# PERTURBATION SERIES FOR JACOBI MATRICES AND THE QUANTUM RABI MODEL

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**Abstract.** We investigate eigenvalue perturbations for a class of infinite tridiagonal matrices which define unbounded self-adjoint operators with discrete spectrum. In particular we obtain explicit estimates for the convergence radius of the perturbation series and error estimates for the Quantum Rabi Model including the resonance case. We also give expressions for coefficients near resonance in order to evaluate the quality of the rotating wave approximation due to Jaynes and Cummings.

**Keywords:** Jacobi matrix, unbounded self-adjoint operators, quasi-degenerate eigenvalue perturbation, perturbation series, quantum Rabi model, rotating wave approximation.

Mathematics Subject Classification: 81Q10, 47B36, 15A18.

# 1. GENERAL PRESENTATION

# 1.1. INTRODUCTION

The main motivation of this paper is the Quantum Rabi Model (QRM) which is the simplest physical example of interactions between radiation and matter. We refer to [19] for physical explanations (see also [4]) and to [23] for a list of recent research works in relation with the QRM. It appears (see [3,21]) that the QRM Hamiltonian is unitarily equivalent to the direct sum  $J^{\omega}_{\Delta}(g) \oplus J^{\omega}_{-\Delta}(g)$ , where  $\Delta$ ,  $\omega$  and g are real parameters (see Section 1.5) and  $J^{\omega}_{s}(g)$  is the self-adjoint operator defined in  $\ell^2$  by the matrix

$$J_{s}^{\omega}(g) = \begin{pmatrix} -\frac{s}{2} & g\sqrt{1} & 0 & 0 & 0 & \cdots \\ g\sqrt{1} & \omega + \frac{s}{2} & g\sqrt{2} & 0 & 0 & \cdots \\ 0 & g\sqrt{2} & 2\omega - \frac{s}{2} & g\sqrt{3} & 0 & \cdots \\ 0 & 0 & g\sqrt{3} & 3\omega + \frac{s}{2} & g\sqrt{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$
 (1.1)

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The QRM has become a subject of numerous experimental works in the domain of the Cavity Quantum Optics. In practice the value of the coupling constant g is small and it is natural to investigate an eigenvalue by means of the Taylor series with respect to g. Let us notice that all diagonal entries of the matrix (1.1) are distinct if s is not a multiple of  $\omega$ . Thus the most interesting phenomena appear when s is a multiple of  $\omega$ . For simplicity, in this paper, we consider the situation  $s = \omega$  and our analysis will concern the following problems:

- (i) to prove that the eigenvalue branches are analytic functions of g and to give an explicit bound for the convergence radius,
- (ii) to give explicit estimates of the error due to a cut-off of the Taylor's series,
- (iii) to give a method of computing the coefficients and to express corrections of low order.

The results concerning points (i) and (ii) are given in Theorem 1.3. Concerning the point (i), we must control the spectrum with respect to g in order to avoid eigenvalue crossing. The result concerning the point (ii) is obtained in a standard way: the Cauchy's integral formula (see Section 2.3) gives the bounds on the coefficients and clearly the estimates become better when the convergence radius is greater. Theorem 1.3 is preceded by Theorem 1.2 which describes results on perturbations of a simple eigenvalue.

The expressions for coefficients are given in Theorem 1.4 for perturbations of a simple eigenvalue and in Theorem 1.5 for perturbations of a double eigenvalue. The case of the matrix (1.1) with  $s = \omega$  has been intensively studied in physics literature because of the rotating wave approximation introduced in the famous paper of Jaynes and Cummings [10]. The reason of this popularity has been double: the Jaynes–Cummings model is explicitly solvable (see Section 1.5) and the experimental results had confirmed a high quality of this approximation. However more recent experiments have allowed to enlarge the values of the coupling constant g and have shown limits of this approximation.

Our interest in this problem comes from the paper [7], where the authors investigate the quality of the Jaynes–Cummings approximation and propose the corrections for the eigenvalues of (1.1). The authors of [7] evoke the difficulties to control an infinite matrix and propose to look at a small block with a hope to obtain correct approximations. In this paper we propose a simple method of reducing the initial problem to an analogical problem for a finite block (see Section 6). In Section 7 we show how to compute the coefficients and in Section 1.5 we comment on the Jaynes–Cummings approximation. Moreover in Section 5 we explain what is the minimal size of the block in order to recover a given coefficient of the Taylor's series. It appears that the coefficients proposed in [7] are not correct because the block is too small.

The purpose of this paper is to study these questions for a more general class of self-adjoint operators in  $\ell^2$  of the form J(g) = D + gB where D is diagonal and B is tridiagonal (see Section 1.2). Thus our results can be also applied to other models, e.g. to the two-photon version of the QRM (see [8]).

# 1.2. DEFINITION OF J(g)

We denote by  $\ell^2$  the Hilbert space of square summable complex valued sequences with the norm  $||(x_j)_{j\in\mathbb{N}^*}|| = (\sum_{j=1}^{\infty} |x_j|^2)^{1/2}$  and the scalar product  $\langle x, y \rangle = \sum_{j=1}^{\infty} \overline{x}_j y_j$ . The canonical basis of  $\ell^2$  is denoted  $\{e_i\}_{i\in\mathbb{N}^*}$  (i.e.  $e_i = (\delta_{i,j})_{j\in\mathbb{N}^*}$ ) and  $\ell_{\text{fin}}^2$  denotes the subspace of finite linear combinations of vectors from  $\{e_i\}_{i\in\mathbb{N}^*}$ . We denote by  $\sigma(L)$ the spectrum of a linear operator L.

Let  $(d_i)_{i=1}^{\infty}$ ,  $(b_i)_{i=1}^{\infty}$ ,  $(b'_i)_{i=1}^{\infty}$  be real valued sequences and  $g \in \mathbb{R}$ . We denote by J(g) the closure of the linear symmetric operator defined on  $\ell_{\text{fin}}^2$  by the matrix

$$\begin{pmatrix} d_1 + gb_1' & gb_1 & 0 & 0 & \cdots \\ gb_1 & d_2 + gb_2' & gb_2 & 0 & \cdots \\ 0 & gb_2 & d_3 + gb_3' & b_3 & \cdots \\ 0 & 0 & gb_3 & d_4 + gb_4' & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix},$$
(1.2)

i.e. J(g) = D + gB with D and B satisfying

$$De_i = d_i e_i, \tag{1.3}$$

$$Be_i = b'_i e_i + b_i e_{i+1} + b_{i-1} e_{i-1}, (1.4)$$

where by convention  $b_{i-1}e_{i-1} = 0$  if i = 1.

We make the following assumptions:

(H1) there exists  $\rho_0 > 0$  such that  $2\rho_0^2 < \liminf_{i \to \infty} \frac{d_i^2}{b_i^2 + b_{i-1}^2}$ ,

- (H2) the sequence  $(b'_i)_{i=1}^{\infty}$  is bounded,
- (H3)  $d_i \xrightarrow[i \to \infty]{} \infty$ .

**Lemma 1.1.** If (H1)–(H3) hold, then the operator J(g) is self-adjoint, bounded from below and has discrete spectrum for all  $g \in [-\rho_0, \rho_0]$ .

*Proof.* See [5] or [9].

#### 1.3. CONVERGENCE RADIUS AND ERROR ESTIMATES

Further on  $(d_i)_{i=1}^{\infty}$ ,  $(b_i)_{i=1}^{\infty}$ ,  $(b'_i)_{i=1}^{\infty}$  are real sequences satisfying (H1)–(H3) and J(g) is the corresponding self-adjoint operator defined for  $g \in [-\rho_0, \rho_0]$ . Our first result concerns perturbations of a simple eigenvalue of D. For this purpose we fix  $k \in \mathbb{N}^*$  and make the assumption

$$d_k \neq d_i \quad \text{for} \quad i \in \mathbb{N}^* \setminus \{k\}. \tag{1.5}$$

Since  $\sigma(J(g) - (d + gb)I) = \sigma(J(g)) - (d + gb)$ , our analysis of J(g) can be reduced to an analysis of J(g) - (d + gb)I and in particular we can use  $d = d_k$ ,  $b = b'_k$ . Thus, without any loss of generality we can assume  $d_k = b'_k = 0$ . Moreover we denote

$$\beta_i := |b_{i-1}| + |b_i| + |b'_i|. \tag{1.6}$$

**Theorem 1.2.** We fix  $k \in \mathbb{N}^*$  and assume  $d_k = b'_k = 0$ . Let  $\rho > 0$  be such that

$$\rho < \inf_{i \neq k} \frac{|d_i|}{\beta_i + \beta_k},\tag{1.7}$$

where  $\beta_i$  are given by (1.6). We also assume that (H1)–(H3) hold and  $\rho \leq \rho_0$ .

(i) If  $-\rho < g < \rho$  then the interval  $[-\beta_k \rho, \beta_k \rho]$  contains exactly one eigenvalue of J(g),

$$[-\beta_k \rho, \beta_k \rho] \cap \sigma(J(g)) = \{\lambda_k(J(g))\}.$$
(1.8)

(ii) The eigenvalue  $\lambda_k(J(g))$  is simple and  $g \to \lambda_k(J(g))$  is real analytic, i.e.

$$\lambda_k(J(g)) = \sum_{\nu=1}^{\infty} c_{k,\nu} g^{\nu} \quad if \quad -\rho < g < \rho.$$
(1.9)

(iii) The coefficients in (1.9) satisfy the estimates  $|c_{k,\nu}| \leq \beta_k \rho^{1-\nu}$  and one has

$$\left|\lambda_k(J(g)) - \sum_{1 \le \nu \le N} c_{k,\nu} g^{\nu}\right| \le \frac{\beta_k |g|^{N+1}}{(\rho - |g|)\rho^{N-1}} \quad if \quad -\rho < g < \rho.$$
(1.10)

Proof. See Section 6.

Our second result concerns perturbations of a double eigenvalue of D. For this purpose we fix  $k \in \mathbb{N}^*$  and make the assumption

$$d_{k+1} = d_k \neq d_j \quad \text{for} \quad j \in \mathbb{N}^* \setminus \{k, k+1\}.$$

$$(1.11)$$

Without loss of generality we can replace J(g) by J(g) - (d + gb)I with  $d = d_k$ ,  $b = (b'_k + b'_{k+1})/2$  and further on we assume

$$d_{k+1} = d_k = 0$$
 and  $b'_{k+1} = -b'_k$ . (1.12)

We introduce the quantities

$$\mu_k := \left(b_k^2 + b_k'^2\right)^{1/2},\tag{1.13}$$

$$\beta_{k-1}' := |b_{k-2}| + |b_{k-1}'|, \qquad (1.14)$$

$$\beta_{k+2}' := |b_{k+2}| + |b_{k+2}'|, \qquad (1.15)$$

$$\gamma_k := 3 \max\{|b_{k-1}|, |b_{k+1}|\} + 2 \max\{\mu_k, \beta'_{k-1}, \beta'_{k+2}\},$$
(1.16)

$$\gamma'_{k} := \max\left\{ \left| \frac{b_{k-1}}{d_{k-1}} \right|, \left| \frac{b_{k+1}}{d_{k+2}} \right| \right\}$$
(1.17)

and

$$\beta'_{i} := |b_{i-1}| + |b_{i}| + |b'_{i}| \quad \text{if} \quad i \notin [k-1, k+2].$$
(1.18)

**Theorem 1.3.** Assume that (H1)–(H3) hold and  $k \in \mathbb{N}^*$  is fixed. Assume moreover that (1.11)–(1.12) hold and  $0 < \rho \leq \rho_0$  satisfies the conditions

$$\rho \le \inf_{i \notin \{k,k+1\}} \frac{|d_i|}{2(\beta'_i + \mu_k)},$$
(1.19)

$$4\rho\mu_k \le \inf_{i \notin \{k,k+1\}} |d_i|, \tag{1.20}$$

$$\rho \gamma_k \gamma'_k e^{2\rho \gamma'_k} < \mu_k, \tag{1.21}$$

where  $\mu_k$ ,  $\gamma_k$ ,  $\gamma'_k$ ,  $\beta'_i$  are given by (1.13)–(1.18).

(i) If  $-\rho < g < \rho$  and  $g \neq 0$ , then

$$[-2\mu_k \rho, 2\mu_k \rho] \cap \sigma(J(g)) = \{\lambda_k(J(g)), \lambda_{k+1}(J(g))\},$$
(1.22)

where the eigenvalues  $\lambda_k(J(g))$ ,  $\lambda_{k+1}(J(g))$  are simple and satisfy

$$\begin{cases} \lambda_k(J(g)) < 0 < \lambda_{k+1}(J(g)) & \text{if } g > 0, \\ \lambda_{k+1}(J(g)) < 0 < \lambda_k(J(g)) & \text{if } g < 0. \end{cases}$$
(1.23)

(ii) If j = 0, 1 and  $\mu_{k+1} := -\mu_k$ , then one has

$$\lambda_{k+j}(J(g)) = -\mu_{k+j}g + \sum_{\nu=2}^{\infty} c_{k+j,\nu}g^{\nu} \ if \ -\rho < g < \rho.$$
(1.24)

(iii) The coefficients in (1.24) satisfy the estimates  $|c_{k+j,\nu}| \leq \mu_k \rho^{1-\nu}$  for j = 0, 1 and

$$\left|\lambda_{k+j}(J(g)) + \mu_{k+j}g - \sum_{2 \le \nu \le N} c_{k+j,\nu}g^{\nu}\right| \le \frac{\mu_k |g|^{N+1}}{(\rho - |g|)\rho^{N-1}} \quad \text{if} \quad -\rho < g < \rho.$$
(1.25)

*Proof.* See Section 6.

### 1.4. COEFFICIENTS OF THE PERTURBATION SERIES

**Theorem 1.4.** Let J(g) be as in Theorem 1.2.

(i) If  $b'_j = 0$  holds for all  $j \in \mathbb{N}^*$ , then  $c_{k,\nu} = 0$  when  $\nu$  is odd and (1.9) holds with

$$c_{k,2} = -\frac{b_k^2}{d_{k+1}} - \frac{b_{k-1}^2}{d_{k-1}}$$
(1.26)

$$c_{k,4} = \frac{b_k^4}{d_{k+1}^3} + \frac{b_{k-1}^4}{d_{k-1}^3} + \frac{b_k^2 b_{k-1}^2}{d_{k-1}^2 d_{k+1}} + \frac{b_k^2 b_{k-1}^2}{d_{k+1}^2 d_{k-1}} - \frac{b_k^2 b_{k+1}^2}{d_{k+1}^2 d_{k+2}} - \frac{b_{k-1}^2 b_{k-2}^2}{d_{k-1}^2 d_{k-2}}.$$
 (1.27)

(ii) In the general case one has

$$\lambda_k(J(g)) = c_{2,k}(g) g^2 + c_{4,k}(g) g^4 + O(g^6), \qquad (1.28)$$

where  $c_{2,k}(g)$  and  $c_{4,k}(g)$  are given by using  $d_i + gb'_i$  instead of  $d_i$  in (1.26)–(1.27).

*Proof.* The assertions of Theorem 1.4 can be deduced from general formulas given e.g. in [16]. However we give an independent proof in Section 7.3.  $\Box$ 

Next we assume that J(g) is as in Theorem 1.3. We denote

$$d_i^0(g) := d_i + gb'_i \text{ for } i \in \mathbb{N}^*, \qquad (1.29)$$

$$b_k^1(g) := b'_k + g \frac{b_{k-1}^2}{d_k^0(g) - d_{k-1}^0(g)}, \qquad (1.30)$$

$$b_{k+1}^{1}(g) := b_{k+1}' + g \frac{b_{k+1}^{2}}{d_{k+1}^{0}(g) - d_{k+2}^{0}(g)}, \qquad (1.31)$$

$$\widehat{b}_{k}^{1}(g) := b_{k} \left( 1 - \frac{g^{2} b_{k-1}^{2}}{2(d_{k}^{0}(g) - d_{k-1}^{0}(g))^{2}} - \frac{g^{2} b_{k+1}^{2}}{2(d_{k+1}^{0}(g) - d_{k+2}^{0}(g))^{2}} \right)$$
(1.32)

and introduce the matrix

$$B_k^1(g) := \begin{pmatrix} b_k^1(g) & \widehat{b}_k^1(g) \\ \widehat{b}_k^1(g) & b_{k+1}^1(g) \end{pmatrix}.$$
 (1.33)

**Theorem 1.5.** Let J(g) be as in Theorem 1.3,  $\mu_k = (b_k^2 + b'_k^2)^{1/2}$  and  $\mu_{k+1} := -\mu_k$ .

(i) Let  $B_k^1(g)$  be given by (1.33) and for j = 0, 1, let  $\lambda_{k+j}^1(g)$  denote the eigenvalue of  $B_k^1(g)$  satisfying  $\lambda_{k+j}^1(g) \xrightarrow[q \to 0]{} -\mu_{k+j}$ . Then

$$\lambda_{k+j}(J(g)) = g \,\lambda_{k+j}^1(g) + O(g^4). \tag{1.34}$$

(ii) If  $b'_k = 0$ , then the estimate (1.34) implies

$$\lambda_{k+j}(J(g)) = -\mu_{k+j}g - g^2 \left(\frac{b_{k-1}^2}{2d_{k-1}} + \frac{b_{k+1}^2}{2d_{k+2}}\right) + O(g^3).$$
(1.35)

(iii) At the end of Section 7.2 we give expressions for  $\lambda_{k+j}(J(g))$ , j = 0, 1, with the error  $O(g^5)$ .

*Proof.* See Section 7.2.

# 1.5. JAYNES–CUMMINGS APPROXIMATION

The simplest interaction between a two-level atom and a classical light field is described by the Rabi model [14, 15]. The quantized version can be reduced to  $J^{\omega}_{\Delta}(g) \oplus J^{\omega}_{-\Delta}(g)$ , where  $\Delta$  is the separation energy between two atomic levels and  $\omega$  is the frequency of the quantized one-mode electromagnetic field. In [10], Jaynes and Cummings proposed to approximate  $J^{\omega}_{s}(g)$  by

$$\widetilde{J}_{s}^{\omega}(g) = \begin{pmatrix} -\frac{s}{2} & 0 & 0 & 0 & 0 & \cdots \\ 0 & \omega + \frac{s}{2} & g\sqrt{2} & 0 & 0 & \cdots \\ 0 & g\sqrt{2} & 2\omega - \frac{s}{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & 3\omega + \frac{s}{2} & g\sqrt{4} & \cdots \\ 0 & 0 & 0 & g\sqrt{4} & 4\omega - \frac{s}{2} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$
(1.36)

under the assumption that  $s \approx \omega$  and g is small. Since  $\widetilde{J}_s^{\omega}(g)$  is the direct sum

$$\frac{s}{2} + \widetilde{J}_s^{\omega}(g) = (0) \oplus \bigoplus_{m \in \mathbb{N}^*} \begin{pmatrix} 2m\omega + (s-\omega) & g\sqrt{2m} \\ g\sqrt{2m} & 2m\omega \end{pmatrix},$$
(1.37)

we can find explicitly all its eigenvalues. Physical reasons for this approximation in semi-classical and fully quantized version were usually given by means of the time dependent perturbation theory (see [1, 6, 20]). The time independent approach was proposed in [7].

Following [7] let us consider the case  $\omega = s$ . In this case, the eigenvalues of (1.36) are

$$(2m - \frac{1}{2})\omega \pm g\sqrt{2m}, \quad m = 0, 1, 2, \dots$$

On the other hand we can use Theorem 1.5 without the hypothesis  $d_k = d_{k+1} = 0$ . The corresponding shift of the diagonal entries in (1.35) gives the expressions

$$d_k \pm g|b_k| - \frac{g^2}{2} \left( \frac{b_{k-1}^2}{d_{k-1} - d_k} + \frac{b_{k+1}^2}{d_{k+2} - d_k} \right) + O(g^3)$$

for the couple  $\lambda_k(J(g))$ ,  $\lambda_{k+1}(J(g))$ . In the case of the QRM with  $s = \omega$ , one has  $b_k = \sqrt{k}$ ,  $d_{2m} - d_{2m-1} = d_{2m+2} - d_{2m+1} = 2\omega$  and the corresponding eigenvalue couple  $\{\lambda_{2m}(J^{\omega}_{\omega}(g)), \lambda_{2m+1}(J^{\omega}_{\omega}(g))\}$ , satisfies

$$(2m - \frac{1}{2})\omega \pm g\sqrt{2m} - \frac{g^2}{2\omega} + O(g^3).$$

We observe that these eigenvalues coincide with the eigenvalues of the Jaynes–Cummings model modulo  $O(g^2)$ . We can also use Theorem 1.5 with  $b'_k \neq 0$  in order to cover a situation when the difference  $s - \omega = cg$ . Reasoning similarly as in Section 2.4 it is also possible to consider the case of entries  $b_i$ ,  $b'_i$  which are analytic functions of g. We have not used this framework in order to simplify the expressions for the convergence radius.

## 2. PRELIMINARIES

#### 2.1. INTRODUCTION

Sections 2–5 present a finite dimensional perturbation theory. In these sections we denote by  $\mathcal{L}(V)$  the set of all linear operators defined on a finite dimensional linear space V and  $\{e_i\}_{i=1}^n$  denotes the canonical basis of  $\mathbb{C}^n$ .

We assume that  $J: \mathbb{C} \to \mathcal{L}(\mathbb{C}^n)$  has the form

$$J(g) = D + gB(g), \tag{2.1}$$

where  $D = \text{diag}(d_i)_{i=1}^n$ , i.e.  $De_i = d_i e_i$  for i = 1, ..., n. Sections 2.2 and 2.3 contain two elementary lemmas which are basic ingredients of our further analysis and in Section 2.4 we prove a finite dimensional version of Theorem 1.2. We will use the following notation.

### Notation 2.1.

- (a) For  $\lambda \in \mathbb{C}$  and  $\rho \ge 0$  we denote  $\overline{\mathbb{D}}(\lambda, \rho) := \{\lambda' \in \mathbb{C} : |\lambda' \lambda| \le \rho\}$ . If  $\rho > 0$  then  $\mathbb{D}(\lambda, \rho) := \{\lambda' \in \mathbb{C} : |\lambda' \lambda| < \rho\}$  and  $\partial \mathbb{D}(\lambda, \rho) := \{\lambda' \in \mathbb{C} : |\lambda' \lambda| = \rho\}$ .
- (b) We denote by  $\langle \cdot, \cdot \rangle$  the scalar product of  $\mathbb{C}^n$  and write  $B(g) = (b_{i,j}(g))_{i,j=1}^n$  with

$$b_{i,j}(g) = \langle \mathbf{e}_i, B(g) \mathbf{e}_j \rangle$$

(c) For  $\rho > 0$  and i = 1, ..., n, we denote  $\beta_i(\rho) := \sup_{g \in \overline{\mathbb{D}}(0,\rho)} \sum_{1 \le j \le n} |b_{i,j}(g)|.$ 

#### 2.2. AN AUXILIARY RESULT

**Lemma 2.2.** We fix  $k \in \{1, \ldots, n\}$ . Let  $\rho > 0$  be such that  $\beta_k(\rho) > 0$  and denote

$$\phi_k(\rho) := \min_{i \neq k} \frac{|d_k - d_i|}{\rho \beta_k(\rho) + \rho \beta_i(\rho)}.$$
(2.2)

If  $\phi_k(\rho) > 1$  and  $|g| < \rho$ , then

$$\partial \mathbb{D}(d_k, \rho \beta_k(\rho)) \cap \sigma(J(g)) = \emptyset.$$
(2.3)

*Proof.* The Gershgorin's theorem (see [18, Theorem 3.11]) ensures  $\sigma(J(g)) \subset \overline{\mathbb{D}}_1 \cup \ldots \cup \overline{\mathbb{D}}_n$ , where

$$\overline{\mathbb{D}}_i := \overline{\mathbb{D}}\Big(d_i + gb_{i,i}(g), \sum_{j \neq i} |gb_{i,j}(g)|\Big).$$

Since  $\overline{\mathbb{D}}_i \subset \overline{\mathbb{D}}(d_i, |g| \beta_i(|g|))$ , it remains to show that for every *i* one has

$$|g| < \rho \implies \partial \mathbb{D}(d_k, \rho \beta_k(\rho)) \cap \overline{\mathbb{D}}(d_i, |g| \beta_i(\rho)) = \emptyset.$$
(2.4)

Since  $|g| < \rho \implies \overline{\mathbb{D}}(d_k, |g| \beta_k(\rho)) \subset \mathbb{D}(d_k, \rho \beta_k(\rho))$ , it is clear that (2.4) holds if i = k. Assume now that  $i \neq k$ . Since by definition,  $\Phi_k(\rho) > 1$  implies

$$|d_k - d_i| > \rho\beta_k(\rho) + \rho\beta_i(\rho), \qquad (2.5)$$

we deduce (2.4) from the fact that (2.5) ensures  $\overline{\mathbb{D}}(d_k, \rho\beta_k(\rho)) \cap \overline{\mathbb{D}}(d_i, \rho\beta_i(\rho)) = \emptyset$ .  $\Box$ 

### 2.3. USE OF THE CAUCHY'S FORMULA

**Lemma 2.3.** We fix  $\beta > 0$  and  $\rho > 0$ . If  $\eta : \mathbb{D}(0, \rho) \to \overline{\mathbb{D}}(0, \beta\rho)$  is holomorphic, then  $|\eta^{(\nu)}(0)| \le \beta \rho^{1-\nu} \nu!$  (2.6)

holds for every  $\nu \in \mathbb{N}$ . Moreover for every  $N \in \mathbb{N}$  and  $g \in \mathbb{D}(0, \rho)$  one has

$$\left|\eta(g) - \sum_{0 \le \nu \le N} \frac{\eta^{(\nu)}(0)}{\nu!} g^{\nu} \right| \le \frac{\beta |g|^{N+1}}{(\rho - |g|)\rho^{N-1}}.$$
(2.7)

*Proof.* Denote  $c_{\nu} = \eta^{(\nu)}(0)/\nu!$  and take  $\rho' < \rho$ . Then the Cauchy's formula

$$c_{\nu} = \frac{1}{2\pi \mathrm{i}} \oint_{|g|=\rho'} \eta(g) g^{-1-\nu} \mathrm{d}g$$

allows us to estimate  $|c_{\nu}| \leq \beta \rho \rho'^{-\nu}$  and taking the limit  $\rho' \to \rho$  we obtain

$$|c_{\nu}| \le \beta \rho^{1-\nu}.\tag{2.8}$$

Using (2.8) we can estimate the left hand side of (2.7) by

$$\sum_{\nu \ge N+1} |c_{\nu}g^{\nu}| \le \sum_{\nu \ge N+1} \beta \rho (|g|/\rho)^{\nu} = \beta \rho \frac{|g|^{N+1}}{\rho^{N+1}(1-|g|/\rho)},$$

completing the proof of Lemma 2.3.

#### 2.4. FINITE DIMENSIONAL VERSION OF THEOREM 1.2

Let us fix  $\rho_0 > 0$  and assume that B is holomorphic  $\mathbb{D}(0, \rho_0) \to \mathcal{L}(\mathbb{C}^n)$ , i.e.  $g \to b_{i,j}(g)$ are holomorphic on  $\mathbb{D}(0, \rho_0)$ . We fix  $k \in \{1, \ldots, n\}$  and assume that

$$d_k = 0 \neq d_i \text{ if } i \neq k. \tag{2.9}$$

Assume moreover that  $0 < \rho < \rho_0$  is such that  $\beta_k(\rho) > 0$  and  $\phi_k(\rho) > 1$ . Due to (2.9),  $d_k = 0$  is a simple eigenvalue of J(0) = D and (2.3) allows us to define

$$P_k(J(g)) = \frac{1}{2\pi i} \oint_{|\lambda| = \rho \beta_k(\rho)} (\lambda - J(g))^{-1} d\lambda$$
(2.10)

for  $g \in \mathbb{D}(0, \rho)$ .

Following Kato [11] we observe that  $g \to P_k(J(g))$  is a holomorphic family of eigenprojectors of J(g) satisfying

$$\operatorname{rank} P_k(J(g)) = \operatorname{rank} P_k(J(0)) = 1$$

and  $\lambda_k(J(g)) = \operatorname{tr} (J(g)P_k(J(g)))$  is an eigenvalue of J(g) satisfying

$$\sigma(J(g)) \cap \mathbb{D}(0, \rho\beta_k(\rho)) = \{\lambda_k(J(g))\}.$$

Since  $g \to \lambda_k(g)$  is holomorphic  $\mathbb{D}(0, \rho) \to \mathbb{D}(0, \rho\beta_k(\rho))$ , the estimates (2.6)–(2.7) hold with  $\lambda_k(g)$  and  $\beta_k(\rho)$  instead of  $\eta(g)$  and  $\beta$ .

### 3. QUASI-DEGENERATE CASE IN FINITE DIMENSION

### 3.1. INTRODUCTION

In this section J(g) = D + gB(g) is holomorphic  $\mathbb{D}(0, \rho_0) \to \mathcal{L}(\mathbb{C}^n)$  and  $D = \text{diag}(d_i)_{i=1}^n$ . Moreover we fix  $\hat{n} \in \{1, \ldots, n-1\}$  and we make the assumption

$$i \le \widehat{n} < j \implies d_i \ne d_j.$$
 (3.1)

We write  $\mathbb{C}^n = \widehat{V} \oplus \widetilde{V}$  with

$$\widehat{V} := \operatorname{span}\left\{e_j\right\}_{1 < j < \widehat{n}},\tag{3.2}$$

$$\widehat{V} := \operatorname{span} \left\{ e_j \right\}_{1+\widehat{n} \le j \le n} \tag{3.3}$$

and consider the corresponding decomposition

$$D = \widehat{D} \oplus \widetilde{D} = \operatorname{diag}(d_j)_{j=1}^{\widehat{n}} \oplus \operatorname{diag}(d_j)_{j=1+\widehat{n}}^n,$$
(3.4)

where  $\widehat{D} \in \mathcal{L}(\widehat{V})$  and  $\widetilde{D} \in \mathcal{L}(\widetilde{V})$  are the restrictions of D to  $\widehat{V}$  and  $\widetilde{V}$ , respectively. Then the assumption (3.1) means that  $\widehat{D}$  and  $\widetilde{D}$  have no common eigenvalue.

Analyticity results for degenerate eigenvalues were given in [17], but in this paper we will develop an approach of Schrieffer–Wolff [2] (see also [2, 12, 13, 22]) in order to prove the following result.

**Proposition 3.1.** Assume that (3.1) holds and  $\varepsilon_0 > 0$  is small enough. If  $|g| < \varepsilon_0$  then J(g) is similar to  $\widehat{J}_{\infty}(g) \oplus \widetilde{J}_{\infty}(g)$  where  $\widehat{J}_{\infty}$  is holomorphic  $\mathbb{D}(0, \varepsilon_0) \to \mathcal{L}(\widehat{\mathcal{V}})$  and  $\widetilde{J}_{\infty}$  is holomorphic  $\mathbb{D}(0, \varepsilon_0) \to \mathcal{L}(\widehat{\mathcal{V}})$ . Moreover  $\widehat{J}_{\infty}(0) = \widehat{D}$  and  $\widetilde{J}_{\infty}(0) = \widetilde{D}$ .

Proof. See Sections 3.2–3.4.

Using Proposition 3.1 in the case  $\hat{n} = 2$  we get the following corollary.

**Corollary 3.2.** Assume that (3.1) holds with  $\hat{n} = 2$  and  $d_1 = d_2 = 0$ . Assume moreover that B(0) is self-adjoint and  $b_{1,2}(0) \neq 0$ . If  $0 < \rho < \min\{|d_j| : j \ge 3\}$ , then there exists  $\varepsilon > 0$  such that for  $g \in \mathbb{D}(0, \varepsilon)$  one has

$$\mathbb{D}(0,\rho) \cap \sigma(J(g)) = \{\lambda_1(J(g)), \lambda_2(J(g))\},\tag{3.5}$$

where  $g \to \lambda_j(J(g))$  are holomorphic on  $\mathbb{D}(0,\varepsilon)$  for j = 1, 2 and

$$\lambda_j(J(g)) = \mu_j g + O(g^2), \qquad (3.6)$$

where  $\mu_1$ ,  $\mu_2$  are eigenvalues of  $\widehat{B}(0) := (b_{i,j}(0))_{1 \le i,j \le 2}$ .

*Proof.* Let  $\varepsilon > 0$  be small enough. Then the assertion of Proposition 3.1 ensures

$$\sigma(J(g)) = \sigma(\widehat{J}_{\infty}(g)) \cup \sigma(\widetilde{J}_{\infty}(g))$$
(3.7)

and there exists C > 0 such that

$$\operatorname{dist}\left(\sigma(\widetilde{J}_{\infty}(g)), \{d_3, \dots, d_n\}\right) \le C|g|.$$
(3.8)

Due to (3.8),  $\mathbb{D}(0,\rho) \cap \sigma(\widetilde{J}_{\infty}(g)) = \emptyset$  holds for  $\varepsilon > 0$  small enough and (3.7) ensures

$$\mathbb{D}(0,\rho)\cap\sigma(J(g))\subset\sigma(\widehat{J}_{\infty}(g)).$$

However  $\widehat{J}_{\infty}(g) = g\widehat{B}_{\infty}(g)$  and  $\widehat{B}_{\infty}(g) = \widehat{B}(0) + g\widehat{B}_{\infty}^{(1)}(g)$  follows from (3.39) and (3.28), where  $\widehat{B}_0(g) := (b_{i,j}(g))_{1 \le i,j \le 2}$ . The hypotheses that  $\widehat{B}(0)$  is self-adjoint and  $b_{1,2}(0) \ne 0$  ensure that fact that  $\widehat{B}(0)$  has two distinct eigenvalues  $\mu_1, \mu_2$ , hence  $\sigma(\widehat{B}_{\infty}(g)) = \{\mu_1(g), \mu_2(g)\}$  holds with  $g \to \mu_j(g)$  holomorphic in a neighbourhood of 0 due to the usual perturbation theory presented in Section 2.4.

# 3.2. SCHRIEFFER–WOLFF APPROXIMATION

We will define  $\widehat{J}_{\infty}(g) \oplus \widetilde{J}_{\infty}(g)$  as the limit of a sequence of operators  $(J_l(g))_{l=0}^{\infty}$  of the form

$$J_l(g) = D + gB_l(g).$$
 (3.9)

Using induction with respect to l we begin by setting  $J_0(g) := J(g)$ . Assume now that  $J_l(g)$  is given by (3.9) and

$$B_l(g) = \begin{pmatrix} \widehat{B}_l(g) & R_l^+(g) \\ R_l^-(g) & \widetilde{B}_l(g) \end{pmatrix}$$
(3.10)

where  $\widehat{B}_l: \widehat{V} \to \widehat{V}, \quad \widetilde{B}_l: \widetilde{V} \to \widetilde{V}, \quad R_l^+: \widehat{V} \to \widetilde{V}, \quad R_l^-: \widetilde{V} \to \widehat{V}.$  Then

$$B_l(g) = \widehat{B}_l(g) \oplus \widetilde{B}_l(g) + R_l(g)$$
(3.11)

and  $R_l(g) = (r_{i,j,l}(g))_{i,j=1}^n$  satisfies  $r_{i,j,l} = 0$  if  $(i,j) \in [1,\hat{n}]^2 \cup [\hat{n}+1,n]^2$ . We define  $Q_l(g) = (q_{i,j,l}(g))_{i,j=1}^n$  by the formula

$$q_{i,j,l}(g) = \begin{cases} \frac{\mathrm{i}\,r_{i,j,l}(g)}{d_i - d_j} & \text{if } (i,j) \notin [1,\widehat{n}]^2 \cup [\widehat{n} + 1,n]^2, \\ 0 & \text{otherwise} \end{cases}$$
(3.12)

and observe that (3.12) ensures the equality

$$[D, iQ_l(g)] = -R_l(g), (3.13)$$

where [A, A'] = AA' - A'A is the commutator of  $A, A' \in \mathcal{L}(\mathbb{C}^n)$ . Then we define

$$J_{l+1}(g) = e^{-igQ_l(g)} J_l(g) e^{igQ_l(g)}.$$
(3.14)

**Notation 3.3.** If  $g \in \mathbb{C} \setminus \{0\}$  and  $A, Q \in \mathcal{L}(\mathbb{C}^n)$ , then we denote

$$F_{gQ}(A) := e^{-igQ} A e^{igQ} - A, \qquad (3.15)$$

$$\widetilde{F}_{gQ}(A) := \frac{1}{g} \Big( e^{-igQ} A e^{igQ} - A - g[A, iQ] \Big).$$
(3.16)

Using these notations we can express the equality (3.14) in the form

$$J_{l+1}(g) = D + g \left( B_l(g) + [D, iQ_l(g)] + F_l(g) \right)$$
(3.17)

with

$$F_{l}(g) = \tilde{F}_{gQ_{l}(g)}(D) + F_{gQ_{l}(g)}(B_{l}(g))$$
(3.18)

and combining (3.17) with (3.11)–(3.13) we obtain

$$J_{l+1} = D + g \left( \widehat{B}_l \oplus \widetilde{B}_l + F_l \right).$$
(3.19)

### 3.3. NORM ESTIMATES

# Notation 3.4.

(a) We denote by  $\|\cdot\|_0$  the norm defined on  $\widehat{V}$  by

$$||x||_0 = \langle x, x \rangle^{1/2} \quad \text{for} \quad x \in \widehat{V}.$$
(3.20)

(b) We denote by  $\|\cdot\|'$  the norm defined on  $\widetilde{V}$  by

$$||x||' = \max_{i} |x_i| \quad \text{for} \quad x \in \widetilde{V}.$$
(3.21)

(c) We denote by  $\|\cdot\|$  the norm defined on  $\mathbb{C}^n$  by the formula

$$\|\widehat{x} + \widetilde{x}\| := \max\{\|\widehat{x}\|_0, \|\widetilde{x}\|'\} \quad \text{for} \quad \widehat{x} \in \widehat{V}, \ \widetilde{x} \in \widetilde{V},$$
(3.22)

and  $||A|| = \sup\{||Ax|| : ||x|| = 1\}$  is the corresponding operator norm.

# **Lemma 3.5.** If A and $Q \in \mathcal{L}(\mathbb{C}^n)$ , then

$$||F_{gQ}(A)|| \le e^{2||gQ||} ||[A, gQ]||, \qquad (3.23)$$

$$\|\widetilde{F}_{gQ}(A)\| \le \frac{1}{2} e^{2\|gQ\|} \|[[A,Q],gQ]\|.$$
(3.24)

*Proof.* Using integral remainders of the Taylor's formula for  $s \to e^{-isgQ}Ae^{isgQ}$  we get

$$F_{gQ}(A) = \int_{0}^{1} e^{-isgQ} [A, igQ] e^{isgQ} ds, \qquad (3.25)$$

$$\widetilde{F}_{gQ}(A) = \int_{0}^{1} e^{-isgQ} [[A, iQ], igQ] e^{isgQ} (1-s) ds.$$
(3.26)

We complete the proof using  $\|e^{isgQ}\| \le e^{\|gQ\|}$ .

**Lemma 3.6.** Assume that  $C_0 > 0$  is fixed large enough. Then there exists  $\varepsilon_0 > 0$  such for  $g \in \mathbb{D}(0, \varepsilon_0)$  and  $m \in \mathbb{N}$  one has

$$||R_m(g)|| \le C_0^{1+3m} |g^m|, \qquad (3.27)$$

$$\|\widehat{B}_{m}(g) \oplus \widetilde{B}_{m}(g) - \widehat{B}_{m-1}(g) \oplus \widetilde{B}_{m-1}(g)\| \le C_{0}^{1+3m} |g^{m}|, \qquad (3.28)$$

where for m = 0 we take  $\widehat{B}_{m-1} = 0$  and  $\widetilde{B}_{m-1} = 0$  in (3.28).

*Proof.* First of all we can assume that  $C_0 > 0$  is large enough to ensure

$$||B(g)|| \le C_0 \text{ for } g \in \mathbb{D}(0, \varepsilon_0) \tag{3.29}$$

for a certain  $\varepsilon_0 > 0$  and

$$||Q_l(g)|| \le C_0 ||R_l(g)||.$$
(3.30)

Let  $l \in \mathbb{N}$  be such that the estimates (3.27)–(3.28) hold if  $m \leq l$ . Further on we assume that  $|g| \leq \varepsilon_0$  and  $2C_0^3 \varepsilon_0 \leq 1$ . Then one has  $C_0^{1+3m} |g^m| \leq 2^{-m} C_0$  and

$$||R_m(g)|| \le 2^{-m} C_0 \text{ if } m \le l,$$
 (3.31)

$$\|\widehat{B}_m(g) \oplus \widetilde{B}_m(g) - \widehat{B}_{m-1}(g) \oplus \widetilde{B}_{m-1}(g)\| \le 2^{-m} C_0 \text{ if } m \le l.$$
(3.32)

Using (3.32) we can estimate  $\|\widehat{B}_l(g) \oplus \widetilde{B}_l(g)\|$  by

$$\sum_{m=0}^{l} \|\widehat{B}_m(g) \oplus \widetilde{B}_m(g) - \widehat{B}_{m-1}(g) \oplus \widetilde{B}_{m-1}(g)\| \le 2C_0,$$

hence

$$||B_l(g)|| \le ||\widehat{B}_l(g) \oplus \widetilde{B}_l(g)|| + ||R_l(g)|| \le 3C_0.$$
(3.33)

Next we observe that (3.19) gives

$$F_l = B_{l+1} - \widehat{B}_l \oplus \widetilde{B}_l = \begin{pmatrix} \widehat{B}_{l+1} - \widehat{B}_l & R_{l+1}^+ \\ R_{l+1}^- & \widetilde{B}_{l+1} - \widetilde{B}_l \end{pmatrix}$$
(3.34)

and in order to prove that (3.27)–(3.28) hold for m = l + 1 it suffices to check the estimate

$$||F_l(g)|| \le C_0^{4+3l} |g^{l+1}|.$$
(3.35)

However using A = D and  $[D, igQ_l] = -gR_l$  in (3.24), we can estimate

$$\|\widetilde{F}_{gQ_{l}}(D)\| \leq \frac{1}{2} e^{2\|gQ_{l}(g)\|} \|[R_{l}(g), gQ_{l}(g)]\| \leq e \|R_{l}(g)\| \|gQ_{l}(g)\|$$
(3.36)

due to  $2||gQ_l(g)|| \le 2\varepsilon_0 C_0 ||R_l(g)|| \le 2\varepsilon_0 C_0^2 \le 1$  and  $||[A, A']|| \le 2||A|| ||A'||$ . Similarly, (3.23) allows us to estimate

$$\|F_{gQ}(B_l(g))\| \le 2e \|B_l(g)\| \|gQ_l(g)\|.$$
(3.37)

Combining (3.36), (3.37) with (3.18) and assuming  $C_0 \ge 7e$ , we get

$$\begin{aligned} \|F_l(g)\| &\leq \mathbf{e}(\|R_l(g)\| + 2\|B_l(g)\|)|g| C_0\|R_l(g)| \\ &\leq 7\mathbf{e}C_0^2|g| \|R_l(g)\| \leq C_0^3|g| \|R_l(g)\|. \end{aligned}$$

Thus (3.27) for m = l gives (3.35), completing the proof of (3.27)–(3.28) for m = l + 1.

# 3.4. END OF THE PROOF OF PROPOSITION 3.1

For  $m, l \in \mathbb{N}$  satisfying m < l we denote

$$U_{m,l}(g) = e^{igQ_m} \dots e^{igQ_{l-1}}.$$
(3.38)

Let  $\varepsilon_0 > 0$  be small enough. Due to Lemma 3.6 we can define

$$\widehat{B}_{\infty}(g) = \lim_{l \to \infty} \widehat{B}_l(g), \quad \widetilde{B}_{\infty}(g) = \lim_{l \to \infty} \widetilde{B}_l(g)$$
(3.39)

and the convergence is uniform with respect to  $g \in \mathbb{D}(0, \varepsilon_0)$ . Thus denoting

$$\widehat{J}_{\infty}(g) := \widehat{D} + g\widehat{B}_{\infty}(g), \quad \widetilde{J}_{\infty}(g) := \widetilde{D} + g\widetilde{B}_{\infty}(g),$$

we find that  $J_l(g) = U_{0,l}(g)^{-1}J(g)U_{0,l}(g)$  converges to  $\widehat{J}_{\infty}(g) \oplus \widetilde{J}_{\infty}(g)$  uniformly on  $\mathbb{D}(0, \varepsilon_0)$ . We still assume  $g \in \mathbb{D}(0, \varepsilon_0)$ . Then

$$||U_{m,l}(g)|| \le \exp\left(\sum_{m\le i< l} ||gQ_i(g)||\right) \le C_1$$

and  $||U_{0,l}(g) - U_{0,m}|| \le C_1 ||U_{m,l}(g) - I||$  can be estimated by

$$C_2 \sum_{m \le i < l} \| e^{igQ_i(g)} - I \| \le C_3 \sum_{m \le i < l} \| gQ_i(g) \| \le 2^{-m} C_4 |g|.$$

Thus we can define  $U_{\infty}(g)$  as the limit of  $U_{0,l}(g)$  as  $l \to \infty$  and  $||U_{\infty}(g) - I|| \leq C|g|$ holds if C > 0 is fixed large enough. Assuming moreover  $|g| \leq 1/(2C)$  we conclude that  $U_{0,l}(g)^{-1}$  converges to  $U_{\infty}(g)^{-1}$  as  $l \to \infty$  and  $J_{\infty}(g) = U_{\infty}(g)^{-1}J(g)U_{\infty}(g)$ .

## 4. FINITE DIMENSIONAL VERSION OF THEOREM 1.3

#### 4.1. INTRODUCTION

In this section we consider  $J(g) = D + gB \in \mathcal{L}(\mathbb{C}^n)$ , assuming that  $D = \text{diag}(d_i)_{i=1}^n$ and B is a tridiagonal matrix,

$$B = \begin{pmatrix} b'_1 & b_1 & 0 & 0 & \cdots \\ b_1 & b'_2 & b_2 & 0 & \cdots \\ 0 & b_2 & b'_3 & b_3 & \cdots \\ 0 & 0 & b_3 & b'_4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}.$$
(4.1)

We fix  $k \in \mathbb{N}^*$  and assume

$$d_{k+1} = d_k = 0 \neq d_i \text{ for } i \notin \{k, k+1\} \text{ and } b'_{k+1} = -b'_k.$$
 (4.2)

Next we remark that a suitable permutation of the canonical basis allows us to work in the framework of Section 3 with  $\hat{n} = 2$ , i.e. we can decompose

$$\mathbb{C}^n = \widehat{V} \oplus \widetilde{V} \text{ with } \widehat{V} := \operatorname{span}\{e_k, e_{k+1}\} \text{ and } \widetilde{V} := \widehat{V}^{\perp}.$$
(4.3)

Then  $D = \widehat{D} \oplus \widetilde{D}$  holds with  $\widehat{D} = \text{diag}(0,0), \ \widetilde{D} = \text{diag}(d_i)_{i \notin \{k, k+1\}}$  and

$$B = \begin{pmatrix} \widehat{B} & R^+ \\ R^- & \widetilde{B} \end{pmatrix} \quad \text{with} \quad \widehat{B} = \begin{pmatrix} b'_k & b_k \\ b_k & -b'_k \end{pmatrix}.$$
(4.4)

We observe that  $\sigma(\widehat{B}) = \{-\mu, \mu\}$  holds with

$$\mu := \left(b_k^2 + b_k'^2\right)^{1/2}.\tag{4.5}$$

Due to Corollary 3.2 the spectrum of J(g) near 0 is composed of two eigenvalues

$$\lambda_k(J(g)) = -\mu g + O(g^2), \quad \lambda_{k+1}(J(g)) = \mu g + O(g^2), \tag{4.6}$$

holomorphic on  $\mathbb{D}(0,\varepsilon)$  for a certain  $\varepsilon > 0$ . In the remaining of the section we prove the following proposition.

**Proposition 4.1.** Assume that  $J(g) = \text{diag}(d_i)_{i=1}^n + gB$  holds with B given by (4.1) and real entries  $(d_i)_{i=1}^n$ ,  $(b_i)_{i=1}^{n-1}$ ,  $(b'_i)_{i=1}^n$  satisfying (4.2). Let  $\mu_k = \mu$  be given by (4.5) and let  $(\beta'_i)_{i=1}^n$ ,  $(\gamma_i)_{i=1}^n$ ,  $(\gamma'_i)_{i=1}^n$  be given by (1.14)–(1.18). Assume moreover that  $\rho > 0$ satisfies (1.19)-(1.21).

- (i) If  $-\rho < g < \rho$  and  $g \neq 0$ , then (1.22) and (1.23) hold.
- (ii) The expansion formula (1.24) holds with  $\mu_{k+1} = -\mu_k = -(b_k^2 + b'_k^2)^{1/2}$ . (iii) The coefficients satisfy  $|c_{k+j,\nu}| \le \mu_k \rho^{1-\nu}$  for j = 0, 1 and (1.25) holds.

*Proof.* The proof is given in four steps described in Sections 4.2–4.5.

# 4.2. FIRST STEP OF THE PROOF OF PROPOSITION 4.1

### Notation 4.2.

(a) For  $m \in \mathbb{N}$  we define the linear subspace

$$V_m := \operatorname{span}\{e_{k+i}\}_{i \in [-m, m+1]}.$$
(4.7)

We observe that dim  $V_m = \min\{2m+2, n\}$  and  $V_0 = \widehat{V}$ . (b) We define  $\Pi_m$  as the orthogonal projector on  $V_m$  and  $\Pi'_m := I - \Pi_m$ .

Reasoning as in Section 3.2 we denote  $J_l(g) = D + gB_l$  where  $B_0 = B$  and (3.14) holds with  $Q_l \in \mathcal{L}(\mathbb{C}^n)$  satisfying (3.13). Then using notations 4.2, we can write

$$\widehat{B}_l \oplus \widetilde{B}_l = \Pi_0 B_l \Pi_0 + \Pi'_0 B_l \Pi'_0.$$

$$\tag{4.8}$$

In this section we consider (3.14) with l = 0 and as before  $F_0(g)$  is given by the equality

$$J_1(g) = D + g\big(\widehat{B} \oplus \widetilde{B} + F_0(g)\big). \tag{4.9}$$

Moreover,  $R_0 = B - \widehat{B} \oplus \widetilde{B}$  satisfies  $R_0 = \prod_1 R_0 \prod_1$  and has the form

$$R_{0} = \begin{pmatrix} 0 & b_{k-1} & 0 & 0 \\ b_{k-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & b_{k+1} \\ 0 & 0 & b_{k+1} & 0 \end{pmatrix} \oplus \mathbb{O}_{V_{1}^{\perp}}$$
(4.10)

where  $\mathbb{O}_{V_{1}^{\perp}}$  is the zero map on  $V_{1}^{\perp}$ . Thus  $Q_{0} = \prod_{1} Q_{0} \prod_{1}$  has the form

$$Q_0 = \begin{pmatrix} 0 & \bar{q}_{k-1} & 0 & 0 \\ q_{k-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & \bar{q}_{k+1} \\ 0 & 0 & q_{k+1} & 0 \end{pmatrix} \oplus \mathbb{O}_{V_1^{\perp}}$$
(4.11)

with

$$q_{k+1} := -ib_{k+1}/d_{k+2}, \quad q_{k-1} := ib_{k-1}/d_{k-1}.$$
 (4.12)

We consider  $\widehat{V} \oplus \widetilde{V}$  with the norm defined by (3.20)–(3.22). Then

$$||R_0|| = \max\{|b_{k-1}|, |b_{k+1}|\},$$
(4.13)

$$||Q_0|| = \gamma'_k = \max\{|q_{k-1}|, |q_{k+1}|\}.$$
(4.14)

Lemma 4.3. We have the estimate

$$|F_0(g)|| \le \gamma_k \gamma'_k |g| e^{2\gamma'_k |g|}.$$
 (4.15)

*Proof.* Due to  $Q_0 = \prod_1 Q_0 \prod_1$  we have

$$[B, Q_0] = [B^{\circ}, Q_0] \quad \text{with} \quad B^{\circ} := B - \Pi'_1 B \Pi'_1 \tag{4.16}$$

and  $||F_0(g)||$  can be estimated by

$$e^{2\|gQ_0\|}(\frac{1}{2}\|[R_0, gQ_0]\| + \|B^{\circ}, gQ_0]\|) \le e^{2\|gQ_0\|}\|gQ_0\|(\|R_0\| + 2\|B^{\circ}\|).$$
(4.17)

Due to (4.13)-(4.14), (4.15) follows from (4.17) if we show that

$$||R_0|| + 2||B^\circ|| \le \gamma_k. \tag{4.18}$$

However  $B^{\circ} = R_0 + \Pi_0 B^{\circ} \Pi_0 + \Pi'_0 B^{\circ} \Pi'_0$  holds with  $\Pi_0 B^{\circ} \Pi_0 = \widehat{B} \oplus \mathbb{O}_{V_0^{\perp}}$  and

$$\Pi_0' B^{\circ} \Pi_0' = \mathbb{O}_{V_0} \oplus \begin{pmatrix} 0 & b_{k-2} & 0 & 0 \\ b_{k-2} & b'_{k-1} & 0 & 0 \\ 0 & 0 & b'_{k+2} & b_{k+2} \\ 0 & 0 & b_{k+2} & 0 \end{pmatrix} \oplus \mathbb{O}_{V_2^{\perp}},$$

hence

$$\|\Pi'_0 B^{\circ} \Pi'_0\| \le \max\{|b_{k-2}| + |b'_{k-1}|, |b_{k+2}| + |b'_{k+2}|\}.$$
(4.19)

In order to obtain (4.18), we observe that  $||B^{\circ}||$  can be estimated by

$$||R_0|| + ||\Pi_0 B^{\circ} \Pi_0 + \Pi_0' B^{\circ} \Pi_0'|| = ||R_0|| + \max\{||\Pi_0 B^{\circ} \Pi_0||, ||\Pi_0' B^{\circ} \Pi_0'||\}$$
(4.20)

and it remains to use (4.13), (4.19) and  $\|\Pi_0 B^\circ \Pi_0\| = \mu$  (the last equality is due to the fact  $\widehat{B}$  is unitarily equivalent to diag  $(-\mu, \mu)$  and  $\|\cdot\|_0$  is the euclidean norm).  $\Box$ 

### 4.3. SECOND STEP OF THE PROOF OF PROPOSITION 4.1

**Lemma 4.4.** Assume that  $\lambda \in \mathbb{C} \setminus \{-g\mu, g\mu\}$  is such that  $|\lambda| \leq 2\mu\rho$ , where  $\rho$  satisfies (1.19)–(1.21). Denote

$$J_{1,0}(g) := g\widehat{B} \oplus (\widetilde{D} + g\widetilde{B}).$$
(4.21)

Then

$$\|(J_{1,0}(g) - \lambda)^{-1}\| \le \max\left\{\frac{1}{|\lambda - g\mu|}, \frac{1}{|\lambda + g\mu|}, \frac{1}{\rho\mu}\right\}.$$
(4.22)

*Proof.* We denote  $\widetilde{J}(g) := \widetilde{D} + g\widetilde{B}$  and observe that

$$(J_{1,0}(g) - \lambda)^{-1} = (g\widehat{B} - \lambda)^{-1} \oplus (\widetilde{J}(g) - \lambda)^{-1}.$$
(4.23)

Since  $\widehat{B}$  is unitarily equivalent to diag  $(-\mu, \mu)$  and  $\|\cdot\|_0$  is the Euclidean norm, the corresponding operator norm

$$\|(g\hat{B} - \lambda)^{-1}\|_{0} = \max\left\{\frac{1}{|\lambda - g\mu|}, \frac{1}{|\lambda + g\mu|}\right\}.$$
(4.24)

Due to (4.24) and (4.23), the proof of (4.22) will be complete if we show

$$\|(\widetilde{J}(g) - \lambda)^{-1}\|' \le \frac{1}{\rho\mu},$$
(4.25)

where we used  $\|\cdot\|'$  to denote the operator norm induced by the norm (3.21).

Since (1.20) ensures  $2\rho\mu \le |d_i| - 2\rho\mu \le |d_i| - |\lambda| \le |d_i - \lambda|$  for all  $i \notin \{k, k+1\}$ ,

$$\|(\widetilde{D} - \lambda)^{-1}\|' = \max_{i \notin \{k, k+1\}} \frac{1}{|d_i - \lambda|} \le \frac{1}{2\rho\mu}.$$
(4.26)

Let us introduce  $\widetilde{A}(\lambda) := (\widetilde{D} - \lambda)^{-1} \widetilde{B}$ . We claim that (4.25) follows from

$$\|g\widetilde{A}(\lambda)\|' \le \frac{1}{2}.\tag{4.27}$$

Indeed, we obtain (4.25) using (4.26)–(4.27) to estimate the norm of the resolvent series  $\tilde{c}$ 

$$(\widetilde{J}(g) - \lambda)^{-1} = \sum_{\nu \in \mathbb{N}} \left( -g\widetilde{A}(\lambda) \right)^{\nu} (\widetilde{D} - \lambda)^{-1}.$$

In order to prove (4.27) we observe that  $\widetilde{A}(\lambda) = (\widetilde{\alpha}_{i,j}(\lambda))_{i,j\notin\{k,k+1\}}$  is the matrix with

$$\widetilde{\alpha}_{i,j}(\lambda) = \langle e_i, (D-\lambda)^{-1}Be_j \rangle = \langle (D-\bar{\lambda})^{-1}e_i, Be_j \rangle = \frac{\langle e_i, Be_j \rangle}{d_i - \lambda}$$

and since  $V_0^{\perp}$  is equipped with the norm (3.21),

$$\|\widetilde{A}(\lambda)\|' \le \max_{i \notin \{k,k+1\}} \sum_{j \notin \{k,k+1\}} |\widetilde{\alpha}_{i,j}(\lambda)| = \max_{i \notin \{k,k+1\}} \frac{\beta'_i}{|d_i - \lambda|}.$$
 (4.28)

However, if  $i \notin \{k, k+1\}$ , then (1.19) ensures  $|d_i| \ge 2\rho(\mu + \beta'_i)$  and consequently

$$|d_i - \lambda| \ge |d_i| - |\lambda| \ge |d_i| - 2\rho\mu \ge 2\rho\beta'_i.$$

Thus the right hand side of (4.28) can be estimated by  $\frac{1}{2\rho}$  and  $\|g\widetilde{A}(\lambda)\|' \leq \frac{|g|}{2\rho} \leq \frac{1}{2}$ .  $\Box$ 

# 4.4. THIRD STEP OF THE PROOF OF PROPOSITION 4.1

- **Lemma 4.5.** Assume that  $\rho$  satisfies (1.19)–(1.21).
- (a) If  $|g| \leq \rho$ , then

$$\partial \mathbb{D}(0, 2\rho\mu) \cap \sigma(J(g)) = \emptyset \tag{4.29}$$

(b) Assume that  $\theta \in [0, 2\pi[$  and  $0 < t \le \rho$ . If  $g = te^{i\theta}$  then

$$\partial \mathbb{D}(\pm \mu \rho e^{i\theta}, \mu \rho) \cap \sigma(J(g)) = \emptyset.$$
(4.30)

*Proof.* (a) If  $|\lambda| = 2\mu\rho$  then  $|\lambda \pm g\mu| \ge \mu\rho \ge \mu|g|$  and Lemma 4.4 ensures

$$\|(J_{1,0}(g) - \lambda)^{-1}\| \le 1/(|g|\mu).$$
(4.31)

Denote  $A_{\lambda}(g) := F_0(g)(J_{1,0}(g) - \lambda)^{-1}$ . Then (4.31), (4.15), (1.21) and  $|g| \leq \rho$ , ensure

$$||gA_{\lambda}(g)|| \le ||gF_{0}(g)|| ||(J_{1,0}(g) - \lambda)^{-1}|| \le |g|^{2}\gamma_{k}'\gamma_{k}e^{2\rho\gamma_{k}'}/(\mu|g|) < 1,$$
(4.32)

hence  $\lambda \notin \sigma(J_1(g)) = \sigma(J(g))$  follows from the convergence of the resolvent series

$$(J_1(g) - \lambda)^{-1} = (J_{1,0}(g) - \lambda)^{-1} \sum_{\nu \in \mathbb{N}^*} (-gA_\lambda(g))^\nu$$
(4.33)

(b) If  $\theta \in [0, 2\pi[$  and  $0 < t \le \rho$ , then

dist 
$$(\pm t\mu e^{i\theta}, e^{i\theta}\partial \mathbb{D}(\pm \mu\rho, \mu\rho)) = dist (\pm t\mu, \partial \mathbb{D}(\pm \mu\rho, \mu\rho)) = t\mu.$$
 (4.34)

If  $\lambda \in \partial \mathbb{D}(\pm \mu \rho e^{i\theta}, \mu \rho) = e^{i\theta} \partial \mathbb{D}(\pm \mu \rho, \mu \rho)$  and  $g = t e^{i\theta}$ , then  $|\lambda \pm g\mu| \ge |g|\mu$  holds due to (4.34). Then Lemma 4.4 gives (4.31), (4.32)–(4.33) and  $\lambda \notin \sigma(J_1(g)) = \sigma(J(g))$ .  $\Box$ 

#### 4.5. END OF THE PROOF OF PROPOSITION 4.1

Lemma 4.5(a) allows us to define on  $\mathbb{D}(0, \rho)$  the projectors

$$P(g) = \frac{1}{2\pi i} \oint_{\partial \mathbb{D}(0,2\rho\mu)} (\lambda - J(g))^{-1} d\lambda$$
(4.35)

with rank  $P(g) = \operatorname{rank} P(0) = 2$ , i.e J(g) has at most two eigenvalues in  $\mathbb{D}(0, 2\rho\mu)$ . Our next step is to show that for  $\kappa \in \{1, -1\}$  one has

$$\operatorname{card}\left(\sigma(J(|g|e^{i\theta})) \cap \mathbb{D}(\kappa\rho\mu e^{i\theta},\rho\mu)\right) = 1 \text{ if } 0 < |g| < \rho.$$
(4.36)

Let us choose  $\varepsilon > 0$  small enough. Then the property (4.36) holds if  $0 < |g| \le \varepsilon$  due to (4.6). Due to Lemma 4.5(b), the property (4.30) holds for  $g \in K_{\varepsilon,\theta} := [\varepsilon, \rho] e^{i\theta}$ . Since  $K_{\varepsilon,\theta}$  is compact,  $K_{\varepsilon,\theta}$  has an open connected neighbourhood  $\mathcal{U}_{\varepsilon,\theta}$  such that the property (4.30) still holds for  $g \in \mathcal{U}_{\varepsilon,\theta}$ . Thus

$$P_{\pm}(g) = \frac{1}{2\pi i} \oint_{\partial \mathbb{D}(\pm \rho \mu e^{i\theta}, \rho \mu)} (\lambda - J(g))^{-1} d\lambda$$
(4.37)

are two holomorphic families of projectors defined on  $\mathcal{U}_{\varepsilon,\theta}$ . However (4.6) ensures the fact that rank  $P_{\pm}(g) = 1$  if  $|g| \leq \varepsilon$ , hence rank  $P_{\pm}(g) = 1$  for all  $g \in \mathcal{U}_{\varepsilon,\theta}$ . Thus,

$$g \in \mathcal{U}_{\varepsilon,\theta} \implies \sigma(J(g)) \cap \mathbb{D}(\pm \rho \mu \mathrm{e}^{\mathrm{i}\theta}, \rho \mu) = \{\lambda_{\pm}(g)\}$$

where  $g \to \lambda_{\pm}(g) = \operatorname{tr} J(g) P_{\pm}(g)$  are two distinct eigenvalues of J(g) if  $g \neq 0$ . Thus

$$\sigma(J(g)) \cap \mathbb{D}(0, 2\rho\mu) = \{\lambda_+(g), \lambda_-(g)\}$$
(4.38)

and  $\lambda_+(g)$  (respectively  $\lambda_-(g)$ ) is the holomorphic extension of  $\lambda_{k+1}(J(g))$ (respectively  $\lambda_k(J(g))$ ) defined on  $\mathbb{D}(0,\rho)$ . Since  $\eta(g) = \lambda_{k+1}(J(g)) - \mu g$  is holomorphic  $\mathbb{D}(0,\rho) \to \mathbb{D}(0,\mu\rho)$ , Lemma 2.3 ensures  $|c_{k+j,\nu}| \leq \mu \rho^{1-\nu}$  and (1.25) holds for j = 1. Similarly, using  $\eta(g) = \lambda_k(J(g)) + \mu g$  we obtain (1.25) for j = 0.

# 5. BLOCK APPROXIMATION

### 5.1. INTRODUCTION

Let J(g) be as in Proposition 4.1 and  $c_{k,\nu}$ ,  $c_{k+1,\nu}$  the coefficients of the series (1.24) for  $\lambda_k(J(g))$  and  $\lambda_{k+1}(J(g))$  respectively. In this section we fix  $\nu \in \mathbb{N}^*$  and claim that  $c_{k,\nu}$  and  $c_{k+1,\nu}$  depend only on the entries  $\{(d_{k+i}, b'_{k+i})\}_{i\in[-\nu/2, 1+\nu/2]}$  and  $\{b_{k+i}\}_{i\in[-\nu/2,\nu/2]}$ . In other words, the computation of  $c_{k,\nu}$  and  $c_{k+1,\nu}$ , can be reduced to the computation of the corresponding coefficients for the operator defined by the sub-matrix of the matrix J(g), namely by the block  $(\langle e_{k+i}, J(g)e_{k+j}\rangle)_{(i,j)\in[-\nu/2, 1+\nu/2]^2}$ . For this purpose we prove

**Proposition 5.1.** The coefficients  $c_{k,\nu}$  and  $c_{k+1,\nu}$  depend only on  $\prod_l J \prod_l$ , where  $l \in \mathbb{N}$  is such that  $2l + 1 \geq \nu$ .

*Proof.* The proof is given in three steps described in Sections 5.2–5.4.

### 5.2. GENERALIZED KATO–TEMPLE ESTIMATE

#### Notation 5.2.

(a) Since  $\mu$  and  $-\mu$  are two distinct eigenvalues of  $\widehat{B}_l(0) = \widehat{B}$ , choosing  $\varepsilon_0 > 0$ small enough we ensure the fact that for  $g \in [-\varepsilon_0, \varepsilon_0]$  the matrix  $\widehat{B}_l(g)$  has two eigenvalues  $\widehat{\lambda}_{0,l}(g), \widehat{\lambda}_{1,l}(g)$ , satisfying

$$\widehat{\lambda}_{0,l}(g) = -\mu + O(g), \quad \widehat{\lambda}_{1,l}(g) = \mu + O(g).$$
(5.1)

For  $j \in \{0,1\}$  we denote  $\lambda_{j,l}(g) := g \widehat{\lambda}_{j,l}(g)$ . Thus (5.1) implies

$$\lambda_{0,l}(g) = -\mu g + O(g^2), \quad \lambda_{1,l}(g) = \mu g + O(g^2)$$
 (5.2)

(b) We denote  $J_{l,0}(g) := g\widehat{B}_l(g) \oplus (\widetilde{D} + g\widetilde{B}_l(g))$ . Thus

$$\sigma(J_{l,0}(g)) = \{\lambda_{0,l}(g), \lambda_{1,l}(g)\} \cup \sigma(D + gB_l(g))$$

$$(5.3)$$

holds due to  $\sigma(g\widehat{B}_l(g)) = \{\lambda_{0,l}(g), \lambda_{1,l}(g)\}.$ 

These notations allow us to deduce immediately the following estimate

$$\lambda_{k+j}(J(g)) = \lambda_{j,l}(g) + O(g^{l+1}) \quad (j = 0, 1).$$
(5.4)

Indeed, if  $0 < \rho' < \min_{i \notin \{k,k+1\}} |d_i|$ , then choosing  $\varepsilon_0 > 0$  small enough we ensure

$$\sigma(J_{l,0}(g)) \cap [-\rho', \rho'] = \{\lambda_{0,l}(g), \lambda_{1,l}(g)\} \quad \text{if} \quad g \in [-\varepsilon_0, \varepsilon_0]$$
(5.5)

and  $J_l(g) - J_{l,0}(g) = gR_l(g) = O(g^{l+1})$  implies

$$\operatorname{dist}(\sigma(J_l(g))), \sigma(J_{l,0}(g))) = O(g^{l+1})$$
(5.6)

due to the min-max principle. If  $g \in [-\varepsilon_0, \varepsilon_0]$  then combining (5.6) with (5.5) and Proposition 4.1, we get

$$dist(\{\lambda_k(J(g)), \lambda_{k+1}(J(g))\}, \{\lambda_{0,l}(g), \lambda_{1,l}(g)\}) = O(g^{l+1})$$
(5.7)

and it is clear that (5.4) follows from (5.7) and (5.2).

However writing an analogical decomposition in the case of perturbations of a simple eigenvalue, we find that the standard Kato–Temple inequality (see [18, Theorem 3.8]) ensures error estimates  $O(g^{2l+2})$  for the eigenvalue perturbed by the terms of order  $O(g^{l+1})$  in the k-th line and k-th column. The following lemma states an analogical result in our framework.

**Lemma 5.3.** For j = 0, 1, let  $\lambda_{j,l}(g)$  be defined as in Notation 5.2. Then

$$\lambda_{k+j}(J(g)) = \lambda_{j,l}(g) + O(g^{2l+2}).$$
(5.8)

Proof. Step 1. We claim that  $\widehat{B}_{l+1} = \widehat{B}_l + O(g^{2l+1})$ . Since  $J_l = D + g(\widehat{B}_l \oplus \widetilde{B}_l + R_l)$  holds with  $R_l(g) = O(g^l)$  and  $J_{l+1}$  can be expressed by

$$e^{-igQ_l}J_le^{igQ_l} = J_l + ig[J_l, Q_l] - \frac{g^2}{2!}[[J_l, Q_l], Q_l] - i\frac{g^3}{3!}[[J_l, Q_l], Q_l], Q_l] + \dots$$
(5.9)

with  $[D, iQ_l] = -R_l$  and  $Q_l(g) = O(g^l)$ , we obtain  $J_{l+1} = D + gB_{l+1}$  with

$$B_{l+1} = \widehat{B}_l \oplus \widetilde{B}_l + [\widehat{B}_l \oplus \widetilde{B}_l, igQ_l] + O(g^{2l+1}).$$

Therefore

$$\widehat{B}_{l+1} \oplus \mathbb{O}_{V_0^\perp} = \Pi_0 B_{l+1} \Pi_0 = \widehat{B}_l \oplus \mathbb{O}_{V_0^\perp} + \Pi_0 [\widehat{B}_l \oplus \widetilde{B}_l, igQ_l] \Pi_0 + O(g^{2l+1})$$

and we obtain  $\widehat{B}_{l+1} = \widehat{B}_l + O(g^{2l+1})$  if we check that

$$\Pi_0[B_l \oplus B_l, Q_l]\Pi_0 = 0. \tag{5.10}$$

However  $\mathbb{O}_{V_0^{\perp}} \oplus \widetilde{B}_l = \Pi'_0 B_l \Pi'_0$  and obviously  $\Pi_0[\Pi'_0 B_l \Pi'_0, Q_l] \Pi_0 = 0$ . To complete the proof of (5.10) we observe that  $\widehat{B}_l \oplus \mathbb{O}_{V_0^{\perp}} = \Pi_0 B_l \Pi_0$  and

$$\Pi_0[\Pi_0 B_l \Pi_0, Q_l]\Pi_0 = \Pi_0[\Pi_0 B_l \Pi_0, \Pi_0 Q_l \Pi_0]\Pi_0 = 0,$$

where the last equality follows from the fact that  $\Pi_0 Q_l \Pi_0 = 0$ .

Step 2. We claim that  $\widehat{B}_{l+i} = \widehat{B}_l + O(g^{2l+1})$  holds for all  $i \in \mathbb{N}$ . Indeed, reasoning by induction we can repeat the proof from Step 1. Step 3. To complete the proof of (5.8) we observe that (5.4) ensures

$$\lambda_{k+j}(J(g)) = \lambda_{j,2l+1}(g) + O(g^{2l+2})$$
(5.11)

and choosing  $\varepsilon_0 > 0$  small enough we obtain

$$|\lambda_{j,2l+1}(g) - \lambda_{j,l}(g)| \le ||g(\widehat{B}_{2l+1}(g) - \widehat{B}_{l}(g))|| = O(g^{2l+2})$$

for  $-\varepsilon_0 < g < \varepsilon_0$  due to the min-max principle.

#### 5.3. SECOND STEP OF THE PROOF OF PROPOSITION 5.1

**Lemma 5.4.** For every  $l \in \mathbb{N}$  one has

$$(J_l - J)\Pi'_{l+1} = 0 = \Pi'_{l+1}(J_l - J),$$
(5.12)

$$R_l \Pi'_{l+1} = 0 = \Pi'_{l+1} R_l.$$
(5.13)

*Proof.* If l = 0, then (5.12) holds due to  $J_0 = J$  and (5.13) holds due to (4.10). Reasoning by induction we fix  $l \ge 1$  and assume that (5.12)–(5.13) hold with l - 1 instead of l. However  $R_{l-1}\Pi'_l = 0 = \Pi'_l R_{l-1}$  implies

$$Q_{l-1}\Pi'_l = 0 = \Pi'_l Q_{l-1} \tag{5.14}$$

and consequently  $e^{igQ_{l-1}}\Pi'_m = \Pi'_m$  if  $m \ge l$ . Therefore

$$J_{l}\Pi'_{l+1} = e^{-igQ_{l-1}}J_{l-1}e^{igQ_{l-1}}\Pi'_{l+1} = e^{-igQ_{l-1}}J_{l-1}\Pi'_{l+1} = e^{-igQ_{l-1}}J\Pi'_{l+1}, \quad (5.15)$$

where the last equality is due to (5.12) with l-1 instead of l. However a tridiagonal matrix J satisfies  $J\Pi'_{l+1} = \Pi'_l J\Pi'_{l+1}$  and

$$e^{-igQ_{l-1}}J\Pi'_{l+1} = e^{-igQ_{l-1}}\Pi'_{l}J\Pi'_{l+1} = \Pi'_{l}J\Pi'_{l+1} = J\Pi'_{l+1}.$$
(5.16)

Combining (5.15) with (5.16) we get  $(J_l - J)\Pi'_{l+1} = 0$ . Similarly we get  $\Pi'_{l+1}(J_l - J) = 0$ , hence (5.12) holds and it remains to prove that (5.12) implies (5.13).

Since  $B_l = (J_l - D)/g$ , it is clear that (5.12) implies

$$(B_l - B)\Pi'_{l+1} = 0 = \Pi'_{l+1}(B_l - B).$$
(5.17)

Using

$$R_l = B_l - \Pi_0 B_l \Pi_0 - \Pi_0' B_l \Pi_0' \tag{5.18}$$

and  $(B_l - B)\Pi'_{l+1} = 0$  we get

$$(R_l - R_0)\Pi'_{l+1} = (B_l - B)\Pi'_{l+1} - \Pi_0(B_l - B)\Pi'_{l+1}\Pi_0 - \Pi'_0(B_l - B)\Pi'_{l+1}\Pi'_0 = 0.$$
  
Similarly  $\Pi'_{l+1}(B_l - B) = 0$  implies  $\Pi'_{l+1}(R_l - R_0) = 0.$ 

### 5.4. END OF THE PROOF OF PROPOSITION 5.1

Let J(g) = D + gB and  $J^{\circ}(g) = D^{\circ} + gB^{\circ}$  be two operators satisfying the hypotheses of Proposition 4.1 and assume that

$$\Pi_i (J(g) - J^{\circ}(g)) \Pi_i = 0 \tag{5.19}$$

holds for a certain  $i \in \mathbb{N}$ . Then (1.24) holds and similarly

$$\lambda_{k+j}(J^{\circ}(g)) = -\mu_{k+j}g + \sum_{\nu=2}^{\infty} c_{k+j,\nu}^{\circ}g^{\nu}.$$
(5.20)

Let  $J_l = D + gB_l$ ,  $J_l^{\circ} = D^{\circ} + gB_l^{\circ}$  be constructed similarly as before. Then it suffices to show

$$\Pi_i (B_i(g) - B_i^{\circ}(g)) \Pi_i = 0.$$
(5.21)

Indeed, (5.21) implies  $\widehat{B}_i(g) = \widehat{B}_i^{\circ}(g)$  and Lemma 5.3 ensures

$$\lambda_{k+j}(J(g)) - \lambda_{k+j}(J^{\circ}(g)) = O(g^{2i+2})$$
 for  $j = 0, 1,$ 

hence  $c_{k+j,\nu} = c_{k+j,\nu}^{\circ}$  holds if  $\nu \leq 2i+1$ .

It remains to prove that (5.19) implies (5.21). Using induction we will prove that

$$\Pi_i (J_l - J_l^\circ) \Pi_i = 0 \tag{5.22}$$

holds for l = 0, ..., i. Since  $J_0 = J$  and  $J_0^{\circ} = J^{\circ}$ , (5.22) holds for l = 0 due to (5.19).

Let us assume that (5.22) holds for a certain  $l \leq i - 1$ . Then

$$\Pi_i (B_l - B_l^{\circ}) \Pi_i = 0 \tag{5.23}$$

follows from (5.22) due to  $B_l - B_l^{\circ} = g^{-1}(J_l - J_l^{\circ})$ . Moreover, using (5.23) and

$$R_l - R_l^{\circ} = B_l - B_l^{\circ} - \Pi_0 (B_l - B_l^{\circ}) \Pi_0 - \Pi_0' (B_l - B_l^{\circ}) \Pi_0'$$
(5.24)

we get  $\Pi_i (R_l - R_l^{\circ}) \Pi_i = 0$ . Therefore Lemma 5.4 and  $l \leq i - 1$  ensure

$$R_l - R_l^{\circ} = \Pi_{l+1} (R_l - R_l^{\circ}) \Pi_{l+1} = \Pi_{l+1} \Pi_i (R_l - R_l^{\circ}) \Pi_i \Pi_{l+1} = 0,$$

hence  $R_l = R_l^{\circ}$  and consequently  $Q_l = Q_l^{\circ}$ . Moreover  $l \leq i - 1$  implies that the operators  $e^{igQ_l} = e^{igQ_l^{\circ}}$  commute with  $\Pi_i$ , hence

$$\Pi_i (J_{l+1} - J_{l+1}^{\circ}) \Pi_i = e^{-igQ_l} \Pi_i (J_l - J_l^{\circ}) \Pi_i e^{igQ_l} = 0,$$

i.e. (5.22) holds for l+1 if  $l \leq i-1$ . Thus (5.22) holds for  $l = 1, \ldots, i$  and using (5.22) with l = i we get (5.21), completing the proof of Proposition 5.1.

# 6. PROOF OF THEOREM 1.2 AND 1.3

### 6.1. INTRODUCTION

In this section we show how to deduce Theorem 1.2 and 1.3 from finite dimensional results proved earlier. In both cases we use the min-max principle and deduce the estimates for coefficients of the Taylor series using a finite dimensional block and Proposition 5.1. For this reason we assume  $g \in \mathbb{R}$ .

Our approach uses the operators  $\widehat{J}_n^+(g)$  and  $\widehat{J}_n^-(g) \in \mathcal{L}(\mathbb{C}^n)$ , given by the formula

$$\widehat{J}_n^{\pm}(g) := \operatorname{diag}(d_i)_{i=1}^n + g\widehat{B}_n^{\pm}, \qquad (6.1)$$

where  $\widehat{B}_n^+$ ,  $\widehat{B}_n^-$  are the following tridiagonal matrices

$$\widehat{B}_{n}^{\pm} := \begin{pmatrix} b_{1}' & b_{1} & 0 & & & 0 \\ b_{1} & b_{2}' & b_{2} & & & & \\ 0 & b_{2} & b_{3}' & & & & \\ & \ddots & \ddots & \ddots & & & \\ & & & b_{n-3}' & b_{n-3} & 0 & 0 \\ & & & & b_{n-3}' & b_{n-2}' & 0 \\ & & & & 0 & b_{n-2} & b_{n-2}' & 0 \\ & & & & 0 & b_{n-2} & b_{n-1}' & b_{n-1} \\ 0 & & & 0 & 0 & b_{n-1} & b_{n}' \pm |b_{n}| \end{pmatrix}$$
(6.2)

In order to prove Theorem 1.2 we show that  $\lambda_k(J(g))$  is well approximated by  $\lambda_k(J_n^{\pm}(g))$  for large n. In order to prove Theorem 1.3 we show moreover that  $\lambda_{k+1}(J(g))$  is well approximated by  $\lambda_{k+1}(J_n^{\pm}(g))$  for large n.

### 6.2. AUXILIARY OPERATOR INEQUALITY

**Lemma 6.1.** Let  $B^{\circ}$  be the linear map defined on  $\ell_{\text{fin}}^2$  by the formula

$$B^{\circ}e_{i} = b_{i}^{\circ}e_{i+1} + b_{i-1}^{\circ}e_{i-1}, \qquad (6.3)$$

where  $(b_i^{\circ})_{i=1}^{\infty}$  are real and by convention  $b_{i-1}^{\circ} = 0$  if i = 1. Then for  $x \in \ell_{\text{fin}}^2$  one has

$$\pm \langle x, B^{\circ} x \rangle \leq \langle x, \operatorname{diag}(|b_i^{\circ}| + |b_{i-1}^{\circ}|)_{i=1}^{\infty} x \rangle.$$
(6.4)

*Proof.* If  $x = (x_j)_{j=1}^{\infty}$  then

$$B^{\circ}x = (b_{j}^{\circ}x_{j+1} + b_{j-1}^{\circ}x_{j-1})_{j=1}^{\infty}$$

and

$$\langle x, B^{\circ}x \rangle = \sum_{j} b_{j}^{\circ}x_{j+1}\bar{x}_{j} + \sum_{i} b_{i-1}^{\circ}x_{i-1}\bar{x}_{i}.$$
 (6.5)

Writing i = j + 1 in (6.5), we can estimate  $|\langle x, B^{\circ}x \rangle|$  by

$$\sum_{j} 2|b_{j}^{\circ}| |x_{j+1}x_{j}| \leq \sum_{j} |b_{j}^{\circ}| (|x_{j+1}|^{2} + |x_{j}|^{2}).$$
(6.6)

To complete the proof we write the right hand side of (6.6) in the form

$$\sum_{i} |b_{i}^{\circ}||x_{i+1}|^{2} + \sum_{j} |b_{j}^{\circ}||x_{j}|^{2} = \sum_{j} (|b_{j-1}^{\circ}| + |b_{j}^{\circ}|)|x_{j}|^{2}$$
(6.7)

and observe that the quantity (6.7) is equal to the right hand side of (6.4).

### 6.3. APPLYING THE MIN-MAX PRINCIPLE

**Notation 6.2.** If *L* is a self-adjoint, bounded from below operator with discrete spectrum, then  $(\hat{\lambda}_i(L))_{i=1}^{\infty}$  denotes the sequence of eigenvalues of *L*, enumerated in non-decreasing order, counting multiplicities, i.e.  $\hat{\lambda}_1(L) \leq \hat{\lambda}_2(L) \leq \ldots$ 

Let  $n \in \mathbb{N}$  be fixed large enough. We decompose  $b_i = b_{n,i} + b_{n,i}^{\circ}$ ,  $b'_i = b'_{n,i} + b'_{n,i}^{\circ}$ , where the sequences  $(b_{n,i})_{i=1}^{\infty}$ ,  $(b'_{n,i})_{i=1}^{\infty}$  are the cut-off given by

$$b_{n,i} = \begin{cases} b_i & \text{if } i < n, \\ 0 & \text{if } i \ge n \end{cases} \text{ and } b'_{n,i} = \begin{cases} b'_i & \text{if } i \le n, \\ 0 & \text{if } i > n. \end{cases}$$

Consequently  $B = B_n + B_n^{\circ}$  holds if the operators  $B_n$ ,  $B_n^{\circ}$  are given by

 $B_n e_i = b'_{n,i} e_i + b_{n,i} e_{i+1} + b_{n,i-1} e_{i-1}, \quad B_n^{\circ} e_i = b'_{n,i} e_i + b_{n,i} e_{i+1} + b_{n,i-1} e_{i-1}$ 

and Lemma 6.1 ensures

$$\pm \langle x, B_n^{\circ} x \rangle \le \langle x, D_n^{\circ} x \rangle, \tag{6.8}$$

where we denoted  $D_n^{\circ} := \operatorname{diag}(d_{i,n}^{\circ})_{i \in \mathbb{N}*}$  with

$$d_{i,n}^{\circ} = \begin{cases} 0 & \text{if } i < n, \\ |b_n| & \text{if } i = n, \\ \beta'_i & \text{if } i > n \end{cases}$$

and  $\beta'_i = |b'_i| + |b_i| + |b_{i-1}|$ . Next we consider

$$J_{n}^{\pm}(g) := D + gB_{n} \pm gD_{n}^{\circ} = \widehat{J}_{n}^{\pm}(g) \oplus \operatorname{diag}(d_{i} \pm g\beta_{i}')_{i=n+1}^{\infty},$$
(6.9)

where  $\widehat{J}_n^{\pm}(g)$  is the linear map acting on span $\{e_1, \ldots, e_n\}$  by means of the matrix (6.2).

If i > n > k + 1 and  $\rho$  satisfies (1.19), then  $\rho \beta'_i \leq \frac{1}{2} d_i$  and

$$d_i \pm g\beta'_i \ge \frac{1}{2}d_i \text{ if } -\rho < g < \rho, \tag{6.10}$$

hence  $J^{\pm}(g)$  are self-adjoint, bounded from below and have discrete spectrum. Moreover

$$\begin{cases} \langle x, J_n^-(g)x \rangle \le \langle x, J(g)x \rangle \le \langle x, J_n^+(g)x \rangle & \text{if } g \ge 0, \\ \langle x, J_n^+(g)x \rangle \le \langle x, J(g)x \rangle \le \langle x, J_n^-(g)x \rangle & \text{if } g \le 0 \end{cases}$$
(6.11)

and the min-max principle ensures

. .

$$\begin{cases} \widehat{\lambda}_i(J_n^-(g)) \le \widehat{\lambda}_i(J(g)) \le \widehat{\lambda}_i(J_n^+(g)) & \text{if } g \ge 0, \\ \widehat{\lambda}_i(J_n^+(g)) \le \widehat{\lambda}_i(J(g)) \le \widehat{\lambda}_i(J_n^-(g)) & \text{if } g \le 0. \end{cases}$$
(6.12)

### 6.4. END OF THE PROOF OF THEOREM 1.3

Let us fix  $\rho > 0$  satisfying (1.19)–(1.21) and assume that n > k + 2. We claim that  $\widehat{J}_n^{\pm}(g)$  satisfies the assumptions of Proposition 4.1 for the same value  $\rho$ . Indeed, the entries of  $\widehat{J}_n^{\pm}(g)$  are the same as the entries of J(g) except the fact that  $b'_n$  is replaced by  $b'_n \pm |b_n|$ ,  $b_i$  are replaced by 0 for  $i \ge n$  and  $b'_i$  are replaced by 0 for i > n. Thus the values of  $\beta'_i$  can only decrease after these modifications and the right hand side of (1.19) can only increase. Applying Proposition 4.1 to  $\widehat{J}_n^{\pm}(g)$  we obtain

$$[-2\mu_k\rho, 2\mu_k\rho] \cap \sigma(\widehat{J}_n^{\pm}(g)) = \{\lambda_k(\widehat{J}_n^{\pm}(g)), \lambda_{k+1}(\widehat{J}_n^{\pm}(g))\},$$
(6.13)

where the eigenvalue  $\lambda_{k+j}(\widehat{J}_n^{\pm}(g))$  is simple if  $-\rho < g < \rho, g \neq 0$ , and satisfies

$$\lambda_{k+j}(\widehat{J}_n^{\pm}(g)) = -\mu_{k+j}g + \sum_{\nu=2}^{\infty} c_{k+j,n,\nu}^{\pm}g^{\nu}$$
(6.14)

with  $|c_{k+j,n,\nu}^{\pm}| \leq \mu_k \rho^{1-\nu}$  for j = 0, 1. We observe that (6.9) ensures

$$\sigma(J_n^{\pm}(g)) = \sigma(\widehat{J}_n^{\pm}(g)) \cup \{d_i \pm g\beta_i' : i > n\}.$$
(6.15)

Let  $n_0$  be such that  $d_i \ge 0$  for  $i \ge n_0$  and assume  $n \ge n_0$ . Then (1.19) ensures  $2\rho\mu_k < d_i - \rho\beta'_i$  for i > n and

$$[-2\mu_k\rho, 2\mu_k\rho] \cap \sigma(J_n^{\pm}(g)) = [-2\mu_k\rho, 2\mu_k\rho] \cap \sigma(\widehat{J}_n^{\pm}(g)), \tag{6.16}$$

hence (1.22)–(1.23) hold with  $J_n^{\pm}(g)$  instead of J(g) and  $\lambda_{k+j}(J_n^{\pm}(g)) = \lambda_{k+j}(\widehat{J}_n^{\pm}(g))$ for j = 0, 1. Let us fix  $0 < g < \rho$ . Using (1.22)–(1.23) with  $J_n^{\pm}$  instead of J, we get

$$\widehat{\lambda}_{l-1}(J_n^+) < -2\rho\mu_k \le \widehat{\lambda}_l(J_n^+) < 0 < \widehat{\lambda}_{l+1}(J_n^+) \le 2\rho\mu_k < \widehat{\lambda}_{l+2}(J_n^+), \tag{6.17}$$

where  $l \in \mathbb{N}^*$  is such that  $\lambda_k(J_n^+(g)) = \widehat{\lambda}_l(J_n^+(g))$  and due to the continuity of  $g \to \widehat{\lambda}_l(J_n^+(g))$ , one has  $l = 1 + \operatorname{card}\{i \in \mathbb{N}^* : d_i < d_k\}$ . Similarly

$$\widehat{\lambda}_{l-1}(J_n^-) < -2\rho\mu_k \le \widehat{\lambda}_l(J_n^-) < 0 < \widehat{\lambda}_{l+1}(J_n^-) \le 2\rho\mu_k < \widehat{\lambda}_{l+2}(J_n^-).$$
(6.18)

Thus  $\lambda_{k+j}(J_n^{\pm}(g)) = \widehat{\lambda}_{l+j}(J_n^{\pm}(g))$  for j = 0, 1, and

$$\widehat{\lambda}_{l-1}(J) < -2\rho\mu_k \le \widehat{\lambda}_l(J) < 0 < \widehat{\lambda}_{l+1}(J) \le 2\rho\mu_k < \widehat{\lambda}_{l+2}(J)$$
(6.19)

follows from (6.12). Using (6.19) we obtain (1.22)–(1.23) with  $\lambda_{k+j}(J(g)) = \widehat{\lambda}_{l+j}(J(g))$  for j = 0, 1, and (6.14) ensures

$$\lambda_{k+j}(J(g)) \le \lambda_{k+j}(J_n^+(g)) \le -\mu_{k+j}g + \sum_{2 \le \nu \le N} c_{k+j,n,\nu}^+ g^\nu + C_N |g|^{N+1}, \quad (6.20)$$

$$\lambda_{k+j}(J(g)) \ge \lambda_{k+j}(J_n^-(g)) \ge -\mu_{k+j}g + \sum_{2 \le \nu \le N} c_{k+j,n,\nu}^- g^\nu - C_N |g|^{N+1}$$
(6.21)

for j = 0, 1.

We observe that Proposition 5.1 applied to  $\hat{J}_n^+$  and  $\hat{J}_n^-$  give

$$n > k + \nu \implies c^+_{k+j,n,\nu} = c^-_{k+j,n,\nu}$$
(6.22)

due to the fact that  $\Pi_l(\hat{J}_n^+ - \hat{J}_n^-)\Pi_l = 0$  holds if k + 1 + l < n. Therefore taking n > k + N in (6.20)–(6.21) we obtain

$$\lambda_{k+j}(J(g)) = -\mu_{k+j}g + \sum_{2 \le \nu \le N} c^+_{k+j,n,\nu}g^\nu + O(|g|^{N+1}).$$
(6.23)

Since Proposition 4.1 ensures  $|c_{k+j,n,\nu}^+| \le \mu_k \rho^{1-\nu}$ , we find that for every  $N \in \mathbb{N}^*$ ,

$$\lambda_{k+j}(J(g)) = -\mu_{k+j}g + \sum_{2 \le \nu \le N} c_{k+j,\nu}g^{\nu} + O(|g|^{N+1})$$
(6.24)

holds with  $|c_{k+j,\nu}| \leq \mu_k \rho^{1-\nu}$ . Similar inequalities can be written when  $-\rho < g < 0$ . Thus  $g \to \lambda_{k+j}(J(g))$  is real analytic, its convergence radius is greater or equal  $\rho$  and the remainder estimates (1.25) follow as in the proof of Lemma 2.3.

### 6.5. END OF THE PROOF OF THEOREM 1.2

If  $\rho$  satisfies (1.7), then (6.10) should be replaced by the fact that one can choose a constant  $C = C(\rho)$  large enough to ensure

$$i \ge C \Rightarrow d_i \pm g\beta_i \ge cd_i \tag{6.25}$$

where  $c = c(\rho) > 0$  and  $g \in [-\rho, \rho]$ . It remains to fix  $n_0 \in \mathbb{N}$  large enough and use a similar reasoning under the additional assumption that  $n \ge n_0$ .

#### 7. COMPUTATIONS OF COEFFICIENTS

### 7.1. INTRODUCTION

To begin we recall well known situation of matrices  $2 \times 2$ .

### Notation 7.1.

- (a) Further on we denote  $d_i^0(g) := d_i + gb'_i$ .
- (b) We denote by  $d_i^1(g)$ ,  $d_{i+1}^1(g)$  the eigenvalues of

$$A_i(g) := \begin{pmatrix} d_i^0(g) & gb_i(g) \\ gb_i(g) & d_{i+1}^0(g) \end{pmatrix}.$$
 (7.1)

(c) For  $t \in \mathbb{R}$  we denote  $\mathfrak{U}(t) := \begin{pmatrix} \cos t & -\sin t \\ \sin t & \cos t \end{pmatrix}$ .

If  $d_i \neq d_{i+1}$  then  $d_i^0(g) \neq d_{i+1}^0(g)$  holds for small |g| and the direct calculation gives

$$\begin{cases} d_i^1(g) = d_i^0(g) - r_i(g), \\ d_{i+1}^1(g) = d_{i+1}^0(g) + r_i(g) \end{cases}$$
(7.2)

with

$$r_i(g) = \frac{g^2 b_i^2}{d_{i+1}^0(g) - d_i^0(g)} - \frac{g^4 b_i^4}{(d_{i+1}^0(g) - d_i^0(g))^3} + O(g^6).$$
(7.3)

Moreover

$$\mathfrak{U}(g\theta_i(g))A_i(g)\mathfrak{U}(g\theta_i(g))^{-1} = \operatorname{diag}(d_i^1(g), d_{i+1}^1(g))$$
(7.4)

holds with

$$\theta_i(g) := \frac{1}{2g} \arctan\left(\frac{2gb_i}{d_i^0(g) - d_{i+1}^0(g)}\right).$$
(7.5)

Using  $\arctan t = \sin t + O(t^3) = t + O(t^3)$  and  $\cos t = 1 - \frac{t^2}{2} + O(t^4)$ , we obtain

$$\theta_i(g) = \frac{b_i}{d_i^0(g) - d_{i+1}^0(g)} + O(g^2), \tag{7.6}$$

$$\sin(g\theta_i(g)) = \frac{gb_i}{d_i^0(g) - d_{i+1}^0(g)} + O(g^3), \tag{7.7}$$

$$\cos(g\theta_i(g)) = 1 - \frac{g^2 b_i^2}{2(d_i^0(g) - d_{i+1}^0(g))^2} + O(g^4).$$
(7.8)

# 7.2. PROOF OF THEOREM 1.5

We consider the first similarity transformation using

$$\mathbf{e}^{\mathbf{i}gQ_0} = \begin{pmatrix} c & -s & 0 & 0\\ s & c & 0 & 0\\ 0 & 0 & \dot{c} & -\dot{s}\\ 0 & 0 & \dot{s} & \dot{c} \end{pmatrix} \oplus I_{V_1^{\perp}}, \tag{7.9}$$

where

$$s(g) := \sin(g\theta_{k-1}(g))), \quad c(g) := \cos(g\theta_{k-1}(g))),$$
 (7.10)

$$\dot{s}(g) := \sin(g\theta_{k+1}(g))), \quad \dot{c}(g) := \cos(g\theta_{k+1}(g)))$$
(7.11)

with  $\theta_i(g)$  given by (7.5). The corresponding similarity transformation allows us to diagonalize the blocks  $A_{k-1}(g)$  and  $A_{k+1}(g)$ . Indeed, the direct calculation shows that the matrix  $J_1(g) = e^{-igQ_0(g)}J(g)e^{igQ_0(g)}$  equals

$$\begin{pmatrix} d_{k-2}^{0} & gb_{k-2}c & -gb_{k-2}s & 0 & 0 & 0 \\ * & d_{k-1}^{0} - r_{k-1} & 0 & gb_{k}s\dot{c} & -gb_{k}s\dot{s} & 0 \\ * & * & d_{k}^{0} + r_{k-1} & gb_{k}c\dot{c} & -gb_{k}c\dot{s} & 0 \\ * & * & * & d_{k+1}^{0} - r_{k+1} & 0 & gb_{k+2}\dot{s} \\ * & * & * & * & * & d_{k+2}^{0} + r_{k+1} & gb_{k+2}\dot{c} \\ * & * & * & * & * & * & d_{k+3}^{0} \end{pmatrix}, \quad (7.12)$$

where the stars correspond to the symmetric entries and we have not written the terms which are the same as in J(g). Then  $J_1(g) = D + g(\widehat{B}_1 \oplus \widetilde{B}_1 + R_1)$  holds with

$$gR_1(g) = \begin{pmatrix} 0 & 0 & -gb_{k-2}s & 0 & 0 & 0 \\ * & 0 & 0 & gb_ks\dot{c} & 0 & 0 \\ * & * & 0 & 0 & -gb_kc\dot{s} & 0 \\ * & * & * & * & 0 & 0 & gb_{k+2}\dot{s} \\ * & * & * & * & * & 0 & 0 \\ * & * & * & * & * & * & 0 \end{pmatrix} \oplus \mathbb{O}_{V_2^{\perp}}$$
(7.13)

and

$$g\widehat{B}_{1}(g) = \begin{pmatrix} d_{k}^{0} + r_{k-1} & gb_{k}c\dot{c} \\ gb_{k}c\dot{c} & d_{k+1}^{0} - r_{k+1} \end{pmatrix} = gB_{k}^{1}(g) + O(g^{4}),$$
(7.14)

where  $B_k^1(g)$  is given by (1.33). Indeed, if  $\hat{b}_k^1$ ,  $b_k^1$ ,  $b_{k+1}^1$  are given by (1.30)–(1.32), then using (7.8) we find  $b_k c\dot{c} = \hat{b}_k^1 + O(g^3)$  and using (7.3) we find  $d_k^0 + r_{k-1} = gb_k^1 + O(g^4)$ ,  $d_{k+1}^0 - r_{k+1} = gb_{k+1}^1 + O(g^4)$ . Due to (7.14) the difference between eigenvalues of  $g\hat{B}_1(g)$  and  $gB_k^1(g)$  is  $O(g^4)$  and Theorem 1.5 follows from (5.8) with l = 1.

(iii) Let  $gR_1$  be given by (7.13) and  $Q_1$  obtained from (3.12). Then (5.9) gives

$$J_2 = J_1 + [D, igQ_1] + [g(\widehat{B}_1 \oplus \widetilde{B}_1 + R_1), igQ_1] + \frac{1}{2}[[D, igQ_1], igQ_1] + O(g^5)$$

due to  $R_1 = O(g)$  and  $Q_1 = O(g)$ . Moreover  $[D, igQ_1] = -gR_1$  allows us to simplify

$$J_2 = D + g(\tilde{B}_1 \oplus \hat{B}_1) + [g(\hat{B}_1 \oplus \tilde{B}_1), igQ_1] + \frac{1}{2}[gR_1, igQ_1] + O(g^5)$$

and  $\widehat{B}_2 - \widehat{B}_1$  depends only on  $\frac{1}{2}[gR_1, igQ_1] + O(g^5)$  due to (5.10). Finally we find that

$$g\widehat{B}_{2}(g) = \begin{pmatrix} d_{k}^{0} + r_{k-1} + p_{k} & gb_{k}c\dot{c} \\ gb_{k}c\dot{c} & d_{k+1}^{0} - r_{k+1} + p_{k+1} \end{pmatrix} + O(g^{5})$$
(7.15)

holds with

$$p_k := \langle e_k, \frac{1}{2} [gR_1, igQ_1] e_k \rangle = -g^2 s^2 b_{k-2}^2 / d_{k-2} - g^2 \dot{s}^2 b_k^2 / d_{k+2},$$
(7.16)

$$p_{k+1} := \langle e_{k+1}, \frac{1}{2} [gR_1, igQ_1] e_{k+1} \rangle = -g^2 s^2 b_k^2 / d_{k-1} - g^2 \dot{s}^2 b_{k+2}^2 / d_{k+3}.$$
(7.17)

Then (5.8) ensures  $\lambda_{k+j}(J(g)) = \lambda_{j,2}(g) + O(g^6)$ , where  $\{\lambda_{j,2}(g)\}_{j=0,1}$  are the eigenvalues of  $g\hat{B}_2$  and using (7.15)–(7.17) we obtain  $\lambda_{j,2}(g)$  with the error  $O(g^5)$ .

## 7.3. PROOF OF THEOREM 1.4

Let J(g) be as in Theorem 1.4. We apply the approach of Section 3 in the case  $\hat{n} = 1$ . Consider first the case when  $b'_i = 0$  for all *i*. Under this assumption we can check by induction that the functions  $g \to \langle e_i, J_l(g)e_j \rangle$  are even when i - j is even and odd when i - j is odd. Since  $\lambda_k(J(g)) = \langle e_k, J_l(g)e_k \rangle + O(g^{2l})$ , it is clear that  $g \to \lambda_k(J(g))$  is even. Further on we consider a general case.

# Notation 7.2.

- (a) We write  $d_i^0(g) := d_i + gb'_i$  and recall the assumption  $d_k^0 = 0$ . (b) For  $l \in \mathbb{N}$  we denote  $V_l := \operatorname{span}\{e_{k+j}\}_{-l \leq j \leq l}$  and  $\widehat{V} := V_0 = \mathbb{C}e_k$ .

We begin by diagonalizing  $A_{k-1}(g)$  (see Notation 7.1). For this purpose we use

$$U(g) := \begin{pmatrix} c & -s & 0\\ s & c & 0\\ 0 & 0 & 1 \end{pmatrix} \oplus I_{V_1^{\perp}}.$$

with c and s given by (7.10). Then  $U(g)^{-1}J(g)U(g)$  equals

$$\begin{pmatrix} d_{k-2}^{0} & gb_{k-2}c & -gb_{k-2}s & 0\\ * & d_{k-1}^{0} - r_{k-1} & 0 & gb_{k}s\\ * & * & r_{k-1} & gb_{k}c\\ * & * & * & d_{k+1}^{0} \end{pmatrix}$$
(7.18)

and using  $d_k^0(g) = 0$  in (7.3) we get

$$r_{k-1}(g) = -\frac{g^2 b_{k-1}^2}{d_{k-1}^0(g)} + \frac{g^4 b_{k-1}^4}{d_{k-1}^0(g)^3} + O(g^6).$$
(7.19)

The next step consists in diagonalizing the block  $\begin{pmatrix} r_{k-1} & gb_kc \\ * & d^0_{k+1} \end{pmatrix}$  using

$$\ddot{U}(g) := \begin{pmatrix} 1 & 0 & 0 \\ 0 & \ddot{c} & -\ddot{s} \\ 0 & \ddot{s} & \ddot{c} \end{pmatrix} \oplus I_{V_1^{\perp}},$$
(7.20)

where we denoted  $\ddot{c} := \cos(g\ddot{\theta}), \ \ddot{s} := \sin(g\ddot{\theta})$  with

$$\ddot{\theta} := \frac{1}{2g} \arctan\left(\frac{2gb_k c(g)}{r_{k-1}(g) - d_{k+1}^0(g)}\right) = -\frac{b_k}{d_{k+1}^0(g)} + O(g^2).$$
(7.21)

Then we find that  $J_1 := \ddot{U}^{-1} U^{-1} J U \ddot{U}$  has the form

$$\begin{pmatrix} d_{k-2}^{0} & gb_{k-2}c & -gb_{k-2}s\ddot{c} & gb_{k-2}s\ddot{s} & 0 \\ * & d_{k-1}^{0} - r_{k-1} & gb_{k}s\ddot{s} & gb_{k}s\ddot{c} & 0 \\ * & * & r_{k-1} - \tilde{r}_{k} & 0 & gb_{k+1}\ddot{s} \\ * & * & * & d_{k+1}^{0} + \tilde{r}_{k} & gb_{k+1}\ddot{c} \\ * & * & * & * & d_{k+2}^{0} \end{pmatrix}$$
(7.22)

with

$$\widetilde{r}_k(g) = \frac{g^2 b_k^2 c^2}{d_{k+1}^0 - r_{k-1}} - \frac{g^4 b_k^4 c^4}{(d_{k+1}^0 - r_{k-1})^3} + O(g^6).$$
(7.23)

We claim that the quantity (7.23) can be written in the form

$$\frac{g^2 b_k^2}{d_{k+1}^0(g)} - \frac{g^4 b_k^2 b_{k-1}^2}{d_{k+1}^0(g) d_{k-1}^0(g)^2} - \frac{g^4 b_k^2 b_{k-1}^2}{d_{k+1}^0(g)^2 d_{k-1}^0(g)} - \frac{g^4 b_k^4}{d_{k+1}^0(g)^3} + O(g^6).$$
(7.24)

Indeed, using (7.19) and  $c^2 = 1 - g^2 \theta_{k-1}^2 + O(g^4)$ , we get

$$\frac{c^2}{d_{k+1}^0 - r_{k-1}} = \frac{1 - g^2 (b_{k-1}/d_{k-1}^0)^2 + O(g^4)}{d_{k+1}^0 + g^2 b_{k-1}^2 / d_{k-1}^0 + O(g^4)}$$
$$= \frac{1}{d_{k+1}^0} \left(1 - \left(\frac{gb_{k-1}}{d_{k-1}^0}\right)^2 - \frac{g^2 b_{k-1}^2}{d_{k+1}^0 d_{k-1}^0}\right) + O(g^4)$$

and multiplying this expression by  $g^2 b_k^2$  we get the first three terms of (7.24).

Let us denote  $d_{k,1} := r_{k-1} - \tilde{r}_k$ . Then reasoning similarly as before we can use two rotations to diagonalize the blocks

$$\begin{pmatrix} d_{k-2}^0 & -gb_{k-2}s\ddot{c} \\ * & d_{k,1} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} d_{k,1} & gb_{k+1}\ddot{s} \\ * & d_{k+2}^0 \end{pmatrix}.$$

This similarity gives  $J_2 = D + gB_2$  with  $B_2 = (d_{k,2}) \oplus \widetilde{B}_2 + R_2$  and

$$d_{k,2} = d_{k,1} + \frac{g^2 b_{k-2}^2 s^2 \ddot{c}^2}{d_{k,1} - d_{k-2}^0} - \frac{g^2 b_{k+1}^2 \ddot{s}^2}{d_{k+2}^0 - d_{k,1}} + O(g^6).$$

Using  $s = g\theta_{k-1} + O(g^3)$ , (7.21) and  $d_{k,1} = O(g^2)$ , we get

$$d_{k,2} = d_{k,1} - \frac{g^4 b_{k-1}^2 b_{k-2}^2}{d_{k-1}^0(g)^2 d_{k-2}^0(g)} - \frac{g^4 b_k^2 b_{k+1}^2}{d_{k+1}^0(g)^2 d_{k+2}^0(g)} + O(g^6).$$
(7.25)

If we express  $d_{k,1} := r_{k-1} - \tilde{r}_k$  using (7.19) and (7.24), we find that the quantity (7.25) gives the right hand side of (1.28). To complete the proof it remains to observe that  $||gR_2(g)|| = O(g^3)$  ensures

$$\lambda_k(J(g)) = d_{k,2}(g) + O(g^6)$$

either by the usual Kato–Temple estimate or by repeating the proof of Lemma 5.3 in this case.

#### REFERENCES

- P.K. Aravind, J.O. Hirschfelder, Two-state systems in semiclassical and quantized fields, J. Phys. Chem. 88 (1984), no. 21, 4788–4801.
- [2] S.S. Bharadwaj, R.U. Haq, T.A. Wan, An explicit method for Schrieffer-Wolff transformation, arXiv:1901.08617.
- [3] A. Boutet de Monvel, L. Zielinski, On the spectrum of the quantum Rabi model, [in:] Analysis as a Tool in Mathematical Physics, Springer, 2020, 183–193.
- [4] D. Braak, Q.-H. Chen, M.T. Batchelor, E. Solano, Semi-classical and quantum Rabi models: in celebration of 80 years, J. of Physics A 49 (2016), 300301.

- [5] P.A. Cojuhari, J. Janas, Discreteness of the spectrum for some unbounded Jacobi matrices, Acta Sci. Math. (Szeged) 73 (2007), no. 3–4, 649–667.
- [6] M. Frasca, Third-order correction to localization in a two-level driven system, Phys. Rev. B 71 (2005), 073301.
- [7] S. He, Q.-H. Chen, X.-Z. Ren, T. Liu, K.-L. Wang, First-order corrections to the rotating-wave approximation in the Jaynes-Cummings model, Phys. Rev. A 86 (2012), no. 3, 033837.
- [8] S. He, Y.-Y. Zhang, Q.-H. Chen, X.-Z. Ren, T. Liu, K.-L. Wang, Unified analytical treatments of qubit-oscillator systems, Chinese Physics B 22 (2013), no. 6, 064205.
- J. Janas, S. Naboko, Infinite Jacobi matrices with unbounded entries: asymptotics of eigenvalues and the transformation operator approach, SIAM J. Math. Anal. 36 (2004), no. 2, 643–658.
- [10] E.T. Jaynes, F.W. Cummings, Comparison of quantum and semiclassical radiation theories with application to the beam maser, Proc. IEEE 51 (1963), no. 1, 89–109.
- T. Kato, Perturbation Theory for Linear Operators, Springer-Verlag, Berlin-Heidelberg--New York, 1995.
- [12] D.J. Klein, Degenerate perturbation theory, J. Chem. Phys. 61 (1974), no. 3, 786.
- P.O. Lödwing, A note on the quantum-mechanical perturbation theory, J. Chem. Phys. 19 (1951), no. 11, 1396.
- [14] I.I. Rabi, On the process of space quantization, Phys. Rev. 49 (1936), 324.
- [15] I.I. Rabi, Space quantization in a gyrating magnetic field, Phys. Rev. 51 (1937), 652.
- [16] M. Reed, B. Simon, Methods of Modern Mathematical Physics. IV. Analysis of Operators, Academic Press, 1978.
- [17] F. Rellich, J. Berkowitz, Perturbation Theory of Eigenvalue Problems, Gordon and Breach, 1969.
- [18] Y. Saad, Numerical Methods for Large Eigenvalue Problems, Classics in Applied Mathematics, vol. 66, Manchester University Press, 1992.
- [19] M.O. Scully, M.S. Zubairy, Quantum Optics, Cambridge, 1997.
- [20] J.H. Shirley, Solution of the Schrödinger equation with a Hamiltonian periodic in time, Phys. Rev. 138 (1965), B979.
- [21] É.A. Tur, Jaynes-Cummings model: solution without rotating wave approximation, Optics and Spectroscopy 89 (2000), no. 4, 574–588.
- [22] J.H. Van Vleck, On  $\sigma$ -type doubling and electron spin in the spectra of diatomic molecules, Phys. Rev. **33** (1929), 467.
- [23] Q. Xie, H. Zhong, T.M. Batchelor, C. Lee, The quantum Rabi model: solution and dynamics, J. Phys. A: Math. Theor. 50 (2017), 113001.

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