrix of $\widehat{H}_{l+2i}$ in the basis $\{e_{l+2i}, e_{l+2i+1}\}$ is

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

The spectrum of $\widehat{H}_{l+2i}$ consists of two eigenvalues $d_{l+2i} \pm |V(l+2i, l+2i+1)|$ and the spectrum of H_{GRWA} has the form

$$\{d_0, \dots, d_{l-1}\} \cup \{d_{l+2i} + \nu |V(l+2i, l+2i+1)| \colon i \in \mathbb{N},\, \nu = \pm 1\}.$$

Our proof of Theorem 1.2 is based on the following :

Proposition 3.1. *Assume that $D = \mathrm{diag}(d_j)_{j\in\mathbb{N}}$ with $\{d_j\}_{j\in\mathbb{N}}$ given by* (2.17)-(2.18) *and assume that V is a bounded self-adjoint operator in $\ell^2(\mathbb{N})$, satisfying* (2.24)-(2.25). *Assume that the spectrum of $H = D + V$ is composed of a non-decreasing sequence of eigenvalues $\{\lambda_n(H)\}_{n\in\mathbb{N}}$ such that*

$$\lambda_n(H) = d_n + o(1) \text{ as } n \to \infty. \tag{3.9}$$

Then one has

$$\lambda_{l+2i}(H) = d_{l+2i} - |V(l+2i, l+2i+1)| + O(i^{-1/2} \ln i) \text{ as } i \to \infty, \tag{3.10}$$

$$\lambda_{l+2i+1}(H) = d_{l+2i} + |V(l+2i, l+2i+1)| + O(i^{-1/2} \ln i) \text{ as } i \to \infty. \tag{3.11}$$

Proof. See Section 7.3. □

3.3. **Proof of Theorem 1.2.** In this section we show how the assertion of Theorem 1.2 can be deduced by combining the results of Section 2 with Proposition 3.1. We first observe that Proposition 2.2 ensures the fact that the operator V satisfies (2.24)-(2.25) and (3.9) holds due to Proposition 2.3. Thus, applying Proposition 3.1, we get the estimates (3.10)-(3.11) and in order to complete the proof of Theorem 1.2, it remains to show that the estimate

$$|V(l+2i, l+2i+1)| = |\mathfrak{r}_i| + O(i^{-1/2}) \text{ as } i \to \infty \tag{3.12}$$

holds with $\mathfrak{r}_i$ given by (1.8). For this purpose we observe that

$$V(l+2i, l+2i+1) = \tfrac{\Delta}{2} \langle u_{-1,l+i}, u_{1,i} \rangle + O(i^{-1/2}) \text{ as } i \to \infty \tag{3.13}$$

follows from (2.22) and (2.11).

Step 1. For $n \in \mathbb{N}$ we define $f_n^{\pm}$ as the 2π-periodic function

$$f_n^{\pm}(\theta) := \mathrm{e}^{\mathrm{i}n\theta \mp 2\mathrm{i}gn^{1/2} \sin\theta + \mathrm{i}g^2 \sin\theta\cos\theta} \tag{3.14}$$

and for $i \in \mathbb{N}$ we introduce

$$\gamma_{g,l,i} := \int_{-\pi}^{\pi} \overline{f_{l+i}^{-}(\theta)}\, f_i^{+}(\theta)\, \frac{\mathrm{d}\theta}{2\pi}. \tag{3.15}$$

We claim that

$$V(l+2i, l+2i+1) = \tfrac{\Delta}{2} \gamma_{g,l,i} + O(i^{-1/2}) \text{ as } i \to \infty. \tag{3.16}$$

To begin the proof of (3.16), we write the Parseval's equality,

$$\gamma_{g,l,i} = \sum_{j\in\mathbb{Z}} \overline{u_{-1,l+i}(j)} u_{1,i}(j), \tag{3.17}$$

where $\{u_{\pm 1,n}(j)\}_{j\in\mathbb{Z}}$ denotes the sequence of Fourier coefficients of $f_n^{\pm}$, i.e.

$$u_{\pm 1,n}(j) := \int_{-\pi}^{\pi} f_n^{\pm}(\theta)\, \mathrm{e}^{-\mathrm{i}j\theta}\, \frac{\mathrm{d}\theta}{2\pi} \tag{3.18}$$

and we remark that the expression of $u_{\pm 1,n}(j)$ given by (3.18) is the same as given by (2.12) for $j \geq 0$. Moreover, the integration by parts allows us to estimate

$$(n-j)^{4N} u_{\pm 1,n}(j) = \int_{-\pi}^{\pi} \mathrm{e}^{\mp 2\mathrm{i}gn^{1/2}\sin\theta + \mathrm{i}g^2 \sin\theta\cos\theta} \left(\tfrac{\mathrm{d}}{\mathrm{d}\theta}\right)^{4N} \left(\mathrm{e}^{\mathrm{i}(n-j)\theta}\right) \frac{\mathrm{d}\theta}{2\pi}$$

$$= \int_{-\pi}^{\pi} \left(\tfrac{\mathrm{d}}{\mathrm{d}\theta}\right)^{4N} \left(\mathrm{e}^{\mp 2\mathrm{i}gn^{1/2}\sin\theta + \mathrm{i}g^2 \sin\theta\cos\theta}\right) \mathrm{e}^{\mathrm{i}(n-j)\theta} \frac{\mathrm{d}\theta}{2\pi} = O(n^{2N}),$$

hence

$$j < 0 \Rightarrow |u_{\pm 1,n}(j)| \leq C_N n^{2N} (n-j)^{-4N} \leq C_N n^{-N} |j|^{-N} \tag{3.19}$$

and, combining (3.17) with (3.19), we find that

$$\gamma_{g,l,i} - \langle u_{-1,l+i}, u_{1,i}\rangle = \sum_{\{j\in\mathbb{Z}:\, j<0\}} \overline{u_{-1,l+i}(j)}\, u_{1,i}(j) = O(i^{-N}) \text{ as } i \to \infty \tag{3.20}$$

holds for any $N \in \mathbb{N}$. It is clear that (3.20) and (3.13) imply (3.16).

Step 2. We investigate $\gamma_{g,l,i}$ as $i \to \infty$ when $g > 0$. The direct computation gives

$$\gamma_{g,l,i} = \int_{-\pi}^{\pi} \mathrm{e}^{-2\mathrm{i}g(\sqrt{l+i}+\sqrt{i})\sin\theta} \mathrm{e}^{-\mathrm{i}\theta l} \frac{\mathrm{d}\theta}{2\pi}. \tag{3.21}$$

Using $2g(\sqrt{l+i}+\sqrt{i}) = 4g\sqrt{i} + O(i^{-1/2})$, we get

$$\gamma_{g,l,i} = \int_{-\pi}^{\pi} \mathrm{e}^{-4\mathrm{i}g\sqrt{i}\sin\theta} \mathrm{e}^{-\mathrm{i}\theta l} \frac{\mathrm{d}\theta}{2\pi} + O(i^{-1/2}). \tag{3.22}$$

We assume that $g > 0$. Since the phase function $\theta \to -\sin\theta$ has non-degenerated critical points $-\pi/2$ and $\pi/2$, the stationary phase formula gives

$$\gamma_{g,l,i} = \frac{1}{\sqrt{2\pi \cdot 4g\sqrt{i}}} \sum_{\kappa=\pm 1} \mathrm{e}^{\mathrm{i}\kappa(4g\sqrt{i}-\pi/4)} \mathrm{e}^{\mathrm{i}\kappa\pi l/2} + O(i^{-1/2})$$

$$= \frac{\cos\left(4g\sqrt{i} - \frac{\pi}{4} + \frac{\pi}{2}l\right)}{\sqrt{2\pi g\sqrt{i}}} + O(i^{-1/2})$$

and we obtain (3.12) for $g > 0$ due to

$$\cos\left(4g\sqrt{i} - \tfrac{\pi}{4} + \tfrac{\pi}{2}l\right) = \begin{cases} (-1)^{l/2}\cos\left(4g\sqrt{i} - \frac{\pi}{4}\right) & \text{when } l \text{ is even} \\ (-1)^{(l+1)/2}\sin\left(4g\sqrt{i} - \frac{\pi}{4}\right) & \text{when } l \text{ is odd} \end{cases}$$

Step 3. We investigate $\gamma_{g,l,i}$ as $i \to \infty$ when $g < 0$. Then $-g = |g|$ and the conjugation of (3.22) gives

$$\gamma_{g,l,i} = \overline{\gamma_{|g|,-l,i}} + O(i^{-1/2}) = \frac{\cos\left(4|g|\sqrt{i} - \frac{\pi}{4} - \frac{\pi}{2}l\right)}{\sqrt{2\pi|g|\sqrt{i}}} + O(i^{-1/2})$$

hence (3.12) still holds.

4. Operators related to the first similarity transformation

4.1. **The idea of the first similarity transformation.** In this section we begin the proof of Proposition 3.1. In what follows, $H = D + V$ satisfies the assumptions of Proposition 3.1. Moreover, we assume that n is large enough and $n \in 2\mathbb{N} + l$, which implies

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

In what follows, we denote

$$\widehat{\mathcal{H}}_n := \mathrm{span}\{e_n, e_{n+1}\}, \qquad \widetilde{\mathcal{H}}_n := \widehat{\mathcal{H}}_n^{\perp}, \tag{4.2}$$

$\widehat{\Pi}_n \in \mathcal{B}(\ell^2(\mathbb{N}))$ is the orthogonal projection on $\widehat{\mathcal{H}}_n$ and $\widetilde{\Pi}_n := I - \widehat{\Pi}_n$.

Using the decomposition $\ell^2(\mathbb{N}) = \widehat{\mathcal{H}}_n \oplus \widetilde{\mathcal{H}}_n$, we can express

$$V = \begin{pmatrix} \widehat{V}_n & V_n^+|_{\widetilde{\mathcal{H}}_n} \\ V_n^-|_{\widehat{\mathcal{H}}_n} & \widetilde{V}_n \end{pmatrix} = \widehat{V}_n \oplus \widetilde{V}_n + V_n^- + V_n^+, \tag{4.3}$$

where

$$\widehat{V}_n := \widehat{\Pi}_n V|_{\widehat{\mathcal{H}}_n} \in \mathcal{B}(\widehat{\mathcal{H}}_n), \tag{4.4}$$

$$\widetilde{V}_n := \widetilde{\Pi}_n V|_{\widetilde{\mathcal{H}}_n} \in \mathcal{B}(\widetilde{\mathcal{H}}_n), \tag{4.5}$$

$$V_n^- := \widetilde{\Pi}_n V \widehat{\Pi}_n, \tag{4.6}$$

$$V_n^+ := \widehat{\Pi}_n V \widetilde{\Pi}_n. \tag{4.7}$$

In Section 4.2 we introduce the operators $Q_n \in \mathcal{B}(\ell^2(\mathbb{N}))$ satisfying

$$[D, \mathrm{i}Q_n] = -V_n^- - V_n^+, \tag{4.8}$$

where (4.8) is understood as the equality

$$\mathrm{i}(DQ_n - Q_n D)x = -(V_n^- + V_n^+)x \text{ for } x \in \ell^{2,1}(\mathbb{N}), \tag{4.9}$$

well defined because $\ell^{2,1}(\mathbb{N})$ is an invariant subspace of Q_n due to Lemma 4.1(a).

In Section 5, we use the operator Q_n to define

$$H_n' := \mathrm{e}^{-\mathrm{i}Q_n} H \mathrm{e}^{\mathrm{i}Q_n} \tag{4.10}$$

and we remark that the right hand side of (4.10) is a well defined map $\ell^{2,1}(\mathbb{N}) \to \ell^2(\mathbb{N})$ because $\ell^{2,1}(\mathbb{N})$ is an invariant subspace of $\mathrm{e}^{\mathrm{i}Q_n}$ due to Lemma 4.1(b). In Lemma 5.1 we show that

$$H_n' = D + \widehat{V}_n \oplus \widetilde{V}_n + R_n'$$

holds with $||R_n'|| = O(n^{-1/4})$. However, the error $O(n^{-1/4})$ is too rough to deduce the asymptotic formula of Proposition 3.1 and we will have to consider a second similarity transformation in Sections 6–7. Besides the operator Q_n, we introduce auxiliary cut-offs $\check{Q}_n^{\pm}$, useful for estimates considered in 6.

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

$$Z_n^- = (\mathbb{N} \setminus \{n, n+1\}) \times \{n, n+1\} \tag{4.11}$$

$$Z_n^+ = \{n, n+1\} \times (\mathbb{N} \setminus \{n, n+1\}). \tag{4.12}$$

We observe that

$$(j,k) \in Z_n^- \Rightarrow d_j \neq d_n = d_{n+1} = d_k, \tag{4.13}$$

$$(j,k) \in Z_n^+ \Rightarrow d_k \neq d_n = d_{n+1} = d_j \tag{4.14}$$

and

$$(j,k) \in Z_n^- \cup Z_n^+ \Rightarrow |d_j - d_k| \geq \tfrac{1}{4}|j-k|. \tag{4.15}$$

In what follows, $\hat{C}$, $\hat{c} > 0$ are fixed so that the estimate (2.25) holds and c is fixed so that $0 < c \leq \min\{\frac{1}{2}\hat{c}, \frac{1}{2}\}$. We introduce the matrices $(\check{Q}_n^-(j,k))_{(j,k)\in\mathbb{N}^2}$, $(\check{Q}_n^+(j,k))_{(j,k)\in\mathbb{N}^2}$ by

$$\check{Q}_n^{\pm}(j,k) := \begin{cases} \mathrm{i}\,\dfrac{V(j,k)}{d_j - d_k} & \text{if } (j,k) \in Z_n^{\pm} \text{ and } |j-k| < cn^{1/2} \\ 0 & \text{otherwise} \end{cases} \tag{4.16}$$

We observe that $\check{Q}_n^-(j,k) \neq 0$ implies $j \neq k$ and $k \in \{n, n+1\}$, hence $|j-k| < cn^{1/2} \leq ck^{1/2} < \hat{c}k^{1/2}$ and

$$|\check{Q}_n^-(j,k)| \leq \frac{\hat{C}k^{-1/4}}{|d_j - d_k|} \leq \frac{4\hat{C}k^{-1/4}}{|j-k|} \leq \frac{4\hat{C}n^{-1/4}}{|j-k|} \tag{4.17}$$

follows from (2.25), (4.15) 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

$$\check{Q}_n^+(j,k) = \overline{\check{Q}_n^-(k,j)} \tag{4.18}$$

and

$$|\check{Q}_n^+(j,k)| \leq \frac{4\hat{C}n^{-1/4}}{|j-k|}. \tag{4.19}$$

We claim that we can define $\check{Q}_n^{\pm} \in \mathcal{B}(\ell^2(\mathbb{N}))$ satisfying $(\check{Q}_n^{\pm} e_k)(j) = Q_n^{\pm}(j,k)$ for all $j, k \in \mathbb{N}$ and one has

$$||\check{Q}_n^{\pm}|| = O(n^{-1/4}). \tag{4.20}$$

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

$$||\check{Q}_n^- e_k||^2 = \sum_{j\in\mathbb{N}} |\check{Q}_n^-(j,k)|^2 \leq \sum_{\{j\in\mathbb{N}:\, 0<|j-k|<cn^{1/2}\}} \left(\frac{4\hat{C}n^{-1/4}}{|j-k|}\right)^2$$

$$\leq 16\hat{C}^2 n^{-1/2} \sum_{j\in\mathbb{N}\setminus\{k\}} |j-k|^{-2} \leq Cn^{-1/2},$$

i.e. $||\check{Q}_n^-|| = O(n^{-1/4})$ and (4.18) ensures $\check{Q}_n^+ = (\check{Q}_n^-)^*$, hence $||\check{Q}_n^+|| = ||\check{Q}_n^-||$.

4.3. **Definition of operators Q_n^- and Q_n^+.** We introduce the matrices $(Q_n^-(j,k))_{(j,k)\in\mathbb{N}^2}$, $(Q_n^+(j,k))_{(j,k)\in\mathbb{N}^2}$ by

$$Q_n^\pm(j,k) := \begin{cases} \mathrm{i}\,\dfrac{V(j,k)}{d_j - d_k} & \text{if } (j,k)\in Z_n^\pm \\ 0 & \text{otherwise} \end{cases} \tag{4.21}$$

where $Z_n^\pm$ are given by (4.11)-(4.12). We claim that we can define $Q_n^\pm \in \mathcal{B}(\ell^2(\mathbb{N}))$ satisfying $(Q_n^\pm e_k)(j) = Q_n^\pm(j,k)$ for all $j,k\in\mathbb{N}$ and

$$||Q_n^\pm - \check{Q}_n^\pm|| = O(n^{-1/2}), \tag{4.22}$$

hence, combining (4.20) with (4.22), we get

$$||Q_n^\pm|| = O(n^{-1/4}). \tag{4.23}$$

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

$$||(Q_n^- - \check{Q}_n^-)e_k||^2 = \sum_{\{j\in\mathbb{N}:\,|j-k|\geq cn^{1/2}\}} |Q_n^-(j,k)|^2$$

$$\leq \sum_{\{j\in\mathbb{N}:\,|j-k|\geq cn^{1/2}\}} \frac{16|V(j,k)|^2}{|j-k|^2} \leq \sum_{j\in\mathbb{N}} \frac{16|V(j,k)|^2}{c^2 n} = \frac{16||Ve_k||^2}{c^2 n} \leq \frac{16||V||^2}{c^2 n},$$

i.e. $Q_n^- - \check{Q}_n^- = (Q_n^- - \check{Q}_n^-)\widehat{\Pi}_n \in \mathcal{B}(\ell^2(\mathbb{N}))$ and $||Q_n^- - \check{Q}_n^-|| = O(n^{-1/2})$. Moreover, $Q_n^+ - \check{Q}_n^+ = (Q_n^- - \check{Q}_n^-)^*$ ensures $||Q_n^+ - \check{Q}_n^+|| = ||Q_n^- - \check{Q}_n^-|| = O(n^{-1/2})$.

4.4. **Properties of $Q_n^\pm$ and Q_n.** Let $Q_n^\pm$ be as in Section 4.3 and introduce

$$Q_n := Q_n^- + Q_n^+. \tag{4.24}$$

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

$$[D, \mathrm{i}Q_n^\pm]x = \mathrm{i}(DQ_n^\pm - Q_n^\pm D)x = -V_n^\pm x \text{ for } x\in\ell^{2,1}(\mathbb{N}) \tag{4.25}$$

with $V_n^\pm$ given by (4.6)-(4.7).

(b) $\ell^{2,1}(\mathbb{N})$ 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. (a) One has

$$V_n^\pm(j,k) = \begin{cases} V(j,k) & \text{if } (j,k)\in Z_n^\pm \\ 0 & \text{otherwise} \end{cases} \tag{4.26}$$

hence

$$\mathrm{i}(d_j - d_k)Q_n^\pm(j,k) = -V_n^\pm(j,k) \text{ for } (j,k)\in\mathbb{N}^2. \tag{4.27}$$

Let $\lambda := 1 - d_0$ and introduce $D' = D + \lambda = \mathrm{diag}(d'_j)_{j\in\mathbb{N}}$ with $d'_j := d_j + \lambda$. Then $d'_j \geq d'_0 = 1$ and (4.27) implies

$$\mathrm{i}(D'Q_n^\pm e_k)(j) = \mathrm{i}d'_j(Q_n^\pm e_k)(j) = \mathrm{i}(Q_n^\pm d'_k e_k)(j) - (V_n^\pm e_k)(j), \tag{4.28}$$

hence $D'Q_n^\pm e_k \in \ell^2(\mathbb{N})$ and $Q_n^\pm e_k \in \ell^{2,1}(\mathbb{N})$. Let $\ell^2_{\mathrm{fin}}(\mathbb{N})$ denote the set of finite linear combinations of vectors from $\{e_k\}_{k\in\mathbb{N}}$. Then (4.28) ensures the equality

$$\mathrm{i}D'Q_n^\pm x = \mathrm{i}Q_n^\pm D'x - V_n^\pm x \tag{4.29}$$

for $x\in\ell^2_{\mathrm{fin}}(\mathbb{N})$. If $y\in\ell^2_{\mathrm{fin}}(\mathbb{N})$, then using (4.29) with $x = D'^{-1}y$, we obtain

$$D'Q_n^\pm D'^{-1}y = T_n^\pm y \text{ with } T_n^\pm := Q_n^\pm + \mathrm{i}V_n^\pm D'^{-1}. \tag{4.30}$$

Due to (4.30), for every $y \in \ell^2_{\text{fin}}(\mathbb{N})$ one has

$$Q_n^{\pm} {D'}^{-1} y = {D'}^{-1} T_n^{\pm} y \tag{4.31}$$

and by continuity, (4.31) holds for every $y \in \ell^2(\mathbb{N})$. Consider now $x \in \ell^{2,1}(\mathbb{N})$ and take $y = D'x$ in (4.31). This gives

$$Q_n^{\pm} x = {D'}^{-1} T_n^{\pm} D' x \in \ell^{2,1}(\mathbb{N}) \tag{4.32}$$

and

$$\mathrm{i} D' Q_n^{\pm} x = \mathrm{i} T_n^{\pm} D' x = \mathrm{i} Q_n^{\pm} D' x - V_n^{\pm} x, \tag{4.33}$$

i.e. (4.25) holds for every $x \in \ell^{2,1}(\mathbb{N})$.

(b) Since (4.31) holds for every $y \in \ell^2(\mathbb{N})$, (4.30) holds for every $y \in \ell^2(\mathbb{N})$ and using $Q_n = Q_n^- + Q_n^+$, we deduce

$$D' Q_n {D'}^{-1} y = T_n y \text{ with } T_n := Q_n + \mathrm{i}(V_n^- + V_n^+){D'}^{-1} \tag{4.34}$$

for every $y \in \ell^2(\mathbb{N})$. More generally, it is clear that $(T_n)^m y = D'(Q_n)^m {D'}^{-1} y$ holds for every $m \in \mathbb{N}$, $y \in \ell^2(\mathbb{N})$, and

$$\mathrm{e}^{\mathrm{i}tQ_n} {D'}^{-1} y = \sum_{m=0}^{\infty} \frac{(\mathrm{i}t)^m}{m!} (Q_n)^m {D'}^{-1} y =$$

$$= \sum_{m=0}^{\infty} \frac{(\mathrm{i}t)^m}{m!} {D'}^{-1} (T_n)^m y = {D'}^{-1} \mathrm{e}^{\mathrm{i}tT_n} y \in \ell^{2,1}(\mathbb{N})$$

if $y \in \ell^2(\mathbb{Z})$, hence setting $x = {D'}^{-1} y$, we find that $t \to D' \mathrm{e}^{\mathrm{i}tQ_n} x = \mathrm{e}^{\mathrm{i}tT_n} y$ is $\mathrm{C}^\infty(\mathbb{R}; \ell^2(\mathbb{N}))$ for every $x \in \ell^{2,1}(\mathbb{N})$. □

5. The first similarity transformation

5.1. **Statement of the result.** If L_n, L'_n are linear maps defined on a dense subspace of $\ell^2(\mathbb{N})$ such that $L_n - L'_n$ can be extended to a bounded operator on $\ell^2(\mathbb{N})$, 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 $||L_n - L'_n|| \le C\eta_n$ for all $n \ge n_0$. We will prove the following

Lemma 5.1. *We assume that $H = D + V$ is as in Proposition 3.1, $n \in 2\mathbb{N} + l$ and $\widehat{V}_n$, $\widetilde{V}_n$ are given by (4.4), (4.5). If $Q_n = Q_n^- + Q_n^+$ are as in Section 4.4 and $H'_n := \mathrm{e}^{-\mathrm{i}Q_n} H \mathrm{e}^{\mathrm{i}Q_n}$, then the estimate*

$$H'_n = D + \widehat{V}_n \oplus \widetilde{V}_n + R_n + O(n^{-1/2}) \text{ as } n \to \infty \tag{5.1}$$

holds with

$$R_n := [\tfrac{1}{2} V + \tfrac{1}{2}(\widehat{V}_n \oplus \widetilde{V}_n), \mathrm{i}Q_n]. \tag{5.2}$$

Proof. See Section 5.3. □

5.2. **Taylor's expansion formula.** Assume that B and $Q \in \mathcal{B}(\ell^2(\mathbb{N}))$ and denote

$$F_{tQ}(B) := \mathrm{e}^{-\mathrm{i}tQ}\, B\, \mathrm{e}^{\mathrm{i}tQ} \text{ for } t \in \mathbb{R}, \tag{5.3}$$

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

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

$$\frac{\mathrm{d}^m}{\mathrm{d}t^m} F_{tQ}(B) = \mathrm{e}^{-\mathrm{i}tQ}\, \mathrm{ad}^m_{\mathrm{i}Q}(B)\, \mathrm{e}^{\mathrm{i}tQ} = F_{tQ}(\mathrm{ad}^m_{\mathrm{i}Q}(B)) \tag{5.4}$$

and the Taylor's expansion formula gives

$$F_{tQ}(B) = B + \sum_{m=1}^{N-1} \frac{t^m}{m!} \mathrm{ad}^m_{\mathrm{i}Q}(B) + \mathcal{R}^{t,N}_Q(B) \tag{5.5}$$

with

$$\mathcal{R}^{t,N}_Q(B) := \frac{t^N}{(N-1)!} \int_0^1 F_{stQ}(\mathrm{ad}^N_{\mathrm{i}Q}(B))\, (1-s)^{N-1}\, \mathrm{d}s. \tag{5.6}$$

We can also consider the case when B is an unbounded symmetric operator in $\ell^2(\mathbb{N})$, 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 $\ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})$, then we can introduce $[B, \mathrm{i}Q] \in \mathcal{B}(\ell^2(\mathbb{N}))$ 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 (5.5)-(5.6) still hold for every $N \in \mathbb{N}^*$.

5.3. **Proof of Lemma 5.1.** Using (5.5)-(5.6) with $N = 2$, $t = 1$, we obtain

$$\mathrm{e}^{-\mathrm{i}Q_n} V \mathrm{e}^{\mathrm{i}Q_n} = V + [V, \mathrm{i}Q_n] + \mathcal{R}^{1,2}_{Q_n}(V), \tag{5.7}$$

$$||\mathcal{R}^{1,2}_{Q_n}(V)|| \le ||\mathrm{ad}^2_{\mathrm{i}Q_n}(V)|| \le C||Q_n||^2 \tag{5.8}$$

and using (5.5)-(5.6) with $N = 3$, $t = 1$, we obtain

$$\mathrm{e}^{-\mathrm{i}Q_n} D \mathrm{e}^{\mathrm{i}Q_n} = D + [D, \mathrm{i}Q_n] + \tfrac{1}{2}[[D, \mathrm{i}Q_n], \mathrm{i}Q_n] + \mathcal{R}^{1,3}_{Q_n}(D), \tag{5.9}$$

$$||\mathcal{R}^{1,3}_{Q_n}(D)|| \le ||\mathrm{ad}^3_{\mathrm{i}Q_n}(D)||. \tag{5.10}$$

Using $[D, \mathrm{i}Q_n] = -V_n^- - V_n^+$ (see Lemma 4.1(a)) in (5.9)-(5.10), we obtain

$$\mathrm{e}^{-\mathrm{i}Q_n} D \mathrm{e}^{\mathrm{i}Q_n} = D - V_n^- - V_n^+ - \tfrac{1}{2}[V_n^- + V_n^+, \mathrm{i}Q_n] + \mathcal{R}^{1,3}_{Q_n}(D), \tag{5.11}$$

$$||\mathcal{R}^{1,3}_{Q_n}(D)|| = ||\mathrm{ad}^2_{\mathrm{i}Q_n}(V_n^- + V_n^+)|| \le C||Q_n||^2 \tag{5.12}$$

and summing up (5.11), (5.7), we obtain

$$H_n' = D + V - V_n^- - V_n^+ + [V - \tfrac{1}{2}(V_n^- + V_n^+), \mathrm{i}Q_n] + O(||Q_n||^2). \tag{5.13}$$

Since $Q_n = Q_n^- + Q_n^+$, (4.23) ensures

$$||Q_n|| = O(n^{-1/4}) \tag{5.14}$$

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

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

with R_n given by (5.2).

6. Operators related to the second similarity transformation

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

$$H_n' = D + \widehat{V}_n \oplus \widetilde{V}_n + R_n + O(n^{-1/2}) \tag{6.1}$$

with R_n given by (5.2). Similarly as before, we can decompose

$$R_n = \begin{pmatrix} \widehat{R}_n & R_n^+|_{\widetilde{\mathcal{H}}_n} \\ R_n^-|_{\widehat{\mathcal{H}}_n} & \widetilde{R}_n \end{pmatrix} = \widehat{R}_n \oplus \widetilde{R}_n + R_n^- + R_n^+, \tag{6.2}$$

where

$$\widehat{R}_n := \widehat{\Pi}_n R_n|_{\widehat{\mathcal{H}}_n} \in \mathcal{B}(\widehat{\mathcal{H}}_n), \tag{6.3}$$

$$\widetilde{R}_n := \widetilde{\Pi}_n R_n|_{\widetilde{\mathcal{H}}_n} \in \mathcal{B}(\widetilde{\mathcal{H}}_n), \tag{6.4}$$

$$R_n^- := \widetilde{\Pi}_n R_n \widehat{\Pi}_n, \tag{6.5}$$

$$R_n^+ := \widehat{\Pi}_n R_n \widetilde{\Pi}_n. \tag{6.6}$$

In Section 6.2 we introduce the operators $Q_n' \in \mathcal{B}(\ell^2(\mathbb{N}))$ satisfying

$$[D, \mathrm{i}Q_n'] = -R_n^- - R_n^+ + O(n^{-1/2}) \tag{6.7}$$

where $[D, \mathrm{i}Q_n']x = \mathrm{i}(DQ_n' - Q_n'D)x$ is well defined for $x \in \ell^{2,1}(\mathbb{N})$ due to the fact that $\ell^{2,1}(\mathbb{N})$ is an invariant subspace of Q_n' (see Lemma 6.1(b)). In Section 7 we use the operator Q_n' to define

$$H_n'' := \mathrm{e}^{-\mathrm{i}Q_n'} H_n' \mathrm{e}^{\mathrm{i}Q_n'} \tag{6.8}$$

and we remark that the right hand side of (6.8) is a well defined map $\ell^{2,1}(\mathbb{N}) \to \ell^2(\mathbb{N})$ as $\ell^{2,1}(\mathbb{N})$ is an invariant subspace of $\mathrm{e}^{\mathrm{i}Q_n'}$ due to Lemma 6.1(c). In Section 7.1 we will show that

$$\begin{aligned} H_n'' &= D + \widehat{V}_n \oplus \widetilde{V}_n + \widehat{R}_n \oplus \widetilde{R}_n + O(n^{-1/2} \ln n) \\ &= D + (\widehat{V}_n + \widehat{R}_n) \oplus (\widetilde{V}_n + \widetilde{R}_n) + O(n^{-1/2} \ln n) \end{aligned}$$

6.2. **Definition and properties of operators Q_n'.** In what follows, we denote

$$W_n := \tfrac{1}{2}V + \tfrac{1}{2}(\widehat{V}_n \oplus \widetilde{V}_n), \tag{6.9}$$

$$\check{Q}_n := \check{Q}_n^- + \check{Q}_n^+, \tag{6.10}$$

where $\check{Q}_n^-$, $\check{Q}_n^+$ are as in Section 4.2. We introduce $(\check{Q}_n'(j,k))_{(j,k)\in\mathbb{N}^2}$ defined by

$$\check{Q}_n'(j,k) := \begin{cases} \dfrac{(W_n \check{Q}_n)(j,k)}{d_k - d_j} & \text{if } (j,k) \in Z_n^- \cup Z_n^+ \\ 0 & \text{otherwise} \end{cases} \tag{6.11}$$

Lemma 6.1. *(a) There exist operators $\check{Q}'_n \in \mathcal{B}(\ell^2(\mathbb{N}))$ satisfying $(\check{Q}'_n e_k)(j) = \check{Q}'_n(j,k)$ for all $j,k \in \mathbb{N}$ and*

$$||\check{Q}'_n|| = O(n^{-1/2}\ln n). \tag{6.12}$$

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

$$[D, \mathrm{i}Q'_n]x = \mathrm{i}(DQ'_n - Q'_n D)x = -(\check{R}^-_n + \check{R}^+_n)x \text{ for } x \in \ell^{2,1}(\mathbb{N}) \tag{6.13}$$

holds with

$$\check{R}^-_n := \widetilde{\Pi}_n[W_n, \mathrm{i}\check{Q}_n]\widehat{\Pi}_n, \tag{6.14}$$

$$\check{R}^+_n := \widehat{\Pi}_n[W_n, \mathrm{i}\check{Q}_n]\widetilde{\Pi}_n. \tag{6.15}$$

(c) $\ell^{2,1}(\mathbb{N})$ 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. See Sections 6.3-6.5. □

6.3. **Step 1 of the proof of Lemma 6.1.** Using $\check{Q}_n = \check{Q}^-_n + \check{Q}^+_n$, we can write the decomposition

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

with

$$\check{Q}'^\pm_n(j,k) := \begin{cases} \dfrac{(W_n\check{Q}^\pm_n)(j,k)}{d_k - d_j} & \text{if } (j,k) \in Z^-_n \cup Z^+_n \\ 0 & \text{otherwise} \end{cases} \tag{6.16}$$

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

$$|\check{Q}'^\pm_n(j,k)| \leq \frac{4|(W_n\check{Q}^\pm_n)(j,k)|}{|j-k|}. \tag{6.17}$$

It is clear that (2.24)-(2.25) imply $W_n(j,k) \neq 0 \Rightarrow j \neq k$ and

$$|j-k| < \hat{c}k^{1/2} \Rightarrow |W_n(j,k)| \leq \hat{C}k^{-1/4}. \tag{6.18}$$

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

$$||\check{Q}'^-_n|| = O(n^{-1/2}\ln n). \tag{6.19}$$

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

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

with

$$\mathcal{M}_n(k) := \sum_{\{j\in\mathbb{N}:\, |j-k|\geq cn^{1/2}\}} \frac{16|(W_n\check{Q}^-_n)(j,k)|^2}{|j-k|^2}$$

$$\mathcal{M}'_n(k) := \sum_{\{j\in\mathbb{N}:\, 0<|j-k|<cn^{1/2}\}} \frac{16|(W_n\check{Q}^-_n)(j,k)|^2}{|j-k|^2}.$$

It is clear that

$$\mathcal{M}_n(k) \leq \sum_{j\in\mathbb{N}} \frac{16|(W_n\check{Q}^-_n)(j,k)|^2}{c^2 n} = \frac{16||W_n\check{Q}^-_n e_k||^2}{c^2 n} \leq C_1 n^{-1}. \tag{6.20}$$

Our next claim is the estimate

$$\sup_{\{j\in\mathbb{N}:\, 0<|j-k|<cn^{1/2}\}} |(W_n\check{Q}_n^-)(j,k)| \le Cn^{-1/2}\ln n. \tag{6.21}$$

Indeed, writing

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

and using $\check{Q}_n^-(m,k)\neq 0 \Rightarrow 0<|m-k|<cn^{1/2}$ with (4.17), we get

$$|W_n\check{Q}_n^-)(j,k)| \le \sum_{\{m\in\mathbb{N}:\, 0<|m-k|<cn^{1/2}\}} |W_n(j,m)|\,\frac{4\hat{C}n^{-1/4}}{|m-k|}. \tag{6.22}$$

However, $|j-k|<cn^{1/2}$ and $|m-k|<cn^{1/2}$ imply

$$|j-m|\le |j-k|+|k-m|<2cn^{1/2} \Rightarrow |W_n(j,m)|\le \hat{C}j^{-1/4}\le 2\hat{C}n^{-1/4}, \tag{6.23}$$

due to (6.18) and $j\ge k-|k-j|>k-cn^{1/2}\ge n-\frac{1}{2}n^{1/2}\ge \frac{1}{2}n$ (where we used $k\in\{n,n+1\}$ and $c\le\frac{1}{2}$). Combining (6.22), (6.23), we get

$$\begin{aligned}\sup_{\{j\in\mathbb{N}:\, 0<|j-k|<cn^{1/2}\}} |(W_n\check{Q}_n^-)(j,k)| &\le \sum_{\{m\in\mathbb{N}:\, 0<|m-k|<cn^{1/2}\}} \frac{8\hat{C}^2n^{-1/2}}{|m-k|}\\ &\le 8\hat{C}^2n^{-1/2}\sum_{1\le i\le cn^{1/2}}\frac{2}{i}\le Cn^{-1/2}\ln n,\end{aligned}$$

completing the proof of (6.21).

Using (6.21), we can estimate

$$\mathcal{M}_n'(k)\le \sup_{\{j\in\mathbb{N}:\, 0<|j-k|<cn^{1/2}\}} |(W_n\check{Q}_n^-)(j,k)|^2 \sum_{j\in\mathbb{N}\setminus\{k\}}\frac{16}{|j-k|^2}\le C_2n^{-1}(\ln n)^2.$$

We conclude that $||\check{Q}_n'^-e_k||^2\le \mathcal{M}_n(k)+\mathcal{M}_n'(k)\le C_1n^{-1}+C_2n^{-1}(\ln n)^2$, completing the proof of (6.19).

6.4. **Step 2 of the proof of Lemma 6.1.** In this section, we are going to check that there is $\check{Q}_n'^+\in\mathcal{B}(\ell^2(\mathbb{N}))$ satisfying $(\check{Q}_n'^+e_k)(j)=\check{Q}_n'^+(j,k)$ for all $j,k\in\mathbb{N}$ and

$$||\check{Q}_n'^+|| = O(n^{-1/2}\ln n). \tag{6.24}$$

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

$$\mathcal{Q}_n(k) := \sum_{j\in\mathbb{N}} |\check{Q}_n'^+(j,k)| \le Cn^{-1/2}\ln n \text{ for every } k\in\mathbb{N}, \tag{6.25}$$

$$\mathcal{Q}_n^*(k) := \sum_{j\in\mathbb{N}} |\check{Q}_n'^+(k,j)| \le Cn^{-1/2}\ln n \text{ for every } k\in\mathbb{N}. \tag{6.26}$$

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

$$\mathcal{Q}_n'(k) := \sum_{\{j\in\mathbb{N}:\, |j-k|\ge cn^{1/2}\}} |\check{Q}_n'^+(j,k)|, \tag{6.27}$$

$$\mathcal{Q}_n''(k) := \sum_{\{j\in\mathbb{N}:\, 0<|j-k|<cn^{1/2}\}} |\check{Q}_n'^+(j,k)|. \tag{6.28}$$

Using (4.15) and the Cauchy-Schwarz inequality, we can estimate

$$\mathcal{Q}'_n(k) \leq \sum_{\{j\in\mathbb{N}:\, |j-k|\geq cn^{1/2}\}} \frac{4|(W_n\check{Q}_n^+)(j,k)|}{|j-k|} \leq 4\mathcal{M}_n(k)^{1/2}\mathcal{M}'_n(k)^{1/2} \tag{6.29}$$

with

$$\mathcal{M}_n(k) := \sum_{\{j\in\mathbb{N}:\, |j-k|\geq cn^{1/2}\}} |j-k|^{-2},$$

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

However,

$$\mathcal{M}_n(k) \leq 2\sum_{i\geq cn^{1/2}} \frac{1}{i^2} \leq 2\int_{cn^{1/2}-1}^{\infty} \frac{\mathrm{d}s}{s^2} = \frac{2}{cn^{1/2}-1} \leq C_1 n^{-1/2} \tag{6.30}$$

and

$$\mathcal{M}'_n(k) = ||W_n\check{Q}_n^+ e_k||^2 \leq ||W_n||^2\, ||\check{Q}_n^+||^2 \leq C_2 n^{-1/2}, \tag{6.31}$$

where the last estimate is due to (4.20). Combining (6.29) with (6.30)-(6.31), we get

$$\mathcal{Q}'_n(k) \leq C' n^{-1/2}. \tag{6.32}$$

In order to estimate $\mathcal{Q}''_n(k)$, we assume $0 < |j-k| < cn^{1/2}$ and observe that

$$(W_n\check{Q}_n^+)(j,k) = \sum_{n\leq m\leq n+1} W_n(j,m)\check{Q}_n^+(m,k) \tag{6.33}$$

due to $Q_n^+ = \widehat{\Pi}_n Q_n^+$. Using $|j-k| < cn^{1/2}$, $m \in \{n, n+1\}$ and $|\check{Q}_n^+(m,k)| \leq 4\hat{C}n^{-1/4}$ (due to (4.19) and $\check{Q}_n^+(k,k) = 0$), we obtain

$$\check{Q}_n^+(m,k) \neq 0 \Rightarrow |k-m| < cn^{1/2} \Rightarrow |j-m| \leq |j-k| + |k-m| < 2cn^{1/2}$$

$$\Rightarrow |W_n(j,m)| \leq \hat{C}m^{-1/4} \leq \hat{C}n^{-1/4} \Rightarrow |W_n(j,m)\check{Q}_n^+(m,k)| \leq 4\hat{C}^2 n^{-1/2},$$

hence $|j-k| < cn^{1/2} \Rightarrow |(W_n\check{Q}_n^+)(j,k)| \leq 8\hat{C}^2 n^{-1/2}$ and

$$\mathcal{Q}''_n(k) \leq \sum_{\{j\in\mathbb{N}:\, 0<|j-k|<cn^{1/2}\}} \frac{4|(W_n\check{Q}_n^+)(j,k)|}{|j-k|}$$

$$\leq 32\hat{C}^2 n^{-1/2} \sum_{\{j\in\mathbb{N}:\, 0<|j-k|<cn^{1/2}\}} \frac{1}{|j-k|} \leq C'' n^{-1/2}\ln n,$$

due to $\displaystyle\sum_{1\leq i\leq cn^{1/2}} \frac{1}{i} = O(\ln n)$. This proves the estimate (6.25).

In order to prove (6.26), we can use a similar decomposition $\mathcal{Q}_n^* = \mathcal{Q}'^*_n + \mathcal{Q}''^*_n$ and estimate

$$\mathcal{Q}'^*_n(k) \leq \sum_{\{j\in\mathbb{N}:\, |j-k|\geq cn^{1/2}\}} \frac{4|(W_n\check{Q}_n^+)(k,j)|}{|j-k|}, \tag{6.34}$$

$$\mathcal{Q}''^*_n(k) := \sum_{\{j\in\mathbb{N}:\, 0<|j-k|<cn^{1/2}\}} \frac{4|(W_n\check{Q}_n^+)(k,j)|}{|j-k|}. \tag{6.35}$$

However, the right hand side of (6.34) can be estimated by $\mathcal{M}_n(k)^{1/2}\mathcal{M}_n'^*(k)^{1/2}$ with $\mathcal{M}_n(k)$ as before and

$$\mathcal{M}_n'^*(k) = \sum_{j\in\mathbb{N}} |(W_n\check{Q}_n^+)(k,j)|^2 = ||(W_n\check{Q}_n^+)^* e_k||^2 \le ||W_n||^2||Q_n^+||^2 \le C' n^{-1/2}.$$

Finally, exchanging j and k in the previous reasoning, we get $|j-k| < cn^{1/2} \Rightarrow |(W_n\check{Q}_n^+)(k,j)| \le 8\hat{C}^2 n^{-1/2}$ and we can estimate the right hand side of (6.35) by $C'' n^{-1/2}\ln n$ similarly as before. This completes the proof of (6.26).

6.5. **End of the proof of Lemma 6.1.** By the definition of $\check{Q}_n'$ given in (6.11), we get

$$\mathrm{i}(d_j - d_k)\check{Q}_n'(j,k) = \langle e_j, (-\mathrm{i})(\widetilde{\Pi}_n W_n \check{Q}_n \widehat{\Pi}_n + \widehat{\Pi}_n W_n \check{Q}_n \widetilde{\Pi}_n) e_k\rangle \tag{6.36}$$

Since $(W_n\check{Q}_n)^* = \check{Q}_n W_n$ and $(\check{Q}_n')^*(j,k) = \overline{\check{Q}_n'(k,j)}$, we can write the adjoint matrix in both sides of (6.36) as follows

$$\mathrm{i}(d_j - d_k)(\check{Q}_n')^*(j,k) = \langle e_j, \mathrm{i}(\widetilde{\Pi}_n \check{Q}_n W_n \widehat{\Pi}_n + \widehat{\Pi}_n \check{Q}_n W_n \widetilde{\Pi}_n) e_k\rangle. \tag{6.37}$$

Summing up (6.36) and (6.37), we obtain

$$\mathrm{i}(d_j - d_k)Q_n'(j,k) = -\langle e_j, (\check{R}_n^- + \check{R}_n^+) e_k\rangle = -(\check{R}_n^- + \check{R}_n^+)('j,k) \tag{6.38}$$

by the definition of $\check{R}_n^\pm$ given in (6.14)-(6.15). It is easy to see that one can deduce the assertions of Lemma 6.1(b) and (c) from (6.38), reasoning similarly as in the proof of Lemma 4.1.

7. Proof of Proposition 3.1

7.1. **Step 1 of the proof of Proposition 3.1.** We claim that one has the estimate

$$H_n'' = D + (\widehat{V}_n + \widehat{R}_n) \oplus (\widetilde{V}_n + \widetilde{R}_n) + O(n^{-1/2}\ln n) \text{ as } n\to\infty \tag{7.1}$$

To begin the proof of (7.1), we observe that

$$H_n' = D + \widehat{V}_n \oplus \widetilde{V}_n + R_n + O(n^{-1/2}). \tag{7.2}$$

Using (5.5)-(5.6) with $N=2$, $t=1$, we get

$$\mathrm{e}^{-\mathrm{i}Q_n'} D \mathrm{e}^{\mathrm{i}Q_n'} = D + [D, \mathrm{i}Q_n'] + O(||\mathrm{ad}^2_{\mathrm{i}Q_n'}(D)||). \tag{7.3}$$

Since Lemma 6.1 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

$$\mathrm{e}^{-\mathrm{i}Q_n'} D \mathrm{e}^{\mathrm{i}Q_n'} = D - \check{R}_n^- - \check{R}_n^+ + O(||Q_n'||). \tag{7.4}$$

Using (5.5)-(5.6) with $N=1$, $t=1$, we get

$$\mathrm{e}^{-\mathrm{i}Q_n'}(\widehat{V}_n \oplus \widetilde{V}_n + R_n)\mathrm{e}^{\mathrm{i}Q_n'} = \widehat{V}_n \oplus \widetilde{V}_n + R_n + O(||Q_n'||). \tag{7.5}$$

Due to $||Q_n'|| = O(n^{-1/2}\ln n)$, summing up (7.4) and (7.5), we get

$$H_n'' = D + \widehat{V}_n \oplus \widetilde{V}_n + R_n - \check{R}_n^- - \check{R}_n^+ + O(n^{-1/2}\ln n). \tag{7.6}$$

However

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

and (4.22) ensures $Q_n^\pm - \check{Q}_n^\pm = O(n^{-1/2})$, hence

$$R_n^\pm - \check{R}_n^\pm = O(n^{-1/2}). \tag{7.7}$$

Combining (7.7) and (7.6), we get

$$H_n'' = D + \widehat{V}_n \oplus \widetilde{V}_n + R_n - R_n^- - R_n^+ + O(n^{-1/2}\ln n) \tag{7.8}$$

and (7.1) follows due to $R_n - R_n^- - R_n^+ = \widehat{R}_n \oplus \widetilde{R}_n$.

7.2. **Step 2 of the proof of Proposition 3.1.** We claim that

$$||\widehat{\Pi}_n R_n \widehat{\Pi}_n|| = O(n^{-1/2}\ln n). \tag{7.9}$$

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

$$||\widehat{\Pi}_n W_n Q_n^\pm \widehat{\Pi}_n|| = O(n^{-1/2}\ln n) \tag{7.10}$$

and due to (4.22), it remains to prove the estimate

$$||\widehat{\Pi}_n W_n \check{Q}_n^\pm \widehat{\Pi}_n|| = O(n^{-1/2}\ln n). \tag{7.11}$$

We observe that

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

with

$$(W_n\check{Q}_n^\pm)(j,k) = \sum_{\{m\in\mathbb{N}:\, 0<|m-k|<cn^{1/2}\}} W_n(j,m)\check{Q}_n^\pm(m,k).$$

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

$$|m-k| < cn^{1/2} \Rightarrow |j-m| \le |j-k| + |k-m| < 1 + cn^{1/2} < \hat{c}n^{1/2}$$

$$\Rightarrow |W_n(j,m)| \le \hat{C}j^{-1/4} \le \hat{C}n^{-1/4} \Rightarrow |W_n(j,m)\check{Q}_n^\pm(m,k)| \le \frac{4\hat{C}^2 n^{-1/2}}{|m-k|}$$

and consequently

$$|(W_n\check{Q}_n^\pm)(j,k)| \le \sum_{\{m\in\mathbb{N}:\, 0<|m-k|<cn^{1/2}\}} \frac{4\hat{C}^2 n^{-1/2}}{|m-k|} = O(n^{-1/2}\ln n), \tag{7.12}$$

where the last estimate is due to $\displaystyle\sum_{1\le i\le cn^{1/2}} \frac{1}{i} = O(\ln n)$.

7.3. **End of the proof of Proposition 3.1.** To begin we observe that (4.1) and (3.9) ensure the fact that there is $n_1\in\mathbb{N}$ such that for $n\ge n_1$ one has

$$\lambda_{n-1}(H) < d_n - \tfrac{3}{4} < d_n - \tfrac{1}{4} < \lambda_n(H) \le \lambda_{n+1}(H) < d_n + \tfrac{1}{4} < d_n + \tfrac{3}{4} < \lambda_{n+2}(H). \tag{7.13}$$

Denote $U_n := \mathrm{e}^{\mathrm{i}Q_n}\mathrm{e}^{\mathrm{i}Q_n'}$. Then (7.1) ensures

$$U_n^{-1}HU_n = D + (\widehat{V}_n + \widehat{R}_n) \oplus (\widetilde{V}_n + \widetilde{R}_n) + O(n^{-1/2}\ln n). \tag{7.14}$$

Since (7.9) ensures $||\widehat{R}_n||_{\mathcal{B}(\widehat{\mathcal{H}}_n)} = O(n^{-1/2}\ln n)$, we can write (7.14) in the form

$$U_n^{-1}HU_n = D + \widehat{V}_n \oplus \widetilde{V}_n' + O(n^{-1/2}\ln n) \text{ with } \widetilde{V}_n' := \widetilde{V}_n + \widetilde{R}_n. \tag{7.15}$$

Let us introduce

$$H_n := U_n(D + \widehat{V}_n \oplus \widetilde{V}_n')U_n^{-1}. \tag{7.16}$$

Then

$$H = H_n + O(n^{-1/2}\ln n) \tag{7.17}$$

and due to the min-max principle, there exists $C > 0$ such that for every $n \in \mathbb{N}^*$ one has

$$\sup_{k\in\mathbb{N}} |\lambda_k(H) - \lambda_k(H_n)| \leq Cn^{-1/2} \ln n, \tag{7.18}$$

where $(\lambda_k(H_n))_{k\in\mathbb{N}}$ denotes the non-decreasing sequence of eigenvalues of H_n, counting the multiplicities. However, combining (7.18) with (7.13), we can find $n_1 \in \mathbb{N}$ such that for $n \geq n_1$ one has

$$\lambda_{n-1}(H_n) < d_n - \tfrac{1}{2} < \lambda_n(H_n) \leq \lambda_{n+1}(H_n) < d_n + \tfrac{1}{2} < \lambda_{n+2}(H_n). \tag{7.19}$$

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

$$\hat{\lambda}_n := d_n - |V(n, n+1)| \text{ and } \hat{\lambda}_{n+1} := d_n + |V(n, n+1)|. \tag{7.20}$$

Since $V(n, n+1) = O(n^{-1/4})$, there is $n_2 \in \mathbb{N}$ such that for $n \geq n_2$ one has

$$d_n - \tfrac{1}{2} < \hat{\lambda}_n \leq \hat{\lambda}_{n+1} < d_n + \tfrac{1}{2}. \tag{7.21}$$

However, $\sigma(H_n) = \sigma((\widehat{D}_n + \widehat{V}_n) \oplus (\widetilde{D}_n + \widetilde{V}'_n)) = \sigma(\widehat{D}_n + \widehat{V}_n) \cup \sigma(\widetilde{D}_n + \widetilde{V}'_n)$ implies

$$\{\hat{\lambda}_n, \hat{\lambda}_{n+1}\} \subset \sigma(H_n). \tag{7.22}$$

Combining (7.22) with (7.19), (7.21), we get $\hat{\lambda}_n = \lambda_n(H_n)$, $\hat{\lambda}_{n+1} = \lambda_{n+1}(H_n)$ and using these equalities in (7.18), we deduce

$$\lambda_n(H) = \hat{\lambda}_n + O(n^{-1/2} \ln n) \text{ and } \lambda_{n+1}(H) = \hat{\lambda}_{n+1} + O(n^{-1/2} \ln n), \tag{7.23}$$

completing the proof of (3.10)-(3.11).

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