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# Estimations du spectre discret des opérateurs définis par des matrices infinies non bornées et le modèle quantique de Rabi

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# Thèse de Doctorat

*Mention Mathématiques et leurs interactions*

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**l'Université du Littoral Côte d'Opale**  
*et*  
à *l'Ecole doctorale en Sciences et Technologie*  
**de l'Université Libanaise**

par

**Mirna Mohamad Charif**

pour obtenir le grade de Docteur de l'Université du Littoral Côte d'Opale

***Estimations du spectre discret des opérateurs définis par des matrices infinies non bornées et le modèle quantique de Rabi***

Soutenue le 14 décembre 2022, après avis des rapporteurs, devant le jury d'examen :

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*À mes directeurs bien-aimés !*

*À ma famille*

*Je dédie également ce travail  
à tous ceux qui le méritent*

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## Estimations du spectre discret des opérateurs définis par des matrices infinies non-bornées et le modèle quantique de Rabi

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### Résumé

Le modèle quantique de Rabi, décrivant les interactions entre un système à deux niveaux et un mode du champ quantique, est considéré comme un modèle fondamental dans l'optique quantique, l'électrodynamique de circuits, l'étude de qubits supraconducteurs etc. L'objectif de cette thèse est une étude des valeurs propres des opérateurs auto adjoints définis par le modèle quantique de Rabi.

Une partie de la thèse est consacrée à l'étude asymptotique des grandes valeurs propres pour le modèle quantique de Rabi avec un paramètre supplémentaire  $\epsilon$ , appelé le biais du modèle. On décrit le comportement asymptotique de la  $n$ -ième valeur propre avec l'erreur  $O(n^{-1/2} \ln n)$  lorsque  $n$  tend vers l'infini. Il s'avère que certaines valeurs de  $\epsilon$  présentent une difficulté supplémentaire due au fait que l'on doit considérer une perturbation de valeurs propres doubles et dans ce cas la formule asymptotique comporte un terme oscillant d'ordre  $n^{-1/4}$ . Ces résultats sont nouveaux dans le cas  $\epsilon \neq 0$ . On obtient aussi des résultats analogues pour le modèle de Rabi à deux photons. L'estimation d'erreur  $O(n^{-1} \ln n)$  pour ce modèle est nouveau même dans le cas  $\epsilon = 0$  et la formule asymptotique à trois termes peut être considérée comme une généralisation de l'approximation de l'onde tournant pour le modèle de Rabi à deux photons.

Une autre partie de la thèse est consacrée à la théorie des perturbations pour une classe des opérateurs définis dans l'espace de Hilbert des suites de carré sommable par des matrices tridiagonales non bornées. Afin d'étudier la qualité de l'approximation du modèle de Rabi par le modèle de Jaynes-Cummings (l'approximation de l'onde tournant) on s'intéresse au comportement des valeurs propres en fonction du paramètre de couplage dans le cas de la perturbation des valeurs propres doubles. Grâce à un développement de la théorie de perturbations quasi-dégénérées de Schrieffer-Wolff, on obtient des estimations explicites du rayon de convergence de la série perturbative et des estimations d'erreur.

**Mots clés :** spectre discret, valeurs propres, asymptotiques, matrices infinies, opérateur auto-adjoint, modèle de Rabi

## Estimates of discrete spectrum of operators defined by unbounded infinite matrices and the quantum Rabi model

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### Abstract

The quantum Rabi model, which describes the interactions between a two-level system and a single-mode quantum field, is considered as a fundamental model in quantum optics, circuits quantum dynamics, analysis of superconducting qubits etc. The aim of this thesis is to study eigenvalues of self-adjoint operators defined by the quantum Rabi model.

The first part of the thesis is devoted to the asymptotic analysis of large eigenvalues of the quantum Rabi model with an additional parameter  $\epsilon$ , called the bias of the model. We give the asymptotic behavior of the  $n$ -th eigenvalue with error of the form  $O(n^{-1/2} \ln n)$  as  $n$  tends to infinity. It appears that some values of  $\epsilon$  present an additional difficulty due to the fact that one must consider the perturbations of double eigenvalues and, in this case, the asymptotic formula contains an oscillating term of order  $n^{-1/4}$ . These results are new in the case  $\epsilon \neq 0$ . We also obtain analogue results for the two-photon quantum Rabi model. The error estimate  $O(n^{-1} \ln n)$  for this model is new even in the case  $\epsilon = 0$  and the three-term asymptotic formula can be considered as a generalized rotating wave approximation for the two-photon quantum Rabi model.

Another part of the thesis is devoted to the perturbation theory for operators defined in the Hilbert space of square summable sequences by means of tridiagonal unbounded matrices. In order to study the quality of the approximation of the quantum Rabi model by the JaynesCummings model (the rotating wave approximation), we are interested in the dependence of the eigenvalues on the coupling constant in the case of perturbations of double eigenvalues. Thanks to a development of the Schrieffer-Wolff theory of quasi-degenerate perturbations, we obtain explicit estimates of the convergence radius of the perturbation series and explicit error estimates.

**Keywords :** discrete spectrum, eigenvalues, asymptotics, infinite matrices, self-adjoint operator, Rabi model

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## Publications

### Article accepté

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Le travail décrit dans le Chapitre 5 de titre "Behaviour of large eigenvalues for the two-photon asymmetric quantum Rabi model" est un article écrit en collaboration avec Anne Boutet de Monvel et Lech Zielinski et accepté le 10-06-2022 pour publication dans le journal "St. Petersburg Mathematical" dans le volume dédié à Sergey Naboko.

### Article publié

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Le travail décrit dans le Chapitre 7 de titre "Perturbation series for Jacobi matrices and the quantum Rabi model" est un article écrit en collaboration avec Lech Zielinski et publié dans le journal "Opuscula Mathematica" le 19-04-2021.

[19] Mirna Charif, Lech Zielinski, Perturbation series for Jacobi matrices and the quantum Rabi model, Opuscula Math. 41, no. 3 (2021), 301-333, <https://doi.org/10.7494/OpMath.2021.41.3.301>



# Chapitre 1

## Introduction

### Sommaire

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## 1.1 L'étude asymptotique des opérateurs tridiagonaux non bornés

Considérons la matrice tridiagonale infinie de la forme

$$\hat{J} = \begin{pmatrix} d_1 & b_1 & 0 & 0 & \cdots \\ a_1 & d_2 & b_2 & 0 & \cdots \\ 0 & a_2 & d_3 & b_3 & \cdots \\ 0 & 0 & a_3 & d_4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (1)$$

où  $(d_k)_{k=1}^\infty$ ,  $(a_k)_{k=1}^\infty$  et  $(b_k)_{k=1}^\infty$  sont des suites complexes données. Alors par définition, la matrice  $\hat{J}$  définit une application linéaire  $\mathbb{C}^{\mathbb{N}^*} \rightarrow \mathbb{C}^{\mathbb{N}^*}$  par la formule

$$\begin{cases} (\hat{J}x)_1 = d_1x_1 + b_1x_2, \\ (\hat{J}x)_k = a_{k-1}x_{k-1} + d_kx_k + b_kx_{k+1}. \end{cases} \quad (2)$$

Les matrices tridiagonales infinies sont très utiles dans de nombreux problèmes de mathématiques et d'applications. Des recherches liées à ces matrices sont menées dans les domaines tels que la théorie des équations différentielles, l'analyse numérique et la théorie des polynômes orthogonaux (voir par exemple [9], [21], [122], [128]). En particulier, on peut mentionner les connexions avec les polynômes orthogonaux formels sur le plan complexe, l'équation et les fonctions de Mathieu, l'équation d'Hill, l'équation d'Ince et les fonctions de Bessel : voir [7, 8, 10, 37, 63, 118, 129] et [136].

Elles jouent également un rôle très important dans certains problèmes de physique mathématiques, notamment en physique du solide et en optique quantique. Dans la suite, nous allons donner des exemples des problèmes de la physique où les matrices Jacobi non aléatoires apparaissent.

### 1.1.1 Analyse spectrale d'un opérateur défini par une matrice tridiagonale

Dans la suite, nous nous limitons au cas où la matrice (1) définit un opérateur linéaire  $J$  agissant dans l'espace des suites carrées sommables  $\ell^2$ , c'est-à-dire  $J : \text{Dom}(J) \rightarrow \ell^2$  est défini comme la restriction de  $\hat{J}$  à

$$\text{Dom}(J) := \{(x_k)_{k=1}^\infty \in \ell^2 : (\hat{J}x)_{k=1}^\infty \in \ell^2\}$$

et l'objet de notre étude est le spectre de  $J$ .

Plusieurs auteurs ont étudié le cas de la matrice hermitienne (c'est-à-dire  $d_k \in \mathbb{R}$  et  $b_k = \bar{a}_k$  pour tout  $k \in \mathbb{N}^*$ ) et en particulier le cas où les coefficients sont réels. L'opérateur  $J$  est alors souvent appelé l'opérateur de Jacobi (voir [122]). Dans le contexte non aléatoire, les propriétés spectrales des opérateurs de Jacobi ont été étudiées entre autres par J. Dombrowski ([40], [41], [39]), J. Janas et S. Naboko ([78], [70], [71], [72], [67],

[73], [74], [99], [76], [101], [24], [77], [101],[102], [26], [100]). Les propriétés spectrales des matrices tridiagonales non symétriques ont été étudiées par Beckermann et Kaliaguine ([7, 8]), Djakov et Mityagin ([37, 38]), Egorova et Golinskii ([45, 44]) et d'autres (voir, par exemple [94, 10, 56, 63, 69, 118, 129]). Cependant, la recherche des propriétés spectrales des opérateurs tridiagonaux non auto-adjoints est dure parce que la structure des suites complexes peut être plus compliquée que la structure des suites réelles. En outre le théorème spectral et ses conséquences échouent dans ce cas, et par conséquent les méthodes de recherche efficaces pour les opérateurs non auto-adjoints utilisent les projections de Riez au lieu du Théorème spectral (voir [38, 75]).

En particulier (voir [67], [22]), si la matrice de  $J$  est hermitienne et la partie hors diagonale est majorée par la diagonale dans le sens de la condition suivante :

$$\liminf_{k \rightarrow \infty} \frac{d_k^2}{|a_k|^2 + |a_{k-1}|^2} > 2. \quad (3)$$

alors l'opérateur  $J$  est auto-adjoint. La condition (3) assure que  $J$  est une perturbation de  $\text{diag}(d_k)_{k=1}^{\infty}$  avec borne relative strictement inférieure à 1. Si en plus on suppose que

$$d_k \xrightarrow[k \rightarrow \infty]{} \infty, \quad (4)$$

alors l'opérateur diagonal  $\text{diag}(d_k)_{k=1}^{\infty}$  est un opérateur à résolvante compacte et le spectre de  $J$  est discret (c'est-à-dire le spectre se compose de valeurs propres isolées de multiplicité finie) et inférieurement borné. Ainsi les valeurs propres de  $J$  pouvant être ordonnées dans l'ordre croissant et suivant la convention usuelle on désigne par  $(\lambda_n(J))_{n=1}^{\infty}$  la suite des valeurs propres de  $J$  disposées dans l'ordre croissant et répétées selon leur multiplicité. Il est bien connu qu'il est parfois possible de calculer des formules exactes pour les valeurs propres des matrices de Jacobi (voir, par exemple, [68, 43, 97]), mais ce n'est pas possible en général et il est naturel de poser la question d'une approximation des valeurs propres de  $J$ . De nombreuses méthodes ont été utilisées pour traiter le problème du comportement asymptotique de valeurs propres de  $J$ , en essayant de trouver des résultats optimaux. Dans ce qui suit, on suppose que la matrice (1) est hermitienne, les conditions (3) et (4) sont satisfaites et on mentionne quelques résultats obtenus par des différentes méthodes d'aborder le problème en question.

Pour commencer la présentation de recherches sur le comportement asymptotique de  $\lambda_n(J)$  quand  $n$  tend vers l'infini, on cite le travail fondamental de J. Janas et S. Naboko [75] dans lequel les auteurs ont développé une approche appelée la méthode de diagonalisations successives. Cette méthode est basée sur la construction d'une suite des transformations qui permettent d'obtenir des opérateurs semblables à l'opérateur  $J$  et de plus en plus proches d'un opérateur diagonal. A chaque étape suivante de la construction on obtient un opérateur similaire au précédent et dont la partie diagonale permet de déterminer le comportement asymptotiques des grandes valeurs propres de manière plus précises que précédemment.

Cette méthode a été appliquée dans [27] par Boutet de Monvel, Naboko et Silva pour trouver l'asymptotique des valeurs propres du modèle de Jaynes-Cummings modifié, et par

Janas et Malejki dans [68] et Malejki dans [91], pour trouver l'asymptotique des valeurs propres d'une classe spéciale de matrice de Jacobi.

Dans l'article [75] les auteurs ont également expliqué pourquoi cette thématique de recherches est très importante pour la physique quantique et ils donnent un exemple pratique d'un modèle d'une molécule dans un champ électrique constant (voir Section 1.1.2).

L'idée de construire un opérateur semblable proche d'un opérateur diagonal avait été déjà utilisée pour étudier le comportement asymptotique de grandes valeurs propres du problème de Sturm-Liouville, mais c'est le travail remarquable de G. V. Rozenblum [111] qui fait apparaître l'idée d'approximations successives comme un outil fondamental pour étudier l'asymptotique de grandes valeurs propres.

L'idée de contrôler l'erreur asymptotique en construisant un opérateur semblable a aussi été utilisée pour étudier les opérateurs issus de l'optique quantique (voir [124], [135], [30], [31], [34], [33]).

Pour étudier des différents types de problèmes dans des espaces infinis, on utilise souvent des stratégies d'approximation par des opérateurs agissant en dimension finie, en raison du fait que de nombreux logiciels mathématiques fournissent des fonctionnalités pour la solution des équations matricielles (voir par exemple [23, 84, 96]). Ainsi, il est naturel de poser la question d'une approximation du spectre d'un opérateur par les valeurs propres d'une certaine matrice finie correctement sélectionnée. Les méthodes projectives, qui utilisent des sous-matrices finies pour étudier les propriétés spectrales des opérateurs données par les matrices Jacobi infinies, ont été appliquées avec succès par Arveson ([3, 4]), Ifantis, Kokologiannaki et Petropoulou ([62]), Volkmer ([128]), Boutet de Monvel et Zielinski ([98]), Malejki ([93, 95]), P. Shivakumar, J. Williams et N. Rudraiah [119] et d'autres.

Dans [30, 31], les auteurs ont utilisé une nouvelle méthode de l'approche du problème en considérant une simplification du problème initiale par une troncature des lignes hors diagonales avec le but de remplacer le problème formulé dans  $\ell^2(\mathbb{N})$  par le problème formulé dans  $\ell^2(\mathbb{Z})$ . L'avantage de l'espace  $\ell^2(\mathbb{Z})$  réside dans la possibilité d'utiliser les séries de Fourier pour résoudre le problème analogue. Ensuite, ils ont déduit le résultat souhaité sur  $\ell^2(\mathbb{N})$  grâce à une comparaison de sous matrices du problème formulé dans  $\ell^2(\mathbb{Z})$  avec celui dans  $\ell^2(\mathbb{N})$  en utilisant le résultat de l'article [98].

La méthode de comparaison des valeurs propres des opérateurs de Jacobi agissant dans  $\ell^2(\mathbb{Z})$  avec des valeurs propres de certains opérateurs différentiels ou pseudo-différentiels sur le cercle unité, est une méthode permettant de contrôler l'erreur d'une formule asymptotique de manière efficace dans certains cas. Cette méthode a été appliquée avec succès par Edward [43] dans les cas particuliers d'opérateurs agissant dans  $\ell^2(\mathbb{Z})$  et ensuite par A. Boutet de Monvel et L. Zielinski dans l'étude de l'asymptotique des valeurs propres pour des matrices de Jacobi agissant dans  $\ell^2(\mathbb{N})$  dont l'origine est le modèle de Rabi à deux photons. En utilisant le principe de min-max pour les opérateurs auto-adjoints, ils ont réussi à réduire le problème à l'étude d'un opérateur agissant dans  $\ell^2(\mathbb{Z})$  qui peut être approché par un opérateur différentiel sur le cercle unité avec le contrôle de l'erreur

d'asymptotique basé sur le Lemme de Van der Corput (voir [120]).

Le problème de l'asymptotique des grandes valeurs propres peut être posé également pour certaines classes des matrices tridiagonales définies par blocs. Dans ce cadre général, des résultats ont été obtenus par Malejki ([93]), Braeutigam, Polyakov [16], Baskakov, Garkavenko, Glazkova, Uskova et Zgolich ([6]).

Pour compléter cette présentation des résultats sur le thème du comportement asymptotique des valeurs propres des opérateurs de Jacobi, nous citons le travail de Masson, Repka [97] sur un cas particulier d'opérateur agissant dans  $\ell^2(\mathbb{Z})$  et les travaux sur la densité des valeurs propres des matrices rationnelles [114, 35, 80].

### 1.1.2 Exemples de problèmes liés aux opérateurs tridiagonaux dont le spectre est discret

*L'équation de Mathieu.* Nous considérons le problème de trouver  $\lambda$  de telle sorte que l'équation

$$w''(t) + (\lambda - 2h^2 \cos(2t))w(t) = 0$$

ait une solution impaire de période  $\pi$ . En munissant  $L^2(0, \pi/2)$  de la base orthonormale  $(e_n)_{n=1}^\infty$  de la forme

$$e_n(t) = \frac{2}{\sqrt{\pi}} \sin(2nt),$$

le problème initial est réduit au problème de trouver une valeur propre  $\lambda$  de l'opérateur de Jacobi dont les coefficients sont

$$\begin{cases} d_k = 4k^2, \\ a_k = h^2 \end{cases} \quad (5)$$

*L'équation des ondes sphéroïdales.* Le problème de trouver une valeur propre  $\lambda$  de l'équation d'onde sphéroïdale réduit à la recherche de  $\lambda$  tel que l'équation

$$((1-t^2)w')'(t) + \left( \lambda + \gamma^2(1-t^2) \frac{m^2}{1-t^2} \right) w(t) = 0, \quad t \in [0, 1],$$

ait une solution paire et bornée sur l'intervalle  $(-1, 1)$  ( $\gamma^2$  est un paramètre réel donné et  $m \in \mathbb{N}$ ). En munissant  $L^2(0, 1)$  de la base orthonormée  $(e_n)_{n=1}^\infty$  de la forme

$$e_n(t) = \sqrt{\frac{(2n+1)(n-m)!}{(n+m)!}} P_n^m(t)$$

où  $P_n^m$  est un polynôme de Legendre, on réduit le problème initial au problème de trouver les valeurs propres de l'opérateur de Jacobi  $J_m$  dont les coefficients sont

$$\begin{cases} d_k = (2k+m-2)(2k+m-1) - 2\gamma^2 \frac{(2k+m-2)(2k+m-1) - 1 + m^2}{(4k+2m-5)(4k+2m-1)}, \\ a_k = \frac{\sqrt{(2k-1)2k}\sqrt{(2k+2m-1)(2k+2m)}}{(4k+2m-3)\sqrt{(4k+2m-3)(4k+2m+1)}} \end{cases}$$

Le problème de la recherche des valeurs propres de l'équation de Mathieu et de l'équation des ondes sphéroïdale est étudié dans l'article de Volkmer [128]. Grâce au développement de la méthode de Rayleigh-Ritz, Volkmer a donné des estimations de l'écart entre  $\lambda_n(J)$  et la  $n$ -ième valeur propre des matrices finies obtenues en tronquant la matrice de l'opérateur  $J$ . L'estimation de l'erreur est obtenue en supposant que l'indice  $n$  est fixe et elle n'est pas applicable à l'étude du comportement asymptotique de  $\lambda_n(J)$  quand  $n \rightarrow \infty$ .

*Les matrices de Whittaker–Hill.* (Voir [89], chapitre 7 et voir [37]). Grâce à la méthode de Fourier ou la transformation de la jauge, le problème se traduit de l'opérateur différentiel

$$y'' + (a \cos 2x + b \cos 4x)y$$

à la matrice (1) avec les coefficients

$$d_k = k^2 \text{ ou } (2k + 1)^2, \quad b_k = t - k, \text{ et } a_k = t + k, t \geq 0 \text{ fixé,}$$

voir [126, 64, 89] pour plus de détails.

*L'hamiltonien d'une molécule dans le champ électrique homogène.* Dans le cas de modèles de la physique quantique, l'hamiltonien du modèle physique est l'opérateur auto-adjoint dont les valeurs propres correspondent aux niveaux d'énergie de système qui peuvent être mesurés expérimentalement. En comparant les propriétés théoriques des valeurs propres de l'hamiltonien avec les données mesurées expérimentalement, la validité du modèle en question peut être testée. Dans le cas général, un modèle dépend d'un certains nombres de paramètres physiques qui apparaissent dans le comportement asymptotique de grandes valeurs propres. La connaissance du spectre de l'hamiltonien, grâce aux données expérimentales peut nous permettre d'obtenir des renseignements sur les valeurs des paramètres physiques du modèle considéré.

Janas et Naboko dans l'article [75] donnent un exemple du modèle d'une molécule dans un champ électrique constant. L'hamiltonien de ce modèle s'écrit sous la forme

$$H = \frac{L^2}{2I} + \left( \frac{1}{2I_3} - \frac{1}{2I} \right) L_z^2 - gz, \quad (6)$$

où  $L$  est l'opérateur du moment cinétique,  $L_z$  sa projection sur l'axe de  $z$ ,  $I, I_3$  sont les moments d'inertie correspondants. En utilisant les fonctions sphériques généralisées  $(\phi_{m,j}^n)_{-n \leq j, m \leq n}^{n=0,1,\dots}$  on peut exprimer les valeurs propres de  $H$  à l'aide des valeurs propres des opérateurs de Jacobi  $J_{m,j}$  dont les coefficients sont donnés par

$$\begin{cases} d_k = \frac{h^2}{2I} k(k-1) + \frac{h^2}{2} \left( \frac{1}{I_3} - \frac{1}{I} \right) j^2 - \frac{gmj}{k(k-1)} \\ a_k = \frac{-g}{(2k-1)k} \sqrt{|(k^2 - m^2)(k^2 - j^2)|} \end{cases} \quad (7)$$

où  $h$  est la constante de Planck.

La méthode des diagonalisations successives utilisée dans l'article [75] permet de donner l'expression pour  $\lambda_n(J_{m,k})$  avec précision  $O(n^{-3})$  quand  $n \rightarrow \infty$ .

*Le modèle quantique de Rabi.* L'hamiltonien quantique de Rabi décrit le plus simple modèle d'interactions entre un champ de radiation monomode à fréquence  $\omega$  et un atome à deux niveaux d'énergie. Le problème du comportement asymptotique des valeurs propres de l'hamiltonien de Rabi se réduit à l'étude des valeurs propres de matrice de Jacobi. Dans la section 1.2, on donne plus des détails sur ce problème.

### 1.1.3 L'historique des résultats sur l'asymptotique des grandes valeurs propres

Dans cette section, nous présentons des résultats généraux très importants dans le problème du comportement asymptotique des valeurs propres des opérateurs à spectre discret, décrits et démontrés en détails dans les articles [75], [135] et [94].

Dans [75], J. Janas et S. Naboko ont montré un lemme fondamental concernant le comportement asymptotique du spectre pour une perturbation compacte d'un opérateur discret diagonal dont les éléments diagonaux sont distincts :

**Lemme 1.1.1.** (Lemme 2.1, Janas et Naboko [75]). *Soit  $H$  un espace de Hilbert muni d'une base orthonormale  $\{e_k\}_{k=1}^\infty$  et soit  $D$  un opérateur diagonal auto-adjoint de la forme  $De_k = \nu_k e_k$  où les valeurs propres  $\nu_k$  sont simples et la suite  $\nu_k \rightarrow \infty$  quand  $k \rightarrow \infty$ . Supposons de plus que  $|\nu_j - \nu_i| \geq \varepsilon_0 > 0$  si  $j \neq i$ . Si  $R$  est un opérateur compact (pas nécessairement auto-adjoint) sur  $H$ , alors le spectre de l'opérateur  $T = D + R$  est discret et constitué des valeurs propres complexes  $\lambda_n(T)$  qui vérifient l'estimation  $\lambda_n(T) = \nu_n + O(\|R^* e_n\|)$  quand  $n \rightarrow \infty$ .*

Ce lemme est essentiel pour les méthodes de diagonalisation. Les auteurs dans [75] donnent le comportement asymptotique des valeurs propres pour une classe spéciale de matrice de Jacobi dont les coefficients ont la forme

$$\begin{cases} d_k = k^2 + c_1 k + c_2 k^{-1} + c_3 k^{-2} + O(k^{-3}) \\ a_k = g + c'_1 k^{-1} + c'_2 k^{-2} + O(k^{-3}) \end{cases} \quad (8)$$

en utilisant la méthode de diagonalisations successives et le lemme 1.1.1.

En 2013, Yanovich dans [135] a utilisé le lemme 1.1.1 de Janas et Naboko dans sa démonstration du théorème 1.1.1 qui présente un nouveau résultat pour le problème du comportement asymptotique du spectre pour une perturbation non compacte et bornée d'un opérateur discret diagonal.

**Théorème 1.1.1** (Théorème 2.1, Yanovich [135]). *Soit  $\{e_n : n \geq 1\}$  une base orthonormée dans l'espace de Hilbert  $H$  et  $D$  l'opérateur auto-adjoint vérifiant  $De_n = ne_n$  pour tout  $n \in \mathbb{N}$ . Si  $R$  est un opérateur auto-adjoint borné et sa matrice  $R_{n,k}$  dans la base  $\{e_n : n \geq 1\}$  satisfait à la condition*

$$\lim_{n \rightarrow \infty} R_{n,n+p} = 0 \quad \forall p \in \mathbb{Z},$$

alors le spectre de l'opérateur  $T = D + R$  est discret et la suite de ses valeurs propres vérifie l'estimation suivante :

$$\lambda_n(T) = \mu_n + R_{n,n} + O(s_n) \quad (9)$$

où

$$s_n = \sqrt{\sum_{k \neq n} \frac{|R_{k,n}|^2}{(n-k)^2}}$$

En 2014, Malejki ([94]) a généralisé le lemme 1.1.1 du Janas et Naboko à une classe des matrices complexes dont les éléments diagonaux ne sont pas nécessairement distincts. Pour définir ces classes des matrices on introduit la condition suivante

(CΓ) Soit  $\Gamma_n$ ,  $n \geq 1$  une suite de courbes fermées sur  $\mathbb{C}$  et supposons qu'il existe une suite  $(p_n)$  non négative telle que

$$\{z \in \mathbb{C} : |z| \leq p_n\} \subset \text{int}\Gamma, \quad n \geq 1,$$

et

$$\lim_{n \rightarrow \infty} \frac{|\Gamma_n|}{p_n^2} = 0, \quad \lim_{n \rightarrow \infty} p_n = +\infty,$$

où  $\text{int}\Gamma_n$  désigne l'ensemble entouré de  $\Gamma_n$  et  $|\Gamma_n|$  dénote la longueur de  $\Gamma_n$ .

**Théorème 1.1.2** (Théorème 4.1, Malejki [94]). *Soit  $\{e_n : n \geq 1\}$  une base orthonormée dans l'espace de Hilbert  $H$  et  $D$  l'opérateur auto-adjoint vérifiant  $De_n = d_n e_n$  pour tout  $n \in \mathbb{N}$ . Supposons que la suite complexe  $(d_n)_{n=1}^\infty$  satisfait aux conditions suivantes :*

1.  $|d_n - d_k| \geq \varepsilon_0 > 0$  pour  $d_n \neq d_k$ ;
2. Il existe une suite de courbes de Jordan fermées  $\{\Gamma_n\}_{n \geq 1}$ , vérifiant (CΓ), telle que

$$\text{dist}(\Gamma_n, d_k) \geq \varepsilon_0/4 \quad \text{pour } k, n \geq 1$$

et

$$\int_{\Gamma_n} \|(D - \lambda)^{-1}\|^2 |d\lambda| \leq C, \quad n \geq 1,$$

où  $\varepsilon_0, C > 0$  sont indépendants de  $n$ .

Soit  $K$  un opérateur compact dans  $H$  et  $T = D + K$ . Alors le spectre de  $T$  est discret et constitué des valeurs propres complexes  $\lambda_n(T)$ ,  $n \geq 1$ , qui peuvent être arrangées de façon à ce que l'on ait la formule asymptotique

$$\lambda_n(T) = d_n + O(\|K^* P_n\|) \quad \text{quand } n \rightarrow \infty,$$

où  $P_n$  désigne la projection orthogonale sur l'espace de dimension finie engendré par  $\{e_k : d_n = d_k\}$ .



Dans [94], l'auteur a donné quelques exemples dans lesquels la suite complexe  $(d_n)_{n=1}^{\infty}$  vérifie les hypothèses du théorème 1.1.2,

1.  $|d_{n+1}| > |d_n|$  pour  $n \geq n_0$ ,  $\lim_{n \rightarrow \infty} |d_n| = +\infty$  et  $\left(\frac{|d_{n+1}| + |d_n|}{(|d_{n+1}| - |d_n|)^2}\right)_{n=1}^{\infty}$  est bornée;
2.  $d_n = \epsilon n^\alpha \left(1 + o\left(\frac{1}{n}\right)\right)$ ,  $|\epsilon_n| = \epsilon$  pour  $n \geq 1$ , avec  $\alpha \geq 2$ ;
3.  $d_n = \epsilon_n \left(\left[\frac{n+T-1}{T}\right]\right) \left(1 + o\left(\frac{1}{n}\right)\right)$ ,  $|\epsilon_n| = \epsilon$  pour  $n \geq 1$ , avec  $\alpha \geq 1$  et  $(\epsilon_n)$  est une suite périodique dont la période est égale à  $T$ ,  $\epsilon_n \neq \epsilon_k$  pour  $n \neq k$ , et  $k, n = 1, \dots, T$ , et  $[x] = \max\{k \in \mathbb{N} : k \leq x\}$  pour  $x \in \mathbb{R}$ .

## 1.2 Problème du comportement asymptotique des valeurs propres du QRM

### 1.2.1 Modèle de Rabi

Le modèle quantique de Rabi a été introduit à la fin des années 30 par Isidor Rabi ([105], [106]) pour étudier le comportement d'un spin nucléaire dans un champ magnétique tournant lors d'expériences de résonance magnétique nucléaire (RMN). Rabi a construit son modèle semi-classique de la matière, la matière traitée quantiquement et le champ classiquement. Dans une expérience de RMN, le spin nucléaire est d'abord plongé dans un champ magnétique homogène et constant pour lever la dégénérescence des niveaux "spin down" et "spin up", par effet Zeeman. Un champ magnétique tournant est ensuite ajouté, ce qui induit des transitions entre les états de spin. C'est le couplage avec ce second champ que le modèle de Rabi décrit. Une version totalement quantique peut être obtenue en quantifiant également le champ électromagnétique et sa version la plus simple suppose en outre qu'il est monomode. Il s'agit de la façon la plus simple de coupler un système à deux niveaux à un seul mode du rayonnement. C'est pour cette raison que ce modèle est considéré comme le modèle le plus fondamental, populaire et réussi pour étudier l'interaction entre la matière et le rayonnement électromagnétique. Par conséquent le QRM occupe une place cruciale dans différents domaines de la physique, notamment en optique quantique [52]. Il est utilisé pour décrire l'interaction entre le champ électrique d'une cavité électromagnétique et deux niveaux électroniques d'un atome [107, 132] ou encore l'interaction entre un circuit supraconducteur et un résonateur électronique [90, 13, 18]. Il peut par ailleurs être réalisé dans de nombreux systèmes physiques, y compris les ions piégés [85], les points quantiques [48] et les systèmes quantiques hybrides [130, 5, 66].

Dans les années 60, Jaynes et Cummings ont proposé un modèle simplifié [79] qui revient à négliger le terme counter-rotating (CRT), sous l'approximation dite "l'onde tournante" (Rotating Wave Approximation- RWA). Le QRM est parfois appelé modèle de Jaynes-Cummings sans RWA. L'approximation de l'onde tournante n'est valable que dans l'hypothèse où la constante de couplage est faible par rapport aux autres fréquences du système, c'est le cas dans les expériences d'atomes en cavité dans les domaines optique et micro-onde. Dans les années 80, avec l'avènement, dans des expériences des circuits supraconducteurs caractérisés par des couplages intenses, l'approximation de l'onde tournante

RWA a été mise à défaut [103]. Dans ce cas, le CRT ne peut être négligé. Par conséquent, de nombreux effets intéressants induits par le CRT apparaissent. En conclusion, les développements technologiques ont ravivé l'intérêt pour le modèle Rabi et ses termes CRT, qui peuvent jouer un rôle très important dans les circuits supraconducteurs.

La connaissance de valeurs propres de l'hamiltonien de QRM, qui définissent les niveaux d'énergie du système, est cruciale. D'une part, pour tester la validité du modèle de manière expérimentale et d'autre part, à déterminer les valeurs de paramètres du modèle testé dans une expérience donnée. Il est bien connu que parfois, il est possible de calculer les formules exactes des valeurs propres mais ce n'est pas possible en général. Ainsi, des approches asymptotiques doivent être appliquées. L'étude du comportement asymptotique des grandes valeurs propres de différents modèles de Rabi a été mentionné dans de nombreuses recherches physiques (voir par exemple [50], [86], [109], [134]), mais l'analyse mathématique de cette question a été initiée par E. A. Yanovich dans [123], [124], [135], et A. Boutet de Monvel, S. Naboko, L. O. Silva dans [27], [28] et a été poursuivie par A. Boutet de Monvel et Zielinski dans [31], [34], [30], [33] et elle fait l'objet de cette thèse.

### 1.2.2 Structure de l'hamiltonien de Rabi

Tout système quantique est caractérisé par son hamiltonien, qui est l'opérateur associé à l'énergie totale du système. Le modèle de Rabi quantique décrit l'interaction entre un système à deux niveaux et un champ. Alors l'hamiltonien du modèle de Rabi sera composé de trois termes : un terme qui se réfère au système à deux niveaux, un terme qui décrit le mode quantique de champ et un dernier terme qui donne le couplage entre eux. Il existe une multitude de généralisations du modèle de Rabi, selon les expériences et les réalisations. On présente dans cette section les différentes formes du modèle de Rabi étudiés dans cette thèse.

L'hamiltonien du modèle de Rabi quantique à deux photons est décrit dans la définition 1.2.1-(c). C'est une extension évidente de l'hamiltonien du modèle de Rabi original donné dans la définition 1.2.1-(a), où les transitions atomiques sont induites par l'absorption et l'émission de deux photons plutôt qu'un seul. Ces processus optiques non linéaires ont suscité un intérêt considérables [116, 131], avec des applications telles que les lasers à deux photons et la bistabilité à deux photons [109]. On peut les réaliser pour des atomes de Rydberg dans des cavités supraconductrices hyperfréquences [12, 17] et des boîtes quantiques [121, 36].

Un modèle plus général est décrit dans la définition 1.2.1-(d). On l'appelle le QRM avec un biais statique fini ou le modèle de Rabi quantique asymétrique (AQRM). Ce modèle attire l'attention en relation avec des expériences récentes de couplage ultra-fort par des circuits supraconducteurs [133, 82]. En fait, les expériences avec un faisceau laser dans la cavité concerne le QRM avec un force de couplage  $g \sim 10^{-6}$ , tandis que des expériences avec des circuits qubits peuvent atteindre la valeur  $g \sim 10^{-1}$  et le biais statique  $\epsilon$  apparaît en raison de l'effet tunnel entre les deux états courants [61]. Dans l'absence de biais  $\epsilon$ , l'AQRM se réduit au modèle quantique de Rabi. Ce modèle a été étudié dans plusieurs travaux (voir par exemple [14], [20], [88] et [133]).

Un QRM généralisé, à un et deux photons, dans la définition 1.2.1-(f), a été pris en compte dans les réalisations expérimentales du circuit quantique électrodynamique (QED) par exemple [11] et [49]. Plus récemment, Pedernales et al. ont suggéré qu'un arrière-plan d'un trou noir à  $(1 + 1)$ -dimension nécessite un QRM avec termes à un et deux photons qui peuvent être implémentés dans un ion piégé pour la simulation quantique des particules de Dirac dans l'espace-temps courbe [104]. Ainsi, le QRM avec des couplages à un et deux photons n'est pas seulement un modèle générique dans le circuit QED, mais a également de larges applications dans le domaine de la recherche interdisciplinaire.

### L'hamiltonien du Rayonnement monomode

L'état quantique accessible au mode de rayonnement est représenté par un vecteur appartient à l'espace de Hilbert  $\ell^2(\mathbb{N})$ , de dimension infinie, dont la base canonique est donnée par  $\{e_n\}_{n=0}^\infty$ . Deux opérateurs  $\hat{a}$  et  $\hat{a}^\dagger$  décrivent respectivement l'annihilation et la création d'un photon dans le mode. Ils sont définis sur  $\ell^2(\mathbb{N})$  selon les formules

$$\hat{a} e_n = \sqrt{n} e_{n-1}, \quad \hat{a}^\dagger e_n = \sqrt{n+1} e_{n+1}, \quad n = 0, 1, 2, \dots,$$

avec  $e_{-1} := 0$ .

L'hamiltonien du rayonnement monomode de fréquence  $\omega > 0$  est défini dans  $\ell^2(\mathbb{N})$  comme un opérateur auto-adjoint donné par

$$H_{\text{rad}}^\omega = h\omega \hat{a}^\dagger \hat{a} = h\omega N \quad (10)$$

où  $h$  est la constante de Planck et  $N = \hat{a}^\dagger \hat{a}$  est l'opérateur du nombre vérifiant  $N e_n = n e_n$  pour tout  $n \in \mathbb{N}$ .

### L'hamiltonien du système à deux niveaux

On identifie les deux états propres du système avec la base canonique de  $\mathbb{C}^2$  et on considère les opérateurs linéaires dans l'espace euclidien  $\mathbb{C}^2$  définis par

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad (11)$$

L'hamiltonien du système à deux niveaux, défini dans  $\mathbb{C}^2$  au moyen de la matrice  $2 \times 2$ , s'écrit

$$H_{\text{TLS}}^\epsilon = \frac{1}{2}(\Delta \sigma_z + \epsilon \sigma_x), \quad (12)$$

où  $\Delta$  et  $\epsilon$  sont des paramètres réels.

### L'hamiltonien d'interaction

L'hamiltonien d'interaction du modèle de Rabi à un photon est défini dans l'espace de Hilbert  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  par

$$hg_1 \sigma_x \otimes (\hat{a} + \hat{a}^\dagger),$$

où  $g_1$  est la constante de couplage. En termes d'opérateurs d'élevation et d'abaissement,  $\sigma_{\pm} := \frac{1}{2}(\sigma_x \pm i\sigma_y)$ , le terme d'interaction à un photon peut être écrit comme la somme de quatre termes :

$$hg_1\sigma_x \otimes (\hat{a} + \hat{a}^\dagger) = hg_1(\sigma_- \otimes \hat{a}^\dagger + \sigma_+ \otimes \hat{a}) + hg_1(\sigma_+ \otimes \hat{a}^\dagger + \sigma_- \otimes \hat{a}) \quad (13)$$

Les deux premiers,  $\sigma_- \otimes \hat{a}^\dagger$ ,  $\sigma_+ \otimes \hat{a}$ , sont dit résonants.  $\sigma_+ \otimes \hat{a}$  exprime l'excitation de l'atome et la perte d'un photon, tandis que  $\sigma_- \otimes \hat{a}^\dagger$  représente le phénomène inverse. Les termes  $\sigma_+ \otimes \hat{a}^\dagger$  et  $\sigma_- \otimes \hat{a}$  sont dits non-résonants et représentent l'excitation de l'atome et la création d'un photon pour le premier et la désexcitation de l'atome accompagné de la destruction d'un photon du mode pour le second. Jaynes-Cummings [79] ont proposé la RWA où les termes non-résonantes sont négligés. Le modèle simplifié résultant est l'hamiltonien

$$H_{\text{JC}} = H_{\text{rad}}^\omega + H_{\text{TLS}}^0 + hg_1(\sigma_- \otimes \hat{a}^\dagger + \sigma_+ \otimes \hat{a}), \quad (14)$$

où  $H_{\text{rad}}^\omega$  est donné par (10) et  $H_{\text{TLS}}^0$  est donné par (12) avec  $\epsilon = 0$ .

L'hamiltonien d'interaction du modèle de Rabi à un et deux photons est défini dans l'espace de Hilbert  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  par

$$H_{\text{int}}^{g_1, g_2} = hg_1\sigma_x \otimes (\hat{a} + \hat{a}^\dagger) + hg_2\sigma_x \otimes (\hat{a}^2 + (\hat{a}^\dagger)^2), \quad (15)$$

où  $g_1$  et  $g_2$  sont les constantes de couplage.

### L'hamiltonien du modèle de Rabi

L'hamiltonien du modèle de Rabi qui nous intéresse dans cette thèse est l'opérateur auto-adjoint défini dans  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  de la forme

$$I_{\mathbb{C}^2} \otimes H_{\text{rad}}^\omega + H_{\text{TLS}}^\epsilon \otimes I_{\ell^2(\mathbb{N})} + H_{\text{int}}^{g_1, g_2} \quad (16)$$

avec  $H_{\text{rad}}^\omega$  donné par (10),  $H_{\text{TLS}}^\epsilon$  donné par (12) et  $H_{\text{int}}^{g_1, g_2}$  donné par (15).

**Définition 1.2.1.** (a) L'hamiltonien du modèle de Rabi quantique (QRM) est défini par la formule (16) avec  $g_1 \neq 0, g_2 = 0$  et  $\epsilon = 0$ .

(b) L'hamiltonien de Jaynes-Cummings est donné par (14).

(c) L'hamiltonien du modèle de Rabi quantique à deux photons est défini par la formule (16) avec  $g_1 = 0, g_2 \neq 0$  et  $\epsilon = 0$ .

(d) L'hamiltonien du modèle de Rabi quantique asymétrique (AQRM) ou c'est ce qu'on appelle le QRM avec un biais statique fini, est l'opérateur défini par (16) avec  $g_1 \neq 0, g_2 = 0$  et  $\epsilon \in \mathbb{R}$ .

(e) L'hamiltonien du modèle de Rabi quantique asymétrique à deux photons est l'opérateur défini par (16) avec  $g_1 = 0, g_2 \neq 0$  et  $\epsilon \in \mathbb{R}$ .

(f) L'hamiltonien de QRM à un et deux photons est défini par la formule (16) avec  $g_1 \neq 0$  et  $g_2 \neq 0$ .

### 1.2.3 Quelques systèmes décrits par le modèle de Rabi

Dans cette section, nous décrivons brièvement certaines réalisations expérimentales du modèle quantique de Rabi dans des systèmes physiques différents.

#### Atome unique dans une cavité

L'interaction entre un atome et un mode du champ électromagnétique peut être décrite par le modèle de Rabi. En supposant que seule une transition atomique soit couplée au mode du champ, rendant l'atome modélisable par un système à deux niveaux, le niveau fondamentale  $e_g$  et le niveau excité  $e_e$  avec les énergies  $E_e$  et  $E_g$  respectivement. La cavité est construite à l'aide de niobium supraconducteur miroirs marqués par C sur la figure 1.1, et soutient un champ de rayonnement monomode de fréquence  $\omega$ . Dans l'approximation dipolaire, l'interaction de l'atome et de la cavité peut être décrite par l'hamiltonien défini dans la définition (1.2.1)-(a) avec

$$\Delta = \frac{E_e - E_g}{h}, \quad g_1 = d\sqrt{h\omega/2\varepsilon_0 V}$$

où  $d$  est l'élément de matrice dipolaire pour la transition entre les deux niveaux et  $V$  est le volume de la cavité.

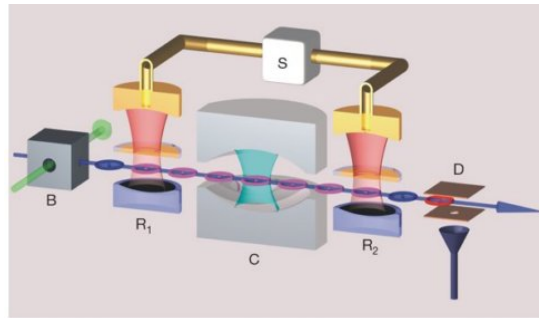


FIGURE 1.1 – Le montage expérimental pour un seul atome dans une cavité. Des atomes de Rydberg sont préparés dans un état particulier dans la boîte B. Ces atomes passent dans une cavité de Ramsey R1 avant de traverser la cavité principale C. Puis ils traversent la cavité R2 alimentée comme R1 par une source micro-onde classique S. En D, un détecteur à ionisation sélectif permet d'identifier l'état de sortie des atomes. Figure tirée de [55].

#### Circuits supraconducteurs

Le modèle quantique de Rabi est également réalisé dans les circuits supraconducteurs. En particulier, dans des expériences récentes où un qubit du flux est couplé à un résonateur LC, le régime d'un couplage ultrafort a été atteint (voir [51]). Le qubit du flux se compose de quatre jonctions de Josephson interrompant une boucle supraconductrice, qui est parcourue par une polarisation du flux externe  $\phi$ . Dans certaines conditions, le paysage

potentiel des qubits est de la forme d'un potentiel double puits, où les deux minima correspondent à des états avec des courants persistants sens horaire et anti-horaire  $\pm I_p$ . Le qubit se comporte donc effectivement comme un bit d'un système à deux niveaux dans la base des deux états persistants, avec hamiltonien effectif donné par (12) avec

$$\epsilon = 8I_p(\phi_0/2 - \phi)$$

où  $\phi_0$  est le flux quantique et  $\Delta/h$  est l'effet tunnel du couplage entre les deux états persistants. Le résonateur est constitué de deux condensateurs et peut être décrit comme l'oscillateur harmonique par l'hamiltonien donné par (10) où  $\omega$  est la fréquence de résonance donnée par

$$\omega = \frac{1}{\sqrt{L_r C_r/2}}$$

L'interaction entre le qubit et le résonateur est décrite par (15) avec  $g_2 = 0$  et  $g_1 = I_p I_{rms} L_k / h$  avec l'inductance cinétique  $L_k = 0,14hR_n / \kappa T_c$  et la fluctuation de courant au point zéro  $I_{rms} = \sqrt{h\omega/2L_r}$ . Pour des valeurs de paramètres typiques dans cette expérience, le rapport  $g_1/\omega \approx 0.1$ .

#### 1.2.4 L'historique des travaux mathématiques sur l'asymptotique des grandes valeurs propres de QRM

Le premier résultat concernant le comportement asymptotique des valeurs propres de QRM a été obtenu par E. A. Yanovich dans [123], [124] et [135]. Dans [135], Yanovich a étudié ce problème pour l'hamiltonien de QRM à un photon donné dans la définition 1.2.1-(a), c'est-à-dire l'opérateur auto-adjoint défini dans  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  :

$$H_\Delta := I_{\mathbb{C}^2} \otimes h\omega \hat{a}^\dagger \hat{a} + \frac{1}{2} \Delta \sigma_z \otimes I_{\ell^2(\mathbb{N})} + hg\sigma_x \otimes (\hat{a} + \hat{a}^\dagger), \quad (17)$$

Il s'avère (voir [123], [32]) que l'hamiltonien de QRM à un photon est unitairement équivalent à la somme directe de deux opérateurs auto-adjoints  $H_\pm$ ,

$$H_\pm = -h\omega + h\omega J_\pm$$

où l'opérateur  $J_+$  (resp.  $J_-$ ) est défini dans une base appropriée par la matrice de Jacobi (1) dont les coefficients sont donnés par

$$\begin{cases} d_k^\pm = k \pm \frac{\Delta}{2h\omega} (-1)^k, \\ a_k = \frac{g}{\omega} \sqrt{k}, \end{cases} \quad (18)$$

Il s'avère que dans le cas particulier  $\Delta = 0$ , l'opérateur  $J_\pm$  peut être diagonalisé à l'aide de la transformation de Bogoliubov. Plus précisément, dans le cas où

$$\begin{cases} d_k = k \\ a_k = \frac{g}{\omega} \sqrt{k}, \end{cases} \quad (19)$$

on trouve que la  $n$ -ième valeur propre est égale  $n - \frac{g^2}{\omega^2}$  (voir [32]).

Dans le cas  $\Delta \neq 0$ , l'estimation d'erreur obtenue par Yanovich dans [135] pour le modèle général est  $O(n^{-1/16})$ , i.e. on obtient la formule asymptotique

$$\lambda_n(H_{\pm}) = h\omega n - \frac{h}{\omega}g^2 + O(n^{-1/16}) \text{ quand } n \rightarrow \infty \quad (20)$$

La preuve de Yanovich est basée sur le lemme 2.1 de l'article [75] de Janas et Naboko. La formule asymptotique pour  $\lambda_n(H_{\pm})$  a été améliorée par Boutet de Monvel et Zielinski dans [31], [34]. L'article [34] donne la formule asymptotique à trois termes

$$\lambda_n(H_{\pm}) = h\omega n - \frac{h}{\omega}g^2 \pm \frac{\Delta \cos(4g\sqrt{n}/\omega - \frac{\pi}{4})}{2\sqrt{2\pi}g/\omega} n^{-\frac{1}{4}} + O(n^{-\frac{1}{2}+\varepsilon}) \text{ quand } n \rightarrow \infty \quad (21)$$

où  $\varepsilon > 0$  est un nombre arbitraire. Cette formule fait apparaître les trois paramètres du modèle  $(\omega, g, \Delta)$  et d'après [32], on peut l'utiliser pour déterminer les valeurs des paramètres  $\omega, g, \Delta$ , à partir du spectre de l'hamiltonien de Rabi. Les mêmes approximations des valeurs propres ont été proposées par Feranchuk, Komarov et Ulyanekov dans [50] et par Irish [65] sous le nom de GRWA (generalized rotating wave approximation). Il existe de nombreux articles consacrés à des problèmes similaires [38], [1], [75], [28], [68], [91], [92], [93], [125].

Dans [33], Boutet de Monvel et Zielinski ont étudié le comportement asymptotique de l'opérateur de l'hamiltonien du QRM à deux photons défini dans  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  :

$$\hat{H}_{\Delta} = I_{\mathbb{C}^2} \otimes \hat{a}^{\dagger}\hat{a} + \frac{\Delta}{2}\sigma_z \otimes I_{\ell^2(\mathbb{N})} + g\sigma_x \otimes (\hat{a}^2 + (\hat{a}^{\dagger})^2), \quad (22)$$

Ils ont supposé  $-\frac{1}{2} < g < \frac{1}{2}$  afin d'assurer que l'opérateur  $\hat{H}_{\Delta}$  soit un opérateur auto-adjoint, borné inférieurement avec spectre discret (voir Sahbani [113]). Il s'avère que dans le cas où  $\Delta = 0$ ,  $\hat{H}_0$  est unitairement équivalent à la somme directe de deux opérateurs auto-adjoints  $\hat{H}_{\pm} : \mathcal{D} \rightarrow \ell^2(\mathbb{N})$ , où

$$\mathcal{D} = \{x \in \ell^2(\mathbb{N}) : \sum_{k \in \mathbb{N}} k^2 |x(k)|^2 < \infty\}$$

et

$$\hat{H}_{\pm} = \hat{a}^{\dagger}\hat{a} \pm g(\hat{a}^2 + (\hat{a}^{\dagger})^2).$$

Les valeurs propres exactes de ces opérateurs sont bien connues (voir [47], [33]),

$$\lambda_n(\hat{H}_{\pm}) = (n + \frac{1}{2})\sqrt{1 - 4g^2} - \frac{1}{2},$$

Il s'avère que dans le cas  $\Delta \neq 0$ , l'hamiltonien de QRM à deux photons  $\hat{H}_{\Delta}$  est unitairement équivalent à la somme directe de quatre opérateurs de Jacobi  $J_{1,0} \oplus J_{-1,0} \oplus J_{1,1} \oplus J_{-1,1}$  définis sur  $\ell^2(\mathbb{N})$  par

$$J_{\nu,\mu} = \begin{pmatrix} d_{\nu,\mu}(0) & b_{\mu}(0) & 0 & 0 & \cdots \\ b_{\mu}(0) & d_{\nu,\mu}(1) & b_{\mu}(1) & 0 & \cdots \\ 0 & b_{\mu}(1) & d_{\nu,\mu}(2) & b_{\mu}(2) & \cdots \\ 0 & 0 & b_{\mu}(2) & d_{\nu,\mu}(3) & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (23)$$

où

$$d_{\nu,\mu}(n) = 2n + \mu + \nu(-1)^n \frac{\Delta}{2}, \quad (24)$$

et

$$b_\mu(n) = g\sqrt{(2n+1+\mu)(2n+2+\mu)}. \quad (25)$$

Le comportement asymptotique de grandes valeurs propres de  $J_{\nu,\mu}$  a été obtenu dans [33] avec l'estimation d'erreur  $O(n^{-1/3})$ ,

$$\lambda_n(J_{\nu,\mu}) = (2n + \mu + \frac{1}{2})\sqrt{1 - 4g^2} - \frac{1}{2} + O(n^{-1/3}) \text{ quand } n \rightarrow \infty$$

Ainsi le spectre du QRM à deux photons  $\hat{H}_\Delta$  se compose de deux suites de valeurs propres

$$\hat{E}_n^\pm = (n + \frac{1}{2})\sqrt{1 - 4g^2} - \frac{1}{2} + O(n^{-1/3}) \text{ quand } n \rightarrow \infty \quad (26)$$

En ce qui concerne ce résultat, nous remarquons ce qui suit :

– puisque les valeurs propres de  $H_0$  (respectivement de  $\hat{H}_0$ ) sont explicitement connues, l'estimation (20) (respectivement (26)) fournit une estimation asymptotique des valeurs propres de  $H_\Delta$  (respectivement de  $\hat{H}_\Delta$ ) avec une erreur  $O(n^{-\alpha})$  où  $\alpha > 0$ , c'est-à-dire

$$\lambda_n(H_\Delta) - \lambda_n(H_0) = O(n^{-\alpha}) \text{ quand } n \rightarrow \infty \quad (27)$$

et

$$\lambda_n(\hat{H}_\Delta) - \lambda_n(\hat{H}_0) = O(n^{-\alpha}) \text{ quand } n \rightarrow \infty \quad (28)$$

– les estimations (27) et (28) montrent un phénomène étrange qui consiste à disparaître l'influence de la perturbation  $H_\Delta - H_0$  et  $\hat{H}_\Delta - \hat{H}_0$  malgré le fait que cette perturbation n'est pas un opérateur compact. En particulier, la différence analogue des  $n$ -ièmes valeurs propres ne converge pas vers 0 quand  $n \rightarrow \infty$  dans le cas des modèles considérés par Boutet de Monvel, Naboko, Silva [27] et [28].

### 1.3 Contribution de recherches menées dans cette thèse

Dans cette section, nous donnons une brève description des contributions de notre travail dans cette thèse.

#### 1.3.1 Comportement asymptotique des grandes valeurs propres du modèle de Rabi asymétrique à un photon.

Dans le travail en collaboration avec mes directeurs de thèse Ahmad Fino et Lech Zielinski, nous avons étudié le comportement asymptotique de la  $n$ -ième valeur propre du



modèle de Rabi asymétrique à un photon, c'est-à-dire pour l'hamiltonien défini dans la définition (1.2.1)-(d) en supposant, sans perte de généralité, que  $h = 1$  et  $\omega = 1$ ,

$$I_{\mathbb{C}^2} \otimes \hat{a}^\dagger \hat{a} + \frac{1}{2}(\Delta \sigma_z + \epsilon \sigma_x) \otimes I_{\ell^2(\mathbb{N})} + g \sigma_x \otimes (\hat{a} + \hat{a}^\dagger), \quad (29)$$

où  $\Delta$ ,  $\epsilon$  et  $g$  sont des paramètres réels. Dans la suite on suppose  $g > 0$ .

Comme nous l'avons mentionné dans la section 1.2.4, ce problème a été étudié dans le cas où  $\epsilon = 0$  par E. A. Yanovich (Tur) dans [135] (voir aussi [124]) où l'estimation d'erreur obtenue est  $O(n^{-\frac{1}{16}})$  et plus tard ce résultat a été amélioré dans [34] qui donne la formule asymptotique à trois termes pour les grandes valeurs propres (21).

Dans le **Chapitre 2** de la thèse, on montre que le spectre de l'opérateur (29) se compose de deux suites  $(E_m^-)_{m \in \mathbb{N}}$ ,  $(E_m^+)_{m \in \mathbb{N}}$ , qui vérifient la formule asymptotique

$$E_m^\pm = m - g^2 \pm \frac{1}{2} \epsilon + O(m^{-1/4}) \text{ quand } m \rightarrow \infty \quad (30)$$

Notre résultat est nouveau pour le modèle de Rabi asymétrique à un photon c'est-à-dire pour le cas où  $\epsilon \in \mathbb{R} \setminus \{0\}$ . Compte tenu de la formule (21), on voit que l'exposant  $-\frac{1}{4}$  ne peut pas être amélioré dans le cas  $\epsilon = 0$ .

Le cas général de l'AQRM à un photon avec  $\omega > 0$  et  $h > 0$  peut être facilement réduit au cas  $\omega = h = 1$ , en utilisant la multiplication de l'opérateur par une constante. Plus précisément, pour l'opérateur

$$I_{\mathbb{C}^2} \otimes h\omega \hat{a}^\dagger \hat{a} + \frac{1}{2}(\Delta \sigma_z + \epsilon \sigma_x) \otimes I_{\ell^2(\mathbb{N})} + hg \sigma_x \otimes (\hat{a} + \hat{a}^\dagger),$$

la formule asymptotique (30) devient

$$E_m^\pm = h\omega m - \frac{h}{\omega} g^2 \pm \frac{1}{2} \epsilon + O(m^{-1/4}) \text{ quand } m \rightarrow \infty$$

Dans notre preuve de (30), on utilise plusieurs idées du travail décrit dans la section 1.3.2, Page 18, par exemple la méthode pour surmonter la difficulté des valeurs propres doubles de l'opérateur (29) avec  $\Delta = 0$ . Cependant, dans le travail décrit dans la section 1.3.2, on utilise une approximation de l'hamiltonien à deux photons avec  $\Delta = 0$  par un opérateur similaire à un opérateur différentiel du premier ordre sur le cercle afin que ses vecteurs propres puissent être exprimés explicitement. Dans le cas de l'hamiltonien à un photon donné par (29) avec  $\Delta = 0$ , une idée pareille donne un opérateur pseudo-différentiel d'ordre 1/2 et il faut construire une approximation de ses vecteurs propres.

L'estimation (30) est un résultat crucial que nous utilisons pour améliorer l'estimation (30). Plus précisément : dans le **Chapitre 3**, on prouve que l'hypothèse  $\epsilon \notin \mathbb{Z}$  implique la formule asymptotique

$$E_m^\pm = m - g^2 \pm \frac{1}{2} \epsilon + O(m^{-1/2} \ln m) \text{ quand } m \rightarrow \infty$$

et dans le **Chapitre 4**, on prouve que dans le cas  $l_0 := \epsilon \in \mathbb{N}$  on a la formule asymptotique à trois termes

$$E_{i+l_0}^- = i + \frac{1}{2} l_0 - g^2 - |\mathfrak{r}_i| + O(i^{-1/2} \ln i) \text{ quand } i \rightarrow \infty \quad (31)$$

$$E_i^+ = i + \frac{1}{2}l_0 - g^2 + |\mathbf{r}_i| + O(i^{-1/2} \ln i) \text{ quand } i \rightarrow \infty \quad (32)$$

avec

$$\mathbf{r}_i := i^{-1/4} \frac{\Delta}{2\sqrt{2\pi g}} \cos\left(4g\sqrt{i} - \frac{\pi}{4} - l_0 \frac{\pi}{2}\right). \quad (33)$$

### 1.3.2 Comportement asymptotique des grandes valeurs propres du modèle de Rabi asymétrique à deux photons.

Dans la suite on se pose la question du comportement asymptotique de la  $n$ -ième valeur propre du modèle de Rabi asymétrique à deux photons, c'est-à-dire pour l'hamiltonien défini dans la définition (1.2.1)-(e) en supposant, sans perte de généralité, que  $h = 1$  et  $\omega = 1$ ,

$$I_{\mathbb{C}^2} \otimes \hat{a}^\dagger \hat{a} + \frac{1}{2}(\Delta \sigma_z + \epsilon \sigma_x) \otimes I_{\ell^2(\mathbb{N})} + g \sigma_x \otimes (\hat{a}^2 + (\hat{a}^\dagger)^2), \quad (34)$$

où  $\Delta$ ,  $\epsilon$  et  $g$  sont des paramètres réels. Dans la suite on suppose  $g > 0$ .

Comme nous l'avons mentionné dans la section 1.2.4, ce problème a été étudié dans le cas où  $\epsilon = 0$  dans [33], où l'estimation de l'erreur obtenue est  $O(n^{-1/3})$ .

Le Chapitre 5 contient un travail en collaboration avec Anne Boutet de Monvel et mon directeur de thèse Lech Zielinski [25], où l'estimation de l'erreur obtenue pour ce modèle est  $O(n^{-1/2})$ . De plus on prouve que l'estimation analogue est toujours valable pour le QRM asymétrique à deux photons.

En supposant que  $0 < g < \frac{1}{2}$ , on montre que l'opérateur (34) est auto-adjoint dans  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$ , son spectre est discret et se compose de deux suites des valeurs propres  $(E_{-1,m})_{m \in \mathbb{N}}$ ,  $(E_{1,m})_{m \in \mathbb{N}}$  qui vérifient la formule asymptotique

$$E_{\nu,m} = \beta m + \beta_\nu + O(m^{-1/2}), \quad \nu = \pm 1 \text{ quand } m \rightarrow \infty \quad (35)$$

où

$$\beta := \sqrt{1 - 4g^2}, \quad (36)$$

$$\beta_\nu = \frac{1}{2}(\beta - 1) + \nu \frac{\epsilon}{2} \text{ pour } \nu = \pm 1. \quad (37)$$

Le cas général de l'AQRM à deux photons avec  $\omega > 0$  et  $h > 0$  peut être facilement réduit au cas  $\omega = h = 1$ , en utilisant la multiplication de l'opérateur par une constante. Plus précisément, l'estimation asymptotique (35) reste valable pour l'opérateur introduit dans la définition (1.2.1)-(e), c'est-à-dire pour

$$I_{\mathbb{C}^2} \otimes h\omega \hat{a}^\dagger \hat{a} + \frac{1}{2}(\Delta \sigma_z + \epsilon \sigma_x) \otimes I_{\ell^2(\mathbb{N})} + hg \sigma_x \otimes (\hat{a}^2 + (\hat{a}^\dagger)^2),$$

sous l'hypothèse  $0 < g < \omega/2$ , la formule asymptotique (35) reste valable avec  $\beta = h\sqrt{\omega^2 - 4g^2}$  et  $\beta_\nu = \frac{1}{2}h(\sqrt{\omega^2 - 4g^2} - \omega) + \nu \frac{\epsilon}{2}$ .

Comme dans l'article [33], notre preuve s'inspire de la transformation de similarité utilisée

dans l'article de J. Janas, S. Naboko [75]. Cependant nous rencontrons une différence majeure par rapport à [33] : dans le cas où  $\epsilon$  est un multiple de  $\beta$  on doit surmonter une difficulté supplémentaire due au fait que dans le cas où  $\Delta = 0$  l'opérateur (34) a des valeurs propres doubles qui ne peuvent pas être découplées lorsque  $\epsilon \neq 0$ .

On observe qu'en utilisant  $U_{\pi/4} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$ , la matrice de rotation d'angle  $\pi/4$  qui vérifie

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

l'opérateur (34) devient similaire à l'opérateur

$$\mathbf{H} := \frac{1}{2}(\Delta \sigma_x - \epsilon \sigma_z) \otimes I_{\ell^2(\mathbb{N})} + I_{\mathbb{C}^2} \otimes \hat{a}^\dagger \hat{a} - g \sigma_z \otimes (\hat{a}^2 + (\hat{a}^\dagger)^2). \quad (38)$$

et le problème est réduit à l'existence d'une base orthonormée  $\{\mathbf{u}_{\nu,m}\}_{(\nu,m) \in \{-1,1\} \times \mathbb{N}}$  dans  $\mathbb{C}^2 \otimes \ell^2$  qui vérifie

$$\mathbf{H} \mathbf{u}_{\nu,m} = E_{\nu,m} \mathbf{u}_{\nu,m} \text{ pour } m \in \mathbb{N}, \nu = \pm 1, \quad (39)$$

où la suite  $(E_{\nu,m})_{m \in \mathbb{N}}$  vérifie l'estimation asymptotique (35). Il est bien connu que dans le cas particulier  $\Delta = 0$ , il existe une base orthonormée  $\{\mathbf{u}_{\nu,m}^0\}_{(\nu,m) \in \{-1,1\} \times \mathbb{N}}$  dans  $\mathbb{C}^2 \otimes \ell^2$  telle que

$$\mathbf{H}_0 \mathbf{u}_{\nu,m}^0 = (\beta m + \beta_\nu) \mathbf{u}_{\nu,m}^0 \text{ pour } m \in \mathbb{N}, \nu = \pm 1, \quad (40)$$

où

$$\mathbf{H}_0 := -\frac{1}{2} \epsilon \sigma_z \otimes I_{\ell^2(\mathbb{N})} + I_{\mathbb{C}^2} \otimes \hat{a}^\dagger \hat{a} - g \sigma_z \otimes (\hat{a}^2 + (\hat{a}^\dagger)^2). \quad (41)$$

Ainsi le problème initial est réduit au problème de la preuve de l'estimation asymptotique

$$\lambda_n(\mathbf{H}) - \lambda_n(\mathbf{H}_0) = O(n^{-1/2}) \text{ quand } n \rightarrow \infty \quad (42)$$

où  $(\lambda_n(\mathbf{H}))_{n=0}^\infty$  (respectivement  $(\lambda_n(\mathbf{H}_0))_{n=0}^\infty$ ) est la suite croissante des valeurs propres de  $\mathbf{H}$  (respectivement  $\mathbf{H}_0$ ), en comptant les multiplicités.

On a choisi de travailler dans l'espace  $\ell^2(\mathbb{Z})$  au lieu de  $\ell^2(\mathbb{N})$  parce que le contrôle de l'erreur dans la formule asymptotique est plus facile quand on peut utiliser la transformée de Fourier.

On observe d'abord que l'opérateur  $\mathbf{H}_0$  peut s'écrire comme la somme directe  $H_{-1} \oplus H_1$ , où  $H_{-1}$  et  $H_1$  sont des opérateurs auto-adjoints dans  $\ell^2(\mathbb{N})$ ,

$$H_\nu := \hat{a}^\dagger \hat{a} + \nu g (\hat{a}^2 + (\hat{a}^\dagger)^2) + \frac{1}{2} \nu \epsilon, \text{ avec } \nu = \pm 1 \quad (43)$$

dont les valeurs propres sont explicitement connues. Notre prochain objectif est d'approximer les opérateurs  $H_{\pm 1}$  agissant dans  $\ell^2(\mathbb{N})$  par les opérateurs  $J_{\pm 1}$  agissant dans  $\ell^2(\mathbb{Z})$ . On remarque que la définition de  $H_{\pm 1}$  contient le terme  $b(m) = \sqrt{(m+1)(m+2)}$  et il est possible de simplifier le problème en utilisant l'estimation

$$\sqrt{(m+1)(m+2)} = m + \frac{3}{2} + O(m^{-1}) \text{ quand } m \rightarrow \infty$$

Ainsi on remplace le terme  $b(m)$  par  $m + \frac{3}{2}$  dans la définition des opérateurs auto-adjoints  $J_{\pm 1}$  qui agissent dans  $\ell^2(\mathbb{Z})$ . Ces opérateurs peuvent être considérés comme les opérateurs

de Jacobi étudiés par Edwards [43]. On utilise ensuite la transformée de Fourier pour changer l'opérateur  $J_{\pm 1}$  en opérateur elliptique différentiel linéaire du premier ordre  $L_{\pm 1}$  auto-adjoint dans  $L^2(\mathbb{T})$  (où  $\mathbb{T} = \mathbb{R}/2\pi$ ). On peut alors exprimer explicitement toutes les valeurs propres et tous les vecteurs propres de  $J_{\pm 1}$ . Les opérateurs  $J_{\pm 1}$  ne sont pas semi-bornés, mais on trouve qu'on peut choisir une suite de valeurs propres  $(\lambda_j(J_{\pm 1}))_{j \in \mathbb{Z}}$  telle que

$$\lambda_j(J_{\pm 1}) = \lambda_j(H_{\pm 1}) \text{ quand } j \in \mathbb{N}.$$

Ensuite on introduit l'opérateur  $\mathbf{J}_0 = J_{-1} \oplus J_1$  avec le but d'approcher les grandes valeurs propres de

$$\mathbf{H} = \mathbf{H}_0 + \frac{1}{2} \Delta \sigma_x \otimes I_{\ell^2} \quad (44)$$

par les grandes valeurs propres de

$$\mathbf{J} = \mathbf{J}_0 + \frac{1}{2} \Delta \sigma_x \otimes I_{\ell^2(\mathbb{Z})}. \quad (45)$$

Afin de comparer les grandes valeurs propres de  $\mathbf{J}$  et  $\mathbf{J}_0$ , nous utilisons la méthode de similarité et un résultat crucial qui assure le fait que les vecteurs propres de  $J_{-1}$  et  $J_1$  sont "asymptotiquement orthogonaux". On montre que l'opérateur  $\mathbf{J}$  est semblable à un certain opérateur  $D + R$ , où  $D = \text{diag}(d_j)_{j \in \mathbb{Z}}$  est l'opérateur diagonal dont les valeurs propres sont celles de  $\mathbf{J}_0$  et  $R$  est un opérateur compact et vérifiant

$$\|R^* e_j\| \leq C(1 + |j|)^{-1/2} \text{ pour tous } j \in \mathbb{Z}. \quad (46)$$

Nous pouvons alors utiliser l'estimation

$$\lambda_j(\mathbf{J}) = \lambda_j(D + R) = d_j + O(\|R^* P_j\|) \text{ quand } j \rightarrow \infty, \quad (47)$$

où  $P_j$  est la projection orthogonale sur le sous-espace linéaire engendré par  $\{e_k : d_k = d_j\}$ . En effet :

- si  $\epsilon/\beta \notin \mathbb{Z}$  alors chaque valeur propre de  $D$  est simple et l'estimation (47) peut être obtenue soit par une adaptation de la preuve du résultat de J. Janas, S. Naboko [75] énoncé dans le Lemme 1.1.1 ou en utilisant le résultat de M. Malejki [94] énoncé dans le Théorème 1.1.2

- si  $\epsilon/\beta \in \mathbb{Z}$  alors chaque valeur propre de  $D$  est double et on obtient (47) utilisant le résultat de M. Malejki [94] énoncé dans le Théorème 1.1.2

Enfin, en utilisant le principe de min-max, on montre que les grandes valeurs propres de  $\mathbf{H}$  et  $\mathbf{J}$  sont proches et on en déduit (35).

Après avoir prouvé (35), on a amélioré le comportement asymptotique des valeurs propres de l'hamiltonien de AQRM à deux photons obtenu dans le cas où  $\epsilon/\beta \in \mathbb{Z}$  en donnant les trois premiers termes de l'asymptotique avec une estimation d'erreur  $O(n^{-1} \ln n)$  et on a montré que cette estimation d'erreur est toujours valable dans le cas où  $\epsilon/\beta \notin \mathbb{Z}$ . Notre amélioration est basée sur l'estimation (35) et elle est obtenue par une approche qui est une adaptation de la théorie des perturbations de Schrieffer-Wolff [57] (voir aussi [83], [87], [127], [57]).

Dans le **Chapitre 6**, en supposant que  $0 < g < \frac{1}{2}$  et  $\epsilon/\beta \notin \mathbb{Z}$ , on prouve que les valeurs propres  $(E_{-1,m})_{m \in \mathbb{N}}$ ,  $(E_{1,m})_{m \in \mathbb{N}}$  de l'opérateur (34), vérifient la formule asymptotique

$$E_{\nu,m} = \beta m + \beta_{\nu} + O(m^{-1} \ln m), \quad \nu = \pm 1 \text{ quand } m \rightarrow \infty$$

avec  $\beta_{\nu} = \beta_0 + \nu\epsilon/2$ .

Dans le **Chapitre 7**, en supposant que  $0 < g < \frac{1}{2}$  et  $l_0 = \epsilon/\beta \in \mathbb{N}$ , on montre que  $(\lambda_n(\mathbf{H}))_{n=1}^{\infty}$ , la suite des valeurs propres de l'opérateur (34) disposées dans l'ordre croissant et répétées selon leurs multiplicité, peut être exprimée comme la réunion des suites  $(E_m^-)_{m \in \mathbb{N}}$  et  $(E_m^+)_{m \in \mathbb{N}}$ , définies de manière suivante

$$E_n^- = \lambda_n(\mathbf{H}) \text{ for } n = 0, \dots, l_0,$$

$$E_{i+l_0}^- = \lambda_{2i+l_0}(\mathbf{H}) \text{ for } i \in \mathbb{N},$$

$$E_i^+ = \lambda_{2i+1+l_0}(\mathbf{H}) \text{ for } i \in \mathbb{N}.$$

De plus on a les formules asymptotiques suivantes

$$E_{i+l_0}^- = \beta i + \beta_0 + \frac{1}{2}\epsilon - |\mathbf{r}_i| + O(i^{-1} \ln i) \text{ quand } i \rightarrow \infty \quad (48)$$

$$E_i^+ = \beta i + \beta_0 + \frac{1}{2}\epsilon + |\mathbf{r}_i| + O(i^{-1} \ln i) \text{ quand } i \rightarrow \infty \quad (49)$$

avec

$$\beta := \sqrt{1 - 4g^2}, \quad \beta_0 := \frac{1}{2}(\beta - 1),$$

$$\begin{aligned} \mathbf{r}_i &:= 0 \text{ si } l_0 \text{ est impair} \\ \mathbf{r}_i &:= i^{-1/2} \frac{\Delta}{2} \sqrt{\frac{\beta}{\pi g}} \cos\left(\left(2\alpha - \frac{\pi}{2}\right)(i + l_0) + (1 - l_0)\alpha\right) \text{ si } l_0 \text{ est pair} \end{aligned} \quad (50)$$

où

$$\alpha = \arctan \sqrt{\frac{1 - 2g}{1 + 2g}}. \quad (51)$$

Dans le cas du QRM à deux photons avec le biais  $l_0 = \epsilon = 0$  on obtient les formules asymptotiques

$$E_m^{\pm} = \beta m + \beta_0 \pm |\mathbf{r}_m| + O(m^{-1} \ln m) \text{ quand } m \rightarrow \infty \quad (52)$$

qui peuvent être considérées comme la généralisation de l'approximation de l'onde tournant (GRWA) pour ce modèle. Compte tenu du fait que  $\mathbf{r}_m$  est un terme oscillant dont l'amplitude est d'ordre  $m^{-1/2}$ , on voit que l'exposant  $-\frac{1}{2}$  dans l'estimation (35) est optimal.

### 1.3.3 Série des perturbations pour les matrices de Jacobi et le modèle quantique de Rabi

Dans le travail en collaboration avec mon directeur de thèse Lech Zielinski, décrit en [Chapitre 8](#), on a étudié le problème des perturbations des valeurs propres pour une classe de matrices tridiagonales infinies qui définissent des opérateurs auto-adjoints non bornés à spectre discret. La motivation principale de ce travail est le modèle quantique de Rabi (QRM). Il s'avère (voir [\(18\)](#) avec  $h = 1$ ) que l'hamiltonien QRM est unitairement équivalent à la somme directe  $J_{\Delta}^{\omega}(g) \oplus J_{-\Delta}^{\omega}(g)$ , où  $\Delta$ ,  $\omega$  et  $g$  sont des paramètres réels et  $J_s^{\omega}(g)$  est l'opérateur auto-adjoint défini dans  $\ell^2(\mathbb{N}^*)$  par la matrice

$$J_s^{\omega}(g) = \begin{pmatrix} -\frac{s}{2} & g\sqrt{1} & 0 & 0 & 0 & \cdots \\ g\sqrt{1} & \omega + \frac{s}{2} & g\sqrt{2} & 0 & 0 & \cdots \\ 0 & g\sqrt{2} & 2\omega - \frac{s}{2} & g\sqrt{3} & 0 & \cdots \\ 0 & 0 & g\sqrt{3} & 3\omega + \frac{s}{2} & g\sqrt{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (53)$$

En pratique, la valeur de la constante de couplage  $g$  est petite et il est naturel d'étudier une valeur propre au moyen de la série de Taylor par rapport à  $g$ . On observe que toutes les entrées diagonales de la matrice [\(53\)](#) sont distinctes si  $s$  n'est pas un multiple de  $\omega$ . Donc les phénomènes les plus intéressants apparaissent lorsque  $s$  est un multiple de  $\omega$ . Pour simplifier notre travail, on considère la situation  $s = \omega$  et notre analyse portera sur les problèmes suivants :

- (i) prouver que les valeurs propres sont des fonctions analytiques de  $g$  et donner une borne explicite du rayon de convergence,
- (ii) donner des estimations explicites de l'erreur due à une coupure de la série de Taylor,
- (iii) donner une méthode de calcul des coefficients et exprimer les corrections d'ordre inférieur.

Concernant le point (i), il faut contrôler le spectre par rapport à  $g$  pour éviter le croisement des valeurs propres. Les résultats pour le point (ii) sont obtenus de manière standard : la formule intégrale de Cauchy donne les bornes des coefficients et il est clair que les estimations deviennent meilleures lorsque le rayon de convergence est plus grand.

Le cas de la matrice [\(53\)](#) avec  $s = \omega$  a été intensivement étudié dans la littérature physique en raison de l'approximation de l'onde tournante introduite dans le célèbre article de Jaynes et Cummings [\[79\]](#). La raison de cette popularité a été double : le modèle de Jaynes-Cummings est explicitement résoluble et les résultats expérimentaux avaient confirmé une haute qualité de cette approximation. Pourtant, des expériences plus récentes ont permis d'agrandir la valeur de la constante de couplage et ont montré la limite de cette approximation.

Notre intérêt pour ce problème vient de l'article [\[60\]](#), où les auteurs étudient la qualité de l'approximation de Jaynes-Cummings et proposent les corrections des valeurs propres de

(53). Les auteurs de [60] évoquent les difficultés à étudier une matrice infinie et proposent de regarder un petit bloc avec l'espoir d'obtenir des approximations correctes. Dans notre travail, on propose une méthode simple pour réduire le problème initial à un problème analogue pour un bloc fini et on montre comment calculer les coefficients. De plus, on explique quelle est la taille minimale du bloc pour récupérer un coefficient donné de la série de Taylor. Il s'avère que les coefficients proposés dans [60] ne sont pas corrects, car le bloc est trop petit.

Le but de notre travail est d'étudier ces questions pour une classe plus générale des opérateurs auto-adjoints dans  $\ell^2(\mathbb{N})$  de la forme  $J(g) = D + gB$  où  $D$  est diagonal et  $B$  est tridiagonal. Ainsi, nos résultats peuvent également être appliqués à d'autres modèles, par exemple aux deux photons version du QRM (voir [61]).

Soient  $(d_i)_{i=1}^\infty$ ,  $(b_i)_{i=1}^\infty$ ,  $(b'_i)_{i=1}^\infty$  des suites à valeurs réelles et  $g \in \mathbb{R}$ . On note  $J(g)$  la fermeture de l'opérateur symétrique linéaire défini par la matrice

$$\begin{pmatrix} d_1 + gb'_1 & gb_1 & 0 & 0 & \cdots \\ gb_1 & d_2 + gb'_2 & gb_2 & 0 & \cdots \\ 0 & gb_2 & d_3 + gb'_3 & gb_3 & \cdots \\ 0 & 0 & gb_3 & d_4 + gb'_4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (54)$$

c'est-à-dire  $J(g) = D + gB$  avec  $D$  et  $B$  donnés par

$$De_i = d_i e_i, \quad (55)$$

$$Be_i = b'_i e_i + b_i e_{i+1} + b_{i-1} e_{i-1}, \quad (56)$$

où par convention  $b_{i-1} e_{i-1} = 0$  si  $i = 1$ .

On fait les hypothèses suivantes

(H1) il existe  $\rho_0 > 0$  tel que  $2\rho_0^2 < \liminf_{i \rightarrow \infty} \frac{d_i^2}{b_i^2 + b_{i-1}^2}$ ,

(H2) la suite  $(b'_i)_{i=1}^\infty$  est bornée,

(H3)  $d_i \xrightarrow{i \rightarrow \infty} \infty$ ,

afin que l'opérateur  $J(g)$  définisse un opérateur auto-adjoint, borné inférieurement et dont le spectre est discret pour tout  $g \in [-\rho_0, \rho_0]$ .

### Premier résultat

Notre premier résultat concerne les perturbations d'une valeur propre simple de  $D$ . Pour cela, on fixe  $k \in \mathbb{N}^*$  et suppose que

$$d_k \neq d_i \text{ pour } i \in \mathbb{N}^* \setminus \{k\}. \quad (57)$$

Puisque  $\sigma(J(g) - (d + gb)I) = \sigma(J(g)) - (d + gb)$ , notre analyse de  $J(g)$  peut être réduite à une analyse de  $J(g) - (d + gb)I$  et en particulier, on peut utiliser  $d = d_k$ ,  $b = b'_k$ . Ainsi, sans aucune perte de la généralité, on peut supposer que  $d_k = b'_k = 0$ . De plus, on note

$$\beta_i := |b_{i-1}| + |b_i| + |b'_i| \quad (58)$$

et on introduit

$$0 < \rho < \inf_{i \neq k} \frac{|d_i|}{\beta_i + \beta_k}. \quad (59)$$

On suppose également que **(H1)**-**(H3)** sont vérifiées et  $\rho \leq \rho_0$ . On montre les résultats suivants :

(i) Si  $-\rho < g < \rho$  alors l'intervalle  $[-\beta_k \rho, \beta_k \rho]$  contient exactement une valeur propre de  $J(g)$ ,

$$[-\beta_k \rho, \beta_k \rho] \cap \sigma(J(g)) = \{\lambda_k(J(g))\}. \quad (60)$$

(ii) La valeur  $\lambda_k(J(g))$  est simple et  $g \rightarrow \lambda_k(J(g))$  est analytique réelle, c'est-à-dire

$$\lambda_k(J(g)) = \sum_{\nu=1}^{\infty} c_{k,\nu} g^\nu \quad \text{si } -\rho < g < \rho. \quad (61)$$

(iii) Les coefficients dans (61) satisfont aux estimations  $|c_{k,\nu}| \leq \beta_k \rho^{1-\nu}$  et on a

$$\left| \lambda_k(J(g)) - \sum_{1 \leq \nu \leq N} c_{k,\nu} g^\nu \right| \leq \frac{\beta_k |g|^{N+1}}{(\rho - |g|) \rho^{N-1}} \quad \text{si } -\rho < g < \rho. \quad (62)$$

(iv) Si  $b'_j = 0$  pour tout  $j \in \mathbb{N}^*$ , alors  $c_{k,\nu} = 0$  lorsque  $\nu$  est impair et (61) est vérifié avec

$$c_{k,2} = -\frac{b_k^2}{d_{k+1}} - \frac{b_{k-1}^2}{d_{k-1}} \quad (63)$$

$$c_{k,4} = \frac{b_k^4}{d_{k+1}^3} + \frac{b_{k-1}^4}{d_{k-1}^3} + \frac{b_k^2 b_{k-1}^2}{d_{k-1}^2 d_{k+1}} + \frac{b_k^2 b_{k-1}^2}{d_{k+1}^2 d_{k-1}} - \frac{b_k^2 b_{k+1}^2}{d_{k+1}^2 d_{k+2}} - \frac{b_{k-1}^2 b_{k-2}^2}{d_{k-1}^2 d_{k-2}}. \quad (64)$$

(v) Dans le cas général, on a

$$\lambda_k(J(g)) = c_{2,k}(g) g^2 + c_{4,k}(g) g^4 + O(g^6), \quad (65)$$

où  $c_{2,k}(g)$  et  $c_{4,k}(g)$  sont donnés en utilisant  $d_i + gb'_i$  au lieu de  $d_i$  dans (63)-(64).

## Deuxième résultat

Notre deuxième résultat concerne les perturbations d'une valeur propre double de  $D$ . Pour cela, on fixe  $k \in \mathbb{N}^*$  et suppose que

$$d_{k+1} = d_k \neq d_j \quad \text{pour } j \in \mathbb{N}^* \setminus \{k, k+1\}. \quad (66)$$



Sans perte de la généralité, on remplace  $J(g)$  par  $J(g) - (d + gb)I$  avec  $d = d_k$ ,  $b = (b'_k + b'_{k+1})/2$  et on suppose que

$$d_{k+1} = d_k = 0 \text{ et } b'_{k+1} = -b'_k. \quad (67)$$

On introduit les quantités

$$\mu_k := (b_k^2 + b_k'^2)^{1/2}, \quad (68)$$

$$\beta'_{k-1} := |b_{k-2}| + |b'_{k-1}|, \quad (69)$$

$$\beta'_{k+2} := |b_{k+2}| + |b'_{k+2}|, \quad (70)$$

$$\gamma_k := 3 \max\{|b_{k-1}|, |b_{k+1}|\} + 2 \max\{\mu_k, \beta'_{k-1}, \beta'_{k+2}\}, \quad (71)$$

$$\gamma'_k := \max\left\{\left|\frac{b_{k-1}}{d_{k-1}}\right|, \left|\frac{b_{k+1}}{d_{k+2}}\right|\right\} \quad (72)$$

et

$$\beta'_i := |b_{i-1}| + |b_i| + |b'_i| \text{ si } i \notin [k-1, k+2]. \quad (73)$$

On suppose que **(H1)**-**(H3)** sont vérifiées et  $0 < \rho \leq \rho_0$  satisfait aux conditions

$$\rho \leq \inf_{i \notin \{k, k+1\}} \frac{|d_i|}{2(\beta'_i + \mu_k)}, \quad (74)$$

$$4\rho\mu_k \leq \inf_{i \notin \{k, k+1\}} |d_i|, \quad (75)$$

$$\rho \gamma_k \gamma'_k e^{2\rho\gamma'_k} < \mu_k, \quad (76)$$

où  $\mu_k, \gamma_k, \gamma'_k, \beta'_i$  sont donnés par (68)-(73). On montre les résultats suivants :

(i) Si  $-\rho < g < \rho$  et  $g \neq 0$ , alors

$$[-2\mu_k\rho, 2\mu_k\rho] \cap \sigma(J(g)) = \{\lambda_k(J(g)), \lambda_{k+1}(J(g))\}, \quad (77)$$

où les valeurs propres  $\lambda_k(J(g)), \lambda_{k+1}(J(g))$  sont simples et vérifient

$$\begin{cases} \lambda_k(J(g)) < 0 < \lambda_{k+1}(J(g)) \text{ if } g > 0, \\ \lambda_{k+1}(J(g)) < 0 < \lambda_k(J(g)) \text{ if } g < 0 \end{cases} \quad (78)$$

(ii) Si  $j = 0, 1$  et  $\mu_{k+1} := -\mu_k$ , alors on a

$$\lambda_{k+j}(J(g)) = -\mu_{k+j}g + \sum_{\nu=2}^{\infty} c_{k+j,\nu}g^\nu \text{ si } -\rho < g < \rho. \quad (79)$$

(iii) Les coefficients dans (79) satisfont aux estimations  $|c_{k+j,\nu}| \leq \mu_k\rho^{1-\nu}$  pour  $j = 0, 1$  et

$$\left| \lambda_{k+j}(J(g)) + \mu_{k+j}g - \sum_{2 \leq \nu \leq N} c_{k+j,\nu}g^\nu \right| \leq \frac{\mu_k|g|^{N+1}}{(\rho - |g|)\rho^{N-1}} \text{ si } -\rho < g < \rho. \quad (80)$$

Ensuite, on désigne

$$d_i^0(g) := d_i + gb'_i \text{ pour } i \in \mathbb{N}^*, \quad (81)$$

$$b_k^1(g) := b'_k + g \frac{b_{k-1}^2}{d_k^0(g) - d_{k-1}^0(g)}, \quad (82)$$

$$b_{k+1}^1(g) := b'_{k+1} + g \frac{b_{k+1}^2}{d_{k+1}^0(g) - d_{k+2}^0(g)}, \quad (83)$$

$$\widehat{b}_k^1(g) := b_k \left( 1 - \frac{g^2 b_{k-1}^2}{2(d_k^0(g) - d_{k-1}^0(g))^2} - \frac{g^2 b_{k+1}^2}{2(d_{k+1}^0(g) - d_{k+2}^0(g))^2} \right) \quad (84)$$

et on introduit la matrice

$$B_k^1(g) := \begin{pmatrix} b_k^1(g) & \widehat{b}_k^1(g) \\ \widehat{b}_k^1(g) & b_{k+1}^1(g) \end{pmatrix}. \quad (85)$$

Pour  $j = 0, 1$ , on désigne par  $\lambda_{k+j}^1(g)$  la valeur propre de  $B_k^1(g)$  qui vérifie

$$\lambda_{k+j}^1(g) \xrightarrow{g \rightarrow 0} -\mu_{k+j}.$$

On montre que

(iv) Pour  $j = 0, 1$ , on a

$$\lambda_{k+j}(J(g)) = g \lambda_{k+j}^1(g) + O(g^4). \quad (86)$$

(v) Si  $b'_k = 0$ , alors l'estimation (86) implique

$$\lambda_{k+j}(J(g)) = -\mu_{k+j}g - g^2 \left( \frac{b_{k-1}^2}{2d_{k-1}} + \frac{b_{k+1}^2}{2d_{k+2}} \right) + O(g^3) \quad (87)$$

où  $j = 0, 1$ , et  $\mu_{k+1} := -\mu_k$ .

Dans le [Chapitre 9](#), on donne la formule détaillée de  $\lambda_{k+j}(J(g))$  avec l'estimation d'erreur  $O(g^6)$ .

### L'approximation de Jaynes-Cummings

Dans [79], Jaynes et Cummings ont proposé d'approcher l'opérateur (53) par

$$\widetilde{J}_s^\omega(g) = \begin{pmatrix} -\frac{s}{2} & 0 & 0 & 0 & 0 & \cdots \\ 0 & \omega + \frac{s}{2} & g\sqrt{2} & 0 & 0 & \cdots \\ 0 & g\sqrt{2} & 2\omega - \frac{s}{2} & 0 & 0 & \cdots \\ 0 & 0 & 0 & 3\omega + \frac{s}{2} & g\sqrt{4} & \cdots \\ 0 & 0 & 0 & g\sqrt{4} & 4\omega - \frac{s}{2} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (88)$$

sous l'hypothèse que  $s \approx \omega$  et  $g$  est petit. Puisque  $\tilde{J}_s^\omega(g)$  est la somme directe

$$\frac{s}{2} + \tilde{J}_s^\omega(g) = (0) \oplus \bigoplus_{m \in \mathbb{N}^*} \begin{pmatrix} 2m\omega + (s - \omega) & g\sqrt{2m} \\ g\sqrt{2m} & 2m\omega \end{pmatrix}, \quad (89)$$

on peut trouver explicitement toutes ses valeurs propres. On peut donner des explications physiques de cette approximation pour le modèle semi-classique. Dans le modèle entièrement quantifié des explications physiques sont généralement données au moyen de la théorie des perturbations dépendante du temps. L'approche indépendante du temps a été proposée dans [60].

Suivant [60], on considère le cas  $\omega = s$ . Dans ce cas, les valeurs propres de (88) sont

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

D'autre part, on peut utiliser notre résultat décrit dans la section (1.3.3) sans l'hypothèse  $d_k = d_{k+1} = 0$ . Le décalage diagonal dans (53) donne les expressions

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

pour le couple  $\lambda_k(J(g)), \lambda_{k+1}(J(g))$ . Dans le cas du QRM avec  $s = \omega$ , on a  $b_k = \sqrt{k}$ ,  $d_{2m} - d_{2m-1} = d_{2m+2} - d_{2m+1} = 2\omega$  et le couple des valeurs propres correspondant  $\{\lambda_{2m}(J_\omega^\omega(g)), \lambda_{2m+1}(J_\omega^\omega(g))\}$ , vérifie

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

On observe que ces valeurs propres coïncident avec les valeurs propres du modèle de Jaynes-Cumming modulo  $O(g^2)$ . On peut aussi utiliser (86) avec  $b'_k \neq 0$  pour couvrir une situation où la différence  $s - \omega = cg$ . Il est également possible de considérer le cas des entrées  $b_i, b'_i$  qui sont des fonctions analytiques de  $g$ , mais nous n'avons pas utilisé ce cadre afin de simplifier les expressions du rayon de convergence.

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# Première partieI

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L'étude asymptotique de grandes  
valeurs propres pour le modèle  
quantique asymétrique de Rabi

## **Sous-partie A:**

**L'étude asymptotique des grandes valeurs propres pour le modèle quantique asymétrique de Rabi à un photon**

## Comportement des grandes valeurs propres pour le Modèle Quantique Asymétrique de Rabi

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# Behaviour of Large Eigenvalues for the Asymmetric Quantum Rabi Model

Mirna Charif<sup>1</sup>, Ahmad Fino<sup>2</sup> and Lech Zielinski<sup>3</sup>

**Abstract.** We prove that the spectrum of the asymmetric quantum Rabi model consists of two eigenvalue sequences  $(E_m^+)_{m=0}^\infty$ ,  $(E_m^-)_{m=0}^\infty$  and we describe their asymptotic behaviour with an error estimate of the form  $O(m^{-1/4})$  when  $m$  tends to infinity.

**Keywords :** unbounded self-adjoint operators, asymptotics of eigenvalues, discrete spectrum, quantum Rabi model

**Mathematics Subject Classification :** 47A75, 47B02, 47B25, 47B36, 81Q10, 81Q15.

## 1 General presentation

### 1.1 Introduction

The quantum Rabi model describes the simplest physical example of interactions between radiation and matter. It has its origin in the semi-classical model of interactions between a Two Level System (TLS) and light, due to I. I. Rabi (see [105], [106]). A fully quantized version, known as the Rotating Wave Approximation (RWA), was introduced in the famous paper of Jaynes and Cummings [79]. The Hamiltonian of the quantum Rabi model (QRM) is given in Definition 1.2(d). It is also known under the name of the Jaynes-Cummings model without RWA and depends on two real parameters :  $g$  and  $\Delta$  (the coupling constant and the level separation energy in the TLS). The Hamiltonian of the asymmetric quantum Rabi model (AQRM) is given in Definition 1.2(c). It is usually referred to as the QRM with a bias and contains an additional parameter  $\epsilon$ , called the bias of the model. The AQRM is a fundamental model in the quantum electrodynamics of superconducting circuits (see [133], [82]). The additional term appears due to the tunnelling between two current states (see [61]). We refer to [15] concerning the historical aspects and to [133] for a list of recent research works and experimental realizations of QRM and AQRM.

Let  $\mathbf{H}_{\text{Rabi}}$  denote the AQRM Hamiltonian from Definition 1.2(c). Its spectrum is discrete and only in the case  $\Delta = 0$ , the spectrum of the corresponding Hamiltonian  $\mathbf{H}_{0,\text{Rabi}}$ , is explicitly known (see Theorem 1.3). Our purpose is to investigate the large  $n$  estimate

$$\lambda_n(\mathbf{H}_{\text{Rabi}}) - \lambda_n(\mathbf{H}_{0,\text{Rabi}}) = O(n^{-\rho}), \quad (1.1)$$

where  $\rho > 0$  and  $(\lambda_n(\mathbf{H}_{\text{Rabi}}))_{n=0}^\infty$  (respectively  $(\lambda_n(\mathbf{H}_{0,\text{Rabi}}))_{n=0}^\infty$ ) is the non-decreasing sequence of eigenvalues of  $\mathbf{H}_{\text{Rabi}}$  (respectively  $\mathbf{H}_{0,\text{Rabi}}$ ), counting the multiplicities. Since  $\lambda_n(\mathbf{H}_{0,\text{Rabi}})$  is explicitly known, the estimate (1.1) gives the asymptotic behaviour of  $\lambda_n(\mathbf{H}_{\text{Rabi}})$  with error  $O(n^{-\rho})$ .

The main result of this paper is Theorem 1.4, which states that the estimate (1.1) holds with  $\rho = \frac{1}{4}$  and this result is new in the case  $\epsilon \neq 0$ . Indeed, the asymptotic behaviour

of  $\lambda_n(\mathbf{H}_{\text{Rabi}})$  was investigated in the case  $\varepsilon = 0$  only (see Section 1.2 for a presentation of known results). It appears that the exponent  $\rho = \frac{1}{4}$  is optimal in the case  $\varepsilon = 0$ .

## 1.2 Overview of earlier results

The problem of the asymptotic behaviour of large eigenvalues of Rabi type models was mentioned e.g. in papers Feranchuk, Komarov, Ulyanenko [50] and Tur [123]. However, concerning the Hamiltonian  $\mathbf{H}_{\text{Rabi}}$  given by (1.10), mathematical results have been obtained only in the case  $\varepsilon = 0$ . In this case,  $\mathbf{H}_{\text{Rabi}}$  is unitarily equivalent to the direct sum  $J_{\Delta/2}(g) \oplus J_{-\Delta/2}(g)$ , where  $J_s(g)$  is the self-adjoint operator defined in  $\ell^2(\mathbb{N})$  by the Jacobi matrix

$$J_s(g) = \begin{pmatrix} s & g\sqrt{1} & 0 & 0 & 0 & \cdots \\ g\sqrt{1} & 1-s & g\sqrt{2} & 0 & 0 & \cdots \\ 0 & g\sqrt{2} & 2+s & g\sqrt{3} & 0 & \cdots \\ 0 & 0 & g\sqrt{3} & 3-s & g\sqrt{4} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (1.2)$$

The analysis of large eigenvalues of Jacobi matrices was initiated by J. Janas and S. Naboko in the paper [75], which contains fundamental ideas of the method of approximative diagonalization and asymptotic estimates (see Theorem 5.7). These ideas were developed by M. Malejki in papers [91], [94], but they do not work for the matrix (1.2). In fact, the perturbation  $J_s(g) - J_0(g) = \text{diag}(s(-1)^n)_{n=0}^{\infty}$  is not compact and it is not clear whether large eigenvalues of  $J_s(g)$  and  $J_0(g)$  are close. For this reason, the results obtained by A. Boutet de Monvel, S. Naboko and L. O. Silva in [27], [28], concern a simpler class of operators, called "modified Jaynes-Cummings models". For this class of operators, the oscillations  $s(-1)^n$  do appear in the asymptotic formula for large eigenvalues.

The first proof of the estimate (1.1) was obtained by E. A. Yanovich (Tur) with  $\rho = \frac{1}{16}$  in [135] (see also [124]). The estimate (1.1) with  $\rho = \frac{1}{4}$  was proved in [34] (see also [31]). The paper [34] gives the three-term asymptotic formula for large eigenvalues of the matrix (1.2), which shows that the exponent  $\rho = \frac{1}{4}$  cannot be improved. Moreover, this three-term asymptotic formula allows one to recover the values of parameters  $\Delta, g$ , from the spectrum of the QRM (see [32]) and it appears that the corresponding approximation is the same as the famous GRWA (generalized rotating wave approximation) introduced by Irish in [65] (and considered earlier in [50]).

We also mention the paper [25], where the asymptotic behaviour of large eigenvalues is investigated for the two-photon asymmetric quantum Rabi model. Our proof of Theorem 1.4 uses several ideas from [25], e.g. a method to overcome the difficulty of the case when  $\mathbf{H}_{0,\text{Rabi}}$  has double eigenvalues. However, the paper [25] uses an approximation of the two-photon Hamiltonian with  $\Delta = 0$  by an operator similar to a first order operator on the circle so that its eigenvectors can be expressed explicitly. In the case of  $\mathbf{H}_{0,\text{Rabi}}$  given by (1.12), a similar idea gives a pseudo-differential operator of order 1/2 and one needs to construct an approximation of its eigenvectors. A construction of this approximation consists the main part of this paper (see Section 3 and 4).



### 1.3 Basic definitions

**Notation 1.1.** (a) We denote by  $\mathbb{Z}$  the set of integers and  $\mathbb{N} := \{j \in \mathbb{Z} : j \geq 0\}$ .

(b) If  $\mathcal{J} \subset \mathbb{Z}$ , then  $\ell^2(\mathcal{J})$  denotes the complex Hilbert space of square-summable sequences  $x : \mathcal{J} \rightarrow \mathbb{C}$  equipped with the scalar product

$$\langle x, y \rangle_{\ell^2(\mathcal{J})} = \sum_{j \in \mathcal{J}} \overline{x(j)} y(j) \quad (1.3)$$

and the norm  $\|x\|_{\ell^2(\mathcal{J})} := \langle x, x \rangle_{\ell^2(\mathcal{J})}^{1/2}$ . We write  $\langle \cdot, \cdot \rangle_{\ell^2(\mathbb{N})} = \langle \cdot, \cdot \rangle$  and  $\|\cdot\|_{\ell^2(\mathbb{N})} = \|\cdot\|$  in the case  $\mathcal{J} = \mathbb{N}$ .

(c)  $\mathcal{B}_+ = \{e_n\}_{n \in \mathbb{N}}$  denotes the canonical basis of  $\ell^2(\mathbb{N})$  (i.e.  $e_n(m) = \delta_{n,m}$ ).

(d) The annihilation and creation operators,  $\hat{a}$  and  $\hat{a}^\dagger$ , are defined as closed linear operators in  $\ell^2(\mathbb{N})$  satisfying

$$\hat{a}^\dagger e_n = \sqrt{n+1} e_{n+1} \text{ for } n \in \mathbb{N} \quad (1.4)$$

$$\hat{a} e_0 = 0 \text{ and } \hat{a} e_n = \sqrt{n} e_{n-1} \text{ for } n \in \mathbb{N} \setminus \{0\}. \quad (1.5)$$

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

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad I_2 := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad (1.6)$$

**Definition 1.2.** (a) The Hamiltonian of the single-mode radiation,  $H_{\text{rad}}$ , is the self-adjoint operator in  $\ell^2(\mathbb{N})$  defined on

$$\ell^{2,1}(\mathbb{N}) := \{x \in \ell^2(\mathbb{N}) : \sum_{j \in \mathbb{N}} (1 + j^2) |x(j)|^2 < \infty\} \quad (1.7)$$

by the formula

$$H_{\text{rad}} e_n = \hat{a}^\dagger \hat{a} e_n = n e_n. \quad (1.8)$$

(b) The Two Level System (TLS) Hamiltonian is the linear operator in  $\mathbb{C}^2$  defined by the matrix

$$H_{\text{TLS}} = \frac{1}{2} \begin{pmatrix} \Delta & \epsilon \\ \epsilon & -\Delta \end{pmatrix} = \frac{1}{2} (\Delta \sigma_z + \epsilon \sigma_x) \quad (1.9)$$

where  $\Delta$  and  $\epsilon$  are real parameters.

(c) We define the AQRM Hamiltonian as the linear mapping  $\mathbf{H}_{\text{Rabi}} : \mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \rightarrow \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  given by

$$\mathbf{H}_{\text{Rabi}} = I_2 \otimes H_{\text{rad}} + H_{\text{TLS}} \otimes I_{\ell^2} + g \sigma_x \otimes (\hat{a} + \hat{a}^\dagger), \quad (1.10)$$

where  $g > 0$ . We can also write

$$\mathbf{H}_{\text{Rabi}} = \mathbf{H}_{0, \text{Rabi}} + \frac{1}{2} \Delta \sigma_z \otimes I_{\ell^2} \quad (1.11)$$

with

$$\mathbf{H}_{0,\text{Rabi}} := I_2 \otimes H_{\text{rad}} + \sigma_x \otimes (g(\hat{a} + \hat{a}^\dagger) + \frac{1}{2}\epsilon I_{\ell^2}). \quad (1.12)$$

(d) The QRM Hamiltonian is given by (1.11)-(1.12) with  $\epsilon = 0$ .

#### 1.4 Statement of the result

We first state the following, well known result (see [61])

**Theorem 1.3.** *Let  $\mathbf{H}_{0,\text{Rabi}}$  be as in Definition 1.2. Then there is an orthonormal basis in  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  of the form  $\{\mathbf{u}_{0,m}^-\}_{m \in \mathbb{N}} \cup \{\mathbf{u}_{0,m}^+\}_{m \in \mathbb{N}}$ , such that*

$$\mathbf{H}_{0,\text{Rabi}} \mathbf{u}_{0,m}^\pm = (m - g^2 \pm \frac{1}{2}\epsilon) \mathbf{u}_{0,m}^\pm \quad (1.13)$$

holds for every  $m \in \mathbb{N}$ .

The main result of this paper is the following

**Theorem 1.4.** *Let  $\mathbf{H}_{\text{Rabi}}$  be as in Definition 1.2. Then there is an orthonormal basis in  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  of the form  $\{\mathbf{u}_m^-\}_{m \in \mathbb{N}} \cup \{\mathbf{u}_m^+\}_{m \in \mathbb{N}}$  such that*

$$\mathbf{H}_{\text{Rabi}} \mathbf{u}_m^\pm = E_m^\pm \mathbf{u}_m^\pm \quad (1.14)$$

holds for every  $m \in \mathbb{N}$  and the eigenvalue sequences  $(E_m^-)_{m=0}^\infty, (E_m^+)_{m=0}^\infty$ , satisfy the large  $m$  asymptotic formula

$$E_m^\pm = m - g^2 \pm \frac{1}{2}\epsilon + O(m^{-1/4}). \quad (1.15)$$

The paper is organized as follows. In Section 2 we give the proof of Theorem 1.3 and the outline of the proof of Theorem 1.4. Our analysis is based on Proposition 2.6, which gives an approximation for the eigenvectors of  $\mathbf{H}_{0,\text{Rabi}}$ . In Section 3 we introduce useful notations and prove auxiliary results. In Section 4 we prove Proposition 2.6 and in Section 5 we complete the proof of Theorem 1.4. In Section 6 we describe useful estimates of oscillatory integrals.

#### 1.5 General notations and conventions

If  $\mathcal{V}$  is a Banach space, then  $\mathcal{B}(\mathcal{V})$  denotes the algebra of bounded operators  $\mathcal{V} \rightarrow \mathcal{V}$  and  $\|\cdot\|_{\mathcal{B}(\mathcal{V})}$  denotes its norm.

If  $L : \mathcal{D}_L \rightarrow \mathcal{H}$  is a linear mapping defined on a dense subspace of the complex Hilbert space  $\mathcal{H}$ , then  $\sigma(L)$  denotes the spectrum of  $L$ . If  $L$  has compact resolvent (i.e. there exists  $\lambda_0 \in \mathbb{C} \setminus \sigma(L)$  such that  $(L - \lambda_0)^{-1}$  is compact) and  $\lambda \in \sigma(L)$ , then  $\lambda$  is an isolated eigenvalue and has finite algebraic multiplicity  $\text{mult}(\lambda) := \text{rank } P_\lambda(L)$ , where  $P_\lambda(L)$  denotes the associated Riesz projector (see Section III.5 in [81]).

We write  $\mathbb{T} := \mathbb{R}/2\pi$  and define  $L^2(\mathbb{T})$  as the Hilbert space of Lebesgue square integrable functions  $]-\pi, \pi[ \rightarrow \mathbb{C}$  equipped with the scalar product

$$\langle f, g \rangle_{L^2(\mathbb{T})} := \int_{-\pi}^{\pi} \overline{f(\theta)} g(\theta) \frac{d\theta}{2\pi}. \quad (1.16)$$

The Fourier transform  $\mathcal{F}_{\mathbb{T}} : L^2(\mathbb{T}) \rightarrow \ell^2(\mathbb{Z})$  is defined by the formula

$$(\mathcal{F}_{\mathbb{T}}f)(j) = \int_{-\pi}^{\pi} f(\theta) e^{-ij\theta} \frac{d\theta}{2\pi}. \quad (1.17)$$

For  $s \in \mathbb{R}$  we write  $\langle s \rangle := (1 + s^2)^{1/2}$  and for  $\mu \geq 0$  we define

$$\ell^{2,\mu}(\mathbb{Z}) := \{x \in \ell^2(\mathbb{Z}) : \|x\|_{\ell^{2,\mu}(\mathbb{Z})} < \infty\} \quad (1.18)$$

with

$$\|x\|_{\ell^{2,\mu}(\mathbb{Z})} = \left( \sum_{j \in \mathbb{Z}} \langle j \rangle^{2\mu} |x(j)|^2 \right)^{1/2}. \quad (1.19)$$

We denote by  $\mathcal{S}(\mathbb{Z})$  the set of fast decaying sequences  $\mathbb{Z} \rightarrow \mathbb{C}$ . By definition

$$\mathcal{S}(\mathbb{Z}) := \bigcap_{\mu \geq 0} \ell^{2,\mu}(\mathbb{Z}). \quad (1.20)$$

For  $x \in \ell^2(\mathbb{Z})$  we denote  $\text{supp } x := \{j \in \mathbb{Z} : x(j) \neq 0\}$  and we define

$$\ell_{\text{fin}}^2(\mathbb{Z}) := \{x \in \ell^2(\mathbb{Z}) : \text{supp } x \text{ is finite}\}. \quad (1.21)$$

If  $\mathcal{J} \subset \mathbb{Z}$  then we identify

$$\ell^2(\mathcal{J}) = \{x \in \ell^2(\mathbb{Z}) : \text{supp } x \subset \mathcal{J}\}. \quad (1.22)$$

In the sequel  $\{e_i\}_{i \in \mathbb{Z}}$  denotes the canonical basis of  $\ell^2(\mathbb{Z})$  (i.e.  $e_i(j) = \delta_{i,j}$  for  $i, j \in \mathbb{Z}$ ). We remark that  $\{e_i\}_{i \in \mathbb{N}}$  is a basis of  $\{x \in \ell^2(\mathbb{Z}) : \text{supp } x \subset \mathbb{N}\} = \ell^2(\mathbb{N})$ , i.e. we can identify  $\{e_i\}_{i \in \mathbb{N}}$  with  $\mathcal{B}_+$ , the canonical basis of  $\ell^2(\mathbb{N})$  introduced in Notation 1.1(c).

If  $\ell^{2,1}(\mathbb{N})$  is defined by (1.7), then  $\ell^{2,1}(\mathbb{N}) = \ell^{2,1}(\mathbb{Z}) \cap \ell^2(\mathbb{N})$  is a Banach space with the norm induced by the norm of  $\|\cdot\|_{\ell^{2,1}(\mathbb{Z})}$ .

We also define  $\mathcal{S}(\mathbb{N}) := \mathcal{S}(\mathbb{Z}) \cap \ell^2(\mathbb{N})$ , the set of fast decaying sequences  $x : \mathbb{N} \rightarrow \mathbb{C}$ .

## 2 Preliminaries

### 2.1 Operators $\mathbf{H}_0$ and $\mathbf{H}$

Our starting point consists in defining operators  $\mathbf{H}_0$  and  $\mathbf{H}$ , which are unitarily similar to  $\mathbf{H}_{0,\text{Rabi}}$  and  $\mathbf{H}_{\text{Rabi}}$  respectively.

**Notation 2.1.** We define the linear mappings  $\mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \rightarrow \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  by

$$\mathbf{H}_0 := I_2 \otimes \hat{a}^\dagger \hat{a} - \sigma_z \otimes \left( g(\hat{a} + \hat{a}^\dagger) + \frac{1}{2} \epsilon I_{\ell^2(\mathbb{N})} \right), \quad (2.1)$$

$$\mathbf{V} := \frac{1}{2} \Delta \sigma_x \otimes I_{\ell^2(\mathbb{N})} \quad (2.2)$$

and

$$\mathbf{H} := \mathbf{H}_0 + \mathbf{V}. \quad (2.3)$$

**Lemma 2.2.**  $\mathbf{H}_0$  and  $\mathbf{H}$  are unitarily similar to  $\mathbf{H}_{0,\text{Rabi}}$  and  $\mathbf{H}_{\text{Rabi}}$  respectively.

*Proof.* Let  $U_{\pi/4} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$  be the matrix of rotation by the angle  $\pi/4$ . Then

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

We observe that the right hand side of (1.12) becomes the right hand side of (2.1) if  $\sigma_x$  is replaced by  $-\sigma_z$ . If moreover  $\sigma_z$  is replaced by  $\sigma_x$ , then the right hand side of (1.11) becomes the right hand side of (2.3).  $\square$

We remark that  $\{(1, 0) \otimes e_j : j \in \mathbb{N}\} \cup \{(0, 1) \otimes e_j : j \in \mathbb{N}\}$  is the canonical basis of  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  and we can identify  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  with  $\ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})$  writing

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

This identification allows us to consider  $\mathbf{H}$  as the linear mapping  $\ell^{2,1}(\mathbb{N}) \times \ell^{2,1}(\mathbb{N}) \rightarrow \ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})$  of the form

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

where  $H_\nu : \ell^{2,1}(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$  is defined for  $\nu = \pm 1$  by

$$H_\nu := \hat{a}^\dagger \hat{a} + \nu g(\hat{a} + \hat{a}^\dagger) + \frac{1}{2}\nu\epsilon \quad (2.5)$$

We can also write

$$\mathbf{V} = \frac{1}{2}\Delta \begin{pmatrix} 0_{\ell^2} & I_{\ell^2} \\ I_{\ell^2} & 0_{\ell^2} \end{pmatrix}, \quad (2.6)$$

where  $0_{\ell^2}$  denotes the null mapping in  $\ell^2(\mathbb{N})$  and

$$\mathbf{H}_0 = H_{-1} \oplus H_1.$$

## 2.2 Proof of Theorem 1.3

**Lemma 2.3.** Let  $\{e_n\}_{n \in \mathbb{N}}$  be the canonical basis of  $\ell^2(\mathbb{N})$  and let  $Q_+$  denote the closure of the symmetric operator  $i(\hat{a}^\dagger - \hat{a})|_{\mathcal{S}(\mathbb{N})}$ . Then

- (a) the operator  $Q_+$  is self-adjoint in  $\ell^2(\mathbb{N})$
- (b) if  $\nu = \pm 1$  and  $\{v_{\nu,n}\}_{n \in \mathbb{N}}$  is the orthonormal basis given by

$$v_{\nu,n} := e^{i\nu g Q_+} e_n, \quad (2.7)$$

then  $H_\nu v_{\nu,n} = (n - g^2 + \frac{1}{2}\nu\epsilon)v_{\nu,n}$  holds for every  $n \in \mathbb{N}$ .

*Proof.* The result is well known, but we indicate the details of its proof below.

(a) See Lemma 3.4 in [58].

(b) Due to Corollary 3.7 in [58],  $\mathcal{S}(\mathbb{N})$  is an invariant subspace of  $e^{itQ_+}$  for every  $t \in \mathbb{R}$  and  $t \rightarrow e^{itQ_+}x$  is a smooth function  $\mathbb{R} \rightarrow \ell^{2,1}(\mathbb{N})$  if  $x \in \mathcal{S}(\mathbb{N})$ .

We claim that for every  $t \in \mathbb{R}$  one has

$$e^{-itQ_+}(\hat{a} + t)e^{itQ_+} = \hat{a}, \quad e^{-itQ_+}(\hat{a}^\dagger + t)e^{itQ_+} = \hat{a}^\dagger. \quad (2.8)$$

Indeed, if  $G(t) := e^{-itQ_+}(t + \hat{a})e^{itQ_+}$  and  $x \in \mathcal{S}(\mathbb{N})$ , then

$$\frac{d}{dt}G(t)x = e^{-itQ_+}(I - [iQ_+, \hat{a}])e^{itQ_+}x = 0 \quad (2.9)$$

follows from  $[iQ_+, \hat{a}] = -[\hat{a}^\dagger, \hat{a}] = I$ . It is clear that (2.9) implies  $G(t) = G(0) = \hat{a}$  and the second equality (2.8) follows similarly. Using (2.8) with  $t = \nu g$ , we get

$$\hat{a}^\dagger \hat{a} = e^{-i\nu g Q_+}(\hat{a}^\dagger + \nu g)(\hat{a} + \nu g)e^{i\nu g Q_+} = e^{-i\nu g Q_+}(H_\nu + g^2 - \frac{1}{2}\nu\varepsilon)e^{i\nu g Q_+},$$

hence  $(H_\nu + g^2 - \frac{1}{2}\nu\varepsilon)v_{\nu,n} = e^{i\nu g Q_+}\hat{a}^\dagger \hat{a}e_n = e^{i\nu g Q_+}ne_n = \nu v_{\nu,n}$ .  $\square$

*Proof of Theorem 1.3.* Denote  $\mathbf{v}_{0,m}^- := (v_{-1,m}, 0)$  and  $\mathbf{v}_{0,m}^+ := (0, v_{1,m})$ . Then

$$(H_{-1} \oplus H_1)\mathbf{v}_{0,m}^\pm = (m - g^2 \pm \frac{1}{2}\varepsilon)\mathbf{v}_{0,m}^\pm \quad (2.10)$$

holds for every  $m \in \mathbb{N}$  and it is clear that the assertion of Theorem 1.3 follows from the fact that  $H_{-1} \oplus H_1$  is unitarily similar to  $\mathbf{H}_{0,\text{Rabi}}$ .

### 2.3 Explicit expression of the $n$ -th eigenvalue of $\mathbf{H}_0$

Let  $(\lambda_n(\mathbf{H}_0))_{n=0}^\infty$  denote the non-decreasing sequence of eigenvalues of  $\mathbf{H}_0$ , counting the multiplicities. The explicit expression for  $\lambda_n(\mathbf{H}_0)$  is given in

**Lemma 2.4.** *Assume that  $\varepsilon \geq 0$ . Denote  $l_0 := \max\{i \in \mathbb{N} : i \leq \varepsilon\}$  and define*

$$\mathbf{v}_n^0 = (v_{-1,n}, 0) \text{ for } n = 0, \dots, l_0, \quad (2.11)$$

$$\mathbf{v}_{l_0+2i}^0 = (v_{-1,l_0+i}, 0) \text{ for } i \in \mathbb{N}, \quad (2.12)$$

$$\mathbf{v}_{l_0+1+2i}^0 = (0, v_{1,i}) \text{ for } i \in \mathbb{N}. \quad (2.13)$$

Then  $\{\mathbf{v}_n^0\}_{n \in \mathbb{N}}$  is an orthonormal basis such that  $\mathbf{H}_0\mathbf{v}_n^0 = d_n\mathbf{v}_n^0$  holds with

$$d_n = n - g^2 - \frac{1}{2}\varepsilon \text{ for } n = 0, \dots, l_0, \quad (2.14)$$

$$d_{l_0+2i} = l_0 + i - g^2 - \frac{1}{2}\varepsilon \text{ for } i \in \mathbb{N}, \quad (2.15)$$

$$d_{l_0+1+2i} = i - g^2 + \frac{1}{2}\varepsilon \text{ for } i \in \mathbb{N}. \quad (2.16)$$

Moreover  $(d_n)_{n=0}^\infty$  is non-decreasing, i.e. one has  $d_n = \lambda_n(\mathbf{H}_0)$  for all  $n \in \mathbb{N}$ .

*Proof.* We observe that  $\{\mathbf{v}_n^0 : n \in \mathbb{N}\} = \{\mathbf{v}_{0,n}^- : n \in \mathbb{N}\} \cup \{\mathbf{v}_{0,n}^+ : n \in \mathbb{N}\}$  holds with  $\mathbf{v}_{0,n}^\pm$  as in (2.10) and (2.10) ensures  $\mathbf{H}_0\mathbf{v}_n^0 = d_n\mathbf{v}_n^0$  with  $(d_n)_{n=0}^\infty$  given by (2.14)-(2.16). It remains to check that the sequence  $(d_n)_{n=0}^\infty$  is non-decreasing. It is obvious that  $(d_n)_{0 \leq n \leq l_0}$ ,  $(d_{l_0+2i})_{i \in \mathbb{N}}$  and  $(d_{l_0+1+2i})_{i \in \mathbb{N}}$  are non-decreasing. Moreover,

$$d_{l_0+1+2i} - d_{l_0+2i} = \varepsilon - l_0 \geq 0,$$

$$d_{l_0+1+2i} - d_{l_0+2+2i} = \varepsilon - (l_0 + 1) < 0$$

hold by the choice of  $l_0$ .  $\square$

## 2.4 Outline of the proof of Theorem 1.4

Using the assertion of Theorem 1.3 and the fact that  $\mathbf{H}_{\text{Rabi}} - \mathbf{H}_{0,\text{Rabi}}$  is bounded, we can conclude (see [81]) that  $\mathbf{H}_{\text{Rabi}}$  is a self-adjoint, bounded from below operator with compact resolvent. Due to the spectral theorem, there is an orthonormal basis  $\{\mathbf{u}_n\}_{n \in \mathbb{N}}$  such that  $\mathbf{H}_{\text{Rabi}}\mathbf{u}_n = \lambda_n(\mathbf{H}_{\text{Rabi}})\mathbf{u}_n$  and it remains to prove that (1.1) holds with  $\rho = \frac{1}{4}$ .

In the sequel we assume that  $\epsilon \geq 0$ . Then, due to Lemma 2.2 and 2.4, it remains to prove the large  $n$  estimate

$$\lambda_n(\mathbf{H}) = d_n + O(n^{-1/4}), \quad (2.17)$$

where  $(d_n)_{n \in \mathbb{N}}$  is given by (2.14)-(2.16). The case of  $\epsilon < 0$  can be treated similarly by exchanging the roles of  $H_{-1}$  and  $H_1$ .

**Notation 2.5.** We define the self-adjoint operators in  $\ell^2(\mathbb{N})$  by

$$H = U\mathbf{H}U^{-1}, \quad (2.18)$$

where  $U : \ell^2(\mathbb{N}) \times \ell^2(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$  is the isometric isomorphism satisfying  $U\mathbf{v}_n^0 = e_n$  for every  $n \in \mathbb{N}$ . Then we can write

$$H = D + V, \quad (2.19)$$

where  $V := UVU^{-1}$  and  $D$  is the diagonal operator satisfying

$$De_n = d_n e_n \text{ for } n \in \mathbb{N}. \quad (2.20)$$

Using this notation we rewrite (2.17) in the form

$$\lambda_n(D + V) = d_n + O(n^{-1/4}) \quad (2.21)$$

and in Section 6 we give the proof of (2.21) by showing that  $H$  is similar to a certain operator  $H' = D + R$ , where  $R$  is compact and satisfies

$$\|R^*e_n\| = O(n^{-1/4}). \quad (2.22)$$

We deduce (2.21) using (2.22) and  $\lambda_n(H) = \lambda_n(H')$  in Theorem 5.7.

The key estimate (2.22) follows from the analysis of the matrix

$$(\langle e_j, Ve_k \rangle)_{j,k \in \mathbb{N}} = (\langle \mathbf{v}_j^0, \mathbf{V}\mathbf{v}_k^0 \rangle_{\ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})})_{j,k \in \mathbb{N}} \quad (2.23)$$

based on the approximation of  $v_{\pm 1,n}$  given in

**Proposition 2.6.** *For  $t, \theta \in \mathbb{R}$ ,  $k \in \mathbb{Z}$ , we define*

$$\varphi(t; \theta, k) := \begin{cases} -2t k^{1/2} \sin \theta + t^2 \sin \theta \cos \theta & \text{if } k \geq 1 \\ 0 & \text{if } k \leq 0 \end{cases} \quad (2.24)$$

*Then the following large  $n$  estimate*

$$\|v_{\pm 1,n} - u_n(\pm g; \cdot)\| = O(n^{-1/2}) \quad (2.25)$$

*holds with  $u_n(t; \cdot) \in \ell^2(\mathbb{N})$  given by the formula*

$$u_n(t; j) := \int_{-\pi}^{\pi} e^{i\varphi(t; \theta, n) + i(n-j)\theta} \frac{d\theta}{2\pi}. \quad (2.26)$$

*Proof.* See Section 4. □

### 3 Auxiliary operators acting in $\ell^2(\mathbb{Z})$

#### 3.1 Matrices of Fourier type operators

The proof of Proposition 2.6 is based on the Fourier transform. For this reason, before starting the proof of Proposition 2.6, we move from  $\ell^2(\mathbb{N})$  to  $\ell^2(\mathbb{Z})$ . At the beginning we introduce a class of matrices  $(\text{op}(p)(j, k))_{j, k \in \mathbb{Z}}$ , which define Fourier type operators acting in  $\ell^2(\mathbb{Z})$ . We recall the notation  $\langle s \rangle := (1 + s^2)^{1/2}$ .

**Notation 3.1.** (a) We write  $\mathbb{T} := \mathbb{R}/2\pi$  and define  $C^\infty(\mathbb{T})$  as the set of all smooth  $2\pi$ -periodic functions  $\mathbb{R} \rightarrow \mathbb{C}$ . We say that  $\{f_\tau\}_{\tau \in \mathcal{T}}$  is bounded in  $C^\infty(\mathbb{T})$  if  $f_\tau \in C^\infty(\mathbb{T})$  for every  $\tau \in \mathcal{T}$  and for every  $\alpha \in \mathbb{N}$  one has

$$\sup_{\tau \in \mathcal{T}} \sup_{\theta \in \mathbb{R}} \left| \frac{d^\alpha}{d\theta^\alpha} f_\tau(\theta) \right| < \infty$$

(b) If  $p(j, \cdot, k) \in C^\infty(\mathbb{T})$  for every  $(j, k) \in \mathbb{Z}^2$ , then we define the matrix  $(\text{op}(p)(j, k))_{j, k \in \mathbb{Z}}$  by the formula

$$\text{op}(p)(j, k) := \int_{-\pi}^{\pi} p(j, \theta, k) e^{i(k-j)\theta} \frac{d\theta}{2\pi}. \quad (3.1)$$

#### 3.2 Non-stationary phase estimates

**Lemma 3.2.** *Assume that  $\{b(j, \cdot, k)\}_{j, k \in \mathbb{Z}}$  and  $\{\phi(\cdot, k)\}_{k \in \mathbb{Z}}$  are bounded in  $C^\infty(\mathbb{T})$ . Assume moreover that  $\phi$  is real valued and denote*

$$C_\phi := \sup_{(\theta, k) \in \mathbb{R} \times \mathbb{Z}} |\partial_\theta \phi(\theta, k)|, \quad (3.2)$$

$$Z_\phi := \{(j, k) \in \mathbb{Z}^2 : |k - j| > 2C_\phi \langle k \rangle^{1/2}\}. \quad (3.3)$$

If

$$p(j, \theta, k) = b(j, \theta, k) e^{i\phi(\theta, k) \langle k \rangle^{1/2}}, \quad (3.4)$$

then for every  $N \in \mathbb{N}$  there is  $C_N > 0$  such that the estimate

$$|\text{op}(p)(j, k)| \leq C_N \langle j \rangle^{-N} \langle k \rangle^{-N} \quad (3.5)$$

holds for  $(j, k) \in Z_\phi$ .

*Proof.* For  $(j, k) \in Z_\phi$  we can write

$$\text{op}(p)(j, k) = \int_{-\pi}^{\pi} e^{i(k-j)(\psi(j, \theta, k) + \theta)} b(j, \theta, k) \frac{d\theta}{2\pi} \quad (3.6)$$

where

$$\psi(j, \theta, k) := \phi(j, \theta, k) \frac{\langle k \rangle^{1/2}}{k - j}. \quad (3.7)$$

However  $\{\psi(j, \cdot, k)\}_{(j,k) \in Z_\phi}$  is bounded in  $C^\infty(\mathbb{T})$  and

$$(j, k) \in Z_\phi \Rightarrow |\partial_\theta \psi(j, \theta, k)| \leq \frac{1}{2} \Rightarrow \partial_\theta (\psi(j, \theta, k) + \theta) \geq \frac{1}{2}.$$

Thus the non-stationary phase estimates (see Lemma 6.1(b)) yield existence of  $C_N > 0$  such that

$$|\text{op}(p)(j, k)| \leq C_N \langle k - j \rangle^{-5N} \quad (3.8)$$

holds for  $(j, k) \in Z_\phi$ . Using  $\langle k - j \rangle^{-N} \leq 2^N \langle j \rangle^{-N} \langle k \rangle^N$  and

$$(j, k) \in Z_\phi \Rightarrow \langle k - j \rangle^{-4N} \leq 2^{-4N} C_\phi^{-4N} \langle k \rangle^{-2N},$$

we can estimate the right hand side of (3.8) by  $C_N 2^{-3N} C_\phi^{-4N} \langle j \rangle^{-N} \langle k \rangle^{-N}$ .  $\square$

**Corollary 3.3.** *If  $p$  satisfies the assumptions of Lemma 3.2, then one can define a linear operator  $\text{op}(p) : \ell_{\text{fin}}^2(\mathbb{Z}) \rightarrow \mathcal{S}(\mathbb{Z})$  by the formula*

$$(\text{op}(p)e_k)(j) = \langle e_j, \text{op}(p)e_k \rangle = \text{op}(p)(j, k), \quad (3.9)$$

where  $\text{op}(p)(j, k)$  is given by (3.1).

*Proof.* It suffices to observe that  $\text{op}(p)(\cdot, k) \in \mathcal{S}(\mathbb{Z})$  holds for every  $k \in \mathbb{Z}$ . Indeed, if  $k \in \mathbb{Z}$  is fixed, then (3.5) holds for  $j > k + 2C_\phi \langle k \rangle^{1/2}$  and for  $j < k - 2C_\phi \langle k \rangle^{1/2}$ .  $\square$

### 3.3 Localization of $u_n(t)$

**Notation 3.4.** (a) For  $t, \theta \in \mathbb{R}$  and  $j, k \in \mathbb{Z}$  we denote

$$\tilde{\varphi}(t; j, \theta, k) := \varphi(t; \theta, k), \quad (3.10)$$

where  $\varphi(t; \theta, k)$  is given by (2.24).

(b) We define  $u_n(t) \in \mathcal{S}(\mathbb{Z})$  by the formula

$$u_n(t) := \text{op}(e^{i\tilde{\varphi}(t)})e_n. \quad (3.11)$$

It is clear that (3.11) defines an extension of  $u_n(t; \cdot)$  introduced in (2.26).

**Corollary 3.5.** *Let  $t_0 > 0$  be fixed.*

(a) *Assume that  $\tilde{C}_{t_0} > 0$  is large enough and for  $n \in \mathbb{N}^*$  denote*

$$Z_n := \{j \in \mathbb{Z} : |j - n| \leq \tilde{C}_{t_0} \langle n \rangle^{1/2}\}. \quad (3.12)$$

*Let  $\Pi_{Z_n}$  be the orthogonal projection on  $\text{span}\{e_k\}_{k \in Z_n}$ . Then for every  $N \in \mathbb{N}$  we can find  $C_{N, t_0} > 0$  such that*

$$\sup_{-t_0 \leq t \leq t_0} \|(I - \Pi_{Z_n})u_n(t)\|_{\ell^{2, N}(\mathbb{Z})} \leq C_{N, t_0} \langle n \rangle^{-N}. \quad (3.13)$$



(b) For every  $N, n \in \mathbb{N}$ , the function  $t \rightarrow u_n(t)$  is differentiable  $[-t_0, t_0] \rightarrow \ell^{2,N}(\mathbb{Z})$ ,

$$\frac{d}{dt}u_n(t) = \text{op}(i\partial_t\tilde{\varphi}(t)e^{i\tilde{\varphi}(t)})e_n \quad (3.14)$$

and we can find  $\tilde{C}_{N,t_0}$  such that

$$\sup_{-t_0 \leq t \leq t_0} \|(I - \Pi_{Z_n})\frac{d}{dt}u_n(t)\|_{\ell^{2,N}(\mathbb{Z})} \leq \tilde{C}_{N,t_0}\langle n \rangle^{-N}. \quad (3.15)$$

*Proof.* (a) We fix  $t_0 > 0$ . Reasoning as in the proof of Lemma 3.2, for every  $N \in \mathbb{N}$  we can find the constant  $C_{N,t_0}$  such that

$$j \in \mathbb{Z} \setminus Z_n \Rightarrow \sup_{-t_0 \leq t \leq t_0} |\langle j \rangle^N (\text{op}(e^{i\tilde{\varphi}(t)})e_n)(j)| \leq C_{N,t_0}\langle n \rangle^{-N}\langle j \rangle^{-2}. \quad (3.16)$$

(b) We fix  $t_0 > 0, n \in \mathbb{N}$  and denote

$$w_n(t, s) := (u_n(t+s) - u_n(t))/s, \quad w_n(t) := \text{op}(i\partial_t\tilde{\varphi}(t)e^{i\tilde{\varphi}(t)})e_n.$$

We claim that the dominated convergence theorem implies

$$\|w_n(t, s) - w_n(t)\|_{\ell^{2,N}(\mathbb{Z})}^2 = \sum_{j \in \mathbb{Z}} \langle j \rangle^{2N} |w_n(t, s; j) - w_n(t; j)|^2 \xrightarrow{s \rightarrow 0} 0. \quad (3.17)$$

Indeed,  $\lim_{s \rightarrow 0} w_n(t, s; j) = \frac{d}{dt}u_n(t; j) = w_n(t; j)$  for every  $j \in \mathbb{N}$  and

$$j \in \mathbb{Z} \setminus Z_n \Rightarrow \sup_{-t_0 \leq s, t \leq t_0} |w_n(t, s; j)| \leq \sup_{-2t_0 \leq t \leq 2t_0} |w_n(t; j)| \leq C_{N,2t_0}\langle j \rangle^{-N-1}\langle n \rangle^{-N},$$

where we get the last estimate similarly as in the proof of Lemma 3.2.  $\square$

### 3.4 An auxiliary result

**Notation 3.6.** For  $\mu \in \mathbb{R}$  we define  $S_1^\mu(\mathbb{T} \times \mathbb{R})$  as the set of smooth functions  $q : \mathbb{R}^2 \rightarrow \mathbb{C}$  satisfying  $q(\theta + 2\pi, k) = q(\theta, k)$  for all  $(\theta, k) \in \mathbb{R}^2$  and such that for every  $\alpha_1, \alpha_2 \in \mathbb{N}$ ,

$$|\partial_\theta^{\alpha_1}\partial_k^{\alpha_2}q(\theta, k)| \leq C_{\alpha_1, \alpha_2}\langle k \rangle^{\mu - \alpha_2} \quad (3.18)$$

holds with a certain constant  $C_{\alpha_1, \alpha_2}$  independent of  $(\theta, k) \in \mathbb{R}^2$ . In the sequel we use the following elementary properties of symbols :

$$q \in S_1^\mu(\mathbb{T} \times \mathbb{R}) \Rightarrow \partial_\theta^{\alpha_1}\partial_k^{\alpha_2}q \in S_1^{\mu - \alpha_2}(\mathbb{T} \times \mathbb{R})$$

$$q_1 \in S_1^{\mu_1}(\mathbb{T} \times \mathbb{R}), \quad q_2 \in S_1^{\mu_2}(\mathbb{T} \times \mathbb{R}) \Rightarrow q_1q_2 \in S_1^{\mu_1 + \mu_2}(\mathbb{T} \times \mathbb{R}).$$

In Section 4.5 we will use the following

**Lemma 3.7.** Assume that  $q \in S_1^{1/2}(\mathbb{T} \times \mathbb{R})$  and define

$$\varphi(t; \theta, k) := tq(\theta, k) + \frac{1}{2}t^2\partial_k q(\theta, k)\partial_\theta q(\theta, k) \quad (3.19)$$

for  $t, \theta, k \in \mathbb{R}$ . If

$$r_0(t; \theta, k) = q(\theta, k + \partial_\theta \varphi(t; \theta, k)) - \partial_t \varphi(t; \theta, k), \quad (3.20)$$

then there is  $C > 0$  such that for all  $\theta, k \in \mathbb{R}$  and  $t \in [-t_0, t_0]$  one has

$$|r_0(t; \theta, k)| \leq C\langle k \rangle^{-1/2}. \quad (3.21)$$

*Proof.* Step 1. Let us write  $\partial_1^{\alpha_1} \partial_2^{\alpha_2} q(\theta, k) := \partial_\theta^{\alpha_1} \partial_k^{\alpha_2} q(\theta, k)$  and denote

$$r_1(t; \theta, k) := q(\theta, k + \partial_\theta \varphi(t; \theta, k)) - q(\theta, k) - \partial_2 q(\theta, k) \partial_\theta \varphi(t; \theta, k). \quad (3.22)$$

We claim that there is a constant  $C_1 > 0$  such that the estimate

$$|r_1(t; \theta, k)| \leq C_1 \langle k \rangle^{-1/2} \quad (3.23)$$

holds for all  $\theta, k \in \mathbb{R}$  and  $t \in [-t_0, t_0]$ . Indeed, since Taylor expansion of order 2, gives

$$r_1(t; \theta, k) = (\partial_\theta \varphi(t; \theta, k))^2 \int_0^1 \partial_2^2 q(\theta, k + s \partial_\theta \varphi(t; \theta, k)) (1-s) ds, \quad (3.24)$$

we deduce (3.23) from (3.24) due to  $(\partial_\theta \varphi(t))^2 \in S_1^1(\mathbb{T} \times \mathbb{R})$  and  $\partial_2^2 q \in S_1^{-3/2}(\mathbb{T} \times \mathbb{R})$ .

Step 2. Using (3.19) in (3.20) we get the expression

$$r_0(t; \theta, k) = q(\theta, k + \partial_\theta \varphi(t; \theta, k)) - q(\theta, k) - t \partial_2 q(\theta, k) \partial_1 q(\theta, k), \quad (3.25)$$

and combining (3.25) with (3.22) we get

$$r_0(t) - r_1(t) = \partial_2 q \partial_\theta (\varphi(t) - tq). \quad (3.26)$$

Since  $\partial_2 q \in S_1^{-1/2}(\mathbb{T} \times \mathbb{R})$  and  $\partial_\theta (\varphi(t) - tq) = \partial_\theta (\frac{1}{2}t^2 \partial_2 q \partial_1 q)$  is bounded due to  $\partial_2 q \partial_1 q \in S_1^0(\mathbb{T} \times \mathbb{R})$ , we can find  $C_2 > 0$  such that for all  $\theta, k \in \mathbb{R}$ ,  $t \in [-t_0, t_0]$ , one has

$$|r_0(t) - r_1(t)| \leq C_2 \langle k \rangle^{-1/2}. \quad (3.27)$$

Combining (3.23) and (3.27), we complete the proof of (3.21).  $\square$

## 4 Proof of Proposition 2.6

### 4.1 Step 1

We move to  $\ell^2(\mathbb{Z}) = \ell^2(\mathbb{Z} \setminus \mathbb{N}) \oplus \ell^2(\mathbb{N})$  by introducing the operator

$$Q := 0_{\ell^2(\mathbb{Z} \setminus \mathbb{N})} \oplus Q_+, \quad (4.1)$$

where  $0_{\ell^2(\mathbb{Z} \setminus \mathbb{N})}$  is the null mapping on  $\ell^2(\mathbb{Z} \setminus \mathbb{N})$ . Then  $Q$  is self-adjoint in  $\ell^2(\mathbb{Z})$  and

$$e^{itQ} = I_{\ell^2(\mathbb{Z} \setminus \mathbb{N})} \oplus e^{itQ_+}.$$

If  $\Pi_{\geq 0} \in \mathcal{B}(\ell^2(\mathbb{Z}))$  denotes the orthogonal projection on  $\ell^2(\mathbb{N})$  and  $u_n(t)$  is given by Notation 3.4(b), then the assertion of Proposition 2.6 says that the large  $n$  estimate

$$\|\Pi_{\geq 0}(u_n(t) - e^{itQ}e_n)\|_{\ell^2(\mathbb{Z})} = O(n^{-1/2}) \quad (4.2)$$

holds for  $t = \pm g$ . In this section we will prove that for every  $t_0 > 0$  one can find  $C_{t_0} > 0$  such that

$$\sup_{-t_0 \leq t \leq t_0} \|u_n(t; \cdot) - e^{itQ}e_n\|_{\ell^2(\mathbb{Z})} \leq C_{t_0} n^{-1/2} \quad (4.3)$$

holds for all  $n \in \mathbb{N}^*$ .

**Notation 4.1.** (a) In the sequel  $\Lambda : \ell^{2,1}(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z})$  is the self-adjoint operator in  $\ell^2(\mathbb{Z})$  satisfying  $\Lambda e_j = j e_j$  for  $j \in \mathbb{Z}$ . Moreover, we denote  $\langle \Lambda \rangle := (1 + \Lambda^2)^{1/2}$ .

(b) If  $h : \mathbb{Z} \rightarrow \mathbb{C}$  then  $h(\Lambda) = \text{diag}(h(j))_{j \in \mathbb{Z}}$  is defined by the functional calculus, i.e.  $h(\Lambda)$  is the closed linear operator satisfying

$$h(\Lambda)e_j = h(j)e_j \text{ for } j \in \mathbb{Z}. \quad (4.4)$$

(c) We define  $S \in \mathcal{B}(\ell^2(\mathbb{Z}))$  as the shift satisfying  $S e_j := e_{j+1}$  for  $j \in \mathbb{Z}$ .

Using these notations we can express the operator  $Q$  in the form

$$Q = i(\Lambda_+^{1/2} S - S^{-1} \Lambda_+^{1/2}), \quad (4.5)$$

where  $\Lambda_+^{1/2} = h(\Lambda)$  with  $h(j) = j_+^{1/2}$ .

## 4.2 Step 2

We fix  $t_0 > 0$  and consider all estimates uniformly with respect to  $t \in [-t_0, t_0]$ . If  $\mu \in \mathbb{R}$ , then we write

$$w_n(t) = O(n^{-\mu}) \text{ for } t \in [-t_0, t_0]$$

if and only if there is  $\tilde{C}_{t_0} > 0$  such that for all  $n \in \mathbb{N}^*$  one has

$$\sup_{-t_0 \leq t \leq t_0} \|w_n(t)\|_{\ell^2(\mathbb{Z})} \leq \tilde{C}_{t_0} n^{-\mu}. \quad (4.6)$$

At the beginning we observe that Corollary 3.5 allows us to write

$$u_n(t) - e^{itQ}e_n = \int_0^t \frac{d}{ds} (e^{i(t-s)Q} u_n(s)) ds = -i \int_0^t e^{i(t-s)Q} \left( Q + i \frac{d}{ds} \right) u_n(s) ds,$$

hence it suffices to prove the estimate

$$\left(Q + i \frac{d}{dt}\right) u_n(t) = O(n^{-1/2}) \text{ for } t \in [-t_0, t_0]. \quad (4.7)$$

We claim that (4.7) follows from the estimate

$$\left(\tilde{Q} + i \frac{d}{dt}\right) u_n(t) = O(n^{-1/2}) \text{ for } t \in [-t_0, t_0] \quad (4.8)$$

where

$$\tilde{Q} := i\Lambda_+^{1/2}(S - S^{-1}). \quad (4.9)$$

To prove this claim, it suffices to show the estimate

$$(\tilde{Q} - Q)u_n(t) = O(n^{-1/2}) \text{ for } t \in [-t_0, t_0]. \quad (4.10)$$

We first observe that  $(Q - \tilde{Q})\langle\Lambda\rangle^{1/2} \in \mathcal{B}(\ell^2(\mathbb{Z}))$ . Indeed, using  $h(j) := j_+^{1/2}$  and  $h_1(j) := h(j-1)$  we get  $S^{-1}h(\Lambda) - h(\Lambda)S^{-1} = S^{-1}(h(\Lambda) - h(S\Lambda S^{-1})) = S^{-1}(h - h_1)(\Lambda)$  and  $(h - h_1)(\Lambda)\langle\Lambda\rangle^{1/2} \in \mathcal{B}(\ell^2(\mathbb{Z}))$  follows from  $(h - h_1)(j) = O(\langle j \rangle^{-1/2})$ .

Due to  $(Q - \tilde{Q})\langle\Lambda\rangle^{1/2} \in \mathcal{B}(\ell^2(\mathbb{Z}))$ , (4.10) holds if we know the estimate

$$\langle\Lambda\rangle^{-1/2}u_n(t) = O(n^{-1/2}) \text{ for } t \in [-t_0, t_0]. \quad (4.11)$$

However, if  $\Pi_{Z_n}$  is as in Corollary 3.5, then  $(I - \Pi_{Z_n})u_n(t) = O(n^{-N})$  for every  $N \in \mathbb{N}$  and (4.11) follows from  $\langle\Lambda\rangle^{-1/2}\Pi_{Z_n} = O(n^{-1/2})$ .

### 4.3 Step 3

We claim that instead of (4.8), it suffices to prove the estimate

$$\Pi_{Z_n} \left(\tilde{Q} + i \frac{d}{dt}\right) u_n(t) = O(n^{-1/2}) \text{ for } t \in [-t_0, t_0] \quad (4.12)$$

where  $\Pi_{Z_n}$  is as in Corollary 3.5 and  $\tilde{Q}$  is given by (4.9).

Indeed, due to (3.15), it suffices to show that

$$(I - \Pi_{Z_n})\tilde{Q}u_n(t) = O(n^{-1/2}) \text{ for } t \in [-t_0, t_0] \quad (4.13)$$

By definition  $((S - S^{-1})x)(j) = x(j-1) - x(j+1)$  and

$$x(j) = e^{-ij\theta} \Rightarrow (i(S - S^{-1})x)(j) = i(e^{i\theta} - e^{-i\theta})x(j) = (-2 \sin \theta) x(j),$$

hence

$$i(S - S^{-1})u_n(t) = \text{op}(p(t))e_n \text{ with } p(t; j, \theta, k) := (-2 \sin \theta) e^{i\tilde{\varphi}(t; j, \theta, k)} \quad (4.14)$$

Therefore  $\tilde{Q}u_n(t) = \Lambda_+^{1/2} \text{op}(p(t))e_n$  and it remains to observe that reasoning as in the proof of Corollary 3.5 we find that for every  $N \in \mathbb{N}$  one has

$$\langle\Lambda\rangle^{1/2}(I - \Pi_{Z_n})\text{op}(p(t))e_n = O(n^{-N}) \text{ for } t \in [-t_0, t_0] \quad (4.15)$$

#### 4.4 Step 4

**Notation 4.2.** (a) We define  $q \in S_1^{1/2}(\mathbb{T} \times \mathbb{R})$  by the formula

$$q(\theta, k) = -2\chi_0(k)|k|^{1/2} \sin \theta, \quad (4.16)$$

where  $\chi_0 \in C^\infty(\mathbb{R})$  is a fixed function such that  $\chi_0(k) = 0$  if  $k \leq 0$ ,  $\chi_0(k) = 1$  if  $k \geq 1$  and  $0 \leq \chi_0(k) \leq 1$  for  $k \in [0, 1]$ .

(b) We define  $\varphi : \mathbb{R} \times \mathbb{R}^2 \rightarrow \mathbb{R}$  by

$$\varphi(t; \theta, k) := tq(\theta, k) + \frac{1}{2}t^2 \partial_k q(\theta, k) \partial_\theta q(\theta, k) \quad (4.17)$$

with  $q$  given by (4.16). By direct calculation we check that for  $k \geq 1$  one has

$$\varphi(t; \theta, k) = -2tk^{1/2} \sin \theta + t^2 \sin \theta \cos \theta \quad (4.18)$$

and  $\varphi(t; \theta, k) = 0$  if  $k \leq 0$ , i.e.  $\varphi$  satisfies (2.24) for  $k \in \mathbb{Z}$ .

(c) We define  $\tilde{\varphi} : \mathbb{R} \times \mathbb{R}^3 \rightarrow \mathbb{R}$  by

$$\tilde{\varphi}(t; j, \theta, k) := \varphi(t; \theta, k) \quad (4.19)$$

with  $\varphi$  given by (4.17). Obviously  $u_n(t) = \text{op}(e^{i\tilde{\varphi}(t)})e_n$  still holds.

Assume that  $r_0$  is given by (3.20) with  $\varphi$  as in (4.17). Let

$$f_n(t; \theta) := r_0(t; \theta, n)e^{i\varphi(t; \theta, n) + in\theta}.$$

Then  $\mathcal{F}_\mathbb{T} f_n(t) = \text{op}(\tilde{r}_0(t)e^{i\tilde{\varphi}(t)})e_n$  holds with

$$\tilde{r}_0(t; j, \theta, k) := r_0(t; \theta, k) \quad (4.20)$$

and

$$\|\text{op}(\tilde{r}_0(t)e^{i\tilde{\varphi}(t)})e_n\|_{\ell^2(\mathbb{Z})} = \|\mathcal{F}_\mathbb{T} f_n(t)\|_{\ell^2(\mathbb{Z})} = \|f_n(t)\|_{L^2(\mathbb{T})} = O(n^{-1/2}), \quad (4.21)$$

where the last estimates result from (3.21).

We observe that using (3.14) and (4.14), we obtain the expression

$$\left(\tilde{Q} + i\frac{d}{dt}\right)u_n(t) = \text{op}(\tilde{b}(t)e^{i\tilde{\varphi}(t)})e_n \quad (4.22)$$

with

$$\tilde{b}(t; j, \theta, k) := q(\theta, j) - \partial_t \varphi(t; \theta, k), \quad (4.23)$$

hence the estimate (4.12) can be written in the form

$$\Pi_{Z_n} \text{op}(\tilde{b}(t)e^{i\tilde{\varphi}(t)})e_n = O(n^{-1/2}) \text{ for } t \in [-t_0, t_0]. \quad (4.24)$$

We introduce  $b(t) := \tilde{b}(t) - \tilde{r}_0(t)$  and observe that due to (4.21), the estimate

$$\Pi_{Z_n} \text{op}(b(t)e^{i\tilde{\varphi}(t)})e_n = O(n^{-1/2}) \text{ for } t \in [-t_0, t_0] \quad (4.25)$$

is equivalent to (4.12). Moreover, using (4.23) and (3.20), we find

$$b(t; j, \theta, k) = (\tilde{b} - \tilde{r}_0)(t; j, \theta, k) = q(\theta, j) - q(\theta, \partial_\theta \varphi(t; \theta, k) + k). \quad (4.26)$$

**4.5 End of the proof of Proposition 2.6**

It remains to prove (4.25) with  $b$  given by (4.26). Using Taylor's expansion of order 2 we can express

$$-b = b_1 + b_2 \quad (4.27)$$

with

$$b_1(t; j, \theta, k) := \partial_2 q(\theta, j)(\partial_\theta \varphi(t; \theta, k) + k - j) \quad (4.28)$$

$$b_2(t; j, \theta, k) := q_2(t; j, \theta, k)(\partial_\theta \varphi(t; \theta, k) + k - j)^2, \quad (4.29)$$

where

$$q_2(t; j, \theta, k) := \int_0^1 \partial_2^2 q(\theta, j + s(\partial_\theta \varphi(t; \theta, k) + k - j)) (1 - s) ds. \quad (4.30)$$

In order to prove

$$\text{op}(b_1(t)e^{i\tilde{\varphi}(t)})e_n = O(n^{-1/2}) \text{ for } t \in [-t_0, t_0] \quad (4.31)$$

we denote

$$q_1(t; j, \theta, k) := \partial_2 q(\theta, j) \quad (4.32)$$

$$\psi(t; j, \theta, k) := \varphi(t; \theta, k) + (k - j)\theta. \quad (4.33)$$

Using (4.32)-(4.33), we can write (4.28) in the form  $b_1 = q_1 \partial_\theta \psi$ , hence

$$\text{op}(b_1(t)e^{i\tilde{\varphi}(t)})(j, k) = \int_{-\pi}^{\pi} (q_1 \partial_\theta \psi e^{i\psi})(t; j, \theta, k) \frac{d\theta}{2\pi}. \quad (4.34)$$

Writing  $\partial_\theta \psi e^{i\psi} = -i\partial_\theta(e^{i\psi})$  in the right hand side of (4.34), we can integrate by parts and express (4.34) in the form

$$i \int_{-\pi}^{\pi} (\partial_\theta q_1 e^{i\psi})(t; j, \theta, k) \frac{d\theta}{2\pi} = (\mathcal{F}_{\mathbb{T}} f_k(t))(j) \quad (4.35)$$

with  $f_k(t; \theta) := i\partial_1 \partial_2 q(\theta, k)e^{i\varphi(t; \theta, k) + ik\theta}$  and

$$\|\text{op}(b_1(t)e^{i\tilde{\varphi}(t)})e_n\|_{\ell^2(\mathbb{Z})} = \|\mathcal{F}_{\mathbb{T}} f_n(t)\|_{\ell^2(\mathbb{Z})} = \|f_n(t)\|_{L^2(\mathbb{T})} = O(n^{-1/2}), \quad (4.36)$$

where the last estimate follows from  $\partial_1 \partial_2 q \in S_1^{-1/2}(\mathbb{T} \times \mathbb{R})$ .

It remains to prove

$$\Pi_{Z_n} \text{op}(b_2(t)e^{i\tilde{\varphi}(t)})e_n = O(n^{-1/2}). \quad (4.37)$$

For this purpose we first observe that  $b_2 = q_2(\partial_\theta \psi)^2$  and

$$\int_{-\pi}^{\pi} q_2 (\partial_\theta \psi)^2 e^{i\psi} = -i \int_{-\pi}^{\pi} q_2 \partial_\theta \psi \partial_\theta (e^{i\psi}) = i \int_{-\pi}^{\pi} \partial_\theta (q_2 \partial_\theta \psi) e^{i\psi}, \quad (4.38)$$

where the last equality follows from the integration by parts. However, (4.38) ensures

$$\text{op}(b_2(t)e^{i\tilde{\varphi}(t)}) = \text{op}(i \partial_\theta (q_2 \partial_\theta \psi)(t) e^{i\tilde{\varphi}(t)}). \quad (4.39)$$

Using  $\varphi(t; \cdot) \in S_1^{1/2}(\mathbb{T} \times \mathbb{R})$  and  $\partial_2^2 q \in S_1^{-3/2}(\mathbb{T} \times \mathbb{R})$  in the expression of  $q_2$  we obtain

$$\sup_{j \in Z_n} |(\partial_\theta(q_2 \partial_\theta \psi))(t; j, \theta, n)| = O(n^{-1}). \quad (4.40)$$

To complete the proof we observe that (4.37) follows from (4.39) and

$$\|\Pi_{Z_n \text{ op}} (\partial_\theta(q_2 \partial_\theta \psi))(t) e^{i\tilde{\varphi}(t)} e_n\|_{\ell^2(\mathbb{Z})} \leq \sum_{j \in Z_n} |(\partial_\theta(q_2 \partial_\theta \psi))(t; j, \theta, n)| = O(n^{-1/2}),$$

where the last estimate is due to (4.40) and  $\text{card } Z_n = O(n^{1/2})$ .

## 5 Proof of Theorem 1.4

### 5.1 Asymptotic orthogonality between eigenvectors of $H_{-1}$ and $H_1$

**Lemma 5.1.** *Let  $\{v_{\pm 1, j}\}_{j \in \mathbb{N}}$  be as in Lemma 2.3. If  $c > 0$  is fixed small enough, then*

$$|k - j| < c(j^{1/2} + k^{1/2}) \Rightarrow |\langle v_{-1, k}, v_{1, j} \rangle| \leq C_0 \langle j \rangle^{-1/4} \quad (5.1)$$

holds with a certain constant  $C_0$ , independent of  $k, j \in \mathbb{N}$ .

*Proof.* Due to Proposition 2.6,

$$\langle v_{-1, k}, v_{1, j} \rangle = \langle e^{-igQ} e_k, e^{igQ} e_j \rangle_{\ell^2(\mathbb{Z})} = \gamma_{k, j} + O(k^{-1/2} + j^{-1/2}) \quad (5.2)$$

holds with  $\gamma_{k, j} := \langle u_k(-g), u_j(g) \rangle_{\ell^2(\mathbb{Z})}$ . Let

$$f_n^\pm(\theta) := e^{\mp 2ign^{1/2} \sin \theta + ig^2 \sin \theta \cos \theta + in\theta}. \quad (5.3)$$

Then  $u_n(\pm g) = \mathcal{F}_\mathbb{T} f_n^\pm$  and

$$\gamma_{k, j} := \langle \mathcal{F}_\mathbb{T} f_k^-, \mathcal{F}_\mathbb{T} f_j^+ \rangle_{\ell^2(\mathbb{Z})} = \langle f_k^-, f_j^+ \rangle_{L^2(\mathbb{T})} = \int_{-\pi}^{\pi} e^{-i(j^{1/2} + k^{1/2})\Psi(j, \theta, k)} \frac{d\theta}{2\pi}$$

holds with

$$\Psi(j, \theta, k) := 2g \sin \theta + \frac{(k - j)\theta}{j^{1/2} + k^{1/2}}.$$

Denote  $\mathcal{I}_0 := [-5\pi/6, -\pi/6] \cup [\pi/6, 5\pi/6]$ . Then

$$\theta \in \mathcal{I}_0 \Rightarrow |\partial_\theta^2 \Psi(j, \theta, k)| = |2g \sin \theta| \geq g > 0$$

and van der Corput Lemma (see Section 6) ensures

$$\int_{\mathcal{I}_0} e^{-i(j^{1/2} + k^{1/2})\Psi(j, \theta, k)} \frac{d\theta}{2\pi} = O((j^{1/2} + k^{1/2})^{-1/2}).$$

Denote  $\tau_{j, k} := (k - j)/(j^{1/2} + k^{1/2})$  and assume that  $|\tau_{j, k}| \leq g/2$ . Then

$$\theta \in [-\pi, \pi] \setminus \mathcal{I}_0 \Rightarrow |\partial_\theta \Psi(j, \theta, k)| \geq |2g \cos \theta| - |\tau_{j, k}| \geq g/2 > 0$$

and the non-stationary phase estimate (see Lemma 6.1(a)) ensures

$$\int_{[-\pi, \pi] \setminus \mathcal{I}_0} e^{-i(j^{1/2} + k^{1/2})\Psi(j, \theta, k)} \frac{d\theta}{2\pi} = O((j^{1/2} + k^{1/2})^{-1}).$$

□

**Corollary 5.2.** *For  $j, k \in \mathbb{N}$  we denote  $V(j, k) := \langle e_j, Ve_k \rangle$ . If  $c > 0$  is small enough, then there exists  $C > 0$  such that*

$$|m - n| < cn^{1/2} \Rightarrow |V(m, n)| \leq C\langle n \rangle^{-1/4}. \quad (5.4)$$

*Proof.* By definition of  $V$ , if  $i, j \in \mathbb{N}$  then

$$V(l_0 + 2i, l_0 + 2j) = \frac{\Delta}{2} \langle (v_{-1, l_0 + i}, 0), (0, v_{-1, l_0 + j}) \rangle_{\ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})} = 0 \quad (5.5)$$

$$V(l_0 + 2i + 1, l_0 + 2j + 1) = \frac{\Delta}{2} \langle (0, v_{1, i}), (v_{1, j}, 0) \rangle_{\ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})} = 0 \quad (5.6)$$

$$V(l_0 + 2i, l_0 + 2j + 1) = \frac{\Delta}{2} \langle (v_{-1, l_0 + i}, 0), (v_{1, j}, 0) \rangle_{\ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})} = \frac{\Delta}{2} \langle v_{-1, l_0 + i}, v_{1, j} \rangle. \quad (5.7)$$

To complete the proof we fix  $j_0 \in \mathbb{N}$  large enough and consider  $k = l_0 + i$ ,  $m = l_0 + 2i$ ,  $n = l_0 + 2j + 1$  with  $j \geq j_0$ . Then one has

$$|m - n| < cn^{1/2} \Rightarrow |j - k| < c(j^{1/2} + k^{1/2}),$$

hence  $|V(m, n)| = \left| \frac{\Delta}{2} \gamma_{j, k} \right| \leq C_0 \left| \frac{\Delta}{2} \right| \langle j \rangle^{-1/4} \leq C\langle n \rangle^{-1/4}$  if  $n \geq l_0 + 2j_0 + 1$ . □

## 5.2 The auxiliary operator $K$

**Notation 5.3.** In the sequel  $K \in \mathcal{B}(\ell^2(\mathbb{N}))$  is the operator defined by

$$\langle e_j, Ke_k \rangle_{\ell^2} = K(j, k) = \begin{cases} \frac{V(j, k)}{d_j - d_k} & \text{if } d_j \neq d_k \\ 0 & \text{if } d_j = d_k \end{cases} \quad (5.8)$$

where  $V(j, k) := \langle e_j, Ve_k \rangle$  for  $j, k \in \mathbb{N}$ .

**Lemma 5.4.** *The operator  $K$  is compact and anti-Hermitian in  $\ell^2(\mathbb{N})$ . Moreover, there is  $C > 0$  such that*

$$\|Ke_n\| \leq C\langle n \rangle^{-1/4} \text{ for all } n \in \mathbb{N}. \quad (5.9)$$

*Proof.* Step 1. We first observe that  $K(k, j) = -\overline{K(j, k)}$ , i.e. the matrix  $(K(j, k))_{j, k \in \mathbb{Z}}$  is anti-Hermitian and (5.4) ensures

$$n \geq c^{-2}|k|^2 \Rightarrow |V(n + k, n)| \leq Cn^{-1/4}. \quad (5.10)$$



Let  $c_0 > 0$  be fixed small enough. Then  $d_j \neq d_k \Rightarrow |d_j - d_k| \geq c_0 \langle j - k \rangle$  and

$$K(j, k) \neq 0 \Rightarrow d_j \neq d_k \Rightarrow |K(j, k)| \leq c_0^{-1} \frac{|V(j, k)|}{\langle j - k \rangle}. \quad (5.11)$$

We also observe that Parseval's equality ensures

$$\sum_{j \in \mathbb{N}} |V(j, k)|^2 = \sum_{j \in \mathbb{N}} |\langle \mathbf{v}_j^0, \mathbf{Vv}_k^0 \rangle_{\ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})}|^2 = \|\mathbf{Vv}_k^0\|_{\ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})}^2 \leq C_0. \quad (5.12)$$

Step 2. For  $N \in \mathbb{N}$  we define  $K_N \in \mathcal{B}(\ell^2(\mathbb{N}))$  by

$$K_N(j, k) = \langle e_j, K_N e_k \rangle_{\ell^2(\mathbb{N})} = \begin{cases} K(j, k) & \text{if } |j - k| < N \\ 0 & \text{if } |j - k| \geq N \end{cases} \quad (5.13)$$

Since  $K_N$  is a finite band matrix and each diagonal  $K_N(k + n, n) \rightarrow 0$  when  $n \rightarrow \infty$  due to (5.10), the operator  $K_N$  is compact. If  $\widetilde{K}_N(m, n) := K(m, n) - K_N(m, n)$ , then

$$\sum_{j \in \mathbb{N}} |\widetilde{K}_N(j, k)| \leq c_0^{-1} \sum_{\{j \in \mathbb{N}: |j-k| \geq N\}} \frac{|V(j, k)|}{\langle j - k \rangle} \quad (5.14)$$

and using Cauchy-Schwarz inequality we can estimate the right-hand side of (5.14) by  $c_0^{-1} C_0^{1/2} \delta_N^{1/2}$ , where we have denoted  $\delta_N := 2 \sum_{m > N} \langle m \rangle^{-2}$  and  $C_0$  is as in (5.12). Thus the Schur boundedness test ensures  $K - K_N \in \mathcal{B}(\ell^2(\mathbb{Z}))$  and

$$\|K - K_N\| \leq c_0^{-1} C_0^{1/2} \delta_N^{1/2} \xrightarrow{N \rightarrow \infty} 0. \quad (5.15)$$

Since  $K = K - K_0 \in \mathcal{B}(\ell^2(\mathbb{N}))$  and  $K_N$  are compact, (5.15) implies that  $K$  is compact.

Step 3. We can estimate

$$\|K e_n\|^2 = \sum_{j \in \mathbb{N}} |K(j, n)|^2 \leq c_0^{-2} (M_n + M'_n),$$

where

$$M_n := \sum_{|j-n| \geq cn^{1/2}} \frac{|V(j, n)|^2}{\langle j - n \rangle^2} \leq \langle cn^{1/2} \rangle^{-2} \sum_{j \in \mathbb{N}} |V(j, n)|^2 \leq C_1 n^{-1}$$

due to (5.12) and

$$M'_n = \sum_{|j-n| < cn^{1/2}} \frac{|V(j, n)|^2}{\langle j - n \rangle^2} \leq C^2 n^{-1/2} \sum_{m \in \mathbb{N}} \langle m - n \rangle^{-2} \leq C'_1 n^{-1/2}$$

due to (5.4). □

### 5.3 Similarity transformation

**Notation 5.5.** In the sequel  $W$  denotes the operator defined in  $\mathcal{B}(\ell^2(\mathbb{N}))$  by

$$\langle e_j, We_k \rangle = W(j, k) = (d_j - d_k)K(j, k) - V(j, k). \quad (5.16)$$

**Lemma 5.6.** (a) *If  $\epsilon \notin \mathbb{N}$  then  $W = 0$ . If  $\epsilon \in \mathbb{N}$  then  $W$  is compact, self-adjoint and there is  $C > 0$  such that*

$$\|We_n\| \leq Cn^{-1/4} \text{ for } n \in \mathbb{N}^*. \quad (5.17)$$

(b) *The operator  $I + K$  is invertible and  $\ell^{2,1}(\mathbb{N})$  is an invariant subspace of  $I + K$ .*

(c) *The operator  $R := (KV - W)(I + K)^{-1}$  is compact and one has*

$$H = (I + K)^{-1}(D + R)(I + K). \quad (5.18)$$

*Proof.* (a) We first observe that  $V(j, j) = 0$  implies  $W(j, j) = 0$  and

$$d_j \neq d_k \implies W(j, k) = 0. \quad (5.19)$$

If  $\epsilon \notin \mathbb{N}$  then  $j \neq k$  implies  $d_j \neq d_k$  and  $W(j, k) = 0$  follows. If  $\epsilon \in \mathbb{N}$  then  $W(j, k) \neq 0$  implies  $d_j = d_k$  and  $|j - k| = 1$ , hence all non zero entries of the matrix  $(W(j, k))_{j, k \in \mathbb{Z}}$  have the form  $W(j, j + 1) = W(j + 1, j) = -V(j + 1, j)$  and  $W$  is compact because  $V(j + 1, j) \rightarrow 0$  when  $j \rightarrow \infty$ .

(b) Since the operator  $iK$  is self-adjoint, the operator  $i + iK = i(I + K)$  is invertible and

$$d_j(Ke_k)(j) = (d_j - d_k)(Ke_k)(j) + (KDe_k)(j) = ((W + V + KD)e_k)(j) \quad (5.20)$$

implies that  $d_j(Kx)(j) = ((W + V + KD)x)(j)$  holds when  $x \in \ell^{2,1}(\mathbb{N})$ . Since  $d_j \sim \frac{1}{2}j$  as  $j \rightarrow \infty$ , we can conclude that  $x \in \ell^{2,1}(\mathbb{N}) \implies DKx \in \ell^2(\mathbb{N}) \implies Kx \in \ell^{2,1}(\mathbb{N})$  and

$$DK = W + V + KD \text{ on } \ell^{2,1}(\mathbb{N}). \quad (5.21)$$

(c) Due to (5.21) we can write  $V + KD = DK - W$  on  $\ell^{2,1}(\mathbb{N})$  and

$$\begin{aligned} (I + K)H &= D + V + KD + KV = D + DK - W + KV = \\ &= D(I + K) - W + KV = (D + R)(I + K). \end{aligned}$$

Applying  $(I + K)^{-1}$  from the left, we obtain (5.18). Moreover  $R$  is compact because  $K$  and  $W$  are compact.  $\square$

### 5.4 End of the proof of (1.15)

Let  $K$  and  $R$  be as in Lemma 5.6. We denote

$$H' := D + R. \quad (5.22)$$

We claim that  $\sigma(H') = \sigma(H)$  and the corresponding eigenvalues have the same multiplicity. Indeed, (5.18) ensures

$$H - z = (I + K)^{-1}(H' - z)(I + K) \text{ for } z \in \mathbb{C} \quad (5.23)$$

and taking  $z_0 \in \mathbb{C} \setminus (\sigma(H) \cup \sigma(H'))$  we find that

$$(I + K)|_{\ell^{2,1}(\mathbb{N})} = (H' - z_0)^{-1}(I + K)(H - z_0)$$

is invertible in  $\mathcal{B}(\ell^{2,1}(\mathbb{N}))$ . Thus  $H - z$  is invertible  $\ell^{2,1}(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$  if and only if  $H' - z$  is invertible  $\ell^{2,1}(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$ , i.e.  $\sigma(H') = \sigma(H)$  and

$$(H - z)^{-1} = (I + K)^{-1}(H' - z)^{-1}(I + K) \text{ for } z \in \mathbb{C} \setminus \sigma(H). \quad (5.24)$$

Finally, the equality  $\text{rank } P_\lambda(H) = \text{rank } P_\lambda(H')$  follows from the fact that (5.24) implies

$$P_\lambda(H) = (I + K)^{-1}P_\lambda(H')(I + K).$$

Let  $(\lambda_n(H))_{n \in \mathbb{N}} = (\lambda_n(H'))_{n \in \mathbb{N}}$  be the non-decreasing sequence of eigenvalues of  $H$  (and of  $H'$ ), counting the multiplicities. We need to prove the large  $n$  estimate

$$\lambda_n(H) = \lambda_n(H') = d_n + O(n^{-1/4}). \quad (5.25)$$

For this purpose we first observe that there exist constants  $C, C'$  such that

$$\|R^*e_n\| \leq C(\|K^*e_n\| + \|We_n\|) \leq C'n^{-1/4} \quad (5.26)$$

holds for all  $n \in \mathbb{N}^*$ . It is easy to see that we obtain (5.25) using (5.26) and

**Theorem 5.7.** *Let  $(d_n)_{n \in \mathbb{N}}$  be given by (2.14)-(2.16) and let  $\widehat{\Pi}_n$  denote the orthogonal projection on the linear subspace generated by  $\{e_m : d_m = d_n\}$ . If  $R$  is as in Lemma 5.6 and  $H' = D + R$ , then one has the large  $n$  estimate*

$$\lambda_n(H') = d_n + O(\|R^*\widehat{\Pi}_n\|_{\mathcal{B}(\ell^2(\mathbb{N}))}). \quad (5.27)$$

*Proof.* If  $\epsilon \notin \mathbb{N}$  then  $\|R^*\widehat{\Pi}_n\| = \|R^*e_n\|$  and the estimate (5.27) was proved in Lemma 2.1 of the paper Janas and Naboko [75]. If  $\epsilon \in \mathbb{N}$  then the eigenvalues are double for  $n \geq l_0$  and the estimate (5.27) can be easily deduced from the result of Malejki [94] similarly as in section 4.4 of Chapter 5.  $\square$

## 6 Estimates of oscillatory integrals

**Lemma 6.1.** *We us fix  $c_0 > 0$  and  $\theta_0, \theta_1 \in \mathbb{R}$  satisfying  $\theta_0 < \theta_1$ . Let  $\mathcal{T}$  be an arbitrary set of parameters. For every  $\tau \in \mathcal{T}$  we consider smooth functions  $h_\tau : [\theta_0, \theta_1] \rightarrow \mathbb{C}$ ,  $\Psi_\tau : [\theta_0, \theta_1] \rightarrow \mathbb{R}$  and for  $\lambda \in \mathbb{R}$  we denote*

$$M_\tau(\lambda) := \int_{\theta_0}^{\theta_1} e^{i\lambda\Psi_\tau(\theta)} h_\tau(\theta) d\theta. \quad (6.1)$$

We assume that the derivative satisfies  $|\Psi'_\tau(\theta)| \geq c_0$  for every  $\theta \in [\theta_0, \theta_1]$  and  $\tau \in \mathcal{T}$ .

(a) If  $\{h_\tau\}_{\tau \in \mathcal{T}}$  is bounded in  $C^1([\theta_0, \theta_1])$  and  $\{\Psi_\tau\}_{\tau \in \mathcal{T}}$  is bounded in  $C^2([\theta_0, \theta_1])$ , then there is a constant  $C_0$  such that the estimate

$$|M_\tau(\lambda)| \leq C_0 |\lambda|^{-1} \quad (6.2)$$

holds for all  $\tau \in \mathcal{T}$  and  $\lambda \in \mathbb{R} \setminus \{0\}$ .

(b) If  $[\theta_0, \theta_1] = [-\pi, \pi]$ ,  $\{h_\tau\}_{\tau \in \mathcal{T}}$  is bounded in  $C^\infty(\mathbb{T})$ ,  $\{\Psi'_\tau\}_{\tau \in \mathcal{T}}$  is bounded in  $C^\infty(\mathbb{T})$  and  $\Psi_\tau(\pi) - \Psi_\tau(-\pi) \in 2\pi\mathbb{Z}$  holds for every  $\tau \in \mathcal{T}$ , then for every  $N \in \mathbb{N}$  one can find a constant  $C_N > 0$  such that

$$|M_\tau(m)| \leq C_N m^{-N} \quad (6.3)$$

holds for all  $\tau \in \mathcal{T}$  and  $m \in \mathbb{N}^*$ .

*Proof.* (a) The integration by parts gives

$$i\lambda M_\tau(\lambda) = \int_{\theta_0}^{\theta_1} (e^{i\lambda\Psi_\tau})' \frac{h_\tau}{\Psi'_\tau} = \int_{\theta_0}^{\theta_1} e^{i\lambda\Psi_\tau} \mathcal{L}_\tau(h_\tau) + \left[ e^{i\lambda\Psi_\tau} \frac{h_\tau}{\Psi'_\tau} \right]_{\theta_0}^{\theta_1} \quad (6.4)$$

where  $\mathcal{L}_\tau$  is the differential operator defined by  $\mathcal{L}_\tau(f) := -(f/\Psi'_\tau)'$ . To complete the proof of (6.2), it suffices to observe that the right hand side of (6.4) is bounded uniformly with respect to  $\tau \in \mathcal{T}$  and  $\lambda \in \mathbb{R}^*$ .

(b) If  $[\theta_0, \theta_1] = [-\pi, \pi]$  and  $\lambda = m \in \mathbb{N}$ , then the last term in the right hand side of (6.4) disappears due to the assumptions of  $2\pi$ -periodicity and we obtain

$$(im)^N M_\tau(\lambda) = \int_{-\pi}^{\pi} e^{im\Psi_\tau} \mathcal{L}_\tau^N(h_\tau) \quad (6.5)$$

after  $N$  integrations by parts. To complete the proof of (6.3), we observe that the right-hand side of (6.5) is bounded uniformly with respect to  $\tau \in \mathcal{T}$  and  $m \in \mathbb{N}^*$ .  $\square$

**Lemma 6.2. (J. van der Corput)** *Assume that  $c_0 > 0$ . If  $\Psi: [\theta_0, \theta_1] \rightarrow \mathbb{R}$  is smooth and its second derivative satisfies  $|\Psi''| \geq c_0$ , then there is a constant  $C_0$  depending only on  $c_0$ , such that for all  $\lambda \in \mathbb{R}^*$  one has*

$$\left| \int_{\theta_0}^{\theta_1} e^{i\lambda\Psi(\theta)} d\theta \right| \leq C_0 |\lambda|^{-1/2}. \quad (6.6)$$

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# Chapitre 3

## Estimations améliorées des grandes valeurs propres pour le Modèle Quantique de Rabi avec un biais non résonant

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# Improved Estimates of Large Eigenvalues for the Quantum Rabi Model with a non-resonant bias

**Abstract.** We consider the asymmetric quantum Rabi model with a bias  $\epsilon \notin \mathbb{Z}$ . The spectrum of this model consists of two eigenvalue sequences  $(E_m^+)_{m=0}^\infty$ ,  $(E_m^-)_{m=0}^\infty$ , and we describe their asymptotic behaviour with an error estimate of the form  $O(m^{-1/2} \ln m)$  when  $m$  tends to infinity.

## 1 Statement of the result

In this Chapter we use notations introduced in Section 1 of Chapter 2. In particular,  $\ell^2(\mathbb{N})$  denotes the Hilbert space of square-summable sequences  $x : \mathbb{N} \rightarrow \mathbb{C}$  and

$$\ell^{2,1}(\mathbb{N}) := \{x \in \ell^2(\mathbb{N}) : \|x\|_{\ell^{2,1}(\mathbb{N})} < \infty\} \quad (1.1)$$

with

$$\|x\|_{\ell^{2,1}(\mathbb{N})} = \left( \sum_{j \in \mathbb{N}} (1 + j^2) |x(j)|^2 \right)^{1/2}. \quad (1.2)$$

The Pauli matrices are denoted  $\sigma_x$ ,  $\sigma_y$ ,  $\sigma_z$ , and we define  $\hat{a}^\dagger$  and  $\hat{a}$  (the creation and annihilation operator) as closed linear operators in  $\ell^2(\mathbb{N})$  satisfying

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

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

where  $\{e_n\}_{n \in \mathbb{N}}$  is the canonical basis of  $\ell^2(\mathbb{N})$ .

The operator  $\mathbf{H}_{0,\text{Rabi}}$  is defined as the linear mapping  $\mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \rightarrow \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  given by

$$\mathbf{H}_{0,\text{Rabi}} := I_2 \otimes \hat{a}^\dagger \hat{a} + \sigma_x \otimes \left( g(\hat{a} + \hat{a}^\dagger) + \frac{\epsilon}{2} I_{\ell^2} \right), \quad (1.5)$$

and the operator  $\mathbf{H}_{\text{Rabi}}$  is defined as the linear mapping  $\mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \rightarrow \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  given by

$$\mathbf{H}_{\text{Rabi}} = \mathbf{H}_{0,\text{Rabi}} + \frac{1}{2} \Delta \sigma_z \otimes I_{\ell^2}. \quad (1.6)$$

where  $g > 0$  is fixed.

In Chapter 2 we proved that there is an orthonormal basis in  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  of the form  $\{\mathbf{u}_m^-\}_{n \in \mathbb{N}} \cup \{\mathbf{u}_m^+\}_{n \in \mathbb{N}}$  such that

$$\mathbf{H}_{\text{Rabi}} \mathbf{u}_m^\pm = E_m^\pm \mathbf{u}_m^\pm \quad (1.7)$$

holds for every  $m \in \mathbb{N}$  and the eigenvalue sequences  $(E_m^-)_{m=0}^\infty$ ,  $(E_m^+)_{m=0}^\infty$ , satisfy the large  $m$  asymptotic formula

$$E_m^\pm = m - g^2 \pm \frac{1}{2} \epsilon + O(m^{-1/4}). \quad (1.8)$$

The purpose of this Chapter is to prove

**Theorem 1.1.** *If  $\epsilon \notin \mathbb{Z}$ , then the eigenvalue sequences  $(E_m^-)_{m=0}^\infty$ ,  $(E_m^+)_{m=0}^\infty$ , satisfy the large  $m$  asymptotic formula*

$$E_m^\pm = m - g^2 \pm \frac{1}{2} \epsilon + O(m^{-1/2} \ln m). \quad (1.9)$$

## 2 Main ideas of the proof

If  $L : \mathcal{D}(L) \rightarrow \mathcal{V}$  is a linear mapping defined on a dense subspace of the complex Banach space  $\mathcal{V}$ , then  $\sigma(L)$  denotes the spectrum of  $L$ . The algebra of bounded operators on  $\mathcal{V}$  is denoted  $\mathcal{B}(\mathcal{V})$  and the norm of  $\mathcal{B}(\ell^2(\mathbb{N}))$  is denoted  $\|\cdot\|$ . If  $T \in \mathcal{B}(\ell^2(\mathbb{N}))$ , then we denote

$$T(j, k) := \langle e_j, T e_k \rangle \text{ for } j, k \in \mathbb{N}. \quad (2.1)$$

Due to Lemma 2.2 in Chapter 2, the operator  $\mathbf{H}_{0, \text{Rabi}}$  is similar to the diagonal operator  $D = \text{diag}(d_j)_{j=0}^\infty$  in  $\ell^2(\mathbb{N})$ , i.e.

$$D e_j = d_j e_j \text{ for } j \in \mathbb{N}, \quad (2.2)$$

where  $(d_j)_{j \in \mathbb{N}}$  is the non-decreasing sequence of eigenvalues of  $\mathbf{H}_{0, \text{Rabi}}$ , counting multiplicities. The operator  $\mathbf{H}_{\text{Rabi}}$  is similar to

$$H = D + V. \quad (2.3)$$

Then the result of Chapter 2 says that one has the large  $n$  estimate

$$\lambda_n(H) = d_n + O(n^{-1/4}) \quad (2.4)$$

and the assertion of Theorem 1.1 says that the large  $n$  asymptotic formula

$$\lambda_n(H) = d_n + O(n^{-1/2} \ln n) \quad (2.5)$$

holds if  $\epsilon \notin \mathbb{Z}$ . However, the assumption  $\epsilon \notin \mathbb{Z}$  insures the fact that

$$c_1 := \inf_{n \in \mathbb{N}} (d_{n+1} - d_n) > 0 \quad (2.6)$$

and using (2.4) we know that there is  $n_1 \in \mathbb{N}$  such that for  $n \geq n_1$  one has

$$\{\lambda_n(H)\} = \sigma(H) \cap ]d_n - \frac{1}{2}c_1, d_n + \frac{1}{2}c_1[. \quad (2.7)$$

In Section 4 we define a sequence of self-adjoint, bounded operators  $(Q_n)_{n=0}^\infty$  and in Section 5 we introduce

$$H'_n := e^{-iQ_n} H e^{iQ_n}.$$

Then for  $n \geq n_1$  we still have

$$\{\lambda_n(H)\} = \sigma(H'_n) \cap ]d_n - \frac{1}{2}c_1, d_n + \frac{1}{2}c_1[ \quad (2.8)$$

and in Section 5 we deduce (2.5) from (2.8), combining the structure of  $H'_n$  with

**Theorem 2.1. (Kato-Temple)** *Assume that the operator  $L$  is self-adjoint in the Hilbert space  $\mathcal{H}$  and has exactly one eigenvalue  $\lambda$  in the interval  $]d', d''[$ . If  $x$  is an element of the domain of  $L$  such that  $\eta := \langle x, Lx \rangle_{\mathcal{H}}$  belongs to  $]d', d''[$ , then*

$$\eta - \frac{\|(L - \eta)x\|^2}{\eta - d'} \leq \lambda \leq \eta + \frac{\|(L - \eta)x\|^2}{d'' - \eta}. \quad (2.9)$$

*Proof.* See [59]. □

To investigate  $H'_n$ , we apply the Taylor's expansion formula as follows. Assume that  $B$  and  $Q \in \mathcal{B}(\ell^2(\mathbb{N}))$  and denote

$$F_{tQ}(B) := e^{-itQ} B e^{itQ} \text{ for } t \in \mathbb{R}. \quad (2.10)$$

We use the notation  $\text{ad}_{iQ}^1(B) := [B, iQ]$  and  $\text{ad}_{iQ}^{m+1}(B) := [\text{ad}_{iQ}^m(B), iQ]$  for  $m \in \mathbb{N}^*$ . Then

$$\frac{d^m}{dt^m} F_{tQ}(B) = e^{-itQ} \text{ad}_{iQ}^m(B) e^{itQ} = F_{tQ}(\text{ad}_{iQ}^m(B)) \quad (2.11)$$

and the Taylor formula gives

$$F_{tQ}(B) = B + \sum_{m=1}^N \frac{t^m}{m!} \text{ad}_{iQ}^m(B) + R_{N,tQ}(B) \quad (2.12)$$

with

$$R_{N,tQ}(B) = \frac{t^{N+1}}{N!} \int_0^1 F_{sQ}(\text{ad}_{iQ}^{N+1}(B)) (1-s)^N ds. \quad (2.13)$$

If  $B$  is a self-adjoint unbounded operator  $\mathcal{D}(B) \rightarrow \ell^2(\mathbb{N})$  such that  $\mathcal{D}(B)$  is an invariant subspace of  $e^{itQ}$  for every  $t \in \mathbb{R}$  and  $t \rightarrow B e^{itQ} x$  is locally bounded  $\mathbb{R} \rightarrow \ell^2(\mathbb{N})$  for every  $x \in \mathcal{D}(B)$ , then

$$\frac{d}{dt} \langle e^{itQ} x, B e^{itQ} y \rangle = \langle B e^{itQ} x, iQ e^{itQ} y \rangle + \langle iQ e^{itQ} x, B Q e^{itQ} y \rangle$$

holds for every  $x, y \in \mathcal{D}(B)$ . If moreover the form  $(x, y) \rightarrow \langle Bx, iQy \rangle + \langle iQx, By \rangle$  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  $[B, iQ] \in \mathcal{B}(\ell^2(\mathbb{N}))$  defined by this form and (2.12)-(2.13) still hold.

### 3 Basic notations and results from Chapter 2

Similarly as in Section 2 of Chapter 2 we introduce the linear mapping  $\ell^{2,1}(\mathbb{N}) \times \ell^{2,1}(\mathbb{N}) \rightarrow \ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})$  by

$$\mathbf{H} = \begin{pmatrix} H_{-1} & \frac{\Delta}{2} I_{\ell^2(\mathbb{N})} \\ \frac{\Delta}{2} I_{\ell^2(\mathbb{N})} & H_1 \end{pmatrix} \quad (3.1)$$

where  $H_{\pm 1} : \ell^{2,1}(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$  are defined by

$$H_{\pm 1} := \hat{a}^\dagger \hat{a} \pm g(\hat{a} + \hat{a}^\dagger) \pm \frac{1}{2} \epsilon. \quad (3.2)$$

We can also write

$$\mathbf{V} = \frac{1}{2} \Delta \begin{pmatrix} 0_{\ell^2(\mathbb{N})} & I_{\ell^2(\mathbb{N})} \\ I_{\ell^2(\mathbb{N})} & 0_{\ell^2(\mathbb{N})} \end{pmatrix}, \quad (3.3)$$

where  $0_{\ell^2(\mathbb{N})}$  denotes the null mapping in  $\ell^2(\mathbb{N})$  and

$$\mathbf{H}_0 = H_{-1} \oplus H_1.$$



Due to Lemma 2.2 in Chapter 2,  $\mathbf{H}$  is similar to  $\mathbf{H}_{\text{Rabi}}$  and  $\mathbf{H}_0$  similar to  $\mathbf{H}_{0,\text{Rabi}}$ . Further on we assume for simplicity that  $\epsilon > 0$ , we introduce

$$l_0 := [\epsilon] = \max\{n \in \mathbb{N} : n \leq \epsilon\}$$

and define  $(d_n)_{n=0}^\infty$  setting

$$d_n = n - g^2 - \frac{1}{2}\epsilon \text{ for } n = 0, \dots, l_0, \quad (3.4)$$

$$d_{l_0+2i} = l_0 + i - g^2 - \frac{1}{2}\epsilon \text{ for } i \in \mathbb{N}, \quad (3.5)$$

$$d_{l_0+1+2i} = i - g^2 + \frac{1}{2}\epsilon \text{ for } i \in \mathbb{N}. \quad (3.6)$$

Then Lemma 2.4 in Chapter 2 ensures that  $(d_n)_{n=0}^\infty = (\lambda_n(H_0))_{n=0}^\infty$  is the non-decreasing sequence of eigenvalues of  $H_0$ , counting multiplicities. It is clear that  $\epsilon \notin \mathbb{Z}$  implies (2.6) and moreover there is  $c_0 > 0$  such that

$$|d_j - d_k| \geq c_0 \langle j - k \rangle, \quad (3.7)$$

where  $\langle s \rangle := (1 + s^2)^{1/2}$ .

Let  $\{\mathbf{v}_n^0\}_{n \in \mathbb{N}}$  be an orthonormal basis of eigenvectors of  $\mathbf{H}_0$  and define  $H$  as the self-adjoint operators in  $\ell^2(\mathbb{N})$  given by

$$H = U\mathbf{H}U^{-1}, \quad (3.8)$$

where  $U : \ell^2(\mathbb{N}) \times \ell^2(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$  is the isometric isomorphism satisfying  $U\mathbf{v}_n^0 = e_n$  for every  $n \in \mathbb{Z}$ . Then  $H = D + V$  holds with  $D = \text{diag}(d_j)_{j=0}^\infty$  and

$$V = U\mathbf{V}U^{-1}. \quad (3.9)$$

Due to Corollary 5.2 in Chapter 2, there exist  $C$  and  $c > 0$  such that

$$|j - k| < ck^{1/2} \Rightarrow |V(j, k)| \leq C\langle k \rangle^{-1/4} \quad (3.10)$$

and

$$V(j, j) = 0 \quad (3.11)$$

holds for every  $j \in \mathbb{N}$  due (5.5)-(5.6) in Chapter 2. Moreover

$$\sum_{j \in \mathbb{N}} |V(j, k)|^2 = \sum_{j \in \mathbb{N}} |\langle e_j, V e_k \rangle|^2 = \|V e_k\|^2 \leq \|V\|^2. \quad (3.12)$$

#### 4 Operators $R_n$ and $Q_n$

In the sequel we consider the orthogonal decomposition

$$\ell^2(\mathbb{N}) = \widehat{\mathcal{H}}_n \oplus \widetilde{\mathcal{H}}_n, \quad (4.1)$$

where

$$\widehat{\mathcal{H}}_n := \mathbb{C}e_n, \quad \widetilde{\mathcal{H}}_n := (\mathbb{C}e_n)^\perp. \quad (4.2)$$

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

We introduce

$$R_n := \widetilde{\Pi}_n V \widehat{\Pi}_n + \widehat{\Pi}_n V \widetilde{\Pi}_n \quad (4.3)$$

and observe that  $R_n(j, k) \neq 0 \Rightarrow$  (either  $j = n \neq k$  or  $k = n \neq j$ ). Moreover,  $V(n, n) = 0$  ensures  $\widehat{\Pi}_n V \widehat{\Pi}_n = 0$  and (4.3) can be written in the form

$$R_n = V - \widetilde{\Pi}_n V \widetilde{\Pi}_n. \quad (4.4)$$

Since  $R_n(j, k) \neq 0 \Rightarrow j \neq k \Rightarrow d_j \neq d_k$ , we can define

$$Q_n(j, k) := \begin{cases} i \frac{R_n(j, k)}{d_j - d_k} & \text{if } R_n(j, k) \neq 0 \\ 0 & \text{if } R_n(j, k) = 0 \end{cases} \quad (4.5)$$

**Lemma 4.1.** (a) *There is  $Q_n \in \mathcal{B}(\ell^2(\mathbb{N}))$  satisfying  $\langle e_j, Q_n e_k \rangle = Q_n(j, k)$  for all  $j, k \in \mathbb{N}$  and*

$$\|Q_n\| = O(n^{-1/4}). \quad (4.6)$$

(b)  $\ell^{2,1}(\mathbb{N})$  is an invariant subspace of  $Q_n$  and one has

$$[D, iQ_n] = -R_n. \quad (4.7)$$

(c)  $\ell^{2,1}(\mathbb{N})$  is an invariant subspace of  $e^{itQ_n}$  and  $t \rightarrow e^{itQ_n} x$  is of class  $C^\infty(\mathbb{R}; \ell^{2,1}(\mathbb{N}))$  if  $x \in \ell^{2,1}(\mathbb{N})$ .

*Proof.* (a) We observe that  $Q_n(n, j) = \overline{Q_n(j, n)}$  and using

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

we can estimate

$$\|Q_n\| \leq \|Q_n \widehat{\Pi}_n\| + \|\widehat{\Pi}_n Q_n\| = 2\|Q_n \widehat{\Pi}_n\| = 2\|Q_n e_n\|.$$

Due to (3.7),

$$\|Q_n e_n\|^2 = \sum_{j \in \mathbb{N}} |Q_n(j, n)|^2 \leq c_0^{-2} \sum_{j \in \mathbb{N}} \frac{|V(j, n)|^2}{\langle j - n \rangle^2} \leq c_0^{-2} (M_n + M'_n),$$

where

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

and

$$M'_n = \sum_{\{j: |j-n| < cn^{1/2}\}} \frac{|V(j, n)|^2}{\langle j - n \rangle^2} \leq C^2 n^{-1/2} \sum_{m \in \mathbb{N}} \langle m - n \rangle^{-2} \leq C_1 n^{-1/2}$$

due to (3.10).

(b) We observe that

$$d_j(Q_n e_k)(j) = (d_j - d_k)(Q_n e_k)(j) + (Q_n D e_k)(j) = ((iR_n + Q_n D)e_k)(j) \quad (4.8)$$

implies that  $d_j(Q_n x)(j) = ((iR_n + Q_n D)x)(j)$  holds when  $x \in \ell^{2,1}(\mathbb{N})$ . Since  $d_j \sim \frac{1}{2}j$  as  $j \rightarrow \infty$ , we can conclude that  $x \in \ell^{2,1}(\mathbb{N}) \Rightarrow DQ_n x \in \ell^2(\mathbb{N}) \Rightarrow Q_n x \in \ell^{2,1}(\mathbb{N})$  and (4.7) holds.

(c) Let us fix  $\lambda_0 > 1 - d_0$  and denote  $D' := D + \lambda_0$ . Then  $D' \geq I$  and we introduce  $Q_{n,1} := iR_n D'^{-1} + Q_n \in \mathcal{B}(\ell^2(\mathbb{N}))$ . We observe that  $Q_{n,1} = D' Q_n D'^{-1}$  and

$$e^{itQ_n} D'^{-1} y = \lim_{N \rightarrow \infty} \sum_{m=0}^N \frac{(it)^m}{m!} Q_n^m D'^{-1} y = \lim_{N \rightarrow \infty} \sum_{m=0}^N \frac{(it)^m}{m!} D'^{-1} Q_{n,1}^m y = D'^{-1} e^{itQ_{n,1}} y \quad (4.9)$$

holds for every  $y \in \ell^2(\mathbb{N})$ . If  $x \in \ell^{2,1}(\mathbb{N})$ , then using  $y = D'x$  in (4.9) we find that  $t \rightarrow e^{itQ_n} x = D'^{-1} e^{itQ_{n,1}} y$  is  $C^\infty(\mathbb{R}; \ell^2(\mathbb{N}))$ . It remains to observe that  $x \rightarrow \|D'^{-1}x\|$  is a norm equivalent to  $\|\cdot\|_{\ell^{2,1}(\mathbb{N})}$ .  $\square$

## 5 Proof of Theorem 1.1

In the sequel  $Q_n$  and  $R_n$  are as in Lemma 4.1. We write  $T_n = T'_n + O(\eta_n)$  if and only if we can find  $C > 0$ ,  $n_0 \in \mathbb{N}$ , such that  $\|T_n - T'_n\| \leq C\eta_n$  holds for all  $n \geq n_0$ . If  $x_n, x'_n \in \ell^2(\mathbb{N})$ , then we write  $x_n = x'_n + O(\eta_n)$  if and only if we can find  $C > 0$ ,  $n_0 \in \mathbb{N}$ , such that  $\|x_n - x'_n\| \leq C\eta_n$  holds for all  $n \geq n_0$ .

**Step 1.** We denote  $H'_n := e^{-iQ_n} H e^{iQ_n}$  and claim that

$$H'_n = D + V - R_n + [V - \frac{1}{2}R_n, iQ_n] + O(\|Q_n\|^2). \quad (5.1)$$

Indeed, using (2.12)-(2.13) with  $N = 1$  and  $Q_n, V$ , instead of  $Q, B$ , we obtain

$$e^{-iQ_n} V e^{iQ_n} = V + [V, iQ_n] + O(\|\text{ad}_{iQ_n}^2(V)\|) \quad (5.2)$$

and  $\|\text{ad}_{iQ_n}^2(V)\| \leq C\|Q_n\|^2$ . Similarly, using (2.12)-(2.13) with  $N = 2$  and  $Q_n, D$ , instead of  $Q, B$ , we obtain

$$e^{-iQ_n} D e^{iQ_n} = D + [D, iQ_n] + \frac{1}{2}[[D, iQ_n], iQ_n] + O(\|\text{ad}_{iQ_n}^3(D)\|). \quad (5.3)$$

and  $[D, iQ_n] = -R_n$  ensures  $\text{ad}_{iQ_n}^3(D) = \text{ad}_{iQ_n}^2(-R_n) = O(\|Q_n\|^2)$ . Summation of (5.2) and (5.3) gives

$$e^{-iQ_n} H e^{iQ_n} = D + V + [D, iQ_n] + W_n + O(\|Q_n\|^2) \quad (5.4)$$

with

$$W_n = [V, iQ_n] + \frac{1}{2}[[D, iQ_n], iQ_n] = [V, iQ_n] - \frac{1}{2}[R_n, iQ_n]. \quad (5.5)$$

We obtain (5.1) using  $[D, iQ_n] = -R_n$  in (5.4) and (5.5) .

**Step 2.** If  $W_n$  is given by (5.5), then

$$W_n(n, n) = O(n^{-1/2} \ln n). \quad (5.6)$$

Denote  $V_n^0 := V - \frac{1}{2}R_n$ . Then  $W_n = [V_n^0, iQ_n]$  and

$$|V_n^0(j, k)| \leq |V(j, k)| \text{ for all } j, k \in \mathbb{N} \quad (5.7)$$

Due to (5.7) and (3.7) we can estimate

$$|(V_n^0 Q_n)(n, n)| \leq \sum_{m \in \mathbb{N}} |V(n, m) Q_n(m, n)| \leq \sum_{m \in \mathbb{N} \setminus \{n\}} \frac{|V(n, m)|^2}{|d_m - d_n|} \leq c_0^{-1} (M_n + M'_n) \quad (5.8)$$

with

$$M_n := \sum_{\{m: |m-n| \geq cn^{1/2}\}} \frac{|V(n, m)|^2}{\langle m - n \rangle} \leq c^{-1} n^{-1/2} \sum_{j \in \mathbb{N}} |V(j, n)|^2 = c^{-1} n^{-1/2} \|V\|^2$$

(see (3.12)) and

$$M'_n := \sum_{\{m: |m-n| < cn^{1/2}\}} \frac{|V(n, m)|^2}{\langle m - n \rangle} \leq C^2 n^{-1/2} \sum_{\{m: |m-n| < cn^{1/2}\}} \langle m - n \rangle^{-1} \leq C'_1 n^{-1/2} \ln n$$

where we used (3.10) and the fact that

$$\sum_{\{m: |m-n| < cn^{1/2}\}} \langle m - n \rangle^{-1} \leq 1 + 2 \sum_{1 \leq i \leq cn^{1/2}} \frac{1}{i} = O(\ln n)$$

**Step 3.** We claim that

$$\langle e_n, H'_n e_n \rangle = d_n + O(n^{-1/2} \ln n) \quad (5.9)$$

and

$$(H'_n - \langle e_n, H'_n e_n \rangle) e_n = O(n^{-1/4}). \quad (5.10)$$

Indeed, using  $\|Q_n\| = O(n^{-1/4})$  and  $V - R_n = \tilde{\Pi}_n V \tilde{\Pi}_n$  in (5.1), we find

$$H'_n e_n = (D + \tilde{\Pi}_n V \tilde{\Pi}_n + W_n) e_n + O(n^{-1/2}) = d_n e_n + W_n e_n + O(n^{-1/2}), \quad (5.11)$$

hence

$$\langle e_n, H'_n e_n \rangle = d_n + \langle e_n, W_n e_n \rangle + O(n^{-1/2})$$

and (5.9) follows from (5.6). Moreover, (5.9) implies

$$(H'_n - \langle e_n, H'_n e_n \rangle) e_n = (H'_n - d_n) e_n + O(n^{-1/2} \ln n) \quad (5.12)$$

and (5.11) ensures

$$(H'_n - d_n)e_n = W_n e_n + O(n^{-1/2}). \quad (5.13)$$

Thus (5.10) follows from (5.12), (5.13) and  $\|W_n\| \leq (2\|V\| + \|R_n\|)\|Q_n\| = O(n^{-1/4})$ .

**End of the proof of Theorem 1.1.** Let  $n_1$  be such that (2.8) holds for  $n \geq n_1$ . Due to (5.9) there is  $n_0 \in \mathbb{N}$  such that for  $n \geq n_0$  one has

$$\langle e_n, H'_n e_n \rangle \in ]d_n - \frac{1}{4}c_1, d_n + \frac{1}{4}c_1[.$$

If  $n \geq \max\{n_0, n_1\}$ , then  $H'_n$  satisfies the assumptions of Theorem 2.1 with  $L = H'_n$ ,  $x = e_n$  and  $]d', d''[ = ]d_n - \frac{1}{2}c_1, d_n + \frac{1}{2}c_1[$ . Therefore (2.9) gives

$$|\lambda_n(H'_n) - \langle e_n, H'_n e_n \rangle| \leq 4c_1^{-1} \|(H'_n - \langle e_n, H'_n e_n \rangle)e_n\|^2 = O(n^{-1/2}). \quad (5.14)$$

Combining (5.14) with (5.9) we get  $\lambda_n(H'_n) = d_n + O(n^{-1/2} \ln n)$ .

# Chapitre 4

## Formule asymptotique à trois termes pour les valeurs propres du modèle de Rabi quantique avec un biais résonant

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# Three-term asymptotic formula for eigenvalues of the quantum Rabi model with a resonant bias

**Abstract.** We obtain the three-term asymptotic formula for large eigenvalues of the asymmetric quantum Rabi model with a bias  $\epsilon \in \mathbb{Z}$ .

## 1 Statement of the result

In this Chapter we use notations introduced in Section 1 of Chapter 2, page 31. The operator  $\mathbf{H}_{0,\text{Rabi}}$  is defined as the linear mapping  $\mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \rightarrow \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  given by

$$\mathbf{H}_{0,\text{Rabi}} := I_2 \otimes \hat{a}^\dagger \hat{a} + \sigma_x \otimes \left( g(\hat{a} + \hat{a}^\dagger) + \frac{\epsilon}{2} I_{\ell^2} \right), \quad (1.1)$$

and the operator  $\mathbf{H}_{\text{Rabi}}$  is defined as the linear mapping  $\mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \rightarrow \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  given by

$$\mathbf{H}_{\text{Rabi}} = \mathbf{H}_{0,\text{Rabi}} + \frac{1}{2} \Delta \sigma_z \otimes I_{\ell^2}. \quad (1.2)$$

where  $g > 0$  is fixed.

In Chapter 2 we proved that there is an orthonormal basis in  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  of the form  $\{\mathbf{u}_m^-\}_{m \in \mathbb{N}} \cup \{\mathbf{u}_m^+\}_{m \in \mathbb{N}}$  such that

$$\mathbf{H}_{\text{Rabi}} \mathbf{u}_m^\pm = E_m^\pm \mathbf{u}_m^\pm \quad (1.3)$$

holds for every  $m \in \mathbb{N}$  and the eigenvalue sequences  $(E_m^-)_{m=0}^\infty, (E_m^+)_{m=0}^\infty$ , satisfy the large  $m$  asymptotic formula

$$E_m^\pm = m - g^2 \pm \frac{1}{2} \epsilon + O(m^{-1/4}). \quad (1.4)$$

The purpose of this Chapter is to prove

**Theorem 1.1.** *Assume that  $\epsilon = l_0 \in \mathbb{N}$ . Then the eigenvalue sequences  $(E_m^-)_{m \in \mathbb{N}}$  and  $(E_m^+)_{m \in \mathbb{N}}$  satisfy the asymptotic estimates*

$$E_{i+l_0}^- = i + \frac{1}{2} l_0 - g^2 - |\mathbf{r}_i| + O(i^{-1/2} \ln i), \quad (1.5)$$

$$E_i^+ = i + \frac{1}{2} l_0 - g^2 + |\mathbf{r}_i| + O(i^{-1/2} \ln i), \quad (1.6)$$

where

$$\mathbf{r}_i := i^{-1/4} \frac{\Delta}{2\sqrt{2\pi g}} \cos \left( 4g\sqrt{i} - \frac{\pi}{4} - l_0 \frac{\pi}{2} \right). \quad (1.7)$$

## 2 Main ingredients of the proof

We keep notations introduced in Chapter 2. In particular,  $\sigma(L)$  denotes the spectrum of  $L$ ,  $\|\cdot\|$  denotes the norm of  $\ell^2(\mathbb{N})$  or the norm of the algebra of bounded operators  $\mathcal{B}(\ell^2(\mathbb{N}))$ . Assume that  $L_n, L'_n$  are linear mappings defined on a dense subspace of  $\ell^2(\mathbb{N})$ . If  $L_n - L'_n$  can be extended to a bounded operator  $\ell^2(\mathbb{N})$ , 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  $\|T_n - T'_n\| \leq C\eta_n$  for all  $n \geq n_0$ .

If  $T \in \mathcal{B}(\ell^2(\mathbb{N}))$ , then we denote

$$T(j, k) := \langle e_j, T e_k \rangle \text{ for } j, k \in \mathbb{N}, \quad (2.1)$$

where  $\{e_m\}_{m \in \mathbb{N}}$  is the canonical basis and  $\langle \cdot, \cdot \rangle$  is the scalar product of  $\ell^2(\mathbb{N})$ .

Further on we assume that  $\epsilon = l_0 \in \mathbb{N}$  and we define  $(d_n)_{n=0}^\infty$  setting

$$d_n = n - g^2 - \frac{1}{2}l_0 \text{ for } n = 0, \dots, l_0, \quad (2.2)$$

$$d_{2i+l_0} = d_{1+2i+l_0} = i - g^2 + \frac{1}{2}l_0 \text{ for } i \in \mathbb{N}. \quad (2.3)$$

Due to Lemma 2.2, Lemma 2.4 and Corollary 5.2 in Chapter 2, the operator  $\mathbf{H}_{0, \text{Rabi}}$  is similar to the diagonal operator  $D = \text{diag}(d_j)_{j=0}^\infty$  in  $\ell^2(\mathbb{N})$ , i.e.

$$D e_j = d_j e_j \text{ for } j \in \mathbb{N}, \quad (2.4)$$

and the operator  $\mathbf{H}_{\text{Rabi}}$  is similar to

$$H = D + V, \quad (2.5)$$

where  $V$  is a bounded self-adjoint operator in  $\ell^2(\mathbb{N})$  satisfying

$$V(j, j) = 0 \text{ for every } j \in \mathbb{N} \quad (2.6)$$

and

$$|j - k| < \hat{c}k^{1/2} \Rightarrow |V(j, k)| \leq \hat{C}k^{-1/4} \quad (2.7)$$

where  $\hat{C}, \hat{c} > 0$  are certain constants independent of  $j, k \in \mathbb{N}$ . In Chapter 2 we used (2.6)-(2.7) to prove the large  $n$  estimate

$$\lambda_n(H) = d_n + O(n^{-1/4}) \quad (2.8)$$

where  $(\lambda_n(H))_{n=0}^\infty$  is the non-decreasing sequence of eigenvalues of  $H$ , counting multiplicities.

We will use the assumption  $\epsilon = l_0 \in \mathbb{N}$  to prove the large  $i$  estimates

$$\lambda_{2i+l_0}(H) = d_{2i+l_0} - |V(2i+l_0, 1+2i+l_0)| + O(i^{-1/2} \ln i), \quad (2.9)$$

$$\lambda_{1+2i+l_0}(H) = d_{1+2i+l_0} + |V(2i+l_0, 1+2i+l_0)| + O(i^{-1/2} \ln i). \quad (2.10)$$

It is clear that the assertion of Theorem 1.1 follows from (2.3), (2.9), (2.10) and



**Proposition 2.1.** *One has the large  $i$  estimate*

$$|V(2i + l_0, 1 + 2i + l_0)| = |\mathfrak{r}_i| + O(i^{-1/2}), \quad (2.11)$$

where  $\mathfrak{r}_i$  is given by (1.7).

*Proof.* See Section 5.3. □

In order to prove the estimates (2.9)-(2.10) we write

$$n = l_0 + 2i \quad (2.12)$$

(where  $i \in \mathbb{N}$ ) and consider the orthogonal decomposition

$$\ell^2(\mathbb{N}) = \widehat{\mathcal{H}}_n \oplus \widetilde{\mathcal{H}}_n, \quad (2.13)$$

where

$$\widehat{\mathcal{H}}_n := \text{span}\{e_n, e_{n+1}\} \quad \text{and} \quad \widetilde{\mathcal{H}}_n := \widehat{\mathcal{H}}_n^\perp. \quad (2.14)$$

In the sequel  $\widehat{\Pi}_n \in \mathcal{B}(\ell^2(\mathbb{N}))$  denotes the orthogonal projection on  $\widehat{\mathcal{H}}_n$  and  $\widetilde{\Pi}_n := I - \widehat{\Pi}_n$ . We use the decomposition (2.13) to express  $V$  in the matrix form

$$V = \begin{pmatrix} \widehat{V}_n & \check{R}_n^* \\ \check{R}_n & \widetilde{V}_n \end{pmatrix} \quad (2.15)$$

where

$$\widehat{V}_n := \widehat{\Pi}_n V|_{\widehat{\mathcal{H}}_n} \in \mathcal{B}(\widehat{\mathcal{H}}_n), \quad (2.16)$$

$$\widetilde{V}_n := \widetilde{\Pi}_n V|_{\widetilde{\mathcal{H}}_n} \in \mathcal{B}(\widetilde{\mathcal{H}}_n), \quad (2.17)$$

$$\check{R}_n^* := \widehat{\Pi}_n V|_{\widetilde{\mathcal{H}}_n} \in \mathcal{B}(\widetilde{\mathcal{H}}_n, \widehat{\mathcal{H}}_n), \quad (2.18)$$

$$\check{R}_n := \widetilde{\Pi}_n V|_{\widehat{\mathcal{H}}_n} \in \mathcal{B}(\widehat{\mathcal{H}}_n, \widetilde{\mathcal{H}}_n). \quad (2.19)$$

Moreover, we can identify  $\widehat{V}_n$  with its matrix in the basis  $\{e_n, e_{n+1}\}$ , i.e. we can write

$$\widehat{V}_n = \begin{pmatrix} 0 & V(n, n+1) \\ V(n+1, n) & 0 \end{pmatrix}. \quad (2.20)$$

We will prove

**Proposition 2.2.** *There exists a sequence of unitary operators  $(U_n)_{n \in \mathbb{N}}$  such that the large  $n$  estimate*

$$U_n^{-1} H U_n = D + \widehat{V}_n \oplus \widetilde{V}'_n + O(n^{-1/2} \ln n) \quad (2.21)$$

holds if  $n - l_0 \in 2\mathbb{N}$ ,  $\widehat{V}_n$  is given by (2.20) and

$$\widetilde{V}'_n = \widetilde{V}_n + O(n^{-1/4}) \quad (2.22)$$

holds with  $\widetilde{V}_n$  given by (2.17).

*Proof.* The estimate (2.21) is proved in Section 5.2 with

$$U_n = e^{iQ_n} e^{iQ'_n}, \quad (2.23)$$

where  $Q_n$  and  $Q'_n$  are bounded self-adjoint operators defined in Section 3 and 4 respectively.  $\square$

**Corollary 2.3.** *The estimates (2.9)-(2.10) follow from the assertion of Proposition 2.2.*

*Proof.* To begin we observe that the assumption  $n - l_0 \in 2\mathbb{N}$  implies

$$d_{n-1} + 1 = d_n = d_{n+1} = d_{n+2} - 1 \quad (2.24)$$

and (2.8) ensures the fact that there is  $n_1 \in \mathbb{N}$  such that for  $n \geq n_1$  one has

$$\lambda_{n-1}(H) < d_n - \frac{3}{4} < d_n - \frac{1}{4} < \lambda_n(H) \leq \lambda_{n+1}(H) < d_n + \frac{1}{4} < d_n + \frac{3}{4} < \lambda_{n+2}(H). \quad (2.25)$$

Moreover, (2.21) ensures

$$H = H_n + O(n^{-1/2} \ln n) \quad (2.26)$$

holds with

$$H_n := U_n(D + \widehat{V}_n \oplus \widetilde{V}'_n)U_n^{-1} \quad (2.27)$$

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

$$\sup_{k \in \mathbb{N}} |\lambda_k(H) - \lambda_k(H_n)| \leq Cn^{-1/2} \ln n, \quad (2.28)$$

where  $(\lambda_k(H_n))_{k \in \mathbb{N}}$  denotes the non-decreasing sequence of eigenvalues of  $H_n$ , counting the multiplicities. However, combining (2.28) with (2.25), we can find  $n_1 \in \mathbb{N}$  such that for  $n \geq n_1$  one has

$$\lambda_{n-1}(H_n) < d_n - \frac{1}{2} < \lambda_n(H_n) \leq \lambda_{n+1}(H_n) < d_n + \frac{1}{2} < \lambda_{n+2}(H). \quad (2.29)$$

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

$$\widehat{\lambda}_n := d_n - |V(n, n+1)| \text{ and } \widehat{\lambda}_{n+1} := d_n + |V(n, n+1)|. \quad (2.30)$$

Moreover, due to (2.7), there is  $n_2 \in \mathbb{N}$  such that for  $n \geq n_2$  one has

$$d_n - \frac{1}{2} < \widehat{\lambda}_n \leq \widehat{\lambda}_{n+1} < d_n + \frac{1}{2}. \quad (2.31)$$

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

$$\{\widehat{\lambda}_n, \widehat{\lambda}_{n+1}\} \subset \sigma(H_n). \quad (2.32)$$

Combining (2.32) with (2.29), (2.31), we get  $\widehat{\lambda}_n = \lambda_n(H_n)$ ,  $\widehat{\lambda}_{n+1} = \lambda_{n+1}(H_n)$  and using these equalities in (2.28), we deduce

$$\lambda_n(H) = \widehat{\lambda}_n + O(n^{-1/2} \ln n) \text{ and } \lambda_{n+1}(H) = \widehat{\lambda}_{n+1} + O(n^{-1/2} \ln n), \quad (2.33)$$

i.e. (2.9)-(2.10) hold.  $\square$

### 3 Operators related to the first similarity transformation

**Notation 3.1.** (a) In the sequel  $\hat{c}, \hat{C}$  are as in (2.7) and  $n - l_0 \in 2\mathbb{N}$ , i.e. (2.24) holds and it is easy to check that

$$d_j \neq d_k \Rightarrow |d_j - d_k| \geq \frac{1}{4}\langle j - k \rangle. \quad (3.1)$$

(b) We introduce  $Z_n^-, Z_n^+ \subset \mathbb{N}^2$  defined as follows

$$Z_n^- = (\mathbb{N} \setminus \{n, n + 1\}) \times \{n, n + 1\} \quad (3.2)$$

$$Z_n^+ = \{n, n + 1\} \times (\mathbb{N} \setminus \{n, n + 1\}). \quad (3.3)$$

We observe that

$$(j, k) \in Z_n^- \Rightarrow d_j \neq d_n = d_k, \quad (3.4)$$

$$(j, k) \in Z_n^+ \Rightarrow d_j = d_n \neq d_k. \quad (3.5)$$

(c) In the sequel we fix  $c$  such that  $0 < c < \frac{1}{4}\hat{c}$  and 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

$$Q_n^\pm(j, k) := \begin{cases} i \frac{V(j, k)}{d_j - d_k} & \text{if } (j, k) \in Z_n^\pm \text{ and } |j - k| < cn^{1/2} \\ 0 & \text{otherwise} \end{cases} \quad (3.6)$$

(d) We define the matrix  $(Q_n(j, k))_{(j,k) \in \mathbb{N}^2}$  by

$$Q_n(j, k) := \begin{cases} i \frac{V(j, k)}{d_j - d_k} & \text{if } (j, k) \in Z_n^+ \cup Z_n^- \\ 0 & \text{otherwise} \end{cases} \quad (3.7)$$

**Lemma 3.2.** *If  $(Q_n^\pm(j, k))_{(j,k) \in \mathbb{N}^2}$  is defined as in Notation 3.1(c), then*

(a) *there is  $C > 0$  such that for all  $j, k \in \mathbb{N}$  one has the estimate*

$$|Q_n^\pm(j, k)| \leq \frac{4\hat{C}n^{-1/4}}{\langle j - k \rangle} \quad (3.8)$$

(b) *there is  $Q_n^\pm \in \mathcal{B}(\ell^2(\mathbb{N}))$  satisfying  $\langle e_j, Q_n^\pm e_k \rangle = Q_n^\pm(j, k)$  for all  $j, k \in \mathbb{N}$  and*

$$\|Q_n^\pm\| = O(n^{-1/4}). \quad (3.9)$$

*Proof.* (a) Due to  $c \leq \hat{c}$ , (3.8) follows from (2.7) and (3.1).

(b) If  $k \in \mathbb{N} \setminus \{n, n + 1\}$ , then  $Q_n^- e_k = 0$ . If  $k \in \{n, n + 1\}$ , then

$$\|Q_n^- e_k\|^2 = \sum_{j \in \mathbb{N}} |Q_n^-(j, k)|^2 \leq \sum_{\{j \in \mathbb{N}: |j-k| < cn^{1/2}\}} \frac{(4\hat{C}n^{-1/4})^2}{\langle j - k \rangle^2}$$

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

hence  $Q_n^- \in \mathcal{B}(\ell^2(\mathbb{N}))$  and  $\|Q_n^-\| = O(n^{-1/4})$ . Since  $(j, k) \in Z_n^+ \Leftrightarrow (k, j) \in Z_n^-$  and  $Q_n^+(j, k) = \overline{Q_n^-(k, j)}$ , one has  $Q_n^+ = (Q_n^-)^* \in \mathcal{B}(\ell^2(\mathbb{N}))$  and  $\|Q_n^+\| = \|Q_n^-\|$   $\square$

**Lemma 3.3.** *If  $(Q_n(j, k))_{(j, k) \in \mathbb{N}^2}$  is defined as in Notation 3.1(d), then*

(a) *there is  $Q_n \in \mathcal{B}(\ell^2(\mathbb{N}))$  satisfying  $\langle e_j, Q_n e_k \rangle = Q_n(j, k)$  for all  $j, k \in \mathbb{N}$  and*

$$\|Q_n^+ + Q_n^- - Q_n\| = O(n^{-1/2}). \quad (3.10)$$

(b)  $\ell^{2,1}(\mathbb{N})$  *is an invariant subspace of  $Q_n$  and one has*

$$-[D, iQ_n] = \tilde{\Pi}_n V \hat{\Pi}_n + \hat{\Pi}_n V \tilde{\Pi}_n. \quad (3.11)$$

(c)  $\ell^{2,1}(\mathbb{N})$  *is an invariant subspace of  $e^{itQ_n}$  and  $t \rightarrow e^{itQ_n} x$  is of class  $C^\infty(\mathbb{R}; \ell^{2,1}(\mathbb{N}))$  if  $x \in \ell^{2,1}(\mathbb{N})$ .*

*Proof.* (a) If  $k \in \mathbb{N} \setminus \{n, n+1\}$ , then  $(Q_n \hat{\Pi}_n - Q_n^-) e_k = 0$ . If  $k \in \{n, n+1\}$ , then

$$\begin{aligned} \|(Q_n \hat{\Pi}_n - Q_n^-) e_k\|^2 &= \sum_{\{j \in \mathbb{N}: |j-k| \geq cn^{1/2}\}} |Q_n(j, k)|^2 \\ &\leq \sum_{\{j \in \mathbb{N}: |j-k| \geq cn^{1/2}\}} \frac{16|V(j, k)|^2}{\langle j - k \rangle^2} \leq \frac{16}{c^2 n} \sum_{j \in \mathbb{N}} |V(j, k)|^2 = \frac{16\|V e_k\|^2}{c^2 n} \leq \frac{C}{n}, \end{aligned}$$

hence  $Q_n \hat{\Pi}_n = Q_n^- + O(n^{-1/2})$ . Using the adjoint formula  $\hat{\Pi}_n Q_n = Q_n^+ + O(n^{-1/2})$ , we obtain

$$Q_n \hat{\Pi}_n + \hat{\Pi}_n Q_n = Q_n^- + Q_n^+ + O(n^{-1/4}). \quad (3.12)$$

However, using  $\hat{\Pi}_n Q_n \hat{\Pi}_n = 0$  and  $\tilde{\Pi}_n Q_n \tilde{\Pi}_n = 0$ , we obtain

$$Q_n = \tilde{\Pi}_n Q_n \hat{\Pi}_n + \hat{\Pi}_n Q_n \tilde{\Pi}_n = Q_n \hat{\Pi}_n + \hat{\Pi}_n Q_n \quad (3.13)$$

and we complete the proof of (a) combining (3.12) and (3.13). We obtain assertions (b) and (c) reasoning as in the proof of Lemma 4.1 in Chapter 3.  $\square$

**Lemma 3.4.** *Let  $Q_n^\pm$  be as in Notation 3.1(c) and*

$$Q_n^0 := Q_n^+ + Q_n^-. \quad (3.14)$$

*If*

$$V_n^0 := \frac{1}{2}V + \frac{1}{2}(\hat{\Pi}_n V \hat{\Pi}_n + \tilde{\Pi}_n V \tilde{\Pi}_n), \quad (3.15)$$

*then one has the following large  $n$  estimate*

$$\hat{\Pi}_n V_n^0 Q_n^0 \hat{\Pi}_n = O(n^{-1/2} \ln n). \quad (3.16)$$

*Proof.* To begin we observe that we still have the large  $k$  estimate

$$\sup_{\{j \in \mathbb{N}: |j-k| < \hat{c}k^{1/2}\}} |V_n^0(j, k)| \leq \hat{C}k^{-1/4}. \quad (3.17)$$

Next we observe that

$$\|\hat{\Pi}_n V_n^0 Q_n^0 \hat{\Pi}_n\| \leq \sum_{n \leq j, k \leq n+1} |(V_n^0 Q_n^0)(j, k)|$$

and

$$(V_n^0 Q_n^0)(j, k) = \sum_{\{m \in \mathbb{N}: |m-k| < cn^{1/2}\}} V_n^0(j, m) Q_n^0(m, k).$$

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

$$|m-k| < cn^{1/2} \Rightarrow |j-m| \leq |j-k| + |k-m| < 1 + cn^{1/2} < \hat{c}n^{1/2} \Rightarrow |V_n^0(j, m)| \leq \hat{C}n^{-1/4} \quad (3.18)$$

holds for every  $n \geq c^{-2}$ . Therefore, using (3.18) and (3.8), we can estimate

$$|(V_n^0 Q_n^0)(j, k)| \leq \sum_{\{m \in \mathbb{N}: |m-k| < cn^{1/2}\}} \frac{4\hat{C}^2 n^{-1/2}}{\langle m-k \rangle} = O(n^{-1/2} \ln n), \quad (3.19)$$

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

#### 4 Operators related to the second similarity transformation

**Notation 4.1.** Assume that  $Q_n^\pm$  is given by Notation 3.1(c) and  $V_n^0$  by (3.15). We introduce the matrices  $(Q_n^+(j, k))_{(j,k) \in \mathbb{N}^2}$  and  $(Q_n^-(j, k))_{(j,k) \in \mathbb{N}^2}$  defined by

$$Q_n^\pm(j, k) := \begin{cases} -\frac{(V_n^0 Q_n^\pm)(j, k)}{d_j - d_k} & \text{if } (j, k) \in Z_n^- \cup Z_n^+ \\ 0 & \text{otherwise} \end{cases} \quad (4.1)$$

**Lemma 4.2.** Let  $(Q_n^+(j, k))_{(j,k) \in \mathbb{N}^2}$  be as in Notation 4.1. Then there is  $Q_n^+ \in \mathcal{B}(\ell^2(\mathbb{N}))$  satisfying  $\langle e_j, Q_n^+ e_k \rangle = Q_n^+(j, k)$  for all  $j, k \in \mathbb{N}$  and

$$\|Q_n^+\| = O(n^{-1/2} \ln n). \quad (4.2)$$

*Proof.* Due to the Schur boundedness test, it suffices to show that there is  $C > 0$  such that for every  $j, k \in \mathbb{N}$ ,  $n \in \mathbb{N}^*$ , the inequalities

$$\mathcal{Q}_n(k) \leq Cn^{-1/2} \ln n \quad \text{and} \quad \mathcal{Q}_n^*(j) \leq Cn^{-1/2} \ln n \quad (4.3)$$

hold with

$$\mathcal{Q}_n(k) := \sum_{j \in \mathbb{N}} |Q_n^+(j, k)|, \quad (4.4)$$

$$\mathcal{Q}_n^*(k) := \sum_{j \in \mathbb{N}} |Q_n^{'+}(k, j)|. \quad (4.5)$$

Let us decompose  $\mathcal{Q}_n = \mathcal{Q}'_n + \mathcal{Q}''_n$  with

$$\mathcal{Q}'_n(k) := \sum_{\{j \in \mathbb{N}: |j-k| \geq cn^{1/2}\}} |Q_n^{'+}(j, k)|, \quad (4.6)$$

$$\mathcal{Q}''_n(k) := \sum_{\{j \in \mathbb{N}: |j-k| < cn^{1/2}\}} |Q_n^{'+}(j, k)|. \quad (4.7)$$

Using (3.1) and the Cauchy-Schwarz inequality, we can estimate

$$\mathcal{Q}'_n(k) \leq \sum_{\{j \in \mathbb{N}: |j-k| \geq cn^{1/2}\}} \frac{4|(V_n^0 Q_n^+)(j, k)|}{\langle j-k \rangle} \leq 4\mathcal{M}_n(k)^{1/2} \mathcal{M}'_n(k)^{1/2} \quad (4.8)$$

with

$$\begin{aligned} \mathcal{M}_n(k) &:= \sum_{\{j \in \mathbb{N}: |j-k| \geq cn^{1/2}\}} \langle j-k \rangle^{-2}, \\ \mathcal{M}'_n(k) &:= \sum_{j \in \mathbb{N}} |(V_n^0 Q_n^+)(j, k)|^2. \end{aligned}$$

However,

$$\mathcal{M}_n(k) \leq 2 \sum_{i \geq cn^{1/2}} \frac{1}{i^2} \leq 2 \int_{cn^{1/2}-1}^{\infty} \frac{ds}{s^2} = \frac{2}{cn^{1/2}-1} \leq C_1 n^{-1/2} \quad (4.9)$$

and using (3.9), we find

$$\mathcal{M}'_n(k) = \|V_n^0 Q_n^+ e_k\|^2 \leq \|V_n^0\|^2 \|Q_n^+\|^2 \leq C_2 n^{-1/2}. \quad (4.10)$$

Combining (4.8) with (4.9)-(4.10), we get  $\mathcal{Q}'_n(k) \leq Cn^{-1/2}$ .

In order to estimate (4.7), we assume  $|j-k| < cn^{1/2}$ . Since  $Q_n^+ = \widehat{\Pi}_n Q_n^+$ , one has

$$(V_n^0 Q_n^+)(j, k) = \sum_{n \leq m \leq n+1} V_n^0(j, m) Q_n^+(m, k). \quad (4.11)$$

and using  $|j-k| < cn^{1/2}$ , we obtain

$$\begin{aligned} Q_n^+(m, k) \neq 0 &\Rightarrow |k-m| < cn^{1/2} \Rightarrow |j-m| \leq |j-k| + |k-m| < 2cn^{1/2} \\ &\Rightarrow |V_n^0(j, m)| \leq \widehat{C} n^{-1/4} \Rightarrow |V_n^0(j, m) Q_n^+(m, k)| \leq 4\widehat{C}^2 n^{-1/2}. \end{aligned}$$

Therefore, the first inequality (4.3) follows from

$$\mathcal{Q}''_n(k) \leq 32\widehat{C}^2 n^{-1/2} \sum_{\{j \in \mathbb{N}: |j-k| < cn^{1/2}\}} \frac{1}{\langle j-k \rangle} = O(n^{-1/2} \ln n), \quad (4.12)$$

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

We can also decompose  $\mathcal{Q}_n^* = \mathcal{Q}_n'^* + \mathcal{Q}_n''^*$  with

$$\mathcal{Q}_n'^*(k) := \sum_{\{j \in \mathbb{N}: |j-k| \geq cn^{1/2}\}} |Q_n'^+(k, j)|, \quad (4.13)$$

$$\mathcal{Q}_n''^*(k) := \sum_{\{j \in \mathbb{N}: |j-k| < cn^{1/2}\}} |Q_n'^+(k, j)|. \quad (4.14)$$

Then  $|\mathcal{Q}_n'^*(k)| \leq 4\mathcal{M}_n(k)^{1/2}\mathcal{M}_n'^*(k)^{1/2}$  with  $M_n(k)$  as before and

$$\mathcal{M}_n'^*(k) = \sum_{j \in \mathbb{N}} |(V_n^0 Q_n^+)(k, j)|^2 = \|(V_n^0 Q_n^+)^* e_k\|^2 \leq Cn^{-1/2}$$

similarly as before. If  $|j - k| < cn^{1/2}$ , then

$$\begin{aligned} Q_n^+(m, j) \neq 0 &\Rightarrow |j - m| < cn^{1/2} \Rightarrow |k - m| \leq |k - j| + |j - m| < 2cn^{1/2} \\ &\Rightarrow |V_n^0(k, m)| \leq \hat{C}n^{-1/4} \Rightarrow |V_n^0(k, m)Q_n^+(m, j)| \leq 4\hat{C}^2 n^{-1/2} \end{aligned}$$

and  $\mathcal{Q}_n''^*(k) = O(n^{-1/2} \ln n)$  follows similarly as before.  $\square$

**Lemma 4.3.** *Let  $(Q_n^-(j, k))_{(j,k) \in \mathbb{N}^2}$  be as in Notation 4.1. Then there is  $Q_n'^- \in \mathcal{B}(\ell^2(\mathbb{N}))$  satisfying  $\langle e_j, Q_n'^- e_k \rangle = Q_n^-(j, k)$  for all  $j, k \in \mathbb{N}$  and*

$$\|Q_n'^-\| = O(n^{-1/2} \ln n). \quad (4.15)$$

*Proof.* If  $k \in \mathbb{N} \setminus \{n, n+1\}$ , then  $Q_n^-(j, k) = 0$ . Thus  $\|Q_n'^-\| \leq \|Q_n'^- e_n\| + \|Q_n'^- e_{n+1}\|$ . Assume now that  $k \in \{n, n+1\}$ . Then

$$\|Q_n'^- e_k\|^2 \leq \mathcal{M}_n(k) + \mathcal{M}_n'(k) \quad (4.16)$$

holds with

$$\begin{aligned} \mathcal{M}_n(k) &:= \sum_{\{j \in \mathbb{N}: |j-k| \geq cn^{1/2}\}} \frac{16|(V_n^0 Q_n^-)(j, k)|^2}{\langle j - k \rangle^2} \\ \mathcal{M}_n'(k) &:= \sum_{\{j \in \mathbb{N}: |j-k| < cn^{1/2}\}} \frac{16|(V_n^0 Q_n^-)(j, k)|^2}{\langle j - k \rangle^2}. \end{aligned}$$

We first observe that

$$\mathcal{M}_n(k) \leq \frac{16}{c^2 n} \sum_{j \in \mathbb{N}} |(V_n^0 Q_n^-)(j, k)|^2 = \frac{16}{c^2 n} \|V_n^0 Q_n^- e_k\|^2 = O(n^{-1}). \quad (4.17)$$

Our next claim is the estimate

$$\sup_{\{j \in \mathbb{N}: |j-k| < cn^{1/2}\}} |(V_n^0 Q_n^-)(j, k)| = O(n^{-1/2} \ln n). \quad (4.18)$$

Since  $Q_n^-(m, k) = 0$  if  $|m - k| \geq cn^{1/2}$ , one has

$$(V_n^0 Q_n^-)(j, k) = \sum_{\{m \in \mathbb{N}: |m-k| < cn^{1/2}\}} V_n^0(j, m) Q_n^-(m, k).$$

However,  $|j - k| < cn^{1/2}$  and  $|m - k| < cn^{1/2}$  imply  $|j - m| \leq |j - k| + |k - m| < 2cn^{1/2}$ , hence  $|V_n^0(j, m)| \leq \hat{C}n^{-1/4}$  and

$$\sup_{\{j \in \mathbb{N}: |j-k| < cn^{1/2}\}} |(V_n^0 Q_n^-)(j, k)| \leq 4\hat{C}^2 n^{-1/2} \sum_{\{m \in \mathbb{N}: |m-k| < cn^{1/2}\}} \frac{1}{\langle m - k \rangle} = O(n^{-1/2} \ln n),$$

i.e. (4.18) holds. However, due to (4.18), we can estimate

$$\mathcal{M}'_n(k) \leq 16 \sup_{\{j \in \mathbb{N}: |j-k| < cn^{1/2}\}} |(V_n^0 Q_n^-)(j, k)|^2 \sum_{j \in \mathbb{N}} \langle j - k \rangle^{-2} = O(n^{-1} (\ln n)^2) \quad (4.19)$$

and combining (4.16) with (4.17) and (4.19), we get  $\|Q_n^- e_k\| = O(n^{-1/2} \ln n)$  for  $k \in \{n, n+1\}$ , completing the proof.  $\square$

**Lemma 4.4.** Assume that  $V_n^0$  is given by (3.15),  $Q_n^\pm$  are as in Notation 3.1(c) and

$$Q_n^0 := Q_n^+ + Q_n^-. \quad (4.20)$$

Assume that  $Q'_n^\pm$  are as in Lemma 4.3 and 4.2,

$$Q'_n := Q_n'^- + Q_n'^+ + (Q_n'^- + Q_n'^+)^* \quad (4.21)$$

and

$$R'_n := \tilde{\Pi}_n [V_n^0, iQ_n^0] \hat{\Pi}_n + \hat{\Pi}_n [V_n^0, iQ_n^0] \tilde{\Pi}_n. \quad (4.22)$$

Then

(a)  $\ell^{2,1}(\mathbb{N})$  is an invariant subspace of  $Q'_n$  and

$$[D, iQ'_n] = -R'_n \quad (4.23)$$

(b)  $\ell^{2,1}(\mathbb{N})$  is an invariant subspace of  $e^{itQ'_n}$  and  $t \rightarrow e^{itQ'_n} x$  is of class  $C^\infty(\mathbb{R}; \ell^{2,1}(\mathbb{N}))$  if  $x \in \ell^{2,1}(\mathbb{N})$ .

*Proof.* Denote  $R_n'^\pm := \tilde{\Pi}_n iV_n^0 Q_n^\pm \hat{\Pi}_n + \hat{\Pi}_n iV_n^0 Q_n^\pm \tilde{\Pi}_n$ . Then we find

$$i((DQ_n'^\pm - Q_n'^\pm D)e_k)(j) = i(d_j - d_k)Q_n'^\pm(j, k) = -(R_n'^\pm e_k)(j). \quad (4.24)$$

and reasoning as in the proof of Lemma 4.1 in Chapter 3, we find that  $\ell^{2,1}(\mathbb{N})$  is an invariant subspace of  $Q_n'^\pm$  and

$$[D, iQ_n'^\pm] = -R_n'^\pm. \quad (4.25)$$

Similarly, using

$$i((D(Q_n'^\pm)^* - (Q_n'^\pm)^* D)e_k) = [D, iQ_n'^\pm]^* e_k = -(R_n'^\pm)^* e_k, \quad (4.26)$$



we find that  $\ell^{2,1}(\mathbb{N})$  is an invariant subspace of  $(Q_n^{\pm})^*$  and

$$-[D, i(Q_n^{\pm})^*] = (R_n^{\pm})^*. \quad (4.27)$$

Combining (4.25)-(4.27), we get

$$-[D, iQ_n'] = R_n'^- + R_n'^+ + (R_n'^- + R_n'^+)^* = R_n'. \quad (4.28)$$

We obtain the assertion (b) reasoning as in the proof of Lemma 4.1 in Chapter 3.  $\square$

## 5 Proof of Theorem 1.1

### 5.1 First similarity transformation

**Lemma 5.1.** *Let  $Q_n$  be as in Notation (3.1)(d) and*

$$H_n' := e^{-iQ_n} H e^{iQ_n}. \quad (5.1)$$

*Then one has the large  $n$  estimate*

$$H_n' := D + \widehat{V}_n \oplus \widetilde{V}_n' + R_n' + O(n^{-1/2} \ln n), \quad (5.2)$$

*where  $R_n'$  is given by (4.22),  $\widehat{V}_n$  is given by (2.16) and*

$$\widetilde{V}_n' = \widetilde{V}_n + O(n^{-1/4}) \quad (5.3)$$

*holds with  $\widetilde{V}_n$  given by (2.17).*

*Proof.* We first observe that the estimate (5.1) from Section 5, Chapter 3 gives

$$H_n' = D + V - R_n + [V - \frac{1}{2}R_n, iQ_n] + O(n^{-1/2}) \quad (5.4)$$

with  $R_n = -[D, iQ_n] = \widetilde{\Pi}_n V \widehat{\Pi}_n + \widehat{\Pi}_n V \widetilde{\Pi}_n$  (see (3.11)). We observe that

$$V - R_n = \widehat{\Pi}_n V \widehat{\Pi}_n + \widetilde{\Pi}_n V \widetilde{\Pi}_n \quad (5.5)$$

and  $V - \frac{1}{2}R_n = V_n^0$  is given by (3.15). Moreover, (3.10) allows us to replace  $Q_n$  by  $Q_n^0$  in the right hand side of (5.5), i.e.

$$H_n' = D + \widehat{\Pi}_n V \widehat{\Pi}_n + \widetilde{\Pi}_n V \widetilde{\Pi}_n + [V_n^0, iQ_n^0] + O(n^{-1/2}). \quad (5.6)$$

Due to (3.16) we obtain

$$[V_n^0, iQ_n^0] = \widetilde{\Pi}_n [V_n^0, iQ_n^0] \widetilde{\Pi}_n + R_n' + O(n^{-1/2} \ln n), \quad (5.7)$$

where  $R_n'$  is given by (4.22). Introducing

$$\widetilde{V}_n' := \widetilde{V}_n + \widetilde{\Pi}_n [V_n^0, iQ_n^0] \widetilde{\Pi}_n, \quad (5.8)$$

we have  $\|\widetilde{V}_n' - \widetilde{V}_n\| \leq C \|Q_n^0\| = O(n^{-1/4})$  and

$$\widehat{\Pi}_n V \widehat{\Pi}_n + \widetilde{\Pi}_n V \widetilde{\Pi}_n + \widetilde{\Pi}_n [V_n^0, iQ_n^0] \widetilde{\Pi}_n = \widehat{V}_n \oplus \widetilde{V}_n'. \quad (5.9)$$

To complete the proof of (5.2), it remains to combine (5.6), (5.7) and (5.9).  $\square$

## 5.2 Proof of Proposition 2.2

Using the Taylor formula given in (2.12)-(2.13) of Chapter 3 with  $N = 1$  we get

$$e^{-iQ'_n} D e^{iQ'_n} = D + [D, iQ'_n] + O(\|\text{ad}_{iQ'_n}^2(D)\|). \quad (5.10)$$

Since  $[D, iQ'_n] = -R'_n$  and  $\text{ad}_{iQ'_n}^2(D) = -[R'_n, iQ'_n] = O(\|Q'_n\|)$ , (5.10) implies

$$e^{-iQ'_n} D e^{iQ'_n} = D - R'_n + O(n^{-1/2} \ln n) \quad (5.11)$$

due to  $\|Q'_n\| = O(n^{-1/2} \ln n)$  (see (4.2) and (4.15)). We also have

$$e^{-iQ'_n} (\widehat{V}_n \oplus \widetilde{V}'_n + R'_n) e^{iQ'_n} = \widehat{V}_n \oplus \widetilde{V}'_n + R'_n + O(n^{-1/2} \ln n). \quad (5.12)$$

Let us denote  $H''_n := e^{-iQ'_n} H'_n e^{iQ'_n}$ . Then (5.2) ensures

$$H''_n = e^{-iQ'_n} (D + \widehat{V}_n \oplus \widetilde{V}'_n + R'_n) e^{iQ'_n} + O(n^{-1/2} \ln n) \quad (5.13)$$

To complete the proof, it remains to observe that (5.11) and (5.12) allow one to write the right hand side of (5.13) in the form  $D + \widehat{V}_n \oplus \widetilde{V}'_n + O(n^{-1/2} \ln n)$ .

## 5.3 Proof of Proposition 2.1

Similarly as in Section 5.1, Chapter 2 we denote  $\mathbb{T} := \mathbb{R}/2\pi$  and introduce

$$\gamma_{k,j} := \langle f_k^-, f_j^+ \rangle_{L^2(\mathbb{T})}. \quad (5.14)$$

where  $f_n^\pm \in L^2(\mathbb{T})$  are given by (5.3), page 47, Chapter 2, i.e.

$$f_n^\pm(\theta) := e^{\mp 2ign^{1/2} \sin \theta + ig^2 \sin \theta \cos \theta + in\theta}. \quad (5.15)$$

Combining (5.5) with (5.2) from Chapter 2, we obtain

$$V(2i + l_0, 1 + 2i + l_0) = \frac{\Delta}{2} \gamma_{i+l_0, i} + O(i^{-1/2}). \quad (5.16)$$

However, the direct calculation gives

$$\gamma_{i+l_0, i} = \int_{-\pi}^{\pi} e^{-i\mu_i \sin \theta} e^{-i\theta l_0} \frac{d\theta}{2\pi} \quad (5.17)$$

with

$$\mu_i := 2g((i + l_0)^{1/2} + i^{1/2}). \quad (5.18)$$

Since the phase function  $\theta \rightarrow \sin \theta$  has non-degenerated critical points  $\pi/2$  and  $-\pi/2$ , one has the large  $i$  asymptotic formula

$$\gamma_{i+l_0, i} = \frac{1}{\sqrt{2\pi\mu_i}} \sum_{\kappa=\pm 1} e^{i\kappa(\mu_i - \pi/4)} e^{-i\kappa\pi l_0/2} + O(\mu_i^{-1}). \quad (5.19)$$

However, using  $\mu_i = 4gi^{1/2} + O(i^{-1/2})$  we get

$$\gamma_{i+l_0, i} = \frac{1}{\sqrt{2\pi g i^{1/2}}} \cos\left(4gi^{1/2} - \frac{\pi}{4} - \frac{\pi}{2}l_0\right) + O(i^{-1/2}). \quad (5.20)$$

The proof is complete due to (5.16) and (5.20).

## **Sous-partie B:**

**L'étude asymptotique des grandes valeurs propres pour le modèle quantique asymétrique de Rabi à deux photons**

# Comportement des grandes valeurs propres pour le Modèle Quantique Asymétrique de Rabi à deux Photons

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# Behaviour of Large Eigenvalues for the Two-photon Asymmetric Quantum Rabi Model

Anne Boutet de Monvel<sup>1</sup>, Mirna Charif<sup>2</sup> and Lech Zielinski<sup>3</sup>

**Abstract.** We investigate the asymptotic behavior of large eigenvalues for the two-photon quantum Rabi model with a finite bias. We prove that the spectrum of this Hamiltonian model consists of two eigenvalues sequences  $(E_n^+)_{n=0}^\infty$ ,  $(E_n^-)_{n=0}^\infty$  and we describe their asymptotic behaviour with an error estimate of the form  $O(n^{-1/2})$  when  $n$  tends to infinity. Our principal tool is the method of near-similarity of operators introduced by G. V. Rozenbljum and developed in works of J. Janas, S. Naboko and E. A. Yanovich (Tur).

**Keywords :** unbounded self-adjoint operators, asymptotics of eigenvalues, discrete spectrum, Quantum Rabi Model.

**Mathematics Subject Classification :** 47A75, 47B02, 47B25, 47B36, 81Q10, 81Q15.

## 1 General presentation of the paper

### 1.1 Introduction

The first model of interactions between a quantum TLS (Two Level System) and a light field was described in [105], [106]. The author of these papers, I. I. Rabi, was awarded the Nobel Prize in Physics in 1944 and (see [15]) the name QRM ( Quantum Rabi Model) is usually used for the model of interaction between a TLS and a single mode radiation. The QRM is considered as a particularly important model in quantum optics : see [133] for numerous references to theoretical and experimental results in the cavity QED. We also mention a famous paper of Jaynes and Cummings [79] describing a simplification of the QRM known under the name of RWA (Rotating Wave Approximation) and the fact that the QRM is sometimes referred to as the Jaynes-Cummings Model without RWA.

The QRM Hamiltonian (see Definition 1.2(d)) is a self-adjoint operator  $\mathbf{H}_{\text{Rabi}}$  with discrete spectrum depending on three parameters : the level separation energy  $\Delta$ , the frequency of the one-mode electromagnetic field  $\omega$  and the coupling constant  $g$ . Its eigenvalues are only known explicitly in the case of the QRM Hamiltonian  $\mathbf{H}_{0,\text{Rabi}}$  corresponding to  $\Delta = 0$ . The question of the behavior of large eigenvalues of  $\mathbf{H}_{\text{Rabi}}$  was posed by A. Boutet de Monvel, S. Naboko and L. O. Silva in [27] (see also [28]). Due to the difficulty of the problem, the authors give a solution for a simpler class of operators ("modified Jaynes-Cummings models"). The first result concerning the asymptotic behaviour of the QRM eigenvalues was obtained by E. A. Yanovich. In the paper [135] he proved the estimate

$$\lambda_n(\mathbf{H}_{\text{Rabi}}) - \lambda_n(\mathbf{H}_{0,\text{Rabi}}) = O(n^{-\alpha}) \text{ as } n \rightarrow \infty \quad (1.1)$$

with the exponent  $\alpha = \frac{1}{16}$ . Here  $(\lambda_n(\mathbf{H}_{\text{Rabi}}))_{n=0}^\infty$  and  $(\lambda_n(\mathbf{H}_{0,\text{Rabi}}))_{n=0}^\infty$  denote the nondecreasing sequences of eigenvalues of  $\mathbf{H}_{\text{Rabi}}$  and  $\mathbf{H}_{0,\text{Rabi}}$ , counting multiplicities (see also [124]). About this result, we notice the following :

- Since the eigenvalues of  $\mathbf{H}_{0,\text{Rabi}}$  are explicitly known, the estimate (1.1) provides the asymptotic estimate of eigenvalues of  $\mathbf{H}_{\text{Rabi}}$  with error term  $O(n^{-\alpha})$ .
- The proof of Yanovich [135] is based on the fundamental Lemma 2.1 from the paper J. Janas, S. Naboko [75] (see Theorem 1.4 below).
- Estimate (1.1) shows that the influence on the eigenvalues of the perturbation  $\mathbf{H}_{\text{Rabi}} - \mathbf{H}_{0,\text{Rabi}}$  vanishes in the large energy limit although this perturbation does not vanish. On the contrary, in the case of models considered in [27], [28], [29],  $\lambda_n(\mathbf{H}_{\text{Rabi}}) - \lambda_n(\mathbf{H}_{0,\text{Rabi}})$  does not converge to 0 as  $n \rightarrow \infty$ .
- In fact the estimate (1.1) is valid with the exponent  $\alpha = \frac{1}{4}$  and this value is optimal (see [34], [32]).

It is natural to ask if similar results hold for other types of Rabi models. The paper [33] gives a proof of the estimate (1.1) with  $\alpha = \frac{1}{3}$  for the Two-photon QRM Hamiltonian described in Definition 1.2(e). This model describes interactions of a TLS with squeezed light (see [54]). We refer to [42] for an overview of works and experimental realizations of the Two-photon QRM (see also [47]).

In the following we consider the “asymmetric quantum Rabi model” (AQRM), which is also referred to as the “QRM with a finite static bias” (see Definitions 1.2(f) and 1.2(g) for the one-photon and two-photon AQRMs). This model attracts attention in relation with recent experiments of the ultra-strong coupling by means of superconducting circuits (see [133], [82]). In fact, the experiments with a laser beam in the cavity concern the QRM with coupling strength  $g \sim 10^{-6}$ , while the experiments with qubit circuits can achieve the values  $g \sim 10^{-1}$  and the static bias appears due to the tunnelling between two current states (see [61]).

This paper is devoted to the “two-photon AQRM” (see Definition 1.2(g)). We prove that estimate (1.1) holds for this model with  $\alpha = \frac{1}{2}$ . As in the paper [33] on the two-photon QRM, our proof is inspired by the similarity transformation used in the paper of J. Janas, S. Naboko [75]. Here are the main differences compared to [33] :

- When  $\epsilon$  is a multiple of  $\sqrt{1 - 4g^2}$  we must overcome an additional difficulty due to the fact that  $\mathbf{H}_{0,\text{Rabi}}$  has double eigenvalues which cannot be decoupled when  $\epsilon \neq 0$ .
- The estimate we get has an error term with exponent  $\alpha = \frac{1}{2}$ . Note that in the case  $\epsilon = 0$  the value  $\alpha = \frac{1}{2}$  has been conjectured to be optimal in [33].

Our approach is based on an approximation of  $\mathbf{H}_{0,\text{Rabi}}$  by an operator unitarily similar to a first order differential operator on the circle (see Section 3) so that the corresponding eigenvalues and eigenvectors can be expressed explicitly in a simple way. The one-photon QRM was considered in [31] and [34] using a similar idea, but the one-photon AQRM leads to pseudo-differential operators of order 1/2 which are more difficult to analyze.

## 1.2 Quantum Rabi Hamiltonians

**Notation 1.1.** (a) If  $\mathcal{J} \subset \mathbb{Z}$  then  $\ell^2(\mathcal{J})$  denotes the complex Hilbert space of square-summable sequences  $x : \mathcal{J} \rightarrow \mathbb{C}$  equipped with the scalar product

$$\langle x, y \rangle_{\ell^2(\mathcal{J})} = \sum_{k \in \mathcal{J}} \overline{x(k)} y(k) \quad (1.2)$$

and the norm  $\|x\|_{\ell^2(\mathcal{J})} := \langle x, x \rangle_{\ell^2(\mathcal{J})}^{1/2}$ .

If  $\mathcal{J} = \mathbb{N} := \{k \in \mathbb{Z} : k \geq 0\}$  then we write  $\ell^2$  instead of  $\ell^2(\mathbb{N})$ .

(b) The photon annihilation and creation operators  $\hat{a}$  and  $\hat{a}^\dagger$  are defined as closed linear operators acting in  $\ell^2$  according to the formulas

$$\hat{a} e_m = \sqrt{m} e_{m-1}, \quad \hat{a}^\dagger e_m = \sqrt{m+1} e_{m+1}, \quad m = 0, 1, 2, \dots, \quad (1.3)$$

where  $\{e_m\}_{m \in \mathbb{N}}$  is the canonical basis in  $\ell^2$  and  $\sqrt{m} e_{m-1} := 0$  if  $m = 0$ .

(c) We consider linear operators in the Euclidean space  $\mathbb{C}^2$  defined by

$$\sigma_x := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_z := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad I_2 := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (1.4)$$

**Definition 1.2.** (a) The Hamiltonian of the single-mode radiation of frequency  $\omega > 0$  is the self-adjoint operator in  $\ell^2$  given by

$$H_{\text{rad}}^\omega = \omega \hat{a}^\dagger \hat{a}. \quad (1.5)$$

It is easy to check that  $H_{\text{rad}}^\omega e_m = \omega m e_m$  holds for all  $m \in \mathbb{N}$ .

(b) The TLS Hamiltonian is defined in  $\mathbb{C}^2$  by means of the  $2 \times 2$  matrix  $\mathbb{C}^2$  of the form

$$H_{\text{TLS}} = \frac{1}{2} \begin{pmatrix} \Delta & \epsilon \\ \epsilon & -\Delta \end{pmatrix} = \frac{1}{2} (\Delta \sigma_z + \epsilon \sigma_x) \quad (1.6)$$

where  $\Delta$  and  $\epsilon$  are real parameters.

(c) the interaction term of the one photon Rabi model has the form

$$\mathbf{H}_{\text{int}} := g \sigma_x \otimes (\hat{a} + \hat{a}^\dagger), \quad (1.7)$$

where  $g \in \mathbb{R}$  is a coupling constant.

(d) The QRM Hamiltonian is a self-adjoint operator in  $\mathbb{C}^2 \otimes \ell^2$  of the form

$$\mathbf{H}_{\text{Rabi}} = H_{\text{TLS}} \otimes I_{\ell^2} + I_2 \otimes H_{\text{rad}}^\omega + \mathbf{H}_{\text{int}}, \quad (1.8)$$

with  $H_{\text{rad}}^\omega$  given by (1.5),  $\mathbf{H}_{\text{int}}$  given by (1.7),  $H_{\text{TLS}}$  given by (1.6) with  $\epsilon = 0$ .

(e) The Two-photon QRM Hamiltonian is defined by the formula (1.8) with  $H_{\text{rad}}^\omega$  given by (1.5),  $H_{\text{TLS}}$  given by (1.6) with  $\epsilon = 0$  and

$$\mathbf{H}_{\text{int}} := g \sigma_x \otimes (\hat{a}^2 + (\hat{a}^\dagger)^2), \quad (1.9)$$

where  $g \in \mathbb{R}$  is a coupling constant.

(f) The (One-photon) AQRM Hamiltonian is defined by the formula (1.8) with  $H_{\text{rad}}^\omega$  given by (1.5),  $\mathbf{H}_{\text{int}}$  given by (1.7),  $H_{\text{TLS}}$  given by (1.6) with  $\epsilon \neq 0$ .

(g) The Two-photon AQRM Hamiltonian is defined by the formula (1.8) with  $H_{\text{rad}}^\omega$  given by (1.5),  $\mathbf{H}_{\text{int}}$  given by (1.9),  $H_{\text{TLS}}$  given by (1.6) with  $\epsilon \neq 0$ .

### 1.3 Statement of the result

The main result of this paper is given in Theorem 1.3. It gives the asymptotic behaviour of eigenvalues of the Two-photon AQRM Hamiltonian described in the Definition 1.2(g) in the case  $\omega = 1$ , i.e. we consider the eigenvalues of the operator defined in  $\mathbb{C}^2 \otimes \ell^2$  by the formula

$$\frac{1}{2}(\Delta\sigma_z + \epsilon\sigma_x) \otimes I_{\ell^2} + I_2 \otimes \hat{a}^\dagger \hat{a} + g\sigma_x \otimes (\hat{a}^2 + (\hat{a}^\dagger)^2), \quad (1.10)$$

where  $\Delta, \epsilon, g$  are real parameters.

**Theorem 1.3** (two-photon asymmetric Rabi model). *Assume that  $0 < g < \frac{1}{2}$ . Then the operator (1.10) is self-adjoint in  $\mathbb{C}^2 \otimes \ell^2$  and its spectrum is discrete. Moreover there is an orthonormal basis  $\{\mathbf{w}_{\nu,m}\}_{(\nu,m) \in \{-1,1\} \times \mathbb{N}}$  of eigenvectors such that the corresponding eigenvalue sequences  $(E_{1,m})_{m \in \mathbb{N}}$  and  $(E_{-1,m})_{m \in \mathbb{N}}$  satisfy the large  $m$  asymptotic estimate*

$$E_{\nu,m} = \beta m + \beta_\nu + O(m^{-1/2}), \quad \nu = \pm 1 \quad (1.11)$$

with

$$\beta := \sqrt{1 - 4g^2}, \quad (1.12)$$

$$\beta_\nu = \frac{1}{2}(\beta - 1) + \nu \frac{\epsilon}{2}, \quad \nu = \pm 1. \quad (1.13)$$

The rest of the paper is devoted to proving this theorem.

**Remark 1.** We assume  $|g| < 1/2$  to insure that the spectrum of  $H_{\pm 1}$  is discrete. Indeed, if  $|g| > 1/2$  then this spectrum is the whole real line  $\mathbb{R}$ . If  $|g| = 1/2$  then the essential spectrum of  $H_{\pm 1}$  is a half-line. These statements are proved in [113].

**Remark 2.** It is well known (see e.g. [61]) that in the case  $\Delta = 0$ , the assertion of Theorem 1.3 holds with  $E_{m,\nu} = \beta m + \beta_\nu$  and  $\beta, \beta_\nu$  given by (1.12)-(1.13).

**Remark 3.** The general case of the Two-Photon AQRM with  $\omega > 0$  can be easily reduced to the case  $\omega = 1$ , using the multiplication of the operator by a constant. In this case, Theorem 1.3 remains true under assumption  $0 < g < \omega/2$  and the asymptotic formula (1.11) remains valid with  $\beta = \sqrt{\omega^2 - 4g^2}$  and  $\beta_\nu = (\beta - \omega)/2 + \nu\epsilon/2$ .



#### 1.4 Method of proof

Denote by  $U_{\pi/4} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$  the rotation of  $\pi/4$  in the plane  $\mathbb{C}^2$ . Then

$$U_{\pi/4} \sigma_z U_{\pi/4}^{-1} = \sigma_x \quad \text{and} \quad U_{\pi/4} \sigma_x U_{\pi/4}^{-1} = -\sigma_z,$$

and it is clear that the operator (1.10) is similar to the operator

$$\mathbf{H} := \frac{1}{2}(\Delta \sigma_x - \epsilon \sigma_z) \otimes I_{\ell^2} + I_2 \otimes \hat{a}^\dagger \hat{a} - g \sigma_z \otimes (\hat{a}^2 + (\hat{a}^\dagger)^2). \quad (1.14)$$

Thus we obtain the assertion of Theorem 1.3 if we prove that there exists an orthonormal basis  $\{\mathbf{u}_{\nu,m}\}_{\nu=\pm 1, m \in \mathbb{N}}$  in  $\mathbb{C}^2 \otimes \ell^2$  such that

$$\mathbf{H} \mathbf{u}_{\nu,m} = E_{\nu,m} \mathbf{u}_{\nu,m} \quad \text{for } m \in \mathbb{N}, \nu = \pm 1, \quad (1.15)$$

where the sequence  $(E_{\nu,m})_{\nu=\pm 1, m \in \mathbb{N}}$  satisfies the large  $m$  asymptotic estimate (1.11). For this purpose we consider the operator (1.14) of parameter  $\Delta = 0$ , that is,

$$\mathbf{H}_0 := -\frac{1}{2} \epsilon \sigma_z \otimes I_{\ell^2} + I_2 \otimes \hat{a}^\dagger \hat{a} - g \sigma_z \otimes (\hat{a}^2 + (\hat{a}^\dagger)^2). \quad (1.16)$$

and we first prove the existence of an orthonormal basis  $\{\mathbf{u}_{\nu,m}^0\}_{(\nu,m) \in \{-1,1\} \times \mathbb{N}}$  in  $\mathbb{C}^2 \otimes \ell^2$  such that

$$\mathbf{H}_0 \mathbf{u}_{\nu,m}^0 = (\beta m + \beta_\nu) \mathbf{u}_{\nu,m}^0 \quad \text{for } m \in \mathbb{N}, \nu = \pm 1, \quad (1.17)$$

We then deduce from (1.17) the assertion of Theorem 1.3 by proving the asymptotic estimate

$$\lambda_n(\mathbf{H}) - \lambda_n(\mathbf{H}_0) = O(n^{-1/2}), \quad (1.18)$$

where  $(\lambda_n(\mathbf{H}))_{n=0}^\infty$  (respectively  $(\lambda_n(\mathbf{H}_0))_{n=0}^\infty$ ) is the non-decreasing sequence of eigenvalues of  $\mathbf{H}$  (respectively  $\mathbf{H}_0$ ), counting the multiplicities.

#### 1.5 Organization of the paper

In Section 2 we first observe that the operator  $\mathbf{H}_0$  can be written as the direct sum  $H_{-1} \oplus H_1$  of two self-adjoint operators in  $\ell^2$  whose eigenvalues are explicitly known. Then we move from  $\ell^2$  to  $\ell^2(\mathbb{Z})$ , replacing  $\mathbf{H}_0$  by  $\mathbf{J}_0 = J_{-1} \oplus J_1$  where  $J_{-1}$  and  $J_1$  are two appropriate self-adjoint operators in  $\ell^2(\mathbb{Z})$ .

In Section 3, we move from  $\ell^2(\mathbb{Z})$  to  $L^2(\mathbb{T})$ . By Fourier transform we change the operators  $J_{\pm 1}$  into first order linear differential elliptic operators  $L_{\pm 1}$  in  $L^2(\mathbb{T})$  and we express explicitly all eigenvalues and eigenvectors of  $J_{\pm 1}$ . The operators  $J_{\pm 1}$  are not semi-bounded, but one can choose two sequences of eigenvalues  $\{\lambda_j(J_{\pm 1})\}_{j \in \mathbb{Z}}$  such that  $\lambda_j(J_{\pm 1}) = \lambda_j(H_{\pm 1})$  when  $j \in \mathbb{N}$ . Our hope is that large eigenvalues of

$$\mathbf{H} = \mathbf{H}_0 + \frac{1}{2} \Delta \sigma_x \otimes I_{\ell^2} \quad (1.19)$$

are well approximated by large eigenvalues of

$$\mathbf{J} = \mathbf{J}_0 + \frac{1}{2} \Delta \sigma_x \otimes I_{\ell^2(\mathbb{Z})}. \quad (1.20)$$

In Section 4 we prove Proposition 4.1, which is the key result of the paper. In order to compare large eigenvalues of  $\mathbf{J}$  and  $\mathbf{J}_0$ , we use a similarity method and the crucial result of Lemma 3.4, which ensures the fact that eigenvectors of  $J_{-1}$  and  $J_1$  are "asymptotically orthogonal".

In Section 5 we show that large eigenvalues of  $\mathbf{H}$  and  $\mathbf{J}$  are close and we deduce Theorem 1.3 from Proposition 4.1.

## 1.6 Main tools

Throughout the paper we are dealing with the discrete spectrum of various operators and we use the following vocabulary. Let  $L$  be an operator acting in the complex Hilbert space  $\mathcal{H}$ . Then we denote by  $\sigma(L)$  its spectrum and we say that  $L$  has discrete spectrum if and only if every point  $\lambda \in \sigma(L)$  is an isolated eigenvalue of finite multiplicity.

Assume that  $L$  has discrete spectrum and  $\mathcal{J}$  is a countable set. We say that  $\{\lambda_j(L)\}_{j \in \mathcal{J}}$  is a *complete eigenvalue sequence* of  $L$  if and only if any  $\lambda \in \sigma(L)$  is some  $\lambda_j(L)$  and if  $m_\lambda := \text{card}\{j \in \mathcal{J} : \lambda_j(L) = \lambda\}$  is the algebraic multiplicity of  $\lambda$ , i.e., the rank of the corresponding Riesz projection (see Section III.5 in [81]). If  $\sigma(L) \subset \mathbb{R}$  and  $\mathcal{J} = \mathbb{N}$  or  $\mathbb{Z}$ , then a complete eigenvalue sequence of  $L$  is called *ordered* if and only if  $\lambda_j(L) \leq \lambda_{j+1}(L)$  holds for every  $j \in \mathcal{J}$ .

If  $L$  has a discrete real spectrum and  $\mathcal{J} = \mathbb{N}$ , then  $\lambda_n(L) \rightarrow \infty$  as  $n \rightarrow \infty$  and there exists a unique complete ordered eigenvalue sequence  $(\lambda_n(L))_{n \in \mathbb{N}}$ . If  $L$  has a discrete real spectrum and  $(\lambda_j(L))_{j \in \mathbb{Z}}$  is a complete ordered sequence of  $L$ , then  $\lambda_j(L) \rightarrow \pm\infty$  as  $j \rightarrow \pm\infty$  and any complete ordered sequence of  $L$  has the form  $(\lambda_{j+\kappa}(L))_{j \in \mathbb{Z}}$  with a certain  $\kappa \in \mathbb{Z}$ . If  $L$  is self-adjoint and  $(\lambda_j(L))_{j \in \mathcal{J}}$  is its complete eigenvalue sequence, then there is an orthonormal basis  $(f_j)_{j \in \mathcal{J}}$  such that  $Lf_j = \lambda_j(L)f_j$  holds for all  $j \in \mathcal{J}$ .

Further on  $\mathcal{B}(\mathcal{H})$  denotes the algebra of linear bounded operators on the Hilbert space  $\mathcal{H}$  and  $\|\cdot\|$  denotes the corresponding operator norm.

At the end of this section we cite basic results which are principal tools allowing one to compare large eigenvalues of operators.

**Theorem 1.4. (J. Janas, S. Naboko)** *Assume that  $L_0$  is a self-adjoint operator in the Hilbert space  $\mathcal{H}$  and there exists an orthonormal basis  $\{e_n\}_{n \in \mathbb{N}}$  such that  $L_0 e_n = d_n e_n$ . Assume moreover that  $|d_n| \leq |d_{n+1}|$  and there exists  $c_0 > 0$  such that  $|d_n - d_m| \geq c_0$  if  $n \neq m$ . If  $R$  is a compact operator in  $\mathcal{H}$ , then the operator  $L = L_0 + R$  has a complete eigenvalue sequence  $(\lambda_n(L))_{n \in \mathbb{N}}$  satisfying the asymptotic formula*

$$\lambda_n(L) = d_n + O(\|R^* e_n\|) \text{ as } n \rightarrow \infty.$$

*Proof.* See Lemma 2.1 in [75]. □

**Theorem 1.5. (G. V. Rozenbljum)** *Let  $A$  and  $B$  be unbounded self-adjoint operators with discrete spectrum in the separable Hilbert space  $\mathcal{H}$ . Assume that  $0 \notin \sigma(A) \cup \sigma(B)$  and there exists  $\alpha \in ]-\infty, 1[$  such that*

$$(A - B)|A|^{-\alpha} \in \mathcal{B}(\mathcal{H}) \quad \text{and} \quad (A - B)|B|^{-\alpha} \in \mathcal{B}(\mathcal{H}). \quad (1.21)$$

(a) If  $A$  and  $B$  are bounded from below and  $(\lambda_n(A))_{n \in \mathbb{N}}$ ,  $(\lambda_n(B))_{n \in \mathbb{N}}$  are complete ordered eigenvalue sequences, then

$$\lambda_n(A) - \lambda_n(B) = O(|\lambda_n(A)|^\alpha) \text{ as } n \rightarrow \infty \quad (1.22)$$

(b) If  $A$  and  $B$  are not semi bounded, then we can choose complete ordered eigenvalue sequences  $(\lambda_j(A))_{j \in \mathbb{Z}}$  and  $(\lambda_j(B))_{j \in \mathbb{Z}}$  so that

$$\lambda_j(A) - \lambda_j(B) = O(|\lambda_j(A)|^\alpha) \text{ as } |j| \rightarrow \infty \quad (1.23)$$

*Proof.* See [111]. □

**Lemma 1.6.** *Let  $A$  and  $B$  be unbounded self-adjoint operators with discrete spectrum in the separable Hilbert space  $\mathcal{H}$ . If (1.21) holds with  $\alpha \leq 0$  and  $A - B \in \mathcal{B}(\mathcal{H})$ , then the assertions of Theorem 1.5 (a) and (b) hold without the hypothesis  $0 \notin \sigma(A) \cup \sigma(B)$ .*

*Proof.* See Section 6.1. □

## 2 Preliminaries

### 2.1 Outline of Section 2

In Section 2.2 we state Lemma 2.2 describing basic properties of auxiliary operators  $H_{-1}$  and  $H_1$  acting in  $\ell^2$ . These operators are well known in the literature (cf. [42], [46], [47]) and are used in Section 2.3 to express  $\mathbf{H}$  as a matrix operator acting in  $\ell^2 \times \ell^2$  and to describe basic properties of  $\mathbf{H}$ .

In Section 2.4 we introduce auxiliary operators  $J_{-1}$  and  $J_1$  acting in  $\ell^2(\mathbb{Z})$ . These operators can be viewed as Jacobi operators investigated by Edwards [43] (see also Masson, Repka [97]) and we will describe their diagonalization in Section 3.

In Section 2.5 we use the operators  $J_{\pm 1}$  to define the operator  $\mathbf{J}$  acting in  $\ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})$ . From Lemma 2.2 at the very beginning, then throughout the text we make the following

**Assumption.** We always assume  $-\frac{1}{2} < g < \frac{1}{2}$ .

### 2.2 Operators $H_{\pm 1}$

**Notation 2.1.** (a) Further on  $\Lambda_+ := \hat{a}^\dagger \hat{a}$  is the self-adjoint operator in  $\ell^2$  defined on

$$\mathcal{D}(\Lambda_+) = \{x \in \ell^2 : \sum_{k \in \mathbb{N}} k^2 |x(k)|^2 < \infty\} \quad (2.1)$$

by the formula  $\Lambda_+ e_m = m e_m$  for  $m \in \mathbb{N}$  where  $\{e_m\}_{m \in \mathbb{N}}$  is the canonical basis of  $\ell^2$ .

(b) For  $\nu = \pm 1$  we denote by  $H_\nu$  the linear mapping  $\mathcal{D}(\Lambda_+) \rightarrow \ell^2$  given by

$$H_\nu := \Lambda_+ + \nu g(\hat{a}^2 + (\hat{a}^\dagger)^2) + \frac{1}{2} \nu \epsilon. \quad (2.2)$$

The direct computation gives the expression

$$H_\nu e_m = (m + \frac{1}{2}\nu\epsilon)e_m + \nu g b(m)e_{m+2} + \nu g b(m-2)e_{m-2} \text{ for } m \in \mathbb{N}, \quad (2.3)$$

where

$$b(m) := \sqrt{(m+1)(m+2)} \text{ for } m \in \mathbb{N} \quad (2.4)$$

and by convention  $b(m-2)e_{m-2} = 0$  when  $m \in \{0, 1\}$ .

**Lemma 2.2.** *Assume that  $\nu = \pm 1$  and  $-\frac{1}{2} < g < \frac{1}{2}$ . Then*

$$H_\nu(I_{\ell^2} + \Lambda_+)^{-1} \in \mathcal{B}(\ell^2), \quad (2.5)$$

$H_\nu$  is self-adjoint in  $\ell^2$  and there is an orthonormal basis  $(u_{\nu,n})_{n \in \mathbb{N}}$  such that

$$H_\nu u_{\nu,n} = (\beta n + \beta_\nu)u_{\nu,n} \text{ for } n \in \mathbb{N}, \quad (2.6)$$

where  $\beta, \beta_\nu$  are given by (1.12)-(1.13).

*Proof.* The result is well known (see e.g. [47], [33]).  $\square$

### 2.3 Basic properties of $\mathbf{H}_0$ and $\mathbf{H}$

The orthonormal basis of the Hilbert space  $\mathcal{H}_0 := \mathbb{C}^2 \otimes \ell^2$  has the form  $\mathfrak{B}_0 := \mathfrak{B}_{-1}^+ \cup \mathfrak{B}_1^+$  where  $\mathfrak{B}_\nu^+ := \{e^{(\nu)} \otimes e_m : m \in \mathbb{N}\}$  for  $\nu = \pm 1$  and  $e^{(-1)} := (1, 0)$ ,  $e^{(1)} := (0, 1)$  are the vectors of the canonical basis of  $\mathbb{C}^2$ . Moreover we identify  $\mathcal{H}_0$  with  $\ell^2 \times \ell^2$  writing

$$e^{(-1)} \otimes e_m = (e_m, 0) \in \ell^2 \times \ell^2, \quad e^{(1)} \otimes e_m = (0, e_m) \in \ell^2 \times \ell^2.$$

This identification allows us to write  $\mathbf{H} : \mathcal{D}(\Lambda_+) \times \mathcal{D}(\Lambda_+) \rightarrow \ell^2 \times \ell^2$  in the matrix form

$$\mathbf{H} = \begin{pmatrix} H_{-1} & \frac{\Delta}{2} I_{\ell^2} \\ \frac{\Delta}{2} I_{\ell^2} & H_1 \end{pmatrix}. \quad (2.7)$$

For simplicity we assume that  $\epsilon \geq 0$ . The case of  $\epsilon < 0$  can be treated similarly by exchanging the roles of  $H_{-1}$  and  $H_1$ .

**Corollary 2.3.** (a) *there is an orthonormal basis  $\{\mathbf{u}_{\nu,m}^0\}_{(\nu,m) \in \{-1,1\} \times \mathbb{N}}$  such that (1.17) holds.*

(b) *Assume  $\epsilon \geq 0$ . If  $l_0 := [\epsilon/\beta] = \max\{n \in \mathbb{N} : n \leq \epsilon/\beta\}$  and  $(\lambda_n^0)_{n \in \mathbb{N}}$  is defined by*

$$\lambda_n^0 = \beta n + \beta_{-1} \text{ for } n = 0, \dots, l_0,$$

$$\lambda_{l_0+2i}^0 = \beta(l_0 + i) + \beta_{-1} \text{ for } i \in \mathbb{N},$$

$$\lambda_{l_0+1+2i}^0 = \beta i + \beta_1 \text{ for } i \in \mathbb{N},$$

*then  $(\lambda_n^0)_{n \in \mathbb{N}}$  is the complete ordered eigenvalue sequence of  $\mathbf{H}_0$ .*

*Proof.* (a) Since  $\mathbf{H}_0 = H_{-1} \oplus H_1$ , the assertion follows from Lemma 2.2.

(b) We observe that  $(\lambda_n^0)_{n \in \mathbb{N}}$  is a permutation of the sequence  $(\beta m + \beta \nu)_{(m, \nu) \in \{-1, 1\} \times \mathbb{N}}$ , which is a complete eigenvalue sequence of  $\mathbf{H}_0$  due to Lemma 2.2. Thus it remains to check that the sequence  $(\lambda_n^0)_{n \in \mathbb{N}}$  is increasing. It is obvious that  $(\lambda_n^0)_{0 \leq n \leq l_0}$ ,  $(\lambda_{l_0+2i}^0)_{i \in \mathbb{N}}$  and  $(\lambda_{l_0+1+2i}^0)_{i \in \mathbb{N}}$  are increasing. Then, using  $\beta_1 - \beta_{-1} = \epsilon$ , we get

$$\lambda_{l_0+1+2i}^0 - \lambda_{l_0+2i}^0 = \beta_1 - \beta_{-1} - \beta l_0 = \beta \left( \frac{\epsilon}{\beta} - l_0 \right) \geq 0,$$

$$\lambda_{l_0+1+2i}^0 - \lambda_{l_0+2+2i}^0 = \beta_1 - \beta_{-1} - \beta(l_0 + 1) = \beta \left( \frac{\epsilon}{\beta} - l_0 - 1 \right) < 0$$

by the choice of  $l_0$ . □

**Lemma 2.4.** *Let  $\mathbf{H}$  be the operator in  $\mathcal{H}_0$  defined by (1.14). Assume that  $-\frac{1}{2} < g < \frac{1}{2}$ . Then  $\mathbf{H}$  is self-adjoint and bounded from below. It has discrete spectrum and its complete ordered eigenvalue sequence  $(\lambda_n(\mathbf{H}))_{n \in \mathbb{N}}$  satisfies*

$$\frac{1}{2}\beta n + O(1) \text{ as } n \rightarrow \infty. \quad (2.8)$$

where  $\beta$  is defined in (1.12).

*Proof.* Since  $\mathbf{H} - \mathbf{H}_0$  is bounded and  $(\mathbf{H} - \mathbf{H}_0)(i + \mathbf{H}_0)^{-1}$  is compact,  $\mathbf{H}$  has no essential spectrum. Indeed,  $\sigma_{\text{ess}}(\mathbf{H}) = \sigma_{\text{ess}}(\mathbf{H}_0) = \emptyset$  due to Weyl's criterion (see Theorem 5.35, Ch. IV in [81]). Thus the spectrum of  $\mathbf{H}$  is discrete, bounded from below and the min-max principle ensures

$$|\lambda_n(\mathbf{H}) - \lambda_n(\mathbf{H}_0)| \leq \|\mathbf{H} - \mathbf{H}_0\|, \quad (2.9)$$

We deduce (2.8) from (2.9) and from the fact that

$$\lambda_n(\mathbf{H}_0) = \frac{1}{2}\beta n + O(1) \text{ as } n \rightarrow \infty, \quad (2.10)$$

which follows from the explicit expressions of  $\lambda_n(\mathbf{H}_0) = \lambda_n^0$  given in Corollary 2.3. □

## 2.4 Operators $J_{\pm 1}$

**Notation 2.5.** We denote by  $\{e_i\}_{i \in \mathbb{Z}}$  the canonical basis of  $\ell^2(\mathbb{Z})$  (i.e.  $e_i(j) = \delta_{i,j}$  for  $i, j \in \mathbb{Z}$ ). If  $\mathcal{J} \subset \mathbb{Z}$  then  $\ell^2(\mathcal{J})$  is identified with the closed subspace of  $\ell^2(\mathbb{Z})$  generated by  $\{e_j\}_{j \in \mathcal{J}}$ , i.e. with  $\{x \in \ell^2(\mathbb{Z}) : x(k) = 0 \text{ for } k \in \mathbb{Z} \setminus \mathcal{J}\}$ . Thus we can write

$$\ell^2(\mathbb{Z}) = \ell^2(\mathbb{Z} \setminus \mathbb{N}) \oplus \ell^2. \quad (2.11)$$

Our next aim is to approximate the operators  $H_{\pm 1}$  acting in  $\ell^2$  by operators  $J_{\pm 1}$  acting in  $\ell^2(\mathbb{Z})$ . For this purpose we will use the fact that  $H_{\pm 1}e_m$  is expressed, by (2.3), as a sum which contains the term  $b(m) = \sqrt{(m+1)(m+2)}$  and one has the following asymptotic estimate :

$$\sqrt{(m+1)(m+2)} = m + \frac{3}{2} + O(m^{-1}) \text{ as } m \rightarrow \infty \quad (2.12)$$

**Notation 2.6.** (a) We denote by  $\Lambda$  the self-adjoint operator in  $\ell^2(\mathbb{Z})$  defined on

$$\mathcal{D}(\Lambda) = \left\{ x \in \ell^2(\mathbb{Z}) : \sum_{k \in \mathbb{Z}} k^2 |x(k)|^2 < \infty \right\} \quad (2.13)$$

by the formula  $\Lambda e_j = j e_j$  for  $j \in \mathbb{Z}$ .

(b) For  $\nu = \pm 1$  we define the linear mapping  $J_\nu : \mathcal{D}(\Lambda) \rightarrow \ell^2(\mathbb{Z})$  by

$$J_\nu e_j = \left( j + \frac{1}{2} \nu \epsilon \right) e_j + \nu g \left( j + \frac{3}{2} \right) e_{j+2} + \nu g \left( j - \frac{1}{2} \right) e_{j-2} \text{ for } j \in \mathbb{Z}. \quad (2.14)$$

**Lemma 2.7.** *Assume that  $\nu = \pm 1$  and  $-\frac{1}{2} < g < \frac{1}{2}$ . Then*

$$J_\nu (I_{\ell^2(\mathbb{Z})} + |\Lambda|)^{-1} \in \mathcal{B}(\ell^2(\mathbb{Z})), \quad (2.15)$$

$J_\nu$  is self-adjoint in  $\ell^2(\mathbb{Z})$  and there is an orthonormal basis  $(v_{\nu,j})_{j \in \mathbb{Z}}$  such that

$$J_\nu v_{\nu,j} = (\beta_j + \beta_\nu) v_{\nu,j} \text{ for } j \in \mathbb{Z} \quad (2.16)$$

where  $\beta, \beta_\nu$  are given by (1.12)-(1.13).

*Proof.* See Section 3. □

## 2.5 Operators $\mathbf{J}$ and $\mathbf{J}_0$

**Notation 2.8.** (a) In the sequel we denote  $\mathcal{H} := \ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})$  and define  $\mathbf{J}$  as the linear mapping  $\mathcal{D}(\Lambda) \times \mathcal{D}(\Lambda) \rightarrow \mathcal{H}$  given by

$$\mathbf{J} := \begin{pmatrix} J_{-1} & \frac{\Delta}{2} I_{\ell^2(\mathbb{Z})} \\ \frac{\Delta}{2} I_{\ell^2(\mathbb{Z})} & J_1 \end{pmatrix} \quad (2.17)$$

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

$$\mathbf{J} = \mathbf{J}_0 + \mathbf{V} \text{ with } \mathbf{V} := \frac{\Delta}{2} \begin{pmatrix} O_{\ell^2(\mathbb{Z})} & I_{\ell^2(\mathbb{Z})} \\ I_{\ell^2(\mathbb{Z})} & O_{\ell^2(\mathbb{Z})} \end{pmatrix}, \quad (2.18)$$

where  $O_{\ell^2(\mathbb{Z})}$  is the null mapping on  $\ell^2(\mathbb{Z})$ .

(c) Let  $(\mathbf{v}_j^0)_{j \in \mathbb{Z}}$  be the orthonormal basis of  $\mathcal{H}$  defined by

$$\mathbf{v}_{2i}^0 = (v_{-1,i}, 0), \quad \mathbf{v}_{2i+1}^0 = (0, v_{1,i-l_0}) \quad (i \in \mathbb{Z}), \quad (2.19)$$

where  $l_0 := \lceil \epsilon/\beta \rceil$  and  $v_{\pm 1,i}$  are as in Lemma 2.7. Then  $\mathbf{J}_0 \mathbf{v}_j^0 = d_j \mathbf{v}_j^0$  holds with

$$d_{2i} = \beta i + \beta_{-1}, \quad d_{2i+1} = \beta(i - l_0) + \beta_1. \quad (2.20)$$

Moreover, similarly as in the proof of Corollary 2.3, the indicated choice of  $l_0$  ensures the fact that the sequence  $(d_j)_{j \in \mathbb{Z}}$  is increasing, i.e. it is a complete ordered eigenvalue sequence for  $\mathbf{J}_0$ . If  $j \geq l_0$  then it can be checked that  $d_{j+l_0} = \lambda_j^0$  are eigenvalues of  $\mathbf{H}_0$  introduced in Corollary 2.3.

In the case  $\epsilon/\beta \notin \mathbb{N}$  each eigenvalue of  $\mathbf{J}_0$  is simple, while in the case  $\epsilon/\beta \in \mathbb{N}$  each eigenvalue of  $\mathbf{J}_0$  is double ( $d_{2i} = d_{2i+1}$ ). Finally we observe that

$$\mathbf{V}\mathbf{v}_{2i}^0 = \mathbf{V}(v_{-1,i}, 0) = \frac{\Delta}{2}(0, v_{-1,i}), \quad (2.21)$$

$$\mathbf{V}\mathbf{v}_{2i+1}^0 = \mathbf{V}(0, v_{1,i-l_0}) = \frac{\Delta}{2}(v_{1,i-l_0}, 0). \quad (2.22)$$

**Corollary 2.9.** *Assume that  $-\frac{1}{2} < g < \frac{1}{2}$ . Then*

(a)  $\mathbf{J}$  is a self-adjoint operator in  $\mathcal{H}$  with discrete spectrum and

$$|\mathbf{J}|(I + |\Lambda| \oplus |\Lambda|)^{-1} \in \mathcal{B}(\mathcal{H}). \quad (2.23)$$

(b) if  $(\lambda_j(\mathbf{J}))_{j \in \mathbb{Z}}$  is a complete ordered eigenvalue sequence, then

$$\lambda_j(\mathbf{J}) = \frac{1}{2}\beta j + O(1) \text{ as } |j| \rightarrow \infty \quad (2.24)$$

*Proof.* (a) Similarly as in the proof of Corollary 2.4 we observe that  $\mathbf{V} = \mathbf{J} - \mathbf{J}_0$  satisfies  $\|\mathbf{V}\| = \frac{1}{2}|\Delta|$  and  $\mathbf{V}(i + \mathbf{J}_0)^{-1}$  is compact, hence  $\mathbf{J}$  is self-adjoint and has discrete spectrum. In order to show (2.23) we first observe that (2.15) implies

$$\mathbf{J}_0(I + |\Lambda| \oplus |\Lambda|)^{-1} \in \mathcal{B}(\mathcal{H}). \quad (2.25)$$

Using  $\mathbf{J}^2 = \mathbf{J}_0^2 + \mathbf{J}_0\mathbf{V} + \mathbf{V}\mathbf{J}_0 + \mathbf{V}^2$  and (2.25) we obtain

$$\|(I + |\Lambda| \oplus |\Lambda|)^{-1}|\mathbf{J}|\|^2 = \|(I + |\Lambda| \oplus |\Lambda|)^{-1}\mathbf{J}^2(I + |\Lambda| \oplus |\Lambda|)^{-1}\| < \infty.$$

(b) Since the complete ordered eigenvalue sequence of  $\mathbf{J}_0$  is given by (2.20), it is clear that  $d_j = \frac{1}{2}\beta j + O(1)$  as  $|j| \rightarrow \infty$  and we deduce (2.24) using Lemma 1.6 with  $A = \mathbf{J}_0$ ,  $B = \mathbf{J}$  and  $\alpha = 0$ .  $\square$

### 3 Diagonalization of $J_{\pm 1}$

#### 3.1 Outline

As before we assume that  $-\frac{1}{2} < g < \frac{1}{2}$ . Recall that the operators  $J_1$  and  $J_{-1}$  are defined in Notation 2.6(b). Following Edwards [43], instead of  $J_\nu$  we consider

$$L_\nu := \mathcal{F}_{\mathbb{T}}^{-1} J_\nu \mathcal{F}_{\mathbb{T}}, \quad (3.1)$$

where  $\mathcal{F}_{\mathbb{T}} : L^2(\mathbb{T}) \rightarrow \ell^2(\mathbb{Z})$  is the Fourier transform

$$(\mathcal{F}_{\mathbb{T}} f)(j) = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\theta) e^{-ij\theta} d\theta \quad (3.2)$$

and  $L^2(\mathbb{T})$  is the Hilbert space of Lebesgue square integrable functions  $]-\pi, \pi] \rightarrow \mathbb{C}$  equipped with the scalar product

$$\langle f, g \rangle_{L^2(\mathbb{T})} := \frac{1}{2\pi} \int_{-\pi}^{\pi} \overline{f(\theta)} g(\theta) d\theta. \quad (3.3)$$

Then  $L_\nu$  is self-adjoint in  $L^2(\mathbb{T})$  and its domain  $\mathcal{D}(L_\nu)$  is the Sobolev space  $H^1(\mathbb{T}) = \mathcal{F}_{\mathbb{T}}^{-1}(\mathcal{D}(\Lambda))$ . Moreover, it appears that  $L_\nu$  is a first order elliptic operator on  $\mathbb{T}$  with coefficients belonging to  $C^\infty(\mathbb{T})$ , where  $f \in C^\infty(\mathbb{T})$  means that  $f : ]-\pi, \pi] \rightarrow \mathbb{C}$  has the  $2\pi$ -periodic extension belonging to  $C^\infty(\mathbb{R})$ . The asymptotic behaviour of the eigenvalues of  $L_\nu$  can be analysed by using the similarity approach of Rozenbljum [111]. In Section 3.2 we modify the approach of Rozenbljum [111] : we introduce the operators  $U_{\Phi_\nu}$  which are unitary in  $L^2(\mathbb{T})$  and such that the operator

$$L_\nu^0 := \beta^{-1} U_{\Phi_\nu}^{-1} L_\nu U_{\Phi_\nu} \quad (3.4)$$

has the form  $L_\nu^0 = D + q_\nu = -\text{id}/d\theta + q_\nu$ , i.e.

$$(L_\nu^0 f)(\theta) = -i \frac{df}{d\theta}(\theta) + q_\nu(\theta) f(\theta), \quad (3.5)$$

where  $q_\nu \in C^\infty(\mathbb{T})$  is given by (3.26). Following [43] we can introduce the orthonormal basis  $(f_{\nu,j}^0)_{j \in \mathbb{Z}}$  of the form

$$f_{\nu,j}^0(\theta) = e^{ij\theta - i(\tilde{q}_\nu(\theta) - \langle q_\nu \rangle \theta)}, \quad (3.6)$$

where  $\tilde{q}_\nu$  is a primitive of  $q_\nu$  and

$$\langle q_\nu \rangle := \frac{1}{2\pi} \int_{-\pi}^{\pi} q_\nu(\theta) d\theta = \frac{\tilde{q}_\nu(\pi) - \tilde{q}_\nu(-\pi)}{2\pi}. \quad (3.7)$$

Then it is easy to see that  $f_{\nu,j}^0 \in C^\infty(\mathbb{T})$  and for every  $j \in \mathbb{Z}$  one has

$$(D + q_\nu) f_{\nu,j}^0 = (j + \langle q_\nu \rangle) f_{\nu,j}^0, \quad (3.8)$$

i.e.  $(j + \langle q_\nu \rangle)_{j \in \mathbb{Z}}$  is a complete eigenvalue sequence of  $D + q_\nu$ . Thus (3.4) ensures

$$L_\nu f_{\nu,j} = \beta(j + \langle q_\nu \rangle) f_{\nu,j} \text{ with } f_{\nu,j} := U_{\Phi_\nu} f_{\nu,j}^0, \quad (3.9)$$

i.e.  $(\beta(j + \langle q_\nu \rangle))_{j \in \mathbb{Z}}$  is a complete eigenvalue sequence of  $L_\nu$  and  $J_\nu$ . Moreover (2.16) holds with  $\beta_\nu = \beta \langle q_\nu \rangle$  and  $v_{\nu,j} = \mathcal{F}_{\mathbb{T}} f_{\nu,j}$ . The special form of  $f_{\nu,j}$  will allow us to deduce a property of asymptotic orthogonality between the basis  $(v_{-1,j})_{j \in \mathbb{Z}}$  and  $(v_{1,j})_{j \in \mathbb{Z}}$  in Lemma 3.4.

### 3.2 A change of variable

**Notation 3.1.** (a) In the sequel  $D$  denotes the self-adjoint operator of differentiation acting  $H^1(\mathbb{T}) \rightarrow L^2(\mathbb{T})$  according to the formula

$$(Df)(\theta) = -if'(\theta), \quad (3.10)$$

where  $f'(\theta) = \frac{df}{d\theta}(\theta)$ .

(b) Assume that  $p, p_0 \in C^\infty(\mathbb{T})$ . If  $p_0$  is real valued, then

$$L = (p(\theta)D_\theta + \text{hc}) + p_0(\theta) \quad (3.11)$$

denotes the symmetric operator acting  $H^1(\mathbb{T}) \rightarrow L^2(\mathbb{T})$  according to the formula

$$(Lf)(\theta) = -i(p(\theta)f'(\theta) + (\bar{p}f)'(\theta)) + p_0(\theta)f(\theta). \quad (3.12)$$



**Lemma 3.2.** *Assume that  $\Phi : ] - \pi, \pi[ \rightarrow ] - \pi, \pi[$  is a bijection such that the derivative  $\Phi' \in C^\infty(\mathbb{T})$  and there is a constant  $c_0 > 0$  such that  $\Phi' \geq c_0$ . We denote by  $U_\Phi$  the unitary operator in  $L^2(\mathbb{T})$  given by the formula*

$$(U_\Phi f)(\xi) = f(\Phi(\xi)) \sqrt{\Phi'(\xi)} \quad (3.13)$$

and define the operator

$$L_\Phi := \frac{1}{2\Phi'(\theta)} D_\theta + \text{hc}. \quad (3.14)$$

Then  $C^\infty(\mathbb{T})$  is invariant for  $U_\Phi^{\pm 1}$  and one has

$$U_\Phi^{-1} L_\Phi U_\Phi = D. \quad (3.15)$$

*Proof.* Assume that  $f \in C^\infty(\mathbb{T})$  and denote  $\tilde{f} = f \circ \Phi$ . Then it is clear that

$$D\tilde{f} = ((Df) \circ \Phi) \Phi' \quad (3.16)$$

belongs to  $C^\infty(\mathbb{T})$  as well as  $U_\Phi f = \sqrt{\Phi'} \tilde{f}$ . Moreover

$$2L_\Phi U_\Phi f = \frac{1}{\Phi'} D(\sqrt{\Phi'} \tilde{f}) + D\left(\frac{1}{\sqrt{\Phi'}} \tilde{f}\right) \quad (3.17)$$

Due to  $\frac{1}{\Phi'} D(\sqrt{\Phi'}) + D\left(\frac{1}{\sqrt{\Phi'}}\right) = 0$ , the right hand side of (3.17) takes the form

$$\frac{1}{\Phi'} \sqrt{\Phi'} D\tilde{f} + \frac{1}{\sqrt{\Phi'}} D\tilde{f} = \frac{2}{\sqrt{\Phi'}} D\tilde{f} \quad (3.18)$$

and due to (3.16), the right hand side of (3.18) takes the form

$$\frac{2}{\sqrt{\Phi'}} ((Df) \circ \Phi) \Phi' = 2U_\Phi Df. \quad (3.19)$$

i.e.  $2L_\Phi U_\Phi f = 2U_\Phi Df$  for  $f \in C^\infty(\mathbb{T})$ . Since the closure of  $D$  is defined on  $H^1(\mathbb{T})$ , the equality (3.15) still holds on functions belonging to  $H^1(\mathbb{T})$ .  $\square$

### 3.3 Diagonalization of $L_\nu$

Let  $J_\nu$  be given by (2.14). Then

$$J_\nu = \Lambda + \nu g \left( S^2 \left( \Lambda + \frac{3}{2} \right) + \left( \Lambda + \frac{3}{2} \right) S^{-2} \right) + \frac{1}{2} \nu \epsilon, \quad (3.20)$$

where  $S \in \mathcal{B}(\ell^2(\mathbb{Z}))$  is the shift operator defined by  $Se_j := e_{j+1}$  for  $j \in \mathbb{Z}$ . Since  $\mathcal{F}_\mathbb{T}^{-1} \Lambda \mathcal{F}_\mathbb{T} = D$  and  $\mathcal{F}_\mathbb{T}^{-1} S \mathcal{F}_\mathbb{T}$  is the operator of multiplication by  $e^{i\theta}$ , we get

$$L_\nu = D_\theta + \nu g \left( e^{2i\theta} \left( D_\theta + \frac{3}{2} \right) + \text{hc} \right) + \frac{1}{2} \nu \epsilon. \quad (3.21)$$

We observe that

$$D_\theta + \nu g \left( e^{2i\theta} D_\theta + \text{hc} \right) = \left( \left( \frac{1}{2} + \nu g \cos(2\theta) \right) D_\theta + \text{hc} \right) - 2\nu g \cos(2\theta) \quad (3.22)$$

and

$$\beta^{-1} L_\nu = (p_\nu(\theta) D_\theta + \text{hc}) + \beta^{-1} \left( \nu g \cos(2\theta) + \frac{1}{2} \nu \epsilon \right) \quad (3.23)$$

holds with

$$p_\nu(\theta) := \beta^{-1} \left( \frac{1}{2} + \nu g \cos(2\theta) \right). \quad (3.24)$$

Introducing

$$\Phi_\nu(\theta) := \int_0^\theta \frac{d\theta'}{2p_\nu(\theta')} = \int_0^\theta \frac{\beta d\theta'}{1 + 2\nu g \cos(2\theta')} \quad (3.25)$$

we find that  $\Phi_\nu(-\theta) = -\Phi_\nu(\theta)$  and calculating the integral we find that  $\Phi_\nu(\pi) = \pi$  holds if  $\beta = \sqrt{1 - 4g^2}$ . It is clear that  $\Phi_\nu$  satisfies the hypotheses of Lemma 3.2 and  $\Phi'_\nu = 1/(2p_\nu)$ . Thus  $p_\nu = 1/(2\Phi'_\nu)$  and due to (3.23), (3.15), we find that (3.4) holds with

$$q_\nu(\eta) = \beta^{-1} \left( \nu g \cos(2\Phi_\nu^{-1}(\eta)) + \frac{1}{2} \nu \epsilon \right). \quad (3.26)$$

As indicated in Section 3.1, the complete eigenvalue sequence of  $D + q_\nu$  is  $(j + \langle q_\nu \rangle)_{j \in \mathbb{Z}}$ , hence the complete eigenvalue sequence of  $L_\nu$  is  $(\beta(j + \langle q_\nu \rangle))_{j \in \mathbb{Z}}$ . We claim that

$$\beta(j + \langle q_\nu \rangle) = \beta j + \beta_\nu \text{ with } \beta_\nu = \frac{1}{2} \nu \epsilon + \frac{1}{2} (\beta - 1). \quad (3.27)$$

Indeed, using (3.26) to compute (3.7), we get

$$\beta \langle q_\nu \rangle = \frac{1}{2} \nu \epsilon + \frac{1}{2\pi} \int_{-\pi}^{\pi} \nu g \cos(2\Phi_\nu^{-1}(\eta)) d\eta \quad (3.28)$$

and the change of variable allows us to write the last term of (3.28) in the form

$$\begin{aligned} \frac{1}{2\pi} \int_{-\pi}^{\pi} \nu g \cos(2\theta) \Phi'_\nu(\theta) d\theta &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{\beta \nu g \cos(2\theta)}{1 + 2\nu g \cos(2\theta)} d\theta \\ &= \frac{1}{2\pi} \int_{-\pi}^{\pi} \frac{1}{2} \left( \beta - \frac{\beta}{1 + 2\nu g \cos(2\theta)} \right) d\theta = \frac{1}{2} (\beta - 1). \end{aligned}$$

We conclude that (3.9) takes the form

$$L_\nu f_{\nu,j} = (\beta j + \beta_\nu) f_{\nu,j} \quad (3.29)$$

with  $\beta_\nu$  given by (1.13) and  $f_{\nu,j} = \sqrt{\Phi'_\nu} (f_{\nu,j}^0 \circ \Phi_\nu)$  has the form

$$f_{\nu,j}(\theta) = \sqrt{\Phi'_\nu(\theta)} e^{ij\Phi_\nu(\theta) + i\phi_\nu(\theta)}, \quad (3.30)$$

where

$$\phi_\nu(\theta) := \langle q_\nu \rangle \Phi_\nu(\theta) - \tilde{q}_\nu(\Phi_\nu(\theta)) \quad (3.31)$$

and  $\tilde{q}_\nu$  is a primitive of  $q_\nu$ .

### 3.4 Asymptotic orthogonality between $(v_{-1,j})_{j \in \mathbb{Z}}$ and $(v_{1,j})_{j \in \mathbb{Z}}$

**Notation 3.3.** For  $j \in \mathbb{Z}$  we consider  $v_{\nu,j} = \mathcal{F}_{\mathbb{T}} f_{\nu,j}$  with  $f_{\nu,j}$  given by (3.30)-(3.31). Then  $(v_{\nu,j})_{j \in \mathbb{Z}}$  is an orthogonal basis of eigenvectors of  $J_{\nu}$  and we define

$$\gamma_{j,k} := \langle v_{-1,j}, v_{1,k} \rangle_{\ell^2(\mathbb{Z})} = \langle f_{-1,j}, f_{1,k} \rangle_{L^2(\mathbb{T})}. \quad (3.32)$$

**Lemma 3.4.** *If  $c > 0$  is small enough and  $g > 0$ , then there exists  $C > 0$  such that*

$$\sup_{\substack{k \in \mathbb{Z} \\ |k| < c|j|}} |\gamma_{j,j+k}| \leq C|j|^{-1/2}. \quad (3.33)$$

*Proof.* Using (3.30)-(3.31) we can express

$$\langle f_{-1,j}, f_{1,j+k} \rangle_{L^2(\mathbb{T})} = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{ij\Psi_{j,k}(\theta)} b(\theta) d\theta \quad (3.34)$$

with

$$b = e^{i(\phi_1 - \phi_{-1})} (\Phi'_1 \Phi'_{-1})^{1/2}, \quad (3.35)$$

$$\Psi_{j,k} = \frac{j+k}{j} \Phi_1 - \Phi_{-1}. \quad (3.36)$$

Denote  $\Psi_0 := \Phi_1 - \Phi_{-1}$ . Then

$$\Psi'_0(\theta) = \frac{\beta}{1 + 2g \cos(2\theta)} - \frac{\beta}{1 - 2g \cos(2\theta)} = 0 \Leftrightarrow \cos(2\theta) = 0, \quad (3.37)$$

i.e.  $\Psi'_0(\theta) \neq 0$  if  $\theta \in [-\pi, \pi] \setminus \{\theta_1, \theta_{-1}, \theta_2, \theta_{-2}\}$ , where  $\theta_{\pm 1} = \pm \frac{\pi}{4}$  and  $\theta_{\pm 2} = \pm \frac{3\pi}{4}$ . However,

$$\Psi''_0(\theta) = \left( \frac{4g\beta}{(1 + 2g \cos(2\theta))^2} + \frac{4g\beta}{(1 - 2g \cos(2\theta))^2} \right) \sin(2\theta) \quad (3.38)$$

and  $\Psi'_0(\theta) = 0 \Rightarrow \cos(2\theta) = 0 \Rightarrow \Psi''_0(\theta) = \pm 8g\beta$ , i.e. the critical points  $\{\theta_i\}_{i=\pm 1, \pm 2}$  are not degenerated. Therefore there exists  $c_0 > 0$  such that  $|\Psi''_0(\theta)| \geq c_0$  holds for every  $\theta \in [\theta_i - c_0, \theta_i + c_0]$ . However  $\Psi_{j,k} = \Psi_0 + \frac{k}{j} \Phi_1$  and denoting  $C_0 = \sup |\Phi''_1|$  we can estimate

$$|\Psi''_{j,k}(\theta)| \geq |\Psi''_0(\theta)| - C_0 \left| \frac{k}{j} \right|$$

and

$$\left| \frac{k}{j} \right| \leq \frac{c_0}{2C_0} \implies |\Psi''_{j,k}(\theta)| \geq \frac{c_0}{2} \text{ for } \theta \in [\theta_i - c_0, \theta_i + c_0]. \quad (3.39)$$

For  $i \in [-2, 2] \cap \mathbb{Z}$  let  $\chi_i \in C^\infty(\mathbb{R})$  be partition of unity such that  $\chi_i(\theta) = 0$  holds for  $\theta \in [-\pi, \pi] \setminus [\theta_i - c_0, \theta_i + c_0]$  when  $i = \pm 1, \pm 2$  and  $\chi_0(\theta) = 0$  for every  $\theta$  in a certain neighbourhood of  $\{\theta_1, \theta_{-1}, \theta_2, \theta_{-2}\}$ . It remains to estimate

$$\gamma_{j,j+k,i} := \int_{-\pi}^{\pi} e^{ij\Psi_{j,k}(\theta)} (b\chi_i)(\theta) d\theta \quad (i = 0, \pm 1, \pm 2) \quad (3.40)$$

Using (3.39) we can find a constant  $C$  such that

$$\left| \frac{k}{j} \right| \leq \frac{c_0}{2C_0} \implies |\gamma_{j,j+k,i}| \leq C|j|^{-1/2} \text{ for } i = \pm 1, \pm 2, \quad (3.41)$$

due to the van der Corput lemma (see Section 6.2).

In order to estimate  $\gamma_{j,j+k,0}$  we observe that

$$c_1 := \inf\{|\Psi'_0(\theta)| : \theta \in [-\pi, \pi] \cap \text{supp } \chi_0\} > 0.$$

However denoting  $C_1 = \sup |\Phi'_1|$  we can estimate

$$|\Psi'_{j,k}(\theta)| \geq |\Psi'_0(\theta)| - C_1 \left| \frac{k}{j} \right|$$

and

$$\left| \frac{k}{j} \right| \leq \frac{c_1}{2C_1} \implies |\Psi'_{j,k}(\theta)| \geq \frac{c_1}{2} \text{ for } \theta \in [-\pi, \pi] \cap \text{supp } \chi_0. \quad (3.42)$$

To complete the proof it remains to check that there is a constant  $C'$  such that

$$\left| \frac{k}{j} \right| \leq \frac{c_1}{2C_1} \implies |\gamma_{j,j+k,0}| \leq C'|j|^{-1}. \quad (3.43)$$

Indeed, if  $\left| \frac{k}{j} \right| \leq \frac{c_1}{2C_1}$  then integrating by parts, we find that

$$- \int_{-\pi}^{\pi} e^{ij\Psi_{j,k}} \frac{d}{d\theta} \left( \frac{b\chi_0}{i\Psi'_{j,k}} \right) d\theta = j \gamma_{j,j+k,0}, \quad (3.44)$$

can be estimated by a constant  $C'$  due to (3.42).  $\square$

## 4 Asymptotic behaviour of eigenvalues of $\mathbf{J}$

### 4.1 Outline of Section 4

In this section we assume  $0 < g < 1/2$  and prove

**Proposition 4.1.** *There is a complete ordered eigenvalue sequence for  $\mathbf{J}$  such that*

$$\lambda_j(\mathbf{J}) = d_j + O(|j|^{-1/2}) \text{ as } |j| \rightarrow \infty, \quad (4.1)$$

where  $(d_j)_{j \in \mathbb{Z}}$  is defined in Notations 2.8(c).

*Proof.* See Section 4.4.  $\square$

In order to simplify our further analysis we replace operators acting in  $\ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})$  by operators acting in  $\ell^2(\mathbb{Z})$ . For this purpose we introduce

**Notation 4.2.** Let  $(\mathbf{v}_j^0)_{j \in \mathbb{Z}}$  denote the orthonormal basis of  $\ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})$  introduced in Notation 2.8(c) and  $U : \ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z})$  is the isometric isomorphism satisfying  $U\mathbf{v}_j^0 = e_j$  for every  $j \in \mathbb{Z}$  (where  $\{e_j\}_{j \in \mathbb{Z}}$  is the canonical basis of  $\ell^2(\mathbb{Z})$ ). We define  $J$  and  $J_0$  as the self-adjoint operators in  $\ell^2(\mathbb{Z})$  given by

$$J := U\mathbf{J}U^{-1}, \quad J_0 := U\mathbf{J}_0U^{-1}. \quad (4.2)$$

Since  $J_0 = \text{diag}(d_j)_{j \in \mathbb{Z}}$  (i.e.  $J_0e_j = d_je_j$  for every  $j \in \mathbb{Z}$ ) and

$$J = J_0 + V \text{ with } V := U\mathbf{V}U^{-1} \quad (4.3)$$

we deduce  $\mathcal{D}(J) = \mathcal{D}(J_0) = \mathcal{D}(\Lambda)$  from the fact that  $d_j \sim \frac{1}{2}\beta j$  as  $|j| \rightarrow \infty$ .

Due to (4.2) it remains to investigate the asymptotic behaviour of eigenvalues of  $J$ . Our analysis uses a compact anti-Hermitian operator  $K$  defined in Section 4.2. In Section 4.3 we prove that

$$J = (I + K)^{-1}(J_0 + R)(I + K) \quad (4.4)$$

holds with a certain compact operator  $R$  and in Section 4.4 we give the asymptotic formula for eigenvalues of  $J_0 + R$ . Due to (4.4) the eigenvalues of  $J_0 + R$  coincide with the eigenvalues of  $J$  and  $\mathbf{J}$ .

## 4.2 The auxiliary operator $K$

**Notation 4.3.** In the sequel  $K \in \mathcal{B}(\ell^2(\mathbb{Z}))$  is the operator defined by

$$\langle e_j, Ke_k \rangle_{\ell^2(\mathbb{Z})} = K(j, k) = \begin{cases} \frac{V(j, k)}{d_j - d_k} & \text{if } d_j \neq d_k \\ 0 & \text{if } d_j = d_k \end{cases} \quad (4.5)$$

where  $V(j, k) = \langle e_j, Ve_k \rangle_{\ell^2(\mathbb{Z})} = \langle \mathbf{v}_j^0, \mathbf{V}\mathbf{v}_k^0 \rangle_{\mathcal{H}}$ .

**Lemma 4.4.** *The operator  $K$  is compact and anti-Hermitian in  $\ell^2(\mathbb{Z})$  (i.e.  $K^* = -K$ ). Moreover there is  $C > 0$  such that*

$$\|Ke_j\|_{\ell^2(\mathbb{Z})} \leq C(1 + |j|)^{-1/2} \text{ for all } j \in \mathbb{Z}. \quad (4.6)$$

*Proof.* Step 1. We claim that for every  $k \in \mathbb{Z}$  we can find  $C_k > 0$  such that

$$|K(j, j+k)|_{\ell^2(\mathbb{Z})} \leq C_k(1 + |j|)^{-1/2} \text{ for all } j \in \mathbb{Z}. \quad (4.7)$$

We first observe that  $K(k, j) = -\overline{K(j, k)}$ , i.e. the matrix  $(K(j, k))_{j, k \in \mathbb{Z}}$  is anti-Hermitian. Combining (2.19) with (2.21) and (2.22) we get

$$\begin{aligned} V(2i, 2j) &= \frac{\Delta}{2} \langle (v_{-1, i}, 0), (0, v_{-1, j}) \rangle_{\mathcal{H}} = 0 \\ V(2i+1, 2j+1) &= \frac{\Delta}{2} \langle (0, v_{1, i-l_0}), (v_{1, j-l_0}, 0) \rangle_{\mathcal{H}} = 0 \end{aligned}$$

$$V(2i, 2j + 1) = \frac{\Delta}{2} \langle (v_{-1,i}, 0), (v_{1,j-l_0}, 0) \rangle_{\mathcal{H}} = \frac{\Delta}{2} \gamma_{i,j-l_0}$$

where  $\gamma_{i,j}$  are given by (3.32). However (3.33) ensures

$$|i| \geq c^{-1}|k| \implies |V(2i + 2k + 1, 2i)| \leq C(1 + |i|)^{-1/2} \quad (4.8)$$

and (4.8) implies (4.7) if  $j = 2i$ . Reasoning similarly we get (4.7) if  $j = 2i + 1$ .

Step 2. Let  $N \in \mathbb{N}$ . We claim that a compact operator  $K_N$  can be defined in  $\ell^2(\mathbb{Z})$  by

$$K_N(j, k) = \langle e_j, K_N e_k \rangle_{\ell^2(\mathbb{Z})} = \begin{cases} K(j, k) & \text{if } |j - k| < 2N \\ 0 & \text{if } |j - k| \geq 2N \end{cases} \quad (4.9)$$

Indeed, since  $B_N := (I + |\Lambda|)^{1/2} K_N \in \mathcal{B}(\ell^2(\mathbb{Z}))$  follows from (4.7), the operator  $K_N = (I + |\Lambda|)^{-1/2} B_N$  is compact.

Step 3. We observe that Parseval's equality ensures

$$\sum_{k \in \mathbb{Z}} |\gamma_{i,i+k-l_0}|^2 = \sum_{j \in \mathbb{Z}} |\gamma_{i,j}|^2 = \sum_{j \in \mathbb{Z}} |\langle v_{-1,i}, v_{1,j} \rangle_{\ell^2(\mathbb{Z})}|^2 = \|v_{-1,i}\|_{\ell^2(\mathbb{Z})}^2 = 1. \quad (4.10)$$

Step 4. Let  $c_0 > 0$  be small enough. Then  $d_j \neq d_k \implies |d_j - d_k| \geq c_0(1 + |j - k|)$  and

$$K(j, k) \neq 0 \implies |K(j, k)| \leq c_0^{-1} \frac{|V(j, k)|}{1 + |j - k|}. \quad (4.11)$$

Let us denote  $\widetilde{K}_N(j, k) := K(j, k) - K_N(j, k)$ . Then

$$\sum_{k \in \mathbb{Z}} |\widetilde{K}_N(2i, 2i + 2k + 1)| \leq \frac{|\Delta|}{2c_0} \sum_{|k| \geq N} \frac{|\gamma_{i,i+k-l_0}|}{1 + |k|}. \quad (4.12)$$

Using Cauchy-Schwarz inequality and (4.10), we can estimate the right hand side of (4.12) by  $c_0^{-1} |\Delta| \delta_N^{1/2}$  with  $\delta_N := \sum_{|k| \geq N} (1 + |k|)^{-2}$ . Since a similar estimate holds when  $(2i, 2i + 2k + 1)$  is replaced by  $(2i + 1, 2i + 2k)$ , we obtain

$$\sup_{j \in \mathbb{Z}} \sum_{k \in \mathbb{Z}} |\widetilde{K}_N(j, k)| \leq c_0^{-1} |\Delta| \delta_N^{1/2}. \quad (4.13)$$

Due to (4.13), the Schur boundedness test ensures  $K - K_N \in \mathcal{B}(\ell^2(\mathbb{Z}))$  and

$$\|K - K_N\| \leq c_0^{-1} |\Delta| \delta_N^{1/2} \xrightarrow{N \rightarrow \infty} 0. \quad (4.14)$$

Since  $K = K - K_N \in \mathcal{B}(\ell^2(\mathbb{Z}))$  and  $K_N$  are compact, (4.14) implies that  $K$  is compact.

Step 5. We observe that

$$\|K e_{2i}\|_{\ell^2(\mathbb{Z})}^2 = \sum_{k \in \mathbb{Z}} |K(2i, 2i + 2k + 1)|^2 \leq c_0^{-2} \Delta^2 (M_i + M'_i)$$

holds with

$$M_i := \sum_{|k-l_0| < c|i|} \frac{|\gamma_{i,i+k-l_0}|^2}{(1 + |k|)^2}, \quad M'_i := \sum_{|k-l_0| \geq c|i|} \frac{|\gamma_{i,i+k-l_0}|^2}{(1 + |k|)^2}.$$

We observe that  $M_i \leq C_1(1 + |i|)^{-1}$  follows from (3.33) and  $\sum_{k \in \mathbb{Z}} (1 + |k|)^{-2} < \infty$ .

Moreover  $M'_i \leq C_2(1 + i^2)^{-1}$  follows from (4.10). Thus the proof of (4.6) is complete if  $j = 2i$  and similarly we obtain (4.6) if  $j = 2i + 1$ .  $\square$

### 4.3 Similarity transformation

**Notation 4.5.** In the sequel  $W$  denotes the operator defined in  $\mathcal{B}(\ell^2(\mathbb{Z}))$  by

$$\langle e_j, We_k \rangle_{\ell^2(\mathbb{Z})} = W(j, k) = (d_j - d_k)K(j, k) - V(j, k) \quad (4.15)$$

**Lemma 4.6.** (a) If  $\epsilon/\beta \notin \mathbb{N}$  then  $W = 0$ . If  $\epsilon/\beta \in \mathbb{N}$  then  $W$  is compact, self-adjoint and there is  $C > 0$  such that

$$\|We_j\| \leq C(1 + |j|)^{-1/2} \text{ for } j \in \mathbb{Z}. \quad (4.16)$$

(b) The operator  $I + K$  is invertible and we can define a compact operator

$$R := (KV - W)(I + K)^{-1}. \quad (4.17)$$

(c) The equality (4.4) holds.

*Proof.* (a) We first observe that  $V(j, j) = 0$  implies  $W(j, j) = 0$ . Moreover,

$$d_j \neq d_k \implies W(j, k) = 0. \quad (4.18)$$

If  $\epsilon/\beta \notin \mathbb{N}$  then  $j \neq k$  implies  $d_j \neq d_k$  and  $W(j, k) = 0$  follows.

If  $\epsilon/\beta \in \mathbb{N}$  then  $W(j, k) \neq 0$  implies  $d_j = d_k$  and  $j - k = 1$ , hence all non zero coefficients of the matrix  $(W(j, k))_{j, k \in \mathbb{Z}}$  must have the form

$$W(2i, 2i + 1) = W(2i + 1, 2i) = -V(2i + 1, 2i) = -\frac{\Delta}{2}\gamma_{i, i-1}, \quad i \in \mathbb{Z}. \quad (4.19)$$

Reasoning similarly as in the proof of Lemma 4.4 we find that  $W$  is compact and (4.16) follows from (4.19) and (3.33).

(b) Since the operator  $iK$  is self-adjoint, the operator  $i + iK = i(I + K)$  is invertible. Moreover  $R$  is compact because  $K$  and  $W$  are compact.

(c) We first observe that the equality

$$d_j(Ke_k)(j) = (d_j - d_k)(Ke_k)(j) + (KJ_0e_k)(j) = ((W + V + KJ_0)e_k)(j) \quad (4.20)$$

implies  $(d_j(Ke_k)(j))_{j \in \mathbb{Z}} \in \ell^2(\mathbb{Z})$ , i.e.  $Ke_k \in \mathcal{D}(J_0)$  for every  $k \in \mathbb{Z}$  and (4.20) means that the equality

$$J_0K = W + V + KJ_0 \quad (4.21)$$

holds on the subspace of finite linear combinations of  $\{e_j\}_{j \in \mathbb{Z}}$ . Since

$$(I + K)J = (I + K)(J_0 + V) = J_0 + KJ_0 + V + KV, \quad (4.22)$$

(4.21) allows us to modify the right hand side of (4.22) writing  $(I + K)J$  in the form

$$(I + K)J = J_0 + J_0K - W + KV = J_0(I + K) - W + KV. \quad (4.23)$$

Applying  $(I + K)^{-1}$  to both sides of (4.23) we obtain (4.4) with  $R$  given by (4.17).  $\square$

#### 4.4 Proof of Proposition 4.1

Let  $R$  be as in Lemma 4.6. Then

$$\|R^*e_j\| \leq C_0(\|K^*e_j\| + \|We_j\|) \leq C(1 + |j|)^{-1/2} \text{ for all } j \in \mathbb{Z} \quad (4.24)$$

and due to (4.4) we get a complete eigenvalues sequence for  $\mathbf{J}$  and  $J$  writing

$$\lambda_j(\mathbf{J}) = \lambda_j(J) = \lambda_j(J_0 + R). \quad (4.25)$$

We deduce (4.1) combining (4.25), (4.24) with

**Proposition 4.7.** *Let  $P_j$  denote the orthogonal projection on the linear subspace generated by  $\{e_k : d_k = d_j\}$ . Then there is a complete ordered eigenvalue sequence  $(\lambda_j(J_0 + R))_{j \in \mathbb{Z}}$  satisfying*

$$\lambda_j(J_0 + R) = d_j + O(\|R^*P_j\|) \text{ as } j \rightarrow \infty. \quad (4.26)$$

If  $\epsilon/\beta \notin \mathbb{N}$  then the inequality  $d_{j+1} - d_j \geq c_0$  holds with a certain  $c_0 > 0$  and  $\|R^*P_j\| = \|R^*e_j\|$ . In this case the estimate (4.26) can be obtained by a suitable adaptation of the proof of a result of J. Janas and S. Naboko [75] (see Theorem 1.4).

But, if  $\epsilon/\beta \in \mathbb{N}$  our proof of (4.26) requires a result of M. Malejki [94] (see Theorem 4.8), a result which can also be used in the first case.

**Theorem 4.8. (M. Malejki)** *Let us fix  $C_0$  and  $\epsilon_0 > 0$ . Let  $(\hat{d}_n)_{n \in \mathbb{N}}$  be a complex sequence satisfying  $|\hat{d}_n - \hat{d}_k| \geq \epsilon_0 > 0$  when  $\hat{d}_n \neq \hat{d}_k$  and assume that  $\{\Gamma_n\}_{n \in \mathbb{N}}$  is a sequence of closed Jordan curves in  $\mathbb{C}$  satisfying*

$$\text{dist}(\Gamma_n, \hat{d}_k) \geq \epsilon_0/4 \text{ for } k, n \in \mathbb{N} \quad (4.27)$$

$$\int_{\Gamma_n} \|(\hat{D} - \lambda)^{-1}\|^2 |d\lambda| \leq C_0 \text{ for } n \in \mathbb{N}, \quad (4.28)$$

where  $\hat{D} = \text{diag}(\hat{d}_n)_{n \in \mathbb{N}}$  denotes the closed diagonal operator in  $\ell^2$ . We also assume that there exists an increasing non-negative sequence  $(p_n)_{n \in \mathbb{N}}$  such that

$$\{z \in \mathbb{C} : |z| \leq p_n\} \subset \text{int}\Gamma_n, \quad n \in \mathbb{N}, \quad (4.29)$$

$$\lim_{n \rightarrow \infty} \frac{|\Gamma_n|}{p_n^2} = 0, \quad \lim_{n \rightarrow \infty} p_n = \infty, \quad (4.30)$$

where  $\text{int}\Gamma_n$  denotes the set surrounded by  $\Gamma_n$  and  $|\Gamma_n|$  means the length of  $\Gamma_n$ .

If  $K$  is compact in  $\ell^2$ , then the spectrum of  $T = \hat{D} + K$  is discrete and there is a complete eigenvalue sequence  $(\lambda_n(T))_{n \in \mathbb{N}}$  satisfying

$$\lambda_n(T) = \hat{d}_n + O(\|K^*P_n\|) \text{ as } n \rightarrow \infty,$$

where  $P_n$  is the orthogonal projection on the linear subspace generated by  $\{e_k : \hat{d}_k = \hat{d}_n\}$ .

*Proof.* See [94]. □



*Proof of Proposition 4.7 in the case  $\epsilon/\beta \in \mathbb{N}$ .* The operator  $J_0 - \beta_{-1}$  is unitarily equivalent with  $\widehat{D} = \text{diag}(\widehat{d}_n)_{n \in \mathbb{N}} = (0, 0, -\beta, -\beta, \beta, \beta, \dots)$ , i.e.  $\widehat{d}_{4k} = \widehat{d}_{4k+1} = k\beta$ ,  $\widehat{d}_{4k+2} = \widehat{d}_{4k+3} = -(k+1)\beta$  for  $k \in \mathbb{N}$ . We consider  $\Gamma_n$  composed of four segments parallel to the real or imaginary axe, forming a square centred in 0,

$$\Gamma_n := [z_n, \bar{z}_n] \cup [\bar{z}_n, -z_n] \cup [-z_n, -\bar{z}_n] \cup [-\bar{z}_n, z_n]$$

with  $z_n := (1 - i)(n + \frac{1}{2})\beta$ . Since  $\Gamma_n \cap \mathbb{R} = \{-(n + \frac{1}{2})\beta, (n + \frac{1}{2})\beta\}$ , it is clear that the conditions (4.27), (4.29), (4.30) hold with  $\epsilon_0 = \beta$  and  $p_n = \beta n$ . In order to apply Theorem 4.8 and to complete the proof, it remains to check (4.28). For this purpose we first observe that

$$[z_n, \bar{z}_n] = \{\lambda \in \mathbb{C} : \text{Re } \lambda = p'_n, \quad |\text{Im } \lambda| \leq p'_n\}$$

holds with  $p'_n := (n + \frac{1}{2})\beta$ . Then for  $\lambda \in [z_n, \bar{z}_n]$  one has

$$\|(\widehat{D} - \lambda)^{-1}\|^2 = \sup_{m \in \mathbb{N}} \frac{1}{|\widehat{d}_m - \lambda|^2} = \sup_{m \in \mathbb{N}} \frac{1}{(\widehat{d}_m - p'_n)^2 + (\text{Im } \lambda)^2}$$

and using  $|\widehat{d}_m - p'_n| \geq \frac{1}{2}\epsilon_0$  we find

$$\int_{[z_n, \bar{z}_n]} \|(\widehat{D} - \lambda)^{-1}\|^2 |d\lambda| \leq \int_{-p'_n}^{p'_n} \frac{1}{\frac{1}{4}\epsilon_0^2 + s^2} ds \leq C_1,$$

where  $C_1$  is independent of  $n$ . If  $\lambda \in [-z_n, -\bar{z}_n]$ , then  $\text{Re } \lambda = -p'_n$  and a similar estimate holds due to  $|\widehat{d}_n + p'_n| \geq \frac{1}{2}\epsilon_0$ . Finally

$$[\bar{z}_n, -z_n] = \{\lambda \in \mathbb{C} : \text{Im } \lambda = p'_n, \quad |\text{Re } \lambda| \leq p'_n\}$$

and  $\pm\lambda \in [\bar{z}_n, -z_n] \Rightarrow \|(\widehat{D} - \lambda)^{-1}\| \leq 1/|\text{Im } \lambda| \leq 1/p'_n$ , hence

$$\int_{\pm[\bar{z}_n, -z_n]} \|(\widehat{D} - \lambda)^{-1}\|^2 |d\lambda| \leq 2/p'_n.$$

*Proof of Proposition 4.7 in the case  $\epsilon/\beta \notin \mathbb{N}$ .* Similarly as before we apply Theorem 4.8 with  $(\widehat{d}_n)_{n=1}^\infty$  satisfying  $\epsilon_0 := \inf_{n \neq m} |\widehat{d}_n - \widehat{d}_m| > 0$  and  $\widehat{d}_{2k+3} < \widehat{d}_{2k+1} < 0 \leq \widehat{d}_{2k} < \widehat{d}_{2k+2}$  for every  $k \in \mathbb{N}$ . Then we can use  $\Gamma_n$  composed of four segments which form a square, each segment being parallel to the real or imaginary axe, the square being symmetric with respect to the real axe and intersecting the real axe in the middle of  $[\widehat{d}_{2k}, \widehat{d}_{2k+2}]$  and in the middle of  $[\widehat{d}_{2k+3}, \widehat{d}_{2k+1}]$ . Then the conditions (4.27)-(4.30) hold similarly as before.

## 5 End of the proof of Theorem 1.3

### 5.1 Outline of Section 5

In this section we write  $\mathbf{H}_\Delta$  instead of  $\mathbf{H}$  given by (2.7),  $\mathbf{J}_\Delta$  instead of  $\mathbf{J}$  given by (2.17) and  $\mathbf{V}_\Delta = \mathbf{J}_\Delta - \mathbf{J}_0$ . In Lemma 5.1 we prove that large eigenvalues of  $\mathbf{H}_\Delta$  are well approximated by eigenvalues of  $\mathbf{J}_\Delta$  modulo a shift  $\kappa(\Delta) \in \mathbb{Z}$ . In Section 5.3 we complete the proof of Theorem 1.3.

## 5.2 Relation between eigenvalues of $\mathbf{J}$ and $\mathbf{H}$

**Lemma 5.1.** *Let  $(\lambda_n(\mathbf{H}_\Delta))_{n \in \mathbb{N}}$  be the complete ordered eigenvalue sequence of  $\mathbf{H}_\Delta$  and let  $(\lambda_j(\mathbf{J}_\Delta))_{j \in \mathbb{Z}}$  be the complete ordered eigenvalue sequence of  $\mathbf{J}_\Delta$  such that (4.1) holds. Then there exists  $\kappa(\Delta) \in \mathbb{Z}$  such that*

$$\lambda_j(\mathbf{J}_\Delta) = \lambda_{j+\kappa(\Delta)}(\mathbf{H}_\Delta) + O(j^{-1}) \text{ as } j \rightarrow \infty. \quad (5.1)$$

*Proof.* Step 1. Let  $\Pi_+ \in \mathcal{B}(\ell^2(\mathbb{Z}))$  denote the orthogonal projection on  $\ell^2$ . Then the operator  $\Pi_- := I_{\ell^2(\mathbb{Z})} - \Pi_+$  is the orthogonal projection on  $\ell^2(\mathbb{Z} \setminus \mathbb{N})$ . We introduce

$$\tilde{J}_\nu := \Pi_- J_\nu \Pi_- + \Pi_+ H_\nu \Pi_+ \quad (5.2)$$

for  $\nu = \pm 1$  and claim that

$$(\tilde{J}_\nu - J_\nu)(I_{\ell^2(\mathbb{Z})} + |\Lambda|) \in \mathcal{B}(\ell^2(\mathbb{Z})). \quad (5.3)$$

Indeed, it suffices to observe that

$$(\tilde{J}_\nu - J_\nu)e_j = 0 \text{ if } j \leq -2 \quad (5.4)$$

$$(\tilde{J}_\nu - J_\nu)e_j = \nu g \tilde{b}(j)e_{j+2} + \nu g \tilde{b}(j-2)e_{j-2} \text{ if } j \geq 2 \quad (5.5)$$

holds with

$$\tilde{b}(j) := \sqrt{(j+1)(j+2)} - j - \frac{3}{2} \quad (5.6)$$

and it is easy to check that  $\tilde{b}(j) = O(j^{-1})$  as  $j \rightarrow \infty$ .

We also observe that the decomposition  $\ell^2(\mathbb{Z}) = \ell^2(\mathbb{Z} \setminus \mathbb{N}) \oplus \ell^2$  allows us to express

$$\tilde{J}_\nu = H_\nu^- \oplus H_\nu, \quad (5.7)$$

where  $H_\nu^- := \Pi_- J_\nu|_{\ell^2(\mathbb{Z} \setminus \mathbb{N})}$  is self-adjoint in  $\ell^2(\mathbb{Z} \setminus \mathbb{N})$  and there is  $C_0 \in \mathbb{R}$  such that

$$\sigma(H_\nu^-) \subset ]-\infty, C_0]. \quad (5.8)$$

Step 2. We introduce the operator

$$\tilde{\mathbf{J}}_\Delta := \tilde{J}_{-1} \oplus \tilde{J}_1 + \mathbf{V}_\Delta \quad (5.9)$$

and using (5.4)-(5.5) with  $\tilde{b}(j) = O(j^{-1})$ , we get

$$(\mathbf{J}_\Delta - \tilde{\mathbf{J}}_\Delta)(I + |\Lambda| \oplus |\Lambda|) \in \mathcal{B}(\mathcal{H}). \quad (5.10)$$

Since  $\mathbf{J}_\Delta - \tilde{\mathbf{J}}_\Delta$  is compact,  $\tilde{\mathbf{J}}_\Delta$  is a self-adjoint operator with discrete spectrum and further on  $(\lambda_j(\tilde{\mathbf{J}}_\Delta))_{j \in \mathbb{Z}}$  is a complete ordered eigenvalue sequence.

We claim that there exists  $l_\Delta \in \mathbb{N}$  and  $\kappa(\Delta) \in \mathbb{Z}$  such that

$$\lambda_n(\mathbf{H}_\Delta) = \lambda_{n+\kappa(\Delta)}(\tilde{\mathbf{J}}_\Delta) \text{ if } n \geq l_\Delta. \quad (5.11)$$

Indeed, we first observe that we can express

$$\tilde{\mathbf{J}}_{\Delta} = \begin{pmatrix} H_{-1}^{-} & O_{\ell^2} & \frac{\Delta}{2} I_{\ell^2(\mathbb{Z}\setminus\mathbb{N})} & O_{\ell^2} \\ O_{\ell^2(\mathbb{Z}\setminus\mathbb{N})} & H_{-1} & O_{\ell^2(\mathbb{Z}\setminus\mathbb{N})} & \frac{\Delta}{2} I_{\ell^2} \\ \frac{\Delta}{2} I_{\ell^2(\mathbb{Z}\setminus\mathbb{N})} & O_{\ell^2} & H_1^{-} & O_{\ell^2} \\ O_{\ell^2(\mathbb{Z}\setminus\mathbb{N})} & \frac{\Delta}{2} I_{\ell^2} & O_{\ell^2(\mathbb{Z}\setminus\mathbb{N})} & H_1 \end{pmatrix} = \mathbf{H}_{\Delta}^{-} \oplus \mathbf{H}_{\Delta},$$

with

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

and combining (5.8) with the min-max principle we get

$$\sigma(\mathbf{H}_{\Delta}^{-}) \subset ]-\infty, C_0 + |\Delta|].$$

Since  $\sigma(\tilde{\mathbf{J}}_{\Delta}) = \sigma(\mathbf{H}_{\Delta}^{-}) \cup \sigma(\mathbf{H}_{\Delta})$ , taking  $C_{\Delta} := 1 + C_0 + |\Delta|$  we obtain

$$\sigma(\tilde{\mathbf{J}}_{\Delta}) \cap [C_{\Delta}, \infty[ = \sigma(\mathbf{H}_{\Delta}) \cap [C_{\Delta}, \infty[,$$

which completes the proof of (5.11).

Step 3. Due to (5.11) it remains to prove

$$\lambda_j(\mathbf{J}_{\Delta}) - \lambda_j(\tilde{\mathbf{J}}_{\Delta}) = O(j^{-1}) \text{ as } j \rightarrow \infty. \quad (5.12)$$

We deduce (5.12) from (1.23) with  $\alpha = -1$  and it suffices to check

$$|\mathbf{J}_{\Delta}|(\mathbf{J}_{\Delta} - \tilde{\mathbf{J}}_{\Delta}) \in \mathcal{B}(\mathcal{H}), \quad |\tilde{\mathbf{J}}_{\Delta}|(\mathbf{J}_{\Delta} - \tilde{\mathbf{J}}_{\Delta}) \in \mathcal{B}(\mathcal{H}). \quad (5.13)$$

However combining (5.10) and (2.23) we obtain the first statement of (5.13). The second statement of (5.13) follows from (5.10) and  $(I + |\Lambda| \oplus |\Lambda|)^{-1} |\tilde{\mathbf{J}}_{\Delta}| \in \mathcal{B}(\mathcal{H})$ , which can be proved similarly as (2.23).  $\square$

### 5.3 End of the proof of Theorem 1.3

Due to Lemma 5.1 one has

$$\lambda_m(\mathbf{H}_{\Delta}) = \lambda_{m-\kappa(\Delta)}(\mathbf{J}_{\Delta}) + O(m^{-1}) \text{ as } m \rightarrow \infty, \quad (5.14)$$

and combining (5.14) with (4.1) we get the estimate

$$|\lambda_m(\mathbf{H}_{\Delta}) - d_{m-\kappa(\Delta)}| \leq C_{\Delta} m^{-1/2}. \quad (5.15)$$

If  $\Delta' \in \mathbb{R}$  then one also has

$$|\lambda_m(\mathbf{H}_{\Delta'}) - d_{m-\kappa(\Delta')}| \leq C_{\Delta'} m^{-1/2} \quad (5.16)$$

and the min-max principle ensures

$$|\lambda_m(\mathbf{H}_{\Delta}) - \lambda_m(\mathbf{H}_{\Delta'})| \leq \|\mathbf{H}_{\Delta} - \mathbf{H}_{\Delta'}\| = \frac{1}{2} |\Delta - \Delta'|. \quad (5.17)$$

Combining (5.15), (5.16) and (5.17), we get the inequality

$$|d_{m-\kappa(\Delta)} - d_{m-\kappa(\Delta')}| \leq (C_\Delta + C_{\Delta'})m^{-1/2} + \frac{1}{2}|\Delta - \Delta'|, \quad (5.18)$$

hence

$$\limsup_{m \rightarrow \infty} |d_{m-\kappa(\Delta)} - d_{m-\kappa(\Delta')}| \leq \frac{1}{2}|\Delta - \Delta'|. \quad (5.19)$$

If  $\kappa(\Delta) \neq \kappa(\Delta')$ , then (5.19) ensures  $\frac{1}{2}|\Delta - \Delta'| \geq c_0$  with

$$c_0 := \limsup_{n \rightarrow \infty} |d_{n+1} - d_n| > 0.$$

Thus  $|\Delta - \Delta'| < c_0$  implies  $\kappa(\Delta) = \kappa(\Delta')$ , i.e. the function  $\Delta \rightarrow \kappa(\Delta)$  is locally constant. We can conclude that  $\kappa(\Delta) = \kappa(0)$  for every  $\Delta \in \mathbb{R}$  and (5.15) takes the form

$$|\lambda_m(\mathbf{H}_\Delta) - d_{m-\kappa(0)}| \leq C_\Delta m^{-1/2}. \quad (5.20)$$

Combining (5.20) with

$$|\lambda_m(\mathbf{H}_0) - d_{m-\kappa(0)}| \leq C_0 m^{-1/2} \quad (5.21)$$

we obtain

$$|\lambda_m(\mathbf{H}_\Delta) - \lambda_m(\mathbf{H}_0)| \leq (C_\Delta + C_0)m^{-1/2}. \quad (5.22)$$

## 6 Appendix

### 6.1 Proof of Lemma 1.6

Let  $\mu \in \mathbb{R} \setminus (\sigma(A) \cup \sigma(B))$ . Then  $(I + |A|^{-\alpha})^{-1}|A - \mu|^{-\alpha}$  and  $(I + |B|^{-\alpha})^{-1}|B - \mu|^{-\alpha}$  are bounded. Since  $(A - B)(I + |A|^{-\alpha})$  and  $(A - B)(I + |B|^{-\alpha})$  are bounded, we get

$$(A - B)|A - \mu|^{-\alpha} \in \mathcal{B}(\mathcal{H}) \quad \text{and} \quad (A - B)|B - \mu|^{-\alpha} \in \mathcal{B}(\mathcal{H}). \quad (6.1)$$

Therefore we can use Theorem 1.5 with  $A - \mu$  instead of  $A$  and  $B - \mu$  instead of  $B$ , i.e. in the case (b) we obtain

$$\lambda_j(A - \mu) - \lambda_j(B - \mu) = O(|\lambda_j(A - \mu)|^\alpha) \text{ as } |j| \rightarrow \infty. \quad (6.2)$$

Since we obtain complete ordered eigenvalue sequences for  $A$  and  $B$  writing  $\lambda_j(A) = \lambda_j(A - \mu) + \mu$  and  $\lambda_j(B) = \lambda_j(B - \mu) + \mu$ , we deduce

$$\lambda_j(A) - \lambda_j(B) = O(|\lambda_j(A) - \mu|^\alpha) \text{ as } |j| \rightarrow \infty \quad (6.3)$$

and using  $|\lambda_j(A)| \rightarrow \infty$  as  $|j| \rightarrow \infty$  we get  $|\lambda_j(A) - \mu|^\alpha \sim |\lambda_j(A)|^\alpha$  as  $|j| \rightarrow \infty$ . This completes the proof of (1.23) and reasoning similarly we obtain (1.22) in the case of operators bounded from below.

## 6.2 Van der Corput Lemma

**Lemma 6.1. (J. van der Corput)** *Let  $c_0 > 0$  and assume that  $\Psi: [t_1, t_2] \rightarrow \mathbb{R}$  is smooth and its second derivative satisfies  $|\Psi''(\theta)| \geq c_0$  for  $t_1 < \theta < t_2$ . Then there is a constant  $C_0$  depending only on  $c_0$  such that the estimate*

$$\left| \int_{t_1}^{t_2} e^{i\mu\Psi(\theta)} b(\theta) \, d\theta \right| \leq \frac{C_0}{\sqrt{|\mu|}} \left( |b(t_1)| + \int_{t_1}^{t_2} |b'(\theta)| \, d\theta \right) \quad (6.4)$$

holds for all  $\mu \in \mathbb{R}^*$  and  $b \in C^1([t_1, t_2])$ .

*Proof.* See [120]. □

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# Chapitre 6

## Estimations améliorées des grandes valeurs propres pour le modèle de Rabi à deux photons avec un biais non résonnant

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# Improved Estimates of Large Eigenvalues for the two-photon Rabi Model with a non-resonant bias

**Abstract.** We consider the asymmetric quantum Rabi model under the assumption that the coupling constant  $g$  satisfies  $0 < g < 1/2$  and the static bias  $\epsilon$  is not a multiple of  $\sqrt{1 - 4g^2}$ . The spectrum of this model consists of two eigenvalue sequences  $(E_m^+)_{m=0}^\infty$ ,  $(E_m^-)_{m=0}^\infty$ , and we describe their asymptotic behaviour with an error estimate of the form  $O(m^{-1} \ln m)$  when  $m$  tends to infinity.

## 1 Statement of the result

In this Chapter we use notations introduced in Section 1 of Chapter 5. In particular,  $\ell^2(\mathbb{N})$  denotes the Hilbert space of square-summable sequences  $x : \mathbb{N} \rightarrow \mathbb{C}$  and

$$\ell^{2,1}(\mathbb{N}) := \{x \in \ell^2(\mathbb{N}) : \|x\|_{\ell^{2,1}(\mathbb{N})} < \infty\} \quad (1.1)$$

with

$$\|x\|_{\ell^{2,1}(\mathbb{N})} = \left( \sum_{j \in \mathbb{N}} (1 + j^2) |x(j)|^2 \right)^{1/2}. \quad (1.2)$$

The Pauli matrices are denoted  $\sigma_x$ ,  $\sigma_y$ ,  $\sigma_z$ , and we define  $\hat{a}^\dagger$  and  $\hat{a}$  (the creation and annihilation operator) as closed linear operators in  $\ell^2(\mathbb{N})$  satisfying

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

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

where  $\{e_n\}_{n \in \mathbb{N}}$  is the canonical basis of  $\ell^2(\mathbb{N})$ .

The operator  $\mathbf{H}_{0,\text{Rabi}}$  is defined as the linear mapping  $\mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \rightarrow \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  given by

$$\mathbf{H}_{0,\text{Rabi}} := I_2 \otimes \hat{a}^\dagger \hat{a} + \sigma_x \otimes \left( g(\hat{a}^2 + (\hat{a}^\dagger)^2) + \frac{\epsilon}{2} I_{\ell^2} \right), \quad (1.5)$$

where  $0 < g < 1/2$  is fixed and the operator  $\mathbf{H}_{\text{Rabi}}$  is defined as the linear mapping  $\mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \rightarrow \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  given by

$$\mathbf{H}_{\text{Rabi}} = \mathbf{H}_{0,\text{Rabi}} + \frac{1}{2} \Delta \sigma_z \otimes I_{\ell^2}. \quad (1.6)$$

In Chapter 5 we proved that there is an orthonormal basis in  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  of the form  $\{\mathbf{u}_m^-\}_{m \in \mathbb{N}} \cup \{\mathbf{u}_m^+\}_{m \in \mathbb{N}}$  such that

$$\mathbf{H}_{\text{Rabi}} \mathbf{u}_m^\pm = E_m^\pm \mathbf{u}_m^\pm \quad (1.7)$$

holds for every  $m \in \mathbb{N}$  and the eigenvalue sequences  $(E_m^-)_{m=0}^\infty$ ,  $(E_m^+)_{m=0}^\infty$ , satisfy the large  $m$  asymptotic formula

$$E_m^\pm = \beta m + \frac{1}{2}(\beta - 1) \pm \frac{\epsilon}{2} + O(m^{-1/2}), \quad (1.8)$$

where

$$\beta := \sqrt{1 - 4g^2}. \quad (1.9)$$

The purpose of this chapter is to prove

**Theorem 1.1.** *If  $\epsilon \notin \beta\mathbb{Z}$ , then the eigenvalue sequences  $(E_m^-)_{m=0}^\infty$ ,  $(E_m^+)_{m=0}^\infty$ , satisfy the large  $m$  asymptotic formula*

$$E_m^\pm = \beta m + \frac{1}{2}(\beta - 1) \pm \frac{\epsilon}{2} + O(m^{-1} \ln m), \quad (1.10)$$

where  $\beta$  is given by (1.9).

We recall that the result of Chapter 5 (i.e. the estimate (1.8)) is equivalent to the large  $n$  estimate

$$\lambda_n(\mathbf{H}_{\text{Rabi}}) - \lambda_n(\mathbf{H}_{0,\text{Rabi}}) = O(n^{-1/2}), \quad (1.11)$$

where  $(\lambda_n(\mathbf{H}_{\text{Rabi}}))_{n=0}^\infty$  (respectively  $(\lambda_n(\mathbf{H}_{0,\text{Rabi}}))_{n=0}^\infty$ ) is the non-decreasing sequence of eigenvalues of  $\mathbf{H}_{\text{Rabi}}$  (respectively  $\mathbf{H}_{0,\text{Rabi}}$ ), counting the multiplicities, while the assertion of Theorem 1.1 is equivalent to the fact that the estimate

$$\lambda_n(\mathbf{H}_{\text{Rabi}}) - \lambda_n(\mathbf{H}_{0,\text{Rabi}}) = O(n^{-1} \ln n) \quad (1.12)$$

holds if  $\epsilon \notin \beta\mathbb{Z}$ .

## 2 Basic notations and results from Chapter 5

**Notation 2.1.** (a) In the sequel we assume  $0 < g < 1/2$ ,  $\epsilon \geq 0$  and denote

$$l_0 = \max\{i \in \mathbb{N} : i \leq \epsilon/\beta\}. \quad (2.1)$$

(b) We introduce the linear mapping  $\ell^{2,1}(\mathbb{N}) \times \ell^{2,1}(\mathbb{N}) \rightarrow \ell^2(\mathbb{N}) \times \ell^2(\mathbb{N})$  by

$$\mathbf{H} = \begin{pmatrix} H_{-1} & \frac{\Delta}{2} I_{\ell^2(\mathbb{N})} \\ \frac{\Delta}{2} I_{\ell^2(\mathbb{N})} & H_1 \end{pmatrix} \quad (2.2)$$

where  $H_{\pm 1} : \ell^{2,1}(\mathbb{N}) \rightarrow \ell^2(\mathbb{N})$  are defined by

$$H_{\pm 1} := \hat{a}^\dagger \hat{a} \pm g(\hat{a}^2 + (\hat{a}^\dagger)^2) \pm \frac{1}{2}\epsilon. \quad (2.3)$$

**Proposition 2.2.** (a)  $\mathbf{H}_{\text{Rabi}}$  is similar to  $\mathbf{H}$  and  $\mathbf{H}_{0,\text{Rabi}}$  is similar to  $\mathbf{H}_0 = H_{-1} \oplus H_1$ .

(b) Let  $(d_n)_{n=0}^\infty$  be the sequence defined as follows

$$d_n^0 = \frac{1}{2}(\beta - 1) + \beta n - \frac{\epsilon}{2} \text{ for } n = 0, \dots, l_0, \quad (2.4)$$

$$d_{l_0+2i}^0 = \frac{1}{2}(\beta - 1) + \beta(l_0 + i) - \frac{\epsilon}{2} \text{ for } i \in \mathbb{N}, \quad (2.5)$$

$$d_{l_0+1+2i}^0 = \frac{1}{2}(\beta - 1) + \beta i + \frac{\epsilon}{2} \text{ for } i \in \mathbb{N}. \quad (2.6)$$

Then  $(d_n^0)_{n=0}^\infty$  is the non-decreasing sequence of eigenvalues of  $\mathbf{H}_0$ , counting multiplicities.



*Proof.* See Section 1.4 and 2.3 of Chapter 5.  $\square$

**Notation 2.3.** a) We denote by  $\ell^2(\mathbb{Z})$  the complex Hilbert space of square-summable sequences  $x : \mathbb{Z} \rightarrow \mathbb{C}$  equipped with the scalar product

$$\langle x, y \rangle_{\ell^2(\mathbb{Z})} = \sum_{j \in \mathbb{Z}} \overline{x(j)} y(j) \quad (2.7)$$

and the norm  $\|x\|_{\ell^2(\mathbb{Z})} := \langle x, x \rangle_{\ell^2(\mathbb{Z})}^{1/2}$ . We identify  $\ell^2(\mathbb{N})$  with the subspace

$$\{x \in \ell^2(\mathbb{Z}) : x(j) = 0 \text{ for } j \in \mathbb{Z} \setminus \mathbb{N}\}$$

and denote by  $\{e_j\}_{j \in \mathbb{Z}}$  the canonical basis of  $\ell^2(\mathbb{Z})$  (i.e.  $e_i(j) = \delta_{i,j}$  for  $i, j \in \mathbb{Z}$ ).

(b) We denote by  $\Lambda$  the self-adjoint operator in  $\ell^2(\mathbb{Z})$  defined on

$$\ell^{2,1}(\mathbb{Z}) := \{x \in \ell^2(\mathbb{Z}) : \sum_{j \in \mathbb{Z}} j^2 |x(j)|^2 < \infty\} \quad (2.8)$$

by the formula  $\Lambda e_j = j e_j$  for  $j \in \mathbb{Z}$ .

(c) We define  $S \in \mathcal{B}(\ell^2(\mathbb{Z}))$  as the shift given by the formula  $S e_j := e_{j+1}$  for  $j \in \mathbb{Z}$ .

(d) We introduce the linear mapping  $\ell^{2,1}(\mathbb{Z}) \times \ell^{2,1}(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})$  by

$$\mathbf{J} = \begin{pmatrix} J_{-1} & \frac{\Delta}{2} I_{\ell^2(\mathbb{Z})} \\ \frac{\Delta}{2} I_{\ell^2(\mathbb{Z})} & J_1 \end{pmatrix} \quad (2.9)$$

where  $J_{\pm 1} : \ell^{2,1}(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z})$  are defined by

$$J_\nu = \Lambda + \nu g \left( S^2 \left( \Lambda + \frac{3}{2} \right) + \left( \Lambda + \frac{3}{2} \right) S^2 \right) + \frac{1}{2} \nu \epsilon. \quad (2.10)$$

We can also write

$$\mathbf{V} = \frac{1}{2} \Delta \begin{pmatrix} 0_{\ell^2(\mathbb{Z})} & I_{\ell^2(\mathbb{Z})} \\ I_{\ell^2(\mathbb{Z})} & 0_{\ell^2(\mathbb{Z})} \end{pmatrix}, \quad (2.11)$$

where  $0_{\ell^2(\mathbb{Z})}$  denotes the null mapping in  $\ell^2(\mathbb{Z})$  and

$$\mathbf{J}_0 = J_{-1} \oplus J_1.$$

**Proposition 2.4.** (a) *There is an orthonormal basis  $(\mathbf{v}_j^0)_{j \in \mathbb{Z}}$  such that*

$$\mathbf{J}_0 \mathbf{v}_j^0 = d_j \mathbf{v}_j^0, \quad (2.12)$$

where the eigenvalue sequence  $(d_j)_{j \in \mathbb{Z}}$  satisfies

$$d_{2i} = \frac{1}{2}(\beta - 1) + \beta i - \frac{\epsilon}{2}, \quad (2.13)$$

$$d_{2i+1} = \frac{1}{2}(\beta - 1) + \beta(i - l_0) + \frac{\epsilon}{2}. \quad (2.14)$$

(b) There exist  $\hat{C}$ ,  $\hat{c} > 0$  and  $n_0 \in \mathbb{N}$  such that

$$|j - k| < \hat{c}n \Rightarrow |\langle \mathbf{v}_j^0, \mathbf{V}\mathbf{v}_k^0 \rangle_{\ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})}| \leq \hat{C}n^{-1/2} \quad (2.15)$$

holds if  $n > n_0$  and for every  $k \in \mathbb{Z}$  one has

$$\langle \mathbf{v}_k^0, \mathbf{V}\mathbf{v}_k^0 \rangle_{\ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})} = 0. \quad (2.16)$$

*Proof.* (a) See Section 2.5 in Chapter 5.

(b) As in the proof of Lemma 4.4 in Chapter 5 we denote

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

for  $i, j \in \mathbb{Z}$  and we get

$$\begin{aligned} V(k, k) &= 0 \text{ for } k \in \mathbb{Z}, \\ V(2i, 2j + 1) &\stackrel{\Delta}{=} \frac{1}{2} \gamma_{i, j - l_0} \text{ for } i, j \in \mathbb{Z}, \end{aligned}$$

where  $\gamma_{j, k}$  is defined in Notation 3.3, Chapter 5. It is easy to check that (2.15) follows from the assertion of Lemma 3.4, Chapter 5.  $\square$

**Proposition 2.5.** (a) We can find  $(\lambda_j(\mathbf{J}))_{j \in \mathbb{Z}}$ , a non-decreasing eigenvalue sequence of  $\mathbf{J}$ , counting the multiplicities, such that one has the large  $j$  asymptotic estimate

$$\lambda_j(\mathbf{J}) = d_j + O(j^{-1/2}). \quad (2.17)$$

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

$$\lambda_n(\mathbf{H}) = \lambda_{n+l_0}(\mathbf{J}) + O(n^{-1}). \quad (2.18)$$

*Proof.* (a) See Proposition 4.1 in Chapter 5.

(b) Due to Lemma 5.1 in Chapter 5, there exists  $\kappa \in \mathbb{Z}$  such that one has the large  $n$  estimate

$$\lambda_n(\mathbf{H}) = \lambda_{n+\kappa}(\mathbf{J}) + O(n^{-1}) \quad (2.19)$$

and in Section 5.3 in Chapter 5, we prove that one has also

$$\lambda_n(\mathbf{H}_0) = \lambda_{n+\kappa}(\mathbf{J}_0) + O(n^{-1}). \quad (2.20)$$

However, it is easy to check that  $d_n^0 = d_{n+l_0}$  holds if  $n \geq l_0$  and (2.20) gives

$$d_{n+l_0} = d_n^0 = d_{n+\kappa} + O(n^{-1}). \quad (2.21)$$

It remains to observe that (2.21) implies  $\kappa = l_0$ . Indeed, if  $\kappa \neq l_0$ , then

$$\limsup_{n \rightarrow \infty} |d_{n+l_0} - d_{n+\kappa}| > 0$$

is a contradiction with (2.21).  $\square$

**Corollary 2.6.** *Instead of (1.12), it suffices to prove that the large  $n$  estimate*

$$\lambda_n(\mathbf{J}) = \lambda_n(\mathbf{J}_0) + O(n^{-1} \ln n) \quad (2.22)$$

holds under the assumption  $\epsilon \notin \beta\mathbb{Z}$ .

*proof.* Combining (2.18) with (2.12), we get

$$\lambda_n(\mathbf{H}) - \lambda_n(\mathbf{H}_0) = O(n^{-1} \ln n),$$

which is equivalent to (1.12).  $\square$

### 3 Main ideas of the proof

If  $L : \mathcal{D}(L) \rightarrow \mathcal{V}$  is a linear mapping defined on a dense subspace of the complex Banach space  $\mathcal{V}$ , then  $\sigma(L)$  denotes the spectrum of  $L$ . The algebra of bounded operators on  $\mathcal{V}$  is denoted  $\mathcal{B}(\mathcal{V})$ . If  $L_n, L'_n$  are linear mappings defined on a dense subspace of  $\mathcal{V}$  and  $L_n - L'_n$  can be extended to a bounded operator  $\mathcal{V}$ , then  $\|L_n - L'_n\|_{\mathcal{B}(\mathcal{V})}$  denotes 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  $\|L_n - L'_n\|_{\mathcal{B}(\mathcal{V})} \leq C\eta_n$  for all  $n \geq n_0$ .

If  $x_n, x'_n \in \mathcal{V}$ , then we write  $x_n = y_n + O(\eta_n)$  if and only if we can find  $C > 0, n_0 \in \mathbb{N}$ , such that  $\|x_n - x'_n\|_{\mathcal{V}} \leq C\eta_n$  holds for all  $n \geq n_0$ .

If  $T \in \mathcal{B}(\ell^2(\mathbb{Z}))$ , then we denote

$$T(j, k) := \langle e_j, T e_k \rangle_{\ell^2(\mathbb{Z})} \text{ for } j, k \in \mathbb{Z}. \quad (3.1)$$

Let  $\{\mathbf{v}_j^0\}_{j \in \mathbb{Z}}$  be as in Proposition 2.4 and define  $J$  as the self-adjoint operators in  $\ell^2(\mathbb{Z})$  given by

$$J = U\mathbf{J}U^{-1}, \quad (3.2)$$

where  $U : \ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z})$  is the isometric isomorphism satisfying  $U\mathbf{v}_j^0 = e_j$  for every  $j \in \mathbb{Z}$ . Then  $J = D + V$  holds with  $D = \text{diag}(d_j)_{j \in \mathbb{Z}}$ , i.e.

$$D e_j = d_j e_j \text{ for } j \in \mathbb{Z}, \quad (3.3)$$

and

$$V = U\mathbf{V}U^{-1}. \quad (3.4)$$

In the sequel we denote

$$V(j, k) := \langle e_j, V e_k \rangle_{\ell^2(\mathbb{Z})} = \langle \mathbf{v}_j^0, \mathbf{V}\mathbf{v}_k^0 \rangle_{\ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})}, \quad (3.5)$$

we fix  $\hat{C}, \hat{c} > 0$  such that (2.15) holds, i.e.

$$|j - k| < \hat{c}|k| \Rightarrow |V(j, k)| \leq \hat{C}|k|^{-1/2} \quad (3.6)$$

and  $(\lambda_j(J))_{j \in \mathbb{Z}}$  is the eigenvalue sequence satisfying the large  $j$  estimate

$$\lambda_j(J) = d_j + O(j^{-1/2}) \quad (3.7)$$

(i.e.  $\lambda_j(J) = \lambda_j(\mathbf{J})$  where  $(\lambda_j(\mathbf{J}))_{j \in \mathbb{Z}}$  is as in Proposition 2.5(a)).

We observe that the assumption  $\epsilon \notin \mathbb{Z}$  insures the fact that

$$c_1 := \inf_{j \in \mathbb{Z}} (d_{j+1} - d_j) > 0 \quad (3.8)$$

and using (3.7) we know that there is  $n_1 \in \mathbb{N}$  such that for  $n \geq n_1$  one has

$$\{\lambda_n(J)\} = \sigma(J) \cap ]d_n - \frac{1}{2}c_1, d_n + \frac{1}{2}c_1[. \quad (3.9)$$

In Section 4 we define a sequence of self-adjoint, bounded operators  $(Q_n)_{n=0}^\infty$  and in Section 5 we introduce

$$J'_n := e^{-iQ_n} J e^{iQ_n}.$$

Then for  $n \geq n_1$  we still have

$$\{\lambda_n(J)\} = \sigma(J'_n) \cap ]d_n - \frac{1}{2}c_1, d_n + \frac{1}{2}c_1[ \quad (3.10)$$

and in Section 5 we deduce (2.22) from (3.10), combining the structure of  $J'_n$  with the Kato-Temple estimate (see Theorem 2.1 in Chapter 3).

#### 4 Operators $R_n$ and $Q_n$

In the sequel we consider the orthogonal decomposition

$$\ell^2(\mathbb{Z}) = \widehat{\mathcal{H}}_n \oplus \widetilde{\mathcal{H}}_n, \quad (4.1)$$

where

$$\widehat{\mathcal{H}}_n := \mathbb{C}e_n, \quad \widetilde{\mathcal{H}}_n := (\mathbb{C}e_n)^\perp. \quad (4.2)$$

Let  $\widehat{\Pi}_n \in \mathcal{B}(\ell^2(\mathbb{Z}))$  denote the orthogonal projection on  $\mathbb{C}e_n$  and  $\widetilde{\Pi}_n := I - \widehat{\Pi}_n$ .

We introduce

$$R_n := \widetilde{\Pi}_n V \widehat{\Pi}_n + \widehat{\Pi}_n V \widetilde{\Pi}_n. \quad (4.3)$$

and observe that  $R_n(j, k) \neq 0 \Rightarrow$  (either  $j = n \neq k$  or  $k = n \neq j$ ). Moreover,  $V(n, n) = 0$  ensures  $\widehat{\Pi}_n V \widehat{\Pi}_n = 0$  and (4.3) can be written in the form

$$R_n = V - \widetilde{\Pi}_n V \widetilde{\Pi}_n. \quad (4.4)$$

Since  $R_n(j, k) \neq 0 \Rightarrow j \neq k \Rightarrow d_j \neq d_k$ , we can define

$$Q_n(j, k) := \begin{cases} -\frac{R_n(j, k)}{i(d_j - d_k)} & \text{if } R_n(j, k) \neq 0 \\ 0 & \text{if } R_n(j, k) = 0 \end{cases} \quad (4.5)$$

**Lemma 4.1.** (a) *There is  $Q_n \in \mathcal{B}(\ell^2(\mathbb{Z}))$  satisfying  $\langle e_j, Q_n e_k \rangle_{\ell^2(\mathbb{Z})} = Q_n(j, k)$  for all  $j, k \in \mathbb{Z}$  and*

$$\|Q_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} = O(n^{-1/2}). \quad (4.6)$$

(b)  $\ell^{2,1}(\mathbb{Z})$  is an invariant subspace of  $Q_n$  and one has

$$[D, iQ_n] = -R_n. \quad (4.7)$$

(c)  $\ell^{2,1}(\mathbb{Z})$  is an invariant subspace of  $e^{itQ_n}$  and  $t \rightarrow e^{itQ_n}x$  is of class  $C^\infty(\mathbb{R}; \ell^{2,1}(\mathbb{Z}))$  if  $x \in \ell^{2,1}(\mathbb{Z})$ .

*Proof.* (a) We observe that  $Q_n(n, j) = \overline{Q_n(j, n)}$  and using

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

we can estimate

$$\|Q_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} \leq \|Q_n \widehat{\Pi}_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} + \|\widehat{\Pi}_n Q_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} = 2\|Q_n \widehat{\Pi}_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} = 2\|Q_n e_n\|_{\ell^2(\mathbb{Z})}.$$

It is clear that the assumption  $\epsilon \notin \beta\mathbb{Z}$  allows us to find  $c_0 > 0$  such that

$$j \neq k \Rightarrow |d_j - d_k| \geq c_0 \langle j - k \rangle, \quad (4.8)$$

where  $\langle s \rangle := (1 + s^2)^{1/2}$  and

$$\|Q_n e_n\|_{\ell^2(\mathbb{Z})}^2 = \sum_{j \in \mathbb{Z}} |Q_n(j, n)|^2 \leq c_0^{-2} \sum_{j \in \mathbb{Z}} \frac{|V(j, n)|^2}{\langle j - n \rangle^2} \leq c_0^{-2} (M_n + M'_n)$$

holds with

$$M_n := \sum_{\{j \in \mathbb{Z}: |j-n| < \hat{c}n\}} \frac{|V(j, n)|^2}{\langle j - n \rangle^2} \leq \hat{c}^2 n^{-1} \sum_{m \in \mathbb{Z}} \langle m - n \rangle^{-2} \leq C_1 n^{-1}$$

due to (2.15) and

$$M'_n := \sum_{\{j \in \mathbb{Z}: |j-n| \geq \hat{c}n\}} \frac{|V(j, n)|^2}{\langle j - n \rangle^2} \leq \hat{c}^{-2} n^{-2} \sum_{j \in \mathbb{Z}} |V(j, n)|^2 = \hat{c}^{-2} n^{-2} \|V e_n\|_{\ell^2(\mathbb{Z})}^2 \leq C_2 n^{-2}.$$

We obtain the assertions (b) and (c), reasoning similarly as in the proof of Lemma 4.1 in Chapter 3.  $\square$

## 5 Proof of Theorem 1.1

In the sequel  $Q_n$  and  $R_n$  are as in Lemma 4.1.

**Step 1.** We denote  $J'_n := e^{-iQ_n} J e^{iQ_n}$ . Then, reasoning as in Section 5, Chapter 3, we obtain

$$J'_n = D + V - R_n + W_n + O(\|Q_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))}^2) \quad (5.1)$$

with

$$W_n = [V, iQ_n] + \frac{1}{2}[[D, iQ_n], iQ_n] = [V, iQ_n] - \frac{1}{2}[R_n, iQ_n]. \quad (5.2)$$

**Step 2.** Let  $W_n$  be given by (5.2). We claim that one has the large  $n$  estimate

$$W_n(n, n) = O(n^{-1} \ln n). \quad (5.3)$$

Indeed,  $W_n = [V_n^0, iQ_n]$  holds with  $V_n^0 := V - \frac{1}{2}R_n$  and

$$|V_n^0(j, k)| \leq |V(j, k)| \text{ for all } j, k \in \mathbb{Z}, \quad (5.4)$$

hence using (5.4) and (4.8), we can estimate

$$|(V_n^0 Q_n)(n, n)| \leq \sum_{m \in \mathbb{Z}} |V(n, m) Q_n(m, n)| \leq c_0^{-1} \sum_{m \in \mathbb{Z}} \frac{|V(m, n)|^2}{\langle m - n \rangle} \leq c_0^{-1} (M_n + M'_n) \quad (5.5)$$

with

$$M_n := \sum_{\{m \in \mathbb{Z}: |m-n| < \hat{c}n\}} \frac{|V(n, m)|^2}{\langle m - n \rangle} \leq \hat{C}^2 n^{-1} \sum_{\{m \in \mathbb{Z}: |m-n| < \hat{c}n\}} \langle m - n \rangle^{-1/2} \leq C_1 n^{-1} \ln n$$

due to (2.15) and

$$M'_n := \sum_{\{m \in \mathbb{Z}: |m-n| \geq \hat{c}n\}} \frac{|V(n, m)|^2}{\langle m - n \rangle} \leq \hat{c}^{-1} n^{-1} \sum_{j \in \mathbb{Z}} |V(j, n)|^2 = \hat{c}^{-1} n^{-1} \|V e_n\|_{\ell^2(\mathbb{Z})}^2 \leq C_2 n^{-1}.$$

**Step 3.** We claim that one has the large  $n$  estimates

$$\langle e_n, J'_n e_n \rangle_{\ell^2(\mathbb{Z})} = d_n + O(n^{-1} \ln n) \quad (5.6)$$

and

$$(J'_n - \langle e_n, J'_n e_n \rangle_{\ell^2(\mathbb{Z})}) e_n = O(n^{-1/2}). \quad (5.7)$$

Indeed, using  $\|Q_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} = O(n^{-1/2})$  and  $V - R_n = \tilde{\Pi}_n V \tilde{\Pi}_n$  in (5.1), we find

$$J'_n e_n = (D + \tilde{\Pi}_n V \tilde{\Pi}_n + W_n) e_n + O(n^{-1}) = d_n e_n + W_n e_n + O(n^{-1}), \quad (5.8)$$

hence

$$\langle e_n, J'_n e_n \rangle_{\ell^2(\mathbb{Z})} = d_n + \langle e_n, W_n e_n \rangle_{\ell^2(\mathbb{Z})} + O(n^{-1})$$

and (5.6) follows from (5.3). Moreover, (5.6) implies

$$(J'_n - \langle e_n, J'_n e_n \rangle_{\ell^2(\mathbb{Z})}) e_n = (J'_n - d_n) e_n + O(n^{-1} \ln n) \quad (5.9)$$

and (5.8) ensures

$$(J'_n - d_n) e_n = W_n e_n + O(n^{-1}). \quad (5.10)$$

Thus (5.7) follows from (5.9), (5.10) and

$$\|W_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} \leq (2\|V\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} + \|R_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))}) \|Q_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} = O(n^{-1/2}).$$

**End of the proof of Theorem 1.1.** Let  $n_1$  be such that (3.10) holds for  $n \geq n_1$ . Due to (5.6) there is  $n_0 \in \mathbb{N}$  such that for  $n \geq n_0$  one has

$$\langle e_n, J'_n e_n \rangle_{\ell^2(\mathbb{Z})} \in ]d_n - \frac{1}{4}c_1, d_n + \frac{1}{4}c_1[.$$

If  $n \geq \max\{n_0, n_1\}$ , then  $J'_n$  satisfies the assumptions of Kato-Temple estimate (see Theorem 2.1 in Chapter 3) with  $L = J'_n$ ,  $x = e_n$  and  $]d', d''[ = ]d_n - \frac{1}{2}c_1, d_n + \frac{1}{2}c_1[$ . Therefore (2.9) in Chapter 3 gives

$$|\lambda_n(J'_n) - \langle e_n, J'_n e_n \rangle_{\ell^2(\mathbb{Z})}| \leq 4c_1^{-1} \| (J'_n - \langle e_n, J'_n e_n \rangle_{\ell^2(\mathbb{Z})}) e_n \|^2 = O(n^{-1}). \quad (5.11)$$

Combining (5.11) with (5.6) we get  $\lambda_n(J'_n) = d_n + O(n^{-1} \ln n)$ .

# Formule asymptotique à trois termes pour les valeurs propres du modèle de Rabi quantique à deux photons avec un biais résonant

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# Three-term Asymptotic Formula for Eigenvalues of the two-photon quantum Rabi model with a resonant bias

**Abstract.** We consider the asymmetric quantum Rabi model under the assumption that the coupling constant  $g$  satisfies  $0 < g < 1/2$  and the static bias  $\epsilon$  is a multiple of  $\sqrt{1 - 4g^2}$ . The spectrum of this model consists of two eigenvalue sequences  $(E_m^+)_{m=0}^\infty$ ,  $(E_m^-)_{m=0}^\infty$ , and we obtain the three-term asymptotic formula with an error estimate of the form  $O(m^{-1} \ln m)$  when  $m$  tends to infinity.

## 1 Statement of the result

In this Chapter we use notations introduced in Section 1 of Chapter 5, i.e.  $\mathbf{H}_{0,\text{Rabi}}$  is defined as the linear mapping  $\mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \rightarrow \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  given by

$$\mathbf{H}_{0,\text{Rabi}} := I_2 \otimes \hat{a}^\dagger \hat{a} + \sigma_x \otimes \left( g(\hat{a}^2 + (\hat{a}^\dagger)^2) + \frac{\epsilon}{2} I_{\ell^2} \right), \quad (1.1)$$

where  $0 < g < 1/2$  is fixed and the operator  $\mathbf{H}_{\text{Rabi}}$  is defined as the linear mapping  $\mathbb{C}^2 \otimes \ell^{2,1}(\mathbb{N}) \rightarrow \mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  given by

$$\mathbf{H}_{\text{Rabi}} = \mathbf{H}_{0,\text{Rabi}} + \frac{1}{2} \Delta \sigma_z \otimes I_{\ell^2}. \quad (1.2)$$

In Chapter 5 we proved that there is an orthonormal basis in  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  of the form  $\{\mathbf{u}_m^-\}_{m \in \mathbb{N}} \cup \{\mathbf{u}_m^+\}_{m \in \mathbb{N}}$  such that

$$\mathbf{H}_{\text{Rabi}} \mathbf{u}_m^\pm = E_m^\pm \mathbf{u}_m^\pm \quad (1.3)$$

holds for every  $m \in \mathbb{N}$  and the eigenvalue sequences  $(E_m^-)_{m=0}^\infty$ ,  $(E_m^+)_{m=0}^\infty$ , satisfy the large  $m$  asymptotic formula

$$E_m^\pm = \beta m + \beta_0 \pm \frac{1}{2} \epsilon + O(m^{-1/2}), \quad (1.4)$$

where

$$\beta := \sqrt{1 - 4g^2}, \quad \beta_0 := \frac{1}{2}(\beta - 1). \quad (1.5)$$

The purpose of this Chapter is to prove

**Theorem 1.1.** *Assume that  $l_0 := \epsilon/\beta \in \mathbb{N}$ . Then the eigenvalue sequences  $(E_m^-)_{m \in \mathbb{N}}$  and  $(E_m^+)_{m \in \mathbb{N}}$  satisfy the asymptotic estimates*

$$E_{i+l_0}^- = \beta i + \beta_0 + \frac{1}{2} \epsilon - |\mathbf{r}_i| + O(i^{-1} \ln i), \quad (1.6)$$

$$E_i^+ = \beta i + \beta_0 + \frac{1}{2} \epsilon + |\mathbf{r}_i| + O(i^{-1} \ln i), \quad (1.7)$$

where  $\beta$ ,  $\beta_0$  are given by (1.5) and

$$\begin{aligned} \mathbf{r}_i &:= 0 \text{ if } l_0 \text{ is odd} \\ \mathbf{r}_i &:= i^{-1/2} \frac{\Delta}{2} \sqrt{\frac{\beta}{\pi g}} \cos \left( (2\alpha - \frac{\pi}{2})(i + l_0) + (1 - l_0)\alpha \right) \text{ if } l_0 \text{ is even} \end{aligned} \quad (1.8)$$

with

$$\alpha = \arctan \sqrt{\frac{1 - 2g}{1 + 2g}}. \quad (1.9)$$

## 2 Main ingredients of the proof

In the sequel we assume  $0 < g < 1/2$ , we denote  $l_0 := \epsilon/\beta \in \mathbb{N}$  (where  $\beta := \sqrt{1 - 4g^2}$ ) and we keep notations introduced in Chapter 5. In particular,

(a) we define  $J_{\pm 1} : \ell^{2,1}(\mathbb{Z}) \rightarrow \ell^2(\mathbb{N})$  by

$$J_{\nu} = \Lambda + \nu g \left( S^2 \left( \Lambda + \frac{3}{2} \right) + \left( \Lambda + \frac{3}{2} \right) S^{-2} \right) + \frac{1}{2} \nu \epsilon, \quad (2.1)$$

where  $S \in \mathcal{B}(\ell^2(\mathbb{Z}))$  is the shift defined by  $Se_j := e_{j+1}$  for  $j \in \mathbb{Z}$ ,

(b) we define  $\mathbf{J} : \ell^{2,1}(\mathbb{Z}) \times \ell^{2,1}(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})$  by

$$\mathbf{J} := J_{-1} \oplus J_1 + \mathbf{V} \quad (2.2)$$

where

$$\mathbf{V} := \frac{1}{2} \Delta \begin{pmatrix} 0_{\ell^2(\mathbb{Z})} & I_{\ell^2(\mathbb{Z})} \\ I_{\ell^2(\mathbb{Z})} & 0_{\ell^2(\mathbb{Z})} \end{pmatrix} \quad (2.3)$$

(c) we introduce sequence the  $(d_j)_{j \in \mathbb{Z}}$  given by

$$d_{2i} = d_{2i+1} = \beta_0 + \beta i - \frac{1}{2} \epsilon = \beta_0 + \beta(i - l_0) + \frac{1}{2} \epsilon. \quad (2.4)$$

Then one has

**Proposition 2.1.** *It suffices to prove that there exists  $(\lambda_j(\mathbf{J}))_{j \in \mathbb{Z}}$ , a non-decreasing eigenvalue sequence of  $\mathbf{J}$ , counting the multiplicities, such that one has the large  $i$  asymptotic estimates*

$$\lambda_{2i}(\mathbf{J}) = d_{2i} - |\mathbf{r}_{i-l_0}| + O(i^{-1} \ln i), \quad (2.5)$$

$$\lambda_{2i+1}(\mathbf{J}) = d_{2i} + |\mathbf{r}_{i-l_0}| + O(i^{-1} \ln i). \quad (2.6)$$

*Proof.* The estimates (2.5)-(2.6) imply the estimate (2.17) in Proposition 2.5(a), Chapter 6 and Proposition 2.5(b), Chapter 6 implies the large  $n$  estimate

$$\lambda_n(\mathbf{H}) = \lambda_{n+l_0}(\mathbf{J}) + O(n^{-1}), \quad (2.7)$$

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

$$E_n^- = \lambda_n(\mathbf{H}) \text{ for } n = 0, \dots, l_0,$$

$$E_{i+l_0}^- = \lambda_{2i+l_0}(\mathbf{H}) \text{ for } i \in \mathbb{N},$$

$$E_i^+ = \lambda_{2i+1+l_0}(\mathbf{H}) \text{ for } i \in \mathbb{N}.$$

Then (2.7) implies

$$E_{i+l_0}^- = \lambda_{2(i+l_0)}(\mathbf{J}) + O(i^{-1}),$$

$$E_i^+ = \lambda_{2(i+l_0)+1}(\mathbf{J}) + O(i^{-1})$$

and (2.5)-(2.6) ensure

$$E_{i+l_0}^- = d_{2(i+l_0)} - |\mathfrak{r}_i| + O(i^{-1} \ln i),$$

$$E_i^+ = d_{2(i+l_0)} + |\mathfrak{r}_i| + O(i^{-1} \ln i),$$

i.e. we get (1.6)-(1.7).  $\square$

Let  $\{\mathbf{v}_j^0\}_{j \in \mathbb{Z}}$  be as in Notation 2.8, Chapter 5 and let  $J$  be the self-adjoint operators in  $\ell^2(\mathbb{Z})$  given by

$$J = U\mathbf{J}U^{-1}, \quad (2.8)$$

where  $U : \ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z})$  is the isometric isomorphism satisfying  $U\mathbf{v}_j^0 = e_j$  for every  $j \in \mathbb{Z}$ . Then

$$J = D + V, \quad (2.9)$$

holds with  $D = \text{diag}(d_j)_{j \in \mathbb{Z}}$ , i.e.

$$De_j = d_j e_j \text{ for } j \in \mathbb{Z}, \quad (2.10)$$

and

$$V = U\mathbf{V}U^{-1}. \quad (2.11)$$

In the sequel we denote

$$V(j, k) := \langle e_j, V e_k \rangle_{\ell^2(\mathbb{Z})} = \langle \mathbf{v}_j^0, \mathbf{V}\mathbf{v}_k^0 \rangle_{\ell^2(\mathbb{Z}) \times \ell^2(\mathbb{Z})}, \quad (2.12)$$

we fix  $\hat{C}$ ,  $\hat{c} > 0$  such that the inequality (3.6) in Chapter 6 holds, i.e.

$$|j - k| < \hat{c}|k| \Rightarrow |V(j, k)| \leq \hat{C}|k|^{-1/2} \quad (2.13)$$

and  $(\lambda_j(J))_{j \in \mathbb{Z}}$  is the eigenvalue sequence satisfying the large  $j$  estimate

$$\lambda_j(J) = d_j + O(j^{-1/2}) \quad (2.14)$$

(i.e.  $\lambda_j(J) = \lambda_j(\mathbf{J})$  where  $(\lambda_j(\mathbf{J}))_{j \in \mathbb{Z}}$  is as in Proposition 4.1, Chapter 5.

We will use the assumption  $\epsilon = l_0 \in \mathbb{N}$  to prove the large  $i$  estimates

$$\lambda_{2i}(J) = d_{2i} - |V(2i, 2i + 1)| + O(i^{-1} \ln i), \quad (2.15)$$

$$\lambda_{2i+1}(J) = d_{2i} + |V(2i, 2i + 1)| + O(i^{-1} \ln i). \quad (2.16)$$

It is clear that the estimates (2.5)-(2.6) follow from (2.15)-(2.16) and

**Proposition 2.2.** *One has the large  $i$  estimate*

$$|V(2i, 2i + 1)| = |\mathfrak{r}_{i-l_0}| + O(i^{-1}), \quad (2.17)$$

where  $\mathfrak{r}_i$  is given by (1.8).

*Proof.* See Section 5.3. □

In order to prove the estimates (2.15)-(2.16) we consider the orthogonal decomposition

$$\ell^2(\mathbb{Z}) = \widehat{\mathcal{H}}_n \oplus \widetilde{\mathcal{H}}_n \quad (2.18)$$

where  $n \in 2\mathbb{Z}$  and

$$\widehat{\mathcal{H}}_n := \text{span}\{e_n, e_{n+1}\}, \quad \widetilde{\mathcal{H}}_n := \widehat{\mathcal{H}}_n^\perp. \quad (2.19)$$

In the sequel  $\widehat{\Pi}_n \in \mathcal{B}(\ell^2(\mathbb{Z}))$  denotes the orthogonal projection on  $\widehat{\mathcal{H}}_n$  and  $\widetilde{\Pi}_n := I - \widehat{\Pi}_n$ . We use the decomposition (2.18) to express  $V$  in the matrix form

$$V = \begin{pmatrix} \widehat{V}_n & \check{R}_n^* \\ \check{R}_n & \widetilde{V}_n \end{pmatrix} \quad (2.20)$$

where

$$\widehat{V}_n := \widehat{\Pi}_n V|_{\widehat{\mathcal{H}}_n} \in \mathcal{B}(\widehat{\mathcal{H}}_n), \quad (2.21)$$

$$\widetilde{V}_n := \widetilde{\Pi}_n V|_{\widetilde{\mathcal{H}}_n} \in \mathcal{B}(\widetilde{\mathcal{H}}_n), \quad (2.22)$$

$$\check{R}_n := \widetilde{\Pi}_n V|_{\widehat{\mathcal{H}}_n} \in \mathcal{B}(\widehat{\mathcal{H}}_n, \widetilde{\mathcal{H}}_n), \quad (2.23)$$

$$\check{R}_n^* := \widehat{\Pi}_n V|_{\widetilde{\mathcal{H}}_n} \in \mathcal{B}(\widetilde{\mathcal{H}}_n, \widehat{\mathcal{H}}_n). \quad (2.24)$$

Moreover, we can identify  $\widehat{V}_n$  with its matrix in the basis  $\{e_n, e_{n+1}\}$ , i.e. we can write

$$\widehat{V}_n = \begin{pmatrix} 0 & V(n, n+1) \\ V(n+1, n) & 0 \end{pmatrix}. \quad (2.25)$$

We will prove

**Proposition 2.3.** *There exists a sequence of unitary operators  $(U_n)_{n \in \mathbb{N}}$  such that the large  $n$  estimate*

$$U_n^{-1} J U_n = D + \widehat{V}_n \oplus \widetilde{V}_n' + O(n^{-1} \ln n) \quad (2.26)$$

holds if  $n \in 2\mathbb{N}$ ,  $\widehat{V}_n$  is given by (2.25) and

$$\widetilde{V}_n' = \widetilde{V}_n + O(n^{-1/2}) \quad (2.27)$$

holds with  $\widetilde{V}_n$  given by (2.22).

*Proof.* The estimate (2.26) is proved in Section 5.2 with

$$U_n = e^{iQ_n} e^{iQ_n'}, \quad (2.28)$$

where  $Q_n$  and  $Q_n'$  are bounded self-adjoint operators defined in Section 3 and 4 respectively. □

**Corollary 2.4.** *The estimates (2.15)-(2.16) follow from the assertion of Proposition 2.3.*

*Proof.* To begin we observe that the assumption  $n \in 2\mathbb{N}$  implies

$$d_{n-1} + \beta = d_n = d_{n+1} = d_{n+2} - \beta \quad (2.29)$$

and (2.14) ensures the fact that there is  $n_1 \in \mathbb{N}$  such that for  $n \geq n_1$  one has

$$\lambda_{n-1}(J) < d_n - \frac{3}{4}\beta < d_n - \frac{1}{4}\beta < \lambda_n(J) \leq \lambda_{n+1}(J) < d_n + \frac{1}{4}\beta < d_n + \frac{3}{4}\beta < \lambda_{n+2}(J). \quad (2.30)$$

Moreover, (2.26) ensures the fact that

$$J = J_n + O(n^{-1} \ln n) \quad (2.31)$$

holds with

$$J_n := U_n(D + \widehat{V}_n \oplus \widetilde{V}'_n)U_n^{-1} \quad (2.32)$$

and we claim that there exists  $(\lambda_j(J_n))_{j \in \mathbb{Z}}$ , a non-decreasing eigenvalue sequence of  $J_n$ , counting multiplicities, such that choosing  $n_0 \in \mathbb{N}$  and  $C > 0$  large enough, one has

$$|\lambda_j(J) - \lambda_j(J_n)| \leq Cn^{-1} \ln n \text{ for every } j \geq n_0. \quad (2.33)$$

Moreover, combining (2.33) with (2.30), we can find  $n_1 \in \mathbb{N}$  such that for  $n \geq n_1$  one has

$$\lambda_{n-1}(J_n) < d_n - \frac{1}{2}\beta < \lambda_n(J_n) \leq \lambda_{n+1}(J_n) < d_n + \frac{1}{2}\beta < \lambda_{n+2}(J). \quad (2.34)$$

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

$$\widehat{\lambda}_n := d_n - |V(n, n+1)| \text{ and } \widehat{\lambda}_{n+1} := d_n + |V(n, n+1)|. \quad (2.35)$$

Moreover, due to (2.13), there is  $n_2 \in \mathbb{N}$  such that for  $n \geq n_2$  one has

$$d_n - \frac{1}{2}\beta < \widehat{\lambda}_n \leq \widehat{\lambda}_{n+1} < d_n + \frac{1}{2}\beta. \quad (2.36)$$

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

$$\{\widehat{\lambda}_n, \widehat{\lambda}_{n+1}\} \subset \sigma(J_n). \quad (2.37)$$

Combining (2.37) with (2.34), (2.36), we get  $\widehat{\lambda}_n = \lambda_n(J_n)$ ,  $\widehat{\lambda}_{n+1} = \lambda_{n+1}(J_n)$  and using these equalities in (2.33), we deduce

$$\lambda_n(J) = \widehat{\lambda}_n + O(n^{-1} \ln n) \text{ and } \lambda_{n+1}(J) = \widehat{\lambda}_{n+1} + O(n^{-1} \ln n), \quad (2.38)$$

i.e. (2.15)-(2.16) hold.  $\square$

### 3 Operators related to the first similarity transformation

**Notation 3.1.** (a) In the sequel  $\hat{c}, \hat{C}$  are as in (2.13) and  $n \in 2\mathbb{N}$ , i.e. (2.29) holds and it is easy to check that

$$d_j \neq d_k \Rightarrow |d_j - d_k| \geq \frac{\beta}{4} \langle j - k \rangle. \quad (3.1)$$

(b) We introduce  $Z_n^-, Z_n^+ \subset \mathbb{Z}^2$  defined as follows

$$Z_n^- = (\mathbb{Z} \setminus \{n, n+1\}) \times \{n, n+1\} \quad (3.2)$$

$$Z_n^+ = \{n, n+1\} \times (\mathbb{Z} \setminus \{n, n+1\}). \quad (3.3)$$

We observe that

$$(j, k) \in Z_n^- \Rightarrow d_j \neq d_n = d_k, \quad (3.4)$$

$$(j, k) \in Z_n^+ \Rightarrow d_j = d_n \neq d_k. \quad (3.5)$$

(c) In the sequel we fix  $c$  such that  $0 < c < \frac{1}{4}\hat{c}$  and we introduce the matrices  $(Q_n^-(j, k))_{(j,k) \in \mathbb{Z}^2}$ ,  $(Q_n^+(j, k))_{(j,k) \in \mathbb{Z}^2}$  by

$$Q_n^\pm(j, k) := \begin{cases} i \frac{V(j, k)}{d_j - d_k} & \text{if } (j, k) \in Z_n^\pm \text{ and } |j - k| < cn \\ 0 & \text{otherwise} \end{cases} \quad (3.6)$$

(d) We define the matrix  $(Q_n(j, k))_{(j,k) \in \mathbb{Z}^2}$  by

$$Q_n(j, k) := \begin{cases} i \frac{V(j, k)}{d_j - d_k} & \text{if } (j, k) \in Z_n^+ \cup Z_n^- \\ 0 & \text{otherwise} \end{cases} \quad (3.7)$$

**Lemma 3.2.** *If  $(Q_n^\pm(j, k))_{(j,k) \in \mathbb{Z}^2}$  is defined as in Notation 3.1(c), then*

(a) *there is  $C > 0$  such that for all  $j, k \in \mathbb{Z}$  one has the estimate*

$$|Q_n^\pm(j, k)| \leq \frac{4\hat{C}n^{-1/2}}{\beta \langle j - k \rangle} \quad (3.8)$$

(b) *there is  $Q_n^\pm \in \mathcal{B}(\ell^2(\mathbb{Z}))$  satisfying  $\langle e_j, Q_n^\pm e_k \rangle_{\ell^2(\mathbb{Z})} = Q_n^\pm(j, k)$  for all  $j, k \in \mathbb{Z}$  and*

$$\|Q_n^\pm\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} = O(n^{-1/2}). \quad (3.9)$$

*Proof.* (a) Due to  $c \leq \hat{c}$ , (3.8) follows from (2.13) and (3.1).

(b) If  $k \in \mathbb{Z} \setminus \{n, n+1\}$ , then  $Q_n^- e_k = 0$ . If  $k \in \{n, n+1\}$ , then

$$\|Q_n^- e_k\|_{\mathcal{B}(\ell^2(\mathbb{Z}))}^2 = \sum_{j \in \mathbb{Z}} |Q_n^-(j, k)|^2 \leq \sum_{\{j \in \mathbb{Z}: |j-k| < cn\}} \frac{(4\hat{C}n^{-1/2})^2}{\beta^2 \langle j - k \rangle^2}$$

$$\leq 16\hat{C}^2 n^{-1} \beta^{-2} \sum_{j \in \mathbb{Z}} \langle j - k \rangle^{-2} \leq C n^{-1},$$

hence  $Q_n^- \in \mathcal{B}(\ell^2(\mathbb{Z}))$  and  $\|Q_n^-\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} = O(n^{-1/2})$ . Since  $(j, k) \in Z_n^+ \Leftrightarrow (k, j) \in Z_n^-$  and  $Q_n^+(j, k) = \overline{Q_n^-(k, j)}$ , one has  $Q_n^+ = (Q_n^-)^* \in \mathcal{B}(\ell^2(\mathbb{Z}))$  and  $\|Q_n^+\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} = \|Q_n^-\|_{\mathcal{B}(\ell^2(\mathbb{Z}))}$   $\square$

**Lemma 3.3.** *If  $(Q_n(j, k))_{(j, k) \in \mathbb{Z}^2}$  is defined as in Notation 3.1(d), then*

(a) *there is  $Q_n \in \mathcal{B}(\ell^2(\mathbb{Z}))$  satisfying  $\langle e_j, Q_n e_k \rangle_{\ell^2(\mathbb{Z})} = Q_n(j, k)$  for all  $j, k \in \mathbb{Z}$  and*

$$\|Q_n^+ + Q_n^- - Q_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} = O(n^{-1}). \quad (3.10)$$

(b)  $\ell^{2,1}(\mathbb{Z})$  *is an invariant subspace of  $Q_n$  and one has*

$$-[D, iQ_n] = \tilde{\Pi}_n V \hat{\Pi}_n + \hat{\Pi}_n V \tilde{\Pi}_n. \quad (3.11)$$

(c)  $\ell^{2,1}(\mathbb{Z})$  *is an invariant subspace of  $e^{itQ_n}$  and  $t \rightarrow e^{itQ_n} x$  is of class  $C^\infty(\mathbb{R}; \ell^{2,1}(\mathbb{Z}))$  if  $x \in \ell^{2,1}(\mathbb{Z})$ .*

*Proof.* (a) If  $k \in \mathbb{Z} \setminus \{n, n+1\}$ , then  $(Q_n \hat{\Pi}_n - Q_n^-) e_k = 0$ . If  $k \in \{n, n+1\}$ , then

$$\begin{aligned} \|(Q_n \hat{\Pi}_n - Q_n^-) e_k\|_{\ell^2(\mathbb{Z})}^2 &= \sum_{\{j \in \mathbb{Z}: |j-k| \geq cn\}} |Q_n(j, k)|^2 \\ &\leq \sum_{\{j \in \mathbb{Z}: |j-k| \geq cn\}} \frac{16|V(j, k)|^2}{\beta^2 \langle j - k \rangle^2} \leq \frac{16}{\beta^2 c^2 n^2} \sum_{j \in \mathbb{Z}} |V(j, k)|^2 = \frac{16\|V e_k\|_{\ell^2(\mathbb{Z})}^2}{\beta^2 c^2 n^2} \leq \frac{C}{n^2}, \end{aligned}$$

hence  $Q_n \hat{\Pi}_n = Q_n^- + O(n^{-1})$ . Using the adjoint formula  $\hat{\Pi}_n Q_n = Q_n^+ + O(n^{-1})$ , we obtain

$$Q_n \hat{\Pi}_n + \hat{\Pi}_n Q_n = Q_n^- + Q_n^+ + O(n^{-1}). \quad (3.12)$$

However,  $\hat{\Pi}_n Q_n \hat{\Pi}_n = 0$  and  $\tilde{\Pi}_n Q_n \tilde{\Pi}_n = 0$  imply

$$Q_n = \tilde{\Pi}_n Q_n \hat{\Pi}_n + \hat{\Pi}_n Q_n \tilde{\Pi}_n = Q_n \hat{\Pi}_n + \hat{\Pi}_n Q_n \quad (3.13)$$

and we complete the proof of (a) combining (3.12) and (3.13). We obtain assertions (b) and (c) reasoning as in the proof of Lemma 4.1 in Chapter 3.  $\square$

**Lemma 3.4.** *Let  $Q_n^\pm$  be as in Notation 3.1(c) and*

$$Q_n^0 := Q_n^+ + Q_n^-. \quad (3.14)$$

*If*

$$V_n^0 := \frac{1}{2}V + \frac{1}{2}(\hat{\Pi}_n V \hat{\Pi}_n + \tilde{\Pi}_n V \tilde{\Pi}_n), \quad (3.15)$$

*then one has the following large  $n$  estimate*

$$\hat{\Pi}_n V_n^0 Q_n^0 \hat{\Pi}_n = O(n^{-1} \ln n). \quad (3.16)$$

*Proof.* To begin we observe that we still have the large  $k$  estimate

$$\sup_{\{j \in \mathbb{Z}: |j-k| < \hat{c}k\}} |V_n^0(j, k)| \leq \hat{C}k^{-1/2}. \quad (3.17)$$

Next we observe that

$$\|\hat{\Pi}_n V_n^0 Q_n^0 \hat{\Pi}_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} \leq \sum_{n \leq j, k \leq n+1} |(V_n^0 Q_n^0)(j, k)|$$

and

$$(V_n^0 Q_n^0)(j, k) = \sum_{\{m \in \mathbb{Z}: |m-k| < cn\}} V_n^0(j, m) Q_n^0(m, k).$$

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

$$|m-k| < cn \Rightarrow |j-m| \leq |j-k| + |k-m| < 1 + cn < \hat{c}n \Rightarrow |V_n^0(j, m)| \leq \hat{C}n^{-1/2} \quad (3.18)$$

holds for every  $n \geq c^{-1}$ . Therefore, using (3.18) and (3.8), we can estimate

$$|(V_n^0 Q_n^0)(j, k)| \leq \sum_{\{m \in \mathbb{Z}: |m-k| < cn\}} \frac{8\hat{C}^2 n^{-1}}{\beta \langle m-k \rangle} = O(n^{-1} \ln n), \quad (3.19)$$

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

#### 4 Operators related to the second similarity transformation

**Notation 4.1.** Assume that  $Q_n^\pm$  is given by Notation 3.1(c) and  $V_n^0$  by (3.15). We introduce the matrices  $(Q_n'^+(j, k))_{(j,k) \in \mathbb{Z}^2}$  and  $(Q_n'^-(j, k))_{(j,k) \in \mathbb{Z}^2}$  defined by

$$Q_n'^{\pm}(j, k) := \begin{cases} \frac{(V_n^0 Q_n^\pm)(j, k)}{d_k - d_j} & \text{if } (j, k) \in Z_n^- \cup Z_n^+ \\ 0 & \text{otherwise} \end{cases} \quad (4.1)$$

**Lemma 4.2.** Let  $(Q_n'^+(j, k))_{(j,k) \in \mathbb{Z}^2}$  be as in Notation 4.1. Then there is  $Q_n'^+ \in \mathcal{B}(\ell^2(\mathbb{Z}))$  satisfying  $\langle e_j, Q_n'^+ e_k \rangle_{\ell^2(\mathbb{Z})} = Q_n'^+(j, k)$  for all  $j, k \in \mathbb{Z}$  and

$$\|Q_n'^+\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} = O(n^{-1} \ln n). \quad (4.2)$$

*Proof.* Due to the Schur boundedness test, it suffices to show that there is  $C > 0$  such that for every  $j, k \in \mathbb{Z}$ ,  $n \in \mathbb{N}^*$ , the inequalities

$$\mathcal{Q}_n(k) \leq Cn^{-1} \ln n \quad \text{and} \quad \mathcal{Q}_n^*(k) \leq Cn^{-1} \ln n \quad (4.3)$$

hold with

$$\mathcal{Q}_n(k) := \sum_{j \in \mathbb{Z}} |Q_n'^+(j, k)|, \quad (4.4)$$



$$\mathcal{Q}_n^*(k) := \sum_{j \in \mathbb{Z}} |Q_n^{'+}(k, j)|. \quad (4.5)$$

Let us decompose  $\mathcal{Q}_n = \mathcal{Q}'_n + \mathcal{Q}''_n$  with

$$\mathcal{Q}'_n(k) := \sum_{\{j \in \mathbb{Z}: |j-k| \geq cn\}} |Q_n^{'+}(j, k)|, \quad (4.6)$$

$$\mathcal{Q}''_n(k) := \sum_{\{j \in \mathbb{Z}: |j-k| < cn\}} |Q_n^{'+}(j, k)|. \quad (4.7)$$

Using (3.1) and the Cauchy-Schwarz inequality, we can estimate

$$\mathcal{Q}'_n(k) \leq \sum_{\{j \in \mathbb{Z}: |j-k| > ck\}} \frac{4|(V_n^0 Q_n^+)(j, k)|}{\beta \langle j-k \rangle} \leq 4\beta^{-1} \mathcal{M}_n(k)^{1/2} \mathcal{M}'_n(k)^{1/2} \quad (4.8)$$

with

$$\begin{aligned} \mathcal{M}_n(k) &:= \sum_{\{j \in \mathbb{Z}: |j-k| \geq cn\}} \langle j-k \rangle^{-2}, \\ \mathcal{M}'_n(k) &:= \sum_{j \in \mathbb{Z}} |(V_n^0 Q_n^+)(j, k)|^2. \end{aligned}$$

However,

$$\mathcal{M}_n(k) \leq 2 \sum_{i \geq cn} \frac{1}{i^2} \leq 2 \int_{cn-1}^{\infty} \frac{ds}{s^2} = \frac{2}{cn-1} \leq C_1 n^{-1} \quad (4.9)$$

and using (3.9), we find

$$\mathcal{M}'_n(k) = \|V_n^0 Q_n^+ e_k\|_{\ell^2(\mathbb{Z})}^2 \leq \|V_n^0\|_{\mathcal{B}(\ell^2(\mathbb{Z}))}^2 \|Q_n^+\|_{\mathcal{B}(\ell^2(\mathbb{Z}))}^2 \leq C_2 n^{-1}. \quad (4.10)$$

Combining (4.8) with (4.9)-(4.10), we get  $\mathcal{Q}'_n(k) \leq Cn^{-1}$ .

In order to estimate (4.7), we assume  $|j-k| < cn$ . Since  $Q_n^+ = \hat{\Pi}_n Q_n^+$ , one has

$$(V_n^0 Q_n^+)(j, k) = \sum_{n \leq m \leq n+1} V_n^0(j, m) Q_n^+(m, k) \quad (4.11)$$

and using  $|j-k| < cn$ , we obtain

$$\begin{aligned} Q_n^+(m, k) \neq 0 &\Rightarrow |k-m| < cn \Rightarrow |j-m| \leq |j-k| + |k-m| < 2cn \\ &\Rightarrow |V_n^0(j, m)| \leq \hat{C} n^{-1/2} \Rightarrow |V_n^0(j, m) Q_n^+(m, k)| \leq 4\beta^{-1} \hat{C}^2 n^{-1}. \end{aligned}$$

Therefore, the first inequality (4.3) follows from

$$\mathcal{Q}''_n(k) \leq 8\beta^{-1} \hat{C}^2 n^{-1} \sum_{\{j \in \mathbb{Z}: |j-k| < cn\}} \frac{1}{\langle j-k \rangle} = O(n^{-1} \ln n), \quad (4.12)$$

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

We can also decompose  $\mathcal{Q}_n^* = \mathcal{Q}_n'^* + \mathcal{Q}_n''^*$  with

$$\mathcal{Q}_n'^*(k) := \sum_{\{j \in \mathbb{Z}: |j-k| \geq cn\}} |Q_n'^+(k, j)|, \quad (4.13)$$

$$\mathcal{Q}_n''^*(k) := \sum_{\{j \in \mathbb{Z}: |j-k| < cn\}} |Q_n'^+(k, j)|. \quad (4.14)$$

Then  $|\mathcal{Q}_n'^*(k)| \leq 4\beta^{-1} \mathcal{M}_n(k)^{1/2} \mathcal{M}_n'^*(k)^{1/2}$  with  $M_n(k)$  as before and

$$\mathcal{M}_n'^*(k) = \sum_{j \in \mathbb{Z}} |(V_n^0 Q_n^+)(k, j)|^2 = \|(V_n^0 Q_n^+)^* e_k\|_{\ell^2(\mathbb{Z})}^2 \leq Cn^{-1}$$

similarly as before. If  $|j - k| < cn$ , then

$$\begin{aligned} Q_n^+(m, j) \neq 0 &\Rightarrow |j - m| < cn \Rightarrow |k - m| \leq |k - j| + |j - m| < 2cn \\ &\Rightarrow |V_n^0(k, m)| \leq \hat{C}n^{-1/2} \Rightarrow |V_n^0(k, m)Q_n^+(m, j)| \leq 4\beta^{-1} \hat{C}^2 n^{-1} \end{aligned}$$

and  $\mathcal{Q}_n''^*(k) = O(n^{-1} \ln n)$  follows similarly as before.  $\square$

**Lemma 4.3.** *Let  $(Q_n^-(j, k))_{(j,k) \in \mathbb{Z}^2}$  be as in Notation 4.1. Then there is  $Q_n'^- \in \mathcal{B}(\ell^2(\mathbb{Z}))$  satisfying  $\langle e_j, Q_n'^- e_k \rangle_{\ell^2(\mathbb{Z})} = Q_n^-(j, k)$  for all  $j, k \in \mathbb{Z}$  and*

$$\|Q_n'^-\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} = O(n^{-1} \ln n). \quad (4.15)$$

*Proof.* If  $k \in \mathbb{Z} \setminus \{n, n+1\}$ , then  $Q_n^-(j, k) = 0$ . Thus

$$\|Q_n'^-\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} \leq \|Q_n'^- e_n\|_{\ell^2(\mathbb{Z})} + \|Q_n'^- e_{n+1}\|_{\ell^2(\mathbb{Z})}. \quad (4.16)$$

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

$$\|Q_n'^- e_k\|_{\ell^2(\mathbb{Z})}^2 \leq \mathcal{M}_n(k) + \mathcal{M}_n'(k) \quad (4.17)$$

holds with

$$\begin{aligned} \mathcal{M}_n(k) &:= \sum_{\{j \in \mathbb{Z}: |j-k| \geq cn\}} \frac{16|(V_n^0 Q_n^-)(j, k)|^2}{\beta^2 \langle j - k \rangle^2} \\ \mathcal{M}_n'(k) &:= \sum_{\{j \in \mathbb{Z}: |j-k| < cn\}} \frac{16|(V_n^0 Q_n^-)(j, k)|^2}{\beta^2 \langle j - k \rangle^2}. \end{aligned}$$

We first observe that

$$\mathcal{M}_n(k) \leq \frac{16}{\beta^2 c^2 n^2} \sum_{j \in \mathbb{Z}} |(V_n^0 Q_n^-)(j, k)|^2 = \frac{16}{\beta^2 c^2 n^2} \|V_n^0 Q_n^- e_k\|_{\ell^2(\mathbb{Z})}^2 = O(n^{-2}). \quad (4.18)$$

Our next claim is the estimate

$$\sup_{\{j \in \mathbb{Z}: |j-k| < cn\}} |(V_n^0 Q_n^-)(j, k)| = O(n^{-1} \ln n). \quad (4.19)$$

Since  $Q_n^-(m, k) = 0$  if  $|m - k| \geq cn$ , one has

$$(V_n^0 Q_n^-)(j, k) = \sum_{\{m \in \mathbb{Z}: |m-k| < cn\}} V_n^0(j, m) Q_n^-(m, k).$$

However,  $|j - k| < cn$  and  $|m - k| < cn$  imply  $|j - m| \leq |j - k| + |k - m| < 2cn$  and  $|V_n^0(j, m)| \leq \hat{C}n^{-1/2}$ , hence

$$\sup_{\{j \in \mathbb{Z}: |j-k| < cn\}} |(V_n^0 Q_n^-)(j, k)| \leq 4\hat{C}^2 n^{-1} \sum_{\{m \in \mathbb{Z}: |m-k| < cn\}} \frac{1}{\beta\langle m - k \rangle} = O(n^{-1} \ln n),$$

i.e. (4.19) holds. However, due to (4.19), we can estimate

$$\mathcal{M}'_n(k) \leq 16 \sup_{\{j \in \mathbb{Z}: |j-k| < cn\}} |(V_n^0 Q_n^-)(j, k)|^2 \sum_{j \in \mathbb{Z}} \beta^{-2} \langle j - k \rangle^{-2} = O(n^{-2} (\ln n)^2) \quad (4.20)$$

and combining (4.17) with (4.18) and (4.20), we get  $\|Q_n^- e_k\|_{\ell^2(\mathbb{Z})} = O(n^{-1} \ln n)$  for  $k \in \{n, n+1\}$ , completing the proof.  $\square$

**Lemma 4.4.** *Assume that  $V_n^0$  is given by (3.15),  $Q_n^\pm$  are as in Notation 3.1 and*

$$Q_n^0 := Q_n^+ + Q_n^-. \quad (4.21)$$

*Assume that  $Q'_n$  are as in Notation 4.1,*

$$Q'_n := Q_n'^- + Q_n'^+ + (Q_n'^- + Q_n'^+)^* \quad (4.22)$$

*and*

$$R'_n := \tilde{\Pi}_n[V_n^0, iQ_n^0] \hat{\Pi}_n + \hat{\Pi}_n[V_n^0, iQ_n^0] \tilde{\Pi}_n. \quad (4.23)$$

*Then*

(a)  $\ell^{2,1}(\mathbb{Z})$  is an invariant subspace of  $Q'_n$  and

$$[D, iQ'_n] = -R'_n \quad (4.24)$$

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

*Proof.* We obtain these assertions reasoning as in the proof of Lemma 4.4 in Chapter 4.  $\square$

## 5 Proof of Theorem 1.1

### 5.1 First similarity transformation

**Lemma 5.1.** *Let  $Q_n$  be as in Notation (3.1)(d) and*

$$J'_n := e^{-iQ_n} J e^{iQ_n}. \quad (5.1)$$

Then one has the large  $n$  estimate

$$J'_n := D + \widehat{V}_n \oplus \widetilde{V}'_n + R'_n + O(n^{-1} \ln n), \quad (5.2)$$

where  $R'_n$  is given by (4.23),  $\widehat{V}_n$  is given by (2.21) and

$$\widetilde{V}'_n = \widetilde{V}_n + O(n^{-1/2}) \quad (5.3)$$

holds with  $\widetilde{V}_n$  given by (2.22).

*Proof.* We first observe that (5.1) from Section 5, Chapter 3 gives

$$J'_n = D + V - R_n + [V - \frac{1}{2}R_n, iQ_n] + O(n^{-1}) \quad (5.4)$$

with  $R_n = -[D, iQ_n] = \widetilde{\Pi}_n V \widehat{\Pi}_n + \widehat{\Pi}_n V \widetilde{\Pi}_n$  (see (3.11)). We observe that

$$V - R_n = \widehat{\Pi}_n V \widehat{\Pi}_n + \widetilde{\Pi}_n V \widetilde{\Pi}_n \quad (5.5)$$

and  $V - \frac{1}{2}R_n = V_n^0$  is given by (3.15). Moreover, (3.10) allows us to replace  $Q_n$  by  $Q_n^0$  in the right hand side of (5.5), i.e.

$$J'_n = D + \widehat{\Pi}_n V \widehat{\Pi}_n + \widetilde{\Pi}_n V \widetilde{\Pi}_n + [V_n^0, iQ_n^0] + O(n^{-1}). \quad (5.6)$$

Due to (3.16) we obtain

$$[V_n^0, iQ_n^0] = \widetilde{\Pi}_n [V_n^0, iQ_n^0] \widetilde{\Pi}_n + R'_n + O(n^{-1} \ln n), \quad (5.7)$$

where  $R'_n$  is given by (4.23). Introducing

$$\widetilde{V}'_n := \widetilde{V}_n + \widetilde{\Pi}_n [V_n^0, iQ_n^0] \widetilde{\Pi}_n, \quad (5.8)$$

we have  $\|\widetilde{V}'_n - \widetilde{V}_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} \leq C \|Q_n^0\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} = O(n^{-1/2})$  and

$$\widehat{\Pi}_n V \widehat{\Pi}_n + \widetilde{\Pi}_n V \widetilde{\Pi}_n + \widetilde{\Pi}_n [V_n^0, iQ_n^0] \widetilde{\Pi}_n = \widehat{V}_n \oplus \widetilde{V}'_n. \quad (5.9)$$

To complete the proof of (5.2), it remains to combine (5.6), (5.7) and (5.9).  $\square$

## 5.2 Proof of Proposition 2.3

Using the Taylor formula (2.12) in Chapter 3 (see page 56), with  $N = 1$  we get

$$e^{-iQ'_n} D e^{iQ'_n} = D + [D, iQ'_n] + O(\|\text{ad}_{iQ'_n}^2(D)\|_{\mathcal{B}(\ell^2(\mathbb{Z}))}). \quad (5.10)$$

Since  $[D, iQ'_n] = -R'_n$  and  $\text{ad}_{iQ'_n}^2(D) = -[R'_n, iQ'_n] = O(\|Q'_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))})$ , (5.10) implies

$$e^{-iQ'_n} D e^{iQ'_n} = D - R'_n + O(n^{-1} \ln n) \quad (5.11)$$

due to  $\|Q'_n\|_{\mathcal{B}(\ell^2(\mathbb{Z}))} = O(n^{-1} \ln n)$  (see (4.2) and (4.15)). We also have

$$e^{-iQ'_n} (\widehat{V}_n \oplus \widetilde{V}'_n + R'_n) e^{iQ'_n} = \widehat{V}_n \oplus \widetilde{V}'_n + R'_n + O(n^{-1} \ln n). \quad (5.12)$$

Let us denote  $J''_n := e^{-iQ'_n} J'_n e^{iQ'_n}$ . Then (5.2) ensures

$$J''_n = e^{-iQ'_n} (D + \widehat{V}_n \oplus \widetilde{V}'_n + R'_n) e^{iQ'_n} + O(n^{-1} \ln n) \quad (5.13)$$

To complete the proof, it remains to observe that (5.11) and (5.12) allow one to write the right hand side of (5.13) in the form  $D + \widehat{V}_n \oplus \widetilde{V}'_n + O(n^{-1} \ln n)$ .

### 5.3 Proof of Proposition 2.2

**Notation 5.2.** (a) We denote  $L^2(\mathbb{T})$  the Hilbert space of Lebesgue square integrable functions  $]-\pi, \pi[ \rightarrow \mathbb{C}$  equipped with the scalar product

$$\langle f, g \rangle_{L^2(\mathbb{T})} := \frac{1}{2\pi} \int_{-\pi}^{\pi} \overline{f(\theta)} g(\theta) d\theta. \quad (5.14)$$

(b) For  $f \in L^2(\mathbb{T})$  we write  $\langle f \rangle := \frac{1}{2\pi} \int_{-\pi}^{\pi} f(\theta) d\theta$ .

(c) For  $\nu = \pm 1$ , we define  $\Phi_\nu \in C^\infty(\mathbb{T})$  by

$$\Phi_\nu(\theta) := \int_0^\theta \frac{\beta d\theta'}{1 + 2\nu g \cos(2\theta')} \quad (5.15)$$

(d) For  $\nu = \pm 1$ , we define  $q_\nu \in C^\infty(\mathbb{T})$  by

$$q_\nu(\theta) = \beta^{-1} \left( \nu g \cos(2\Phi_\nu^{-1}(\theta)) + \frac{1}{2}\nu\epsilon \right). \quad (5.16)$$

(e) For  $\nu = \pm 1$ , we denote

$$f_{\nu,j}(\theta) = \sqrt{\Phi'_\nu(\theta)} e^{ij\Phi_\nu(\theta) + i\phi_\nu(\theta)}, \quad (5.17)$$

where

$$\phi_\nu(\theta) := \langle q_\nu \rangle \Phi_\nu(\theta) - \tilde{q}_\nu(\Phi_\nu(\theta)) \quad (5.18)$$

and  $\tilde{q}_\nu$  is a primitive of  $q_\nu$  and

$$\langle q_\nu \rangle = \frac{\nu\epsilon}{2\beta} + \frac{\beta_0}{\beta}. \quad (5.19)$$

Similarly as in Section 4.2 and Section 3.4, Chapter 5 We have

$$V(2j, 2j+1) = \frac{\Delta}{2} \gamma_{j,j-l_0}, \quad (5.20)$$

where

$$\gamma_{j,j-l_0} = \langle f_{-1,j}, f_{1,j-l_0} \rangle_{L^2(\mathbb{T})} = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{ij\Psi_0(\theta)} h(\theta) d\theta \quad (5.21)$$

with

$$h := e^{-il_0\Phi_1} e^{i(\phi_1 - \phi_{-1})} (\Phi'_1 \Phi'_{-1})^{1/2}, \quad (5.22)$$

and

$$\Psi_0 := \Phi_1 - \Phi_{-1}. \quad (5.23)$$

Then

$$\Psi'_0(\theta) = \frac{\beta}{1 + 2g \cos(2\theta)} - \frac{\beta}{1 - 2g \cos(2\theta)} = 0 \Leftrightarrow \cos(2\theta) = 0, \quad (5.24)$$

i.e.  $\Psi'_0(\theta) \neq 0$  if  $\theta \in [-\pi, \pi] \setminus \{\theta_1, \theta_{-1}, \theta_2, \theta_{-2}\}$ , where  $\theta_{\pm 1} = \pm \frac{\pi}{4}$  and  $\theta_{\pm 2} = \pm \frac{3\pi}{4}$ . However,

$$\Psi''_0(\theta) = \left( \frac{4g\beta}{(1 + 2g \cos(2\theta))^2} + \frac{4g\beta}{(1 - 2g \cos(2\theta))^2} \right) \sin(2\theta) \quad (5.25)$$

and  $\Psi'_0(\theta) = 0 \Rightarrow \cos(2\theta) = 0 \Rightarrow \Psi''_0(\theta) = \pm 8g\beta$ , i.e. the critical points  $\{\theta_i\}_{i=\pm 1, \pm 2}$  are not degenerated such that

$$\Psi''_0(\pi/4) = \Psi''_0(-3\pi/4) = 8g\beta \text{ and } \Psi''_0(-\pi/4) = \Psi''_0(3\pi/4) = -8g\beta,$$

Then the stationary phase formula gives the large  $j$  asymptotic formula

$$\gamma_{j, j-l_0} = G_1 + G_{-1} + O(j^{-1}), \quad (5.26)$$

where for  $\nu = \pm 1$

$$G_\nu = \sum_{\theta \in \{\frac{\nu\pi}{4}, \frac{-\nu 3\pi}{4}\}} \frac{1}{4\sqrt{\pi j g \beta}} h(\theta) e^{ij\Psi_0(\theta)} e^{i\nu\frac{\pi}{4}}, \quad (5.27)$$

**Step 1.** We claim that

$$\Psi_0(\theta) = -\arctan\left(\frac{2g \sin 2\theta}{\beta}\right) \quad (5.28)$$

Indeed, we can write

$$\Psi_0(\theta) = -2g\beta \int_0^{2\theta} \frac{\cos \theta'}{1 - 4g^2 \cos^2 \theta'} d\theta' \quad (5.29)$$

and we have

$$\int \frac{\cos \theta'}{1 - 4g^2 \cos^2 \theta'} d\theta' = \int \frac{\cos \theta'}{(1 - 4g^2) + 4g^2 \sin^2 \theta'} d\theta' = \frac{1}{2g\beta} \arctan\left(\frac{2g \sin \theta}{\beta}\right). \quad (5.30)$$

**Step 2.** We have  $\Phi_\nu(\pm\pi) = \pm\pi$  and  $\Phi_\nu(\pm\frac{\pi}{2}) = \pm\frac{\pi}{2}$ . We claim that

$$\Phi_1(\theta) = \begin{cases} \arctan(\alpha_0 \tan \theta) & \text{if } -\frac{\pi}{2} < \theta < \frac{\pi}{2}, \\ \pi - \arctan(\alpha_0 \tan(\pi - \theta)) & \text{if } \frac{\pi}{2} < \theta < \pi \\ -\pi + \arctan(\alpha_0 \tan(\pi + \theta)) & \text{if } -\pi < \theta < -\frac{\pi}{2}, \end{cases} \quad (5.31)$$

where  $\alpha_0 := \sqrt{\frac{1-2g}{1+2g}}$ . Indeed, if  $-\frac{\pi}{2} < \theta < \frac{\pi}{2}$ , we have

$$\Phi_1(\theta) = \int_0^\theta \frac{\beta}{1 + 2g \cos 2\theta'} d\theta' = \int_0^\theta \frac{U'(\theta')}{1 + U^2(\theta')} d\theta' = \arctan U(\theta), \quad (5.32)$$

with  $U(\theta) = \alpha_0 \tan(\theta)$ . If  $\frac{\pi}{2} < \theta < \pi$ , then

$$\Phi_1(\theta) = \Phi_1\left(\frac{\pi}{2}\right) + \Phi_{-1}\left(\theta - \frac{\pi}{2}\right) = \frac{\pi}{2} + \arctan\left(\alpha_0^{-1} \tan\left(\theta - \frac{\pi}{2}\right)\right) \quad (5.33)$$

$$= \pi - \arctan(\alpha_0 \tan(\pi - \theta)). \quad (5.34)$$

If  $-\pi < \theta < -\frac{\pi}{2}$ , then

$$\Phi_1(\theta) = -\Phi_1(-\theta) = -\pi + \arctan(\alpha_0 \tan(\pi + \theta)). \quad (5.35)$$

**Step 3.** We claim that

$$\tilde{q}_\nu(\Phi_\nu(\theta)) = \frac{\theta}{2} + \left(\frac{\nu\epsilon - 1}{2\beta}\right) \Phi_\nu(\theta), \quad (5.36)$$

Indeed, since  $\tilde{q}$  is an odd function then  $\tilde{q}_\nu(\Phi_\nu(0)) = \tilde{q}_\nu(0) = 0$  and we can write

$$\tilde{q}_\nu(\Phi_\nu(\theta)) = \int_0^{\Phi_\nu(\theta)} q_\nu(\theta) d\theta = \frac{\nu\epsilon}{2\beta} \Phi_\nu(\theta) + \frac{\nu g}{\beta} \int_0^{\Phi_\nu(\theta)} \cos(2\Phi_\nu^{-1}(\theta)) d\theta \quad (5.37)$$

However using the change of variable  $\xi = \Phi_\nu^{-1}(\theta)$  we can express

$$\int_0^{\Phi_\nu(\theta)} \cos(2\Phi_\nu^{-1}(\theta)) d\theta = \int_0^\theta \cos(2\xi) \Phi'_\nu(\xi) d\xi = \frac{\beta\theta}{2\nu g} - \frac{\Phi_\nu(\theta)}{2\nu g} \quad (5.38)$$

Then combining (5.37) with (5.38) we get (5.36).

**Step 4.** We claim that

$$G_\nu = \frac{\sqrt{\beta}(1 + (-1)^{l_0})}{4\sqrt{\pi j g}} e^{-i\nu l_0 \Phi_1(\pi/4)} e^{i\frac{\nu}{2} \Psi_0(\pi/4)} e^{ij\nu \Psi_0(\pi/4)} e^{i\nu \frac{\pi}{4}} \quad (5.39)$$

Indeed, we observe that

$$(\Phi'_1 \Phi'_{-1})^{\frac{1}{2}}(\pm\pi/4) = (\Phi'_1 \Phi'_{-1})^{\frac{1}{2}}(\pm 3\pi/4) = \beta \quad (5.40)$$

and using (5.36) we find

$$\phi_1 - \phi_{-1} = \frac{1}{2}(\Phi_1 - \Phi_{-1}) = \frac{1}{2}\Psi_0 \quad (5.41)$$

and using (5.28) and (5.31) we obtain

$$\Psi_0\left(\frac{-\nu 3\pi}{4}\right) = \Psi_0\left(\frac{\nu\pi}{4}\right) = \nu\Psi_0\left(\frac{\pi}{4}\right) \quad (5.42)$$

and

$$\Phi_1\left(\frac{\nu 3\pi}{4}\right) = \nu\pi - \nu\Phi_1\left(\frac{\pi}{4}\right) = \nu\pi + \nu\Phi_1\left(-\frac{\pi}{4}\right) \quad (5.43)$$

Therefore we deduce

$$h(-\nu 3\pi/4) e^{ij\Psi_0(-\nu 3\pi/4)} = h(\nu\pi/4) e^{ij\Psi_0(\nu\pi/4)} e^{i\nu l_0 \pi} \quad (5.44)$$

Moreover, we can write the right side of (5.44) as

$$\beta(-1)^{l_0} e^{-i\nu l_0 \Phi_1(\pi/4)} e^{i\frac{\nu}{2} \Psi_0(\pi/4)} e^{ij\nu \Psi_0(\pi/4)} \quad (5.45)$$

thus we get (5.39).

**Step 5.** We deduce that we can express

$$G_1 + G_{-1} = \frac{\sqrt{\beta}(1 + (-1)^{l_0})}{2\sqrt{\pi j g}} \cos(j\tilde{\theta}_g + \hat{\theta}_{g,\epsilon}) \quad (5.46)$$

where

$$\tilde{\theta}_g := \Psi_0(\pi/4) = -\arctan(2g/\beta) = -\frac{\pi}{2} + 2\alpha, \quad (5.47)$$

with

$$\alpha = \arctan \alpha_0, \quad (5.48)$$

and

$$\hat{\theta}_{g,\epsilon} = \frac{\tilde{\theta}_g}{2} + \frac{\pi}{4} - l_0 \Phi_1(\pi/4) = (1 - l_0) \alpha. \quad (5.49)$$

Then combining (5.20), (5.26) with (5.46) we get (2.17).



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## Deuxième partieII

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**Théorie des perturbations pour  
une classe des opérateurs définis  
dans l'espace de Hilbert des suites  
de carré sommable par des  
matrices tridiagonales non  
bornées**

## Série de perturbations pour les matrices de Jacobi et le modèle quantique de Rabi

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# Perturbation series for Jacobi matrices and the Quantum Rabi Model

Mirna Charif<sup>1</sup> and Lech Zielinski<sup>2</sup>

**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

## 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 [115] for physical explanations (see also [15]) and to [133] for a list of recent research works in relation with the QRM. It appears (see [123], [32]) that the QRM Hamiltonian is unitarily equivalent to the direct sum  $J_{\Delta}^{\omega}(g) \oplus J_{-\Delta}^{\omega}(g)$ , where  $\Delta$ ,  $\omega$  and  $g$  are real parameters (see Section 1.5) and  $J_s^{\omega}(g)$  is the self-adjoint operator defined in  $\ell^2$  by the matrix

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

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 [79]. 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 [60], where the authors investigate the quality of the Jaynes-Cummings approximation and propose the corrections for the eigenvalues of (1.1). The authors of [60] 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 [60] 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 [61]).

## 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  $\langle x, y \rangle = \sum_{j=1}^{\infty} \bar{x}_j y_j$ . 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

$$\begin{pmatrix} d_1 + gb'_1 & gb_1 & 0 & 0 & \cdots \\ gb_1 & d_2 + gb'_2 & gb_2 & 0 & \cdots \\ 0 & gb_2 & d_3 + gb'_3 & b_3 & \cdots \\ 0 & 0 & gb_3 & d_4 + gb'_4 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (1.2)$$

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

$$De_i = d_i e_i, \quad (1.3)$$

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

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  $2\rho_0^2 < \liminf_{i \rightarrow \infty} \frac{d_i^2}{b_i^2 + b_{i-1}^2}$

**(H2)** the sequence  $(b'_i)_{i=1}^\infty$  is bounded

**(H3)**  $d_i \xrightarrow{i \rightarrow \infty} \infty$ .

**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 [22] or [75]. □

### 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

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

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

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

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

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

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  $J(g)$ ,*

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

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

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

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

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

*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

$$d_{k+1} = d_k \neq d_j \text{ for } j \in \mathbb{N}^* \setminus \{k, k+1\}. \quad (1.11)$$

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

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

We introduce the quantities

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

$$\beta'_{k-1} := |b_{k-2}| + |b'_{k-1}|, \quad (1.14)$$

$$\beta'_{k+2} := |b_{k+2}| + |b'_{k+2}|, \quad (1.15)$$

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

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

and

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

**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

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

$$4\rho\mu_k \leq \inf_{i \notin \{k, k+1\}} |d_i|, \quad (1.20)$$

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

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

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

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

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

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

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

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

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

*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

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

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

(ii) In the general case one has

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

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 Reed-Simon [108]. However we give an independent proof in Section 7.3. □

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

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

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

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

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

and introduce the matrix

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

**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  $\lambda_{k+j}^1(g) \xrightarrow{g \rightarrow 0} -\mu_{k+j}$ . Then

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

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

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

(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 [105], [106]. The quantized version can be reduced to  $J_{\Delta}^{\omega}(g) \oplus J_{-\Delta}^{\omega}(g)$ , where  $\Delta$  is the separation energy between two atomic levels and  $\omega$  is the frequency of the quantized one-mode electromagnetic field. In [79], Jaynes and Cummings proposed to approximate  $J_s^{\omega}(g)$  by

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

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

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

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 [117], [2], [53]). The time independent approach was proposed in [60].

Following [60] 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 (1.1) 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  $b_k = \sqrt{k}$ ,  $d_{2m} - d_{2m-1} = d_{2m+2} - d_{2m+1} = \omega$  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  $J : \mathbb{C} \rightarrow \mathcal{L}(\mathbb{C}^n)$  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  $i = 1, \dots, n$ . Sections 2.2 and 2.2 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 2.1.** (a) For  $\lambda \in \mathbb{C}$  and  $\rho \geq 0$  we denote  $\overline{\mathbb{D}}(\lambda, \rho) := \{\lambda' \in \mathbb{C} : |\lambda' - \lambda| \leq \rho\}$ . 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

$$b_{i,j}(g) = \langle e_i, B(g)e_j \rangle.$$

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

### 2.2 An auxiliary result

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

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

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

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

*Proof.* The Gershgorin's theorem (see Th. 3.11 in [112]) ensures  $\sigma(J(g)) \subset \overline{\mathbb{D}}_1 \cup \dots \cup \overline{\mathbb{D}}_n$ , where

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

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

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

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

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

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

### 2.3 Use of the Cauchy's formula

**Lemma 2.3.** *We fix  $\beta > 0$  and  $\rho > 0$ . If  $\eta: \mathbb{D}(0, \rho) \rightarrow \overline{\mathbb{D}}(0, \beta\rho)$  is holomorphic, then*

$$|\eta^{(\nu)}(0)| \leq \beta\rho^{1-\nu}\nu! \quad (2.6)$$

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

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

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

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

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

$$|c_\nu| \leq \beta\rho^{1-\nu}. \quad (2.8)$$

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

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

completing the proof of Lemma 2.3.  $\square$

## 2.4 Finite dimensional version of Theorem 1.2

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

$$d_k = 0 \neq d_i \text{ if } i \neq k. \quad (2.9)$$

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

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

for  $g \in \mathbb{D}(0, \rho)$ . Following Kato [81] we observe that  $g \rightarrow P_k(J(g))$  is a holomorphic family of eigenprojectors of  $J(g)$  satisfying  $\text{rank } P_k(J(g)) = \text{rank } P_k(J(0)) = 1$  and  $\lambda_k(J(g)) = \text{tr}(J(g)P_k(J(g)))$  is an eigenvalue of  $J(g)$  satisfying

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

Since  $g \rightarrow \lambda_k(g)$  is holomorphic  $\mathbb{D}(0, \rho) \rightarrow \mathbb{D}(0, \rho\beta_k(\rho))$ , 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  $\mathbb{D}(0, \rho_0) \rightarrow \mathcal{L}(\mathbb{C}^n)$  and  $D = \text{diag}(d_i)_{i=1}^n$ . Moreover we fix  $\hat{n} \in \{1, \dots, n-1\}$  and we make the assumption

$$i \leq \hat{n} < j \implies d_i \neq d_j. \quad (3.1)$$

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

$$\widehat{V} := \text{span}\{e_j\}_{1 \leq j \leq \hat{n}}, \quad (3.2)$$

$$\widetilde{V} := \text{span}\{e_j\}_{1+\hat{n} \leq j \leq n} \quad (3.3)$$

and consider the corresponding decomposition

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

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 [110], but in this paper we will develop an approach of Schrieffer-Wolff [57] (see also [83], [87], [127], [57]) in order to prove

**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  $\mathbb{D}(0, \varepsilon_0) \rightarrow \mathcal{L}(\widehat{V})$  and  $\widetilde{J}_\infty$  is holomorphic  $\mathbb{D}(0, \varepsilon_0) \rightarrow \mathcal{L}(\widetilde{V})$ .*

*Proof.* See Sections 3.2–3.4. □

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

**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  $0 < \rho < \min\{|d_j| : j \geq 3\}$ , then there exists  $\varepsilon > 0$  such that for  $g \in \mathbb{D}(0, \varepsilon)$  one has*

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

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

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

where  $\mu_1, \mu_2$  are eigenvalues of  $B(0)$ .

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

$$\sigma(J(g)) = \sigma(\hat{J}_\infty(g)) \cup \sigma(\tilde{J}_\infty(g)) \quad (3.7)$$

and there exists  $C > 0$  such that

$$\text{dist}(\sigma(\tilde{J}_\infty(g)), \{d_3, \dots, d_n\}) \leq C|g|. \quad (3.8)$$

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

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

However  $\hat{J}_\infty(g) = g\hat{B}_\infty(g)$  and  $\hat{B}_\infty(g) = \hat{B}(0) + g\hat{B}_\infty^{(1)}(g)$ . The hypotheses that  $\hat{B}(0)$  is self-adjoint and  $b_{1,2}(0) \neq 0$  ensure that fact that  $\hat{B}(0)$  has two distinct eigenvalues  $\mu_1, \mu_2$ , hence  $\sigma(\hat{B}_\infty(g)) = \{\mu_1(g), \mu_2(g)\}$  holds with  $g \rightarrow \mu_j(g)$  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  $\hat{J}_\infty(g) \oplus \tilde{J}_\infty(g)$  as the limit of a sequence of operators  $(J_l(g))_{l=0}^\infty$  of the form

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

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

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

where  $\hat{B}_l: \hat{V} \rightarrow \hat{V}$ ,  $\tilde{B}_l: \tilde{V} \rightarrow \tilde{V}$ ,  $R_l^+: \hat{V} \rightarrow \tilde{V}$ ,  $R_l^-: \tilde{V} \rightarrow \hat{V}$ . Then

$$B_l(g) = \hat{B}_l(g) \oplus \tilde{B}_l(g) + R_l(g) \quad (3.11)$$

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

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

and observe that (3.12) ensures the equality

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

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

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

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

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

$$\tilde{F}_{gQ}(A) := \frac{1}{g} \left( e^{-igQ} A e^{igQ} - A - g[A, iQ] \right) \quad (3.16)$$

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

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

with

$$F_l(g) = \tilde{F}_{gQ_l(g)}(D) + F_{gQ_l(g)}(B_l(g)) \quad (3.18)$$

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

$$J_{l+1} = D + g(\hat{B}_l \oplus \tilde{B}_l + F_l). \quad (3.19)$$

### 3.3 Norm estimates

**Notation 3.4.** (a) We denote by  $\|\cdot\|_0$  the norm defined on  $\hat{V}$  by

$$\|x\|_0 = (|x_k|^2 + |x_{k+1}|^2)^{1/2}. \quad (3.20)$$

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

$$\|x\|' = \max_{i \notin \{k, k+1\}} |x_i|. \quad (3.21)$$

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

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

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*

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

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

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

$$F_{gQ}(A) = \int_0^1 e^{-isgQ} [A, igQ] e^{isgQ} ds,$$

$$\tilde{F}_{gQ}(A) = \int_0^1 e^{-isgQ} [[A, iQ], igQ] e^{isgQ} (1-s) ds.$$

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

**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*

$$\|R_m(g)\| \leq C_0^{1+3m} |g^m| \quad (3.25)$$

$$\|\hat{B}_m(g) \oplus \tilde{B}_m(g) - \hat{B}_{m-1}(g) \oplus \tilde{B}_{m-1}(g)\| \leq C_0^{1+3m} |g^m| \quad (3.26)$$

where for  $m = 0$  we take  $\hat{B}_{m-1} = 0$  and  $\tilde{B}_{m-1} = 0$  in (3.26).

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

$$\|B(g)\| \leq C_0 \text{ for } g \in \mathbb{D}(0, \varepsilon_0) \quad (3.27)$$

for a certain  $\varepsilon_0 > 0$  and

$$\|Q_l(g)\| \leq C_0 \|R_l(g)\|. \quad (3.28)$$

Let  $l \in \mathbb{N}$  be such that the estimates (3.25)-(3.26) 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

$$\|R_m(g)\| \leq 2^{-m} C_0 \text{ if } m \leq l, \quad (3.29)$$

$$\|\hat{B}_m(g) \oplus \tilde{B}_m(g) - \hat{B}_{m-1}(g) \oplus \tilde{B}_{m-1}(g)\| \leq 2^{-m} C_0 \text{ if } m \leq l. \quad (3.30)$$

Using (3.30) we can estimate  $\|\hat{B}_l(g) \oplus \tilde{B}_l(g)\|$  by

$$\sum_{m=0}^l \|\hat{B}_m(g) \oplus \tilde{B}_m(g) - \hat{B}_{m-1}(g) \oplus \tilde{B}_{m-1}(g)\| \leq 2C_0,$$

hence

$$\|B_l(g)\| \leq \|\hat{B}_l(g) \oplus \tilde{B}_l(g)\| + \|R_l(g)\| \leq 3C_0. \quad (3.31)$$

Next we observe that (3.19) gives

$$F_l = B_{l+1} - \hat{B}_l \oplus \tilde{B}_l = \begin{pmatrix} \hat{B}_{l+1} - \hat{B}_l & R_{l+1}^+ \\ R_{l+1}^- & \tilde{B}_{l+1} - \tilde{B}_l \end{pmatrix} \quad (3.32)$$

and in order to prove that (3.25)-(3.26) hold for  $m = l + 1$  it suffices to check the estimate

$$\|F_l(g)\| \leq C_0^{4+3l} |g|^{l+1}. \quad (3.33)$$

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

$$\|\tilde{F}_{gQ_l}(D)\| \leq \frac{1}{2} e^{2\|gQ_l(g)\|} \|[R_l(g), gQ_l(g)]\| \leq e \|R_l(g)\| \|gQ_l(g)\| \quad (3.34)$$

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

$$\|F_{gQ}(B_l(g))\| \leq 2e \|B_l(g)\| \|gQ_l(g)\|. \quad (3.35)$$

Combining (3.34), (3.35) with (3.18) and assuming  $C_0 \geq 7e$ , we get

$$\begin{aligned} \|F_l(g)\| &\leq e(\|R_l(g)\| + 2\|B_l(g)\|)|g| C_0 \|R_l(g)\| \leq \\ &\leq 7eC_0^2 |g| \|R_l(g)\| \leq C_0^3 |g| \|R_l(g)\|. \end{aligned}$$

Thus (3.25) for  $m = l$  gives (3.33), completing the proof of (3.25)-(3.26) for  $m = l + 1$ .  $\square$

### 3.4 End of the proof of Proposition 3.1

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

$$U_{m,l}(g) = e^{igQ_m} \dots e^{igQ_{l-1}}. \quad (3.36)$$

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

$$\hat{B}_\infty(g) = \lim_{l \rightarrow \infty} \hat{B}_l(g), \quad \tilde{B}_\infty(g) = \lim_{l \rightarrow \infty} \tilde{B}_l(g) \quad (3.37)$$

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

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

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

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

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

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

Thus we can define  $U_\infty(g)$  as the limit of  $U_{0,l}(g)$  as  $l \rightarrow \infty$  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  $l \rightarrow \infty$  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,

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

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

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

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

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

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

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

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

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

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

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

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

**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  $|c_{k+j,\nu}| \leq \mu_k \rho^{1-\nu}$  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

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

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

$$\widehat{B}_l \oplus \widetilde{B}_l = \Pi_0 B_l \Pi_0 + \Pi'_0 B_l \Pi'_0. \quad (4.8)$$

In this section we consider (3.9) with  $l = 0$  and as before  $F_0(g)$  is given by the equality

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

Moreover  $R_0 = B - \widehat{B} \oplus \widetilde{B}$  satisfies  $R_0 = \Pi_1 R_0 \Pi_1$  and has the form

$$R_0 = \begin{pmatrix} 0 & b_{k-1} & 0 & 0 \\ b_{k-1} & 0 & 0 & 0 \\ 0 & 0 & 0 & b_{k+1} \\ 0 & 0 & b_{k+1} & 0 \end{pmatrix} \oplus \mathbb{O}_{V_1^\perp} \quad (4.10)$$

where  $\mathbb{O}_{V_1^\perp}$  is the zero map on  $V_1^\perp$ . Thus  $Q_0 = \Pi_1 Q_0 \Pi_1$  has the form

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

with

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

In particular we have

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

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

**Lemma 4.3.** *We have the estimate*

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

*Proof.* Due to  $Q_0 = \Pi_1 Q_0 \Pi_1$  we have

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

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

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

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

$$\|R_0\| + 2\|B^\circ\| \leq \gamma_k. \quad (4.18)$$

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

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

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

$$\|R_0\| + \|\Pi_0 B^\circ \Pi_0 + \Pi'_0 B^\circ \Pi'_0\| = \|R_0\| + \max\{\|\Pi_0 B^\circ \Pi_0\|, \|\Pi'_0 B^\circ \Pi'_0\|\} \quad (4.20)$$

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  $\text{diag}(-\mu, \mu)$  and  $\|\cdot\|_0$  is the euclidean norm).  $\square$

### 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*

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

Then

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

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

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

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

$$\|(g\widehat{B} - \lambda)^{-1}\|_0 = \max\left\{ \frac{1}{|\lambda - g\mu|}, \frac{1}{|\lambda + g\mu|} \right\}. \quad (4.24)$$

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

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

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

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

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

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

$$\|g\tilde{A}(\lambda)\|' \leq \frac{1}{2}. \quad (4.27)$$

Indeed, we obtain (4.25) using (4.26)-(4.27) to estimate the norm of the resolvent series

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

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

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

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

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

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

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

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

#### 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*

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

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

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

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

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

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

$$\|gA_\lambda(g)\| \leq \|gF_0(g)\| \|(J_{1,0}(g) - \lambda)^{-1}\| \leq |g|^2 \gamma'_k \gamma_k e^{2\rho\gamma'_k} / (\mu|g|) < 1, \quad (4.32)$$

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

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

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

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

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  $g = te^{i\theta}$ , then  $|\lambda \pm g\mu| \geq |g|\mu$  holds due to (4.34). Then Lemma 4.4 gives (4.31), (4.32)-(4.33) and  $\lambda \notin \sigma(J_1(g)) = \sigma(J(g))$ .  $\square$

#### 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

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

with  $\text{rank } P(g) = \text{rank } P(0) = 2$ , 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

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

Let us choose  $\varepsilon > 0$  small enough. Then the property (4.36) holds if  $0 < |g| \leq \varepsilon$  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

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

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

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

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

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

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  $\mathbb{D}(0, \rho) \rightarrow \mathbb{D}(0, \mu\rho)$ , 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  $\Pi_l J \Pi_l$ , 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.  $\square$

### 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

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

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

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

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

$$\sigma(J_{l,0}(g)) = \{\lambda_{0,l}(g), \lambda_{1,l}(g)\} \cup \sigma(\widetilde{D} + g\widetilde{B}_l(g)) \quad (5.3)$$

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

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

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

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

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

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

due to the min-max principle. If  $g \in [-\varepsilon_0, \varepsilon_0]$  then combining (5.6) with (5.5) and Theorem 1.3, we get

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

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 Th. 3.8 in [112]) 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*

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

*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

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

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

$$\Pi_0 [\widehat{B}_l \oplus \widetilde{B}_l, Q_l] \Pi_0 = 0. \quad (5.10)$$

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

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

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

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

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

### 5.3 Second step of the proof of Proposition 5.1

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

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

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

*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  $l \geq 1$  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

$$Q_{l-1}\Pi'_l = 0 = \Pi'_l Q_{l-1} \quad (5.14)$$

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

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

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

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

Using

$$R_l = B_l - \Pi_0 B_l \Pi_0 - \Pi'_0 B_l \Pi'_0 \quad (5.18)$$

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  $\Pi'_{l+1}(R_l - R_0) = 0$ .  $\square$

### 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

$$\Pi_i(J(g) - J^\circ(g))\Pi_i = 0 \quad (5.19)$$

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

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

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

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

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

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

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

$$\Pi_i(J_l - J_l^\circ)\Pi_i = 0 \quad (5.22)$$

holds for  $l = 0, \dots, i$ . 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

$$\Pi_i(B_l - B_l^\circ)\Pi_i = 0 \quad (5.23)$$

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

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

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  $l = 1, \dots, i$  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

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



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

$$\widehat{B}_n^\pm := \begin{pmatrix} b'_1 & b_1 & 0 & & & & & 0 \\ b_1 & b'_2 & b_2 & & & & & \\ 0 & b_2 & b'_3 & & & & & \\ & & & \ddots & \ddots & \ddots & & \\ & & & & b'_{n-3} & b_{n-3} & 0 & 0 \\ & & & & b_{n-3} & b'_{n-2} & b_{n-2} & 0 \\ 0 & & & & 0 & b_{n-2} & b'_{n-1} & b_{n-1} \\ & & & & 0 & 0 & b_{n-1} & b'_n \pm |b_n| \end{pmatrix} \quad (6.2)$$

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*

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

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

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

*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

$$\langle x, B^\circ x \rangle = \sum_j b_j^\circ x_{j+1} \bar{x}_j + \sum_i b_{i-1}^\circ x_{i-1} \bar{x}_i. \quad (6.5)$$

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

$$\sum_j 2|b_j^\circ| |x_{j+1} x_j| \leq \sum_j |b_j^\circ| (|x_{j+1}|^2 + |x_j|^2). \quad (6.6)$$

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

$$\sum_i |b_i^\circ| |x_{i+1}|^2 + \sum_j |b_j^\circ| |x_j|^2 = \sum_j (|b_{j-1}^\circ| + |b_j^\circ|) |x_j|^2 \quad (6.7)$$

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

## 6.3 Applying the min-max principle.

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

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

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

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

$$\pm \langle x, B_n^\circ x \rangle \leq \langle x, D_n^\circ x \rangle, \quad (6.8)$$

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

$$J_n^\pm(g) := D + gB_n \pm gD_n^\circ = \widehat{J}_n^\pm(g) \oplus \text{diag}(d_i \pm g\beta'_i)_{i=n+1}^\infty \quad (6.9)$$

where  $\widehat{J}_n^\pm(g)$  is the linear map acting on  $\text{span}\{e_1, \dots, e_n\}$  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

$$d_i \pm g\beta'_i \geq \frac{1}{2}d_i \text{ if } -\rho < g < \rho, \quad (6.10)$$

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

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

and the min-max principle ensures

$$\begin{cases} \widehat{\lambda}_i(J_n^-(g)) \leq \widehat{\lambda}_i(J(g)) \leq \widehat{\lambda}_i(J_n^+(g)) & \text{if } g \geq 0 \\ \widehat{\lambda}_i(J_n^+(g)) \leq \widehat{\lambda}_i(J(g)) \leq \widehat{\lambda}_i(J_n^-(g)) & \text{if } g \leq 0 \end{cases} \quad (6.12)$$

#### 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  $i \geq n$  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

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

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

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

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

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

Since (1.19) ensures  $2\rho\mu_k < d_i - \rho\beta'_i$ , one has

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

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  $J_n^+$  instead of  $J$ , we get

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

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  $g \rightarrow \widehat{\lambda}_l(J_n^+(g))$ , one has  $l = 1 + \text{card}\{i \in \mathbb{N}^* : d_i < d_k\}$ . Similarly

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

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

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

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

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

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

for  $j = 0, 1$ . We observe that Proposition 5.1 applied to  $\widehat{J}_n^+$  and  $\widehat{J}_n^-$  give

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

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

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

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

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

holds with  $|c_{k+j,\nu}| \leq \mu_k \rho^{1-\nu}$ . Similar inequalities can be written when  $-\rho < g < 0$ . Thus  $g \rightarrow \lambda_{k+j}(J(g))$  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

$$i \geq C \Rightarrow d_i \pm g\beta_i \geq cd_i \quad (6.25)$$

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  $n \geq n_0$ .

## 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

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

(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

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

with

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

Moreover

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

holds with

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

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

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

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

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

## 7.2 Proof of Theorem 1.5

We consider the first similarity transformation using

$$e^{igQ_0} = \begin{pmatrix} c & -s & 0 & 0 \\ s & c & 0 & 0 \\ 0 & 0 & \dot{c} & -\dot{s} \\ 0 & 0 & \dot{s} & \dot{c} \end{pmatrix} \oplus I_{V_1^\perp}, \quad (7.9)$$

where

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

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

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

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

and

$$g\widehat{B}_1(g) = \begin{pmatrix} d_k^0 + r_{k-1} & gb_k c \dot{c} \\ gb_k c \dot{c} & d_{k+1}^0 - r_{k+1} \end{pmatrix} = gB_k^1(g) + O(g^4) \quad (7.14)$$

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

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

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

$$g\widehat{B}_2(g) = \begin{pmatrix} d_k^0 + r_{k-1} + p_k & gb_k c \dot{c} \\ gb_k c \dot{c} & d_{k+1}^0 - r_{k+1} + p_{k+1} \end{pmatrix} + O(g^5) \quad (7.15)$$

holds with

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

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

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  $g\widehat{B}_2$  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  $\widehat{n} = 1$ . Consider first the case when  $b'_i = 0$  for all  $i$ . Under this assumption we can check by induction that the functions  $g \rightarrow \langle e_i, J_l(g)e_j \rangle$  are even when  $i - j$  is even and odd when  $i - j$  is odd. Since  $\lambda_k(J(g)) = \langle e_i, J_l(g)e_j \rangle + O(g^{2l})$ , it is clear that  $g \rightarrow \lambda_k(J(g))$  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  $V_l := \text{span}\{e_{k+j}\}_{-l \leq j \leq l}$  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

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

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

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

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

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

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

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

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

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

with

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

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

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

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

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

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  $\begin{pmatrix} d_{k-2}^0 & -gb_{k-2}s \\ * & d_{k,1} \end{pmatrix}$  and  $\begin{pmatrix} d_{k,1} & gb_{k+1}\ddot{s} \\ * & d_{k+2}^0 \end{pmatrix}$ . This similarity gives  $J_2 = D + gB_2$  with  $B_2 = (d_{k,2}) \oplus \tilde{B}_2 + R_2$  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

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

If we express  $d_{k,1} := r_{k-1} - \tilde{r}_k$  using (7.19) and (7.23), 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.

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# Chapitre 9

## Les cinq coefficients de la série de perturbations des valeurs propres

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## The five coefficients of the perturbation series of eigenvalues

Let  $J(g)$  be the operator defined in Theorem 1.3 of Chapter 8. Our goal in this chapter is to prove proposition 1 which give the detailed formulas of the two eigenvalues of  $J(g)$  close to  $d(k)$  with the error  $O(g^6)$ .

### 1 Statement of the result

**Proposition 1.** *Let  $J(g)$  be the operator defined in Theorem 1.3 of Chapter 8 and assume that all the hypothesis of Theorem 1.3 holds and  $(\lambda_{k+j}(J(g)))_{j=0,1}$  are the eigenvalues of  $J(g)$  satisfy (i),(ii) and (iii) of Theorem 1.3 in Chapter 8. Then we have*

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

where  $(\lambda_{k+j,2}(g))_{j=0,1}$  given by (2.1).

### 2 Proof

Further on, to simplify the writing, we write  $d_i^0$  instead of  $d_i^0(g)$  and the same for the functions which contain  $d_i^0(g)$  we denote it  $f$  instead of  $f(g)$ .

In Section 7.2 of chapter 8, we show that  $J_1(g) = e^{-igQ_0(g)}J(g)e^{igQ_0(g)}$  is equivalent to

$$\begin{pmatrix} d_{k-2}^0 & gb_{k-2}c & -gb_{k-2}s & 0 & 0 & 0 \\ * & d_{k-1}^0 - r_{k-1} & 0 & gb_k s \dot{c} & -gb_k s \dot{s} & 0 \\ * & * & d_k^0 + r_{k-1} & gb_k c \dot{c} & -gb_k c \dot{s} & 0 \\ * & * & * & d_{k+1}^0 - r_{k+1} & 0 & gb_{k+2} \dot{s} \\ * & * & * & * & d_{k+2}^0 + r_{k+1} & gb_{k+2} \dot{c} \\ * & * & * & * & * & d_{k+3}^0 \end{pmatrix}$$

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

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

The operator  $Q_1$  obtained from (5.9) in Chapter 8, i.e,

$$gQ_1(g) = \begin{pmatrix} 0 & 0 & -\frac{igb_{k-2}s}{d_{k-2}} & 0 & 0 & 0 \\ * & 0 & 0 & \frac{igb_k s \dot{c}}{d_{k-1}} & 0 & 0 \\ * & * & 0 & 0 & -\frac{igb_k c \dot{s}}{d_{k+2}} & 0 \\ * & * & * & 0 & 0 & \frac{igb_{k+2} \dot{s}}{d_{k+3}} \\ * & * & * & * & 0 & 0 \\ * & * & * & * & * & 0 \end{pmatrix} \oplus \mathbb{O}_{V_2^\perp}$$

Then (5.9) in Chapter 8 for  $l = 2$  gives

$$J_2 = e^{-igQ_1(g)} J(g) e^{igQ_1(g)} = J_1 + i[J_1, gQ_1] - \frac{1}{2}[[J_1, gQ], gQ] + O(g^6).$$

due to  $Q_1 = O(g)$ . The direct calculation gives us :

$$g\widehat{B}_2(g) = \begin{pmatrix} d_k^0 + r_{k-1} + q_k & gb_k c\dot{c} + h_k \\ gb_k c\dot{c} + h_k & d_{k+1}^0 - r_{k+1} + q_{k+1} \end{pmatrix} + O(g^6)$$

with

$$q_k = -2g^2 \frac{b_{k-2}^2 s^2}{d_{k-2}} - 2g^2 \frac{b_k^2 \dot{s}^2}{d_{k+2}} - g^2 \frac{b_{k-2}^2 s^2 (d_k^0 - d_{k-2}^0)}{d_{k-2}^2} - g^2 \frac{b_k^2 \dot{c}^2 \dot{s}^2 (d_k^0 - d_{k+2}^0)}{d_{k+2}^2},$$

$$q_{k+1} = -2g^2 \frac{b_k^2 s^2}{d_{k-1}} - 2g^2 \frac{b_{k+2}^2 \dot{s}^2}{d_{k+3}} - g^2 \frac{b_k^2 s^2 \dot{c}^2 (d_{k+1}^0 - d_{k-1}^0)}{d_{k-1}^2} - g^2 \frac{b_{k+2}^2 \dot{s}^2 (d_{k+1}^0 - d_{k+3}^0)}{d_{k+3}^2},$$

and

$$h_k = -g^3 \frac{b_k^3 s^2}{2d_{k-1}^2} - g^3 \frac{b_{k-2}^2 b_k s^2}{d_{k-1} d_{k-2}} - g^3 \frac{b_{k+2}^2 b_k \dot{s}^2}{d_{k+3} d_{k+2}} - g^3 \frac{b_{k-2}^2 b_k s^2}{2d_{k-2}^2} - g^3 \frac{b_k^3 \dot{s}^2 \dot{c}^3}{2d_{k+2}^2}.$$

Then (5.8) of chapter 8 ensures that  $\lambda_{k+j}(J(g)) = \lambda_{k+j,2}(g) + O(g^6)$ , where  $\{\lambda_{j,2}(g)\}_{j=0,1}$  are the eigenvalues of  $g\widehat{B}_2$ . Our goal is to find the formulas of  $\lambda_{j,2}(g)$  with the error  $O(g^6)$ .

**Eigenvalues of  $g\widehat{B}_2$**  Let  $\lambda$  be an eigenvalue of  $g\widehat{B}_2$ , then  $\det(g\widehat{B}_2 - \lambda) = 0$ , by making a direct calculation and using the Taylor series expansions around 0 of the functions  $c, \dot{c}, s$  and  $\dot{s}$  we obtain :

$$\begin{aligned} \det(g\widehat{B}_2 - \lambda) &= (d_k^0 + r_{k-1} + q_k - \lambda) (d_{k+1}^0 - r_{k+1} + q_{k+1} - \lambda) - (gb_k c\dot{c} + h_k)^2 \\ &= \lambda^2 + B\lambda + C + O(g^7) \end{aligned}$$

with

$$\begin{aligned} B &= \alpha_2 g^2 + \alpha_4 g^4 + \alpha_5 g^5 + O(g^6); \\ C &= \gamma_2 g^2 + \gamma_3 g^3 + \gamma_4 g^4 + \gamma_5 g^5 + \gamma_6 g^6; \end{aligned}$$

where

$$\begin{aligned}
 \alpha_2 &= -\frac{b_{k-1}^2}{d_k^0 - d_{k-1}^0} + \frac{b_{k+1}^2}{d_{k+2}^0 - d_{k+1}^0}, \\
 \alpha_4 &= \frac{b_{k-1}^4}{(d_k^0 - d_{k-1}^0)^3} - \frac{b_{k+1}^4}{(d_{k+2}^0 - d_{k+1}^0)^3} + \frac{b_{k-2}^2 b^2 k - 1}{d_{k-2}(d_{k-1}^0 - d_k^0)^2} + \frac{b_k^2 b_{k+1}^2}{d_{k+2}(d_{k+1} - d_{k+2}^0)^2} \\
 &+ \frac{b_k^2 b_{k-1}^2}{d_{k-1}(d_{k-1}^0 - d_k^0)^2} + \frac{b_{k+1}^4}{d_{k+3}(d_{k+1}^0 - d_{k+2}^0)^2}, \\
 \alpha_5 &= \frac{b_k^2 b_{k-1}^2 (b'_{k+1} - b'_{k-2})}{d_{k-2}^2 (d_{k-1}^0 - d_k^0)^2} + \frac{b_{k+2}^2 b_{k+1}^2 (b'_{k+1} - b'_{k+3})}{d_{k+3}^2 (d_{k+1}^0 - d_{k+2}^0)^2} + \frac{b_{k-2}^2 b_{k-1}^2 (b'_k - b'_{k-2})}{d_{k-2}^2 (d_{k-1}^0 - d_k^0)^2} \\
 &+ \frac{b_k^2 b_{k+1}^2 (b'_k - b'_{k+2})}{d_{k+2}^2 (d_{k+1}^0 - d_{k+2}^0)^2}, \\
 \gamma_2 &= -b_k'^2 - b_k^2, \\
 \gamma_3 &= -\frac{b'_k b_{k+1}^2}{d_{k+2}^0 - d_{k+1}^0} + \frac{b'_{k+1} b_{k-1}^2}{d_k^0 - d_{k-1}^0}, \\
 \gamma_4 &= -\frac{b_{k-1}^2 b_{k+1}^2}{(d_k^0 - d_{k-1}^0)(d_{k+2}^0 - d_{k+1}^0)} + \frac{b_{k+1}^2 b_k^2}{(d_{k+1}^0 - d_{k+2}^0)^2} + \frac{b_{k-1}^2 b_k^2}{(d_{k+1}^0 - d_k^0)^2}, \\
 \gamma_5 &= \frac{b_{k+1}^4 b'_k}{(d_{k+2}^0 - d_{k+1}^0)^3} - \frac{b_k^2 (b'_k - b'_{k-1})}{d_{k-1}(d_{k-1}^0 - d_k^0)^2} - \frac{b_{k+1}^4 (b'_k - b'_{k+3})}{d_{k+3}(d_{k+1}^0 - d_{k+2}^0)} - \frac{b_{k-1}^4 b'_{k+1}}{(d_k^0 - d_{k-1}^0)^3} \\
 &- \frac{b_{k-2}^2 b_{k-1}^2 (b'_{k+1} - b'_{k-2})}{d_{k-2}(d_{k-1}^0 - d_k^0)^2} - \frac{b_k^2 (b'_{k+1} - b'_{k+2})}{d_{k+2}(d_{k-1}^0 - d_k^0)^2},
 \end{aligned}$$

and

$$\begin{aligned}
 \gamma_6 &= -\frac{b_k^2 b_{k-1}^2 b'_{k+1} (b'_k - b'_{k-2})}{d_{k-2}^2 (d_{k-1}^0 - d_k^0)^2} - \frac{b'_{k+1} b_{k+2}^2 b_{k+1}^2 (b'_k - b'_{k+3})}{d_{k+3}^2 (d_{k+1}^0 - d_{k+2}^0)^2} + \frac{b_{k-1}^2 b_{k+1}^4}{(d_k^0 - d_{k-1}^0)(d_{k+2}^0 - d_{k+1}^0)^3} \\
 &+ \frac{b_{k-1}^4 b_{k+1}^2}{(d_{k+2}^0 - d_{k+1}^0)(d_k^0 - d_{k-1}^0)^3} - \frac{b_{k-1}^4 b_k^2}{d_{k-1}(d_k^0 - d_{k-1}^0)^3} - \frac{b_{k-1}^2 b_{k+1}^4}{d_{k+3}(d_k^0 - d_{k-1}^0)(d_{k+1}^0 - d_{k+2}^0)^2} \\
 &+ \frac{b_{k-2}^2 b_{k+1}^2 b_{k-1}^2}{d_{k-2}(d_{k+2}^0 - d_{k+1}^0)(d_{k-1}^0 - d_k^0)^2} + \frac{b_k^2 b_{k+1}^4}{d_{k+2}(d_{k+2}^0 - d_{k+1}^0)^3} - \frac{b'_{k+1} b_{k-2}^2 b_{k-1}^2 (b'_k - b'_{k-2})}{d_{k-2}^2 (d_{k-1}^0 - d_k^0)^2} \\
 &- \frac{b'_{k+1} b_k^2 b_{k+1}^2 (b'_k - b'_{k+2})}{d_{k+2}^2 (d_{k+1}^0 - d_{k+2}^0)^2} - \frac{b_k b_{k+1}^4}{3(d_{k+1}^0 - d_{k+2}^0)^4} - \frac{b_{k-1}^2 b_{k+1}^2 b_k}{(d_{k-1}^0 - d_k^0)^2 (d_{k+1}^0 - d_{k+2}^0)^2} - \frac{b_{k+1}^4 b_k}{3(d_{k-1}^0 - d_k^0)^4}
 \end{aligned}$$

We introduce  $\Delta = B^2 - 4C$ , it is clear that the formulas of two eigenvalues  $\{\lambda_{j,2}(g)\}_{0,1}$  given by

$$\lambda_{k+j,2}(g) = \frac{-B + (-1)^j \sqrt{\Delta}}{2} + O(g^7)$$

A direct calculation allow us to obtain the formula of  $\Delta$  which takes the form  $\Delta = \theta g^2(1 + \beta(g)g)$  where  $\theta, \beta(g)$  two constants found. Next, we use the expansion limited of

$(1 + \beta(g)g)^{1/2}$  to the neighborhood of 0 to deduce an approximation of  $\sqrt{\Delta}$  with the error  $O(g^6)$ , finally we obtain :

$$\sqrt{\Delta} = \delta_1 g + \delta_2 g^2 + \delta_3 g^3 + \delta_4 g^4 + \delta_5 g^5 + O(g^6).$$

with

$$\begin{aligned} \delta_1 &= \sqrt{-4\gamma_2} = 2(b'_k{}^2 + b_k^2), \\ \delta_2 &= \frac{\gamma_3 \delta_1}{2\gamma_2}, \\ \delta_3 &= -\frac{\delta_1(\alpha_2^2 - 4\gamma_4)}{8\gamma_2} - \frac{\delta_1 \gamma_3^2}{8\gamma_2^2}, \\ \delta_4 &= \frac{\delta_1 \gamma_3}{2\gamma_2} + \frac{\delta_1 \gamma_3^3}{16\gamma_2^3}, \\ \delta_5 &= -\frac{\delta_1(\alpha_4 \alpha_2 - 2\gamma_6)}{4\gamma_2} - \frac{\gamma_3(\alpha_2^2 - 4\gamma_4)\delta_1}{4\gamma_2(\alpha_1^2 - 4\gamma_2)} - \frac{\gamma_3^2 \delta_1}{4\gamma_2^2} + \frac{3\gamma_3^2 \delta_1(\alpha_2^2 - 4\gamma_4)}{16\gamma_2^2}. \end{aligned}$$

And we deduce that

$$\lambda_{k+j,2}(g) = \mu_{k+j}g + \hat{c}_{k+j,2}g^2 + \hat{c}_{k+j,3}g^3 + \hat{c}_{k+j,4}g^4 + \hat{c}_{k+j,5}g^5 + O(g^6) \quad (2.1)$$

with

$$\begin{aligned} \mu_{k+j} &= \frac{(-1)^j \delta_1}{2} = (-1)^j (b'_k{}^2 + b_k^2) \\ \hat{c}_{k+j,2} &= \frac{-\alpha_2 + (-1)^j \delta_2}{2} = \frac{b_{k-1}^2}{2(d_k^0 - d_{k-1}^0)} - \frac{b_{k+1}^2}{2(d_{k+2}^0 - d_{k+1}^0)} + \frac{b'_k b_{k+1}^2}{2\mu_{k+j}(d_{k+2}^0 - d_{k+1}^0)} + \frac{b_{k-1}^2 b'_k}{2\mu_{k+j}(d_k^0 - d_{k-1}^0)}, \\ \hat{c}_{k+j,3} &= -\frac{b_k^2 b_{k+1}^2}{2\mu_{k+j}(d_{k+2}^0 - d_{k+1}^0)^2} - \frac{b_{k-1}^2 b_k^2}{2\mu_{k+j}(d_k^0 - d_{k-1}^0)^2} + \frac{b_{k-1}^4}{8\mu_{k+j}(d_k^0 - d_{k-1}^0)^2} \\ &+ \frac{b_{k+1}^4}{8\mu_{k+j}(d_{k+2}^0 - d_{k+1}^0)^2} + \frac{b_{k-1}^2 b_{k+1}^2}{4(d_k^0 - d_{k-1}^0)(d_{k-2}^0 - d_{k+1}^0)} - \frac{b_{k+1}^4 b_k^2}{2\mu_{k+j}(d_{k+2}^0 - d_{k+1}^0)^2} \\ &- \frac{b_{k-1}^4 b_k^2}{2(d_k^0 - d_{k-1}^0)^2} - \frac{b_{k+1}^2 b_{k-1}^2 b_k^2}{\mu_{k+j}(d_k^0 - d_{k-1}^0)(d_{k+2}^0 - d_{k+1}^0)}, \\ \hat{c}_{k+j,4} &= -\frac{b_{k-1}^4}{2(d_k^0 - d_{k-1}^0)^3} + \frac{b_{k+1}^4}{2(d_{k+2}^0 - d_{k+1}^0)^3} - \frac{b_{k-2}^2 b^2 k - 1}{2d_{k-2}(d_{k-1}^0 - d_k^0)^2} - \frac{b_k^2 b_{k+1}^2}{2d_{k+2}(d_{k+1}^0 - d_{k+2}^0)^2} \\ &- \frac{b_k^2 b_{k-1}^2}{2d_{k-1}(d_{k-1}^0 - d_k^0)^2} - \frac{b_{k+1}^2 b^2 k + 2}{2d_{k+3}(d_{k+1}^0 - d_{k+2}^0)^2} + \frac{b'_k b_{k+1}^2}{2\mu_{k+j}(d_{k+2}^0 - d_{k+1}^0)} \\ &- \frac{b'_{k+1} b_{k-1}^2}{2\mu_{k+j}(d_k^0 - d_{k-1}^0)} - \frac{1}{32 \cdot 8\mu_{k+j}^{2/5}} \cdot \left( \frac{b'_k b_{k+1}^2}{d_{k+2}^0 - d_{k+1}^0} - \frac{b'_{k+1} b_{k-1}^2}{d_k^0 - d_{k-1}^0} \right)^3, \\ \hat{c}_{k+j,5} &= \frac{-\alpha_5 + (-1)^j \delta_5}{2}. \end{aligned}$$

## Résumé

### Estimations du spectre discret des opérateurs définis par des matrices infinies non-bornées et le modèle quantique de Rabi

L'objectif de cette thèse est d'étudier les valeurs propres des opérateurs auto-adjoints en relation avec le modèle proposé par le lauréat du prix Nobel en physique, I. I. Rabi. Le modèle quantique de Rabi, décrivant des interactions entre un système à deux niveaux et un mode du champ quantique. Il s'agit de la façon la plus simple de coupler un système à deux niveaux à un seul mode du rayonnement. C'est pour cette raison que ce modèle est considéré comme le modèle le plus fondamental, populaire et réussi pour étudier l'interaction entre la matière et le rayonnement électromagnétique. Par conséquent le QRM occupe une place cruciale dans différents domaines de la physique, notamment en optique quantique [52]. Il est utilisé pour décrire l'interaction entre le champ électrique d'une cavité électromagnétique et deux niveaux électroniques d'un atome [107, 132] ou encore l'interaction entre un circuit supraconducteur et un résonateur électronique [90, 13, 18]. Il peut par ailleurs être réalisé dans de nombreux systèmes physiques, y compris les ions piégés [85], les points quantiques [48] et les systèmes quantiques hybrides [130, 5, 66].

Comme tout le système quantique, le modèle quantique de Rabi est caractérisé par son hamiltonien, qui est un opérateur auto-adjoint dont les valeurs propres correspondent aux niveaux d'énergie du système. La connaissance des niveaux d'énergie du système est cruciale pour tester la validité du modèle de manière expérimentale ou à déterminer les valeurs de paramètres du modèle testé dans une expérience donnée.

L'hamiltonien du modèle quantique de Rabi contient trois termes. Le premier terme se réfère à un système quantique à deux niveaux et le second décrit le mode quantique du champ. Le troisième terme est le terme de l'interaction dont la forme est motivée par l'idée que chaque création d'un photon accompagne la désexcitation atomique et chaque annihilation d'un photon accompagne l'excitation atomique. Il existe une multitude de généralisations du modèle de Rabi, selon les expériences et les réalisations. On réfère à [115] pour des explications physiques (voir aussi [15]) et à [133] pour une liste de travaux de recherche théoriques et expérimentales en relation avec le modèle quantique de Rabi.

Une partie de cette thèse est consacrée à la théorie de perturbations des valeurs propres pour une classe de matrices tridiagonales infinies qui définissent des opérateurs auto-adjoints non bornés à spectre discret dans l'espace de Hilbert des suites de carré

sommables. On donne le comportement des valeurs propres en fonction du paramètre du couplage  $g$  et on s'intéresse en particulier au cas de la perturbation des valeurs propres doubles. Notre analyse porte sur les problèmes suivants :

- (i) prouver que les branches de valeurs propres sont des fonctions analytiques de  $g$  et donner une borne explicite du rayon de convergence,
- (ii) donner des estimations explicites de l'erreur due à une coupure de la série de Taylor,
- (iii) donner une méthode de calcul des coefficients et exprimer les corrections d'ordre inférieur.

Concernant le point (i), il faut contrôler le spectre par rapport à  $g$  pour éviter le croisement des valeurs propres. Les résultats pour le point (ii) sont obtenus de manière standard : la formule intégrale de Cauchy donne les bornes des coefficients et il est clair que les estimations deviennent meilleures lorsque le rayon de convergence est plus grand.

Notre intérêt pour ce problème vient de l'article [60], où les auteurs étudient la qualité de l'approximation du modèle quantique de Rabi par le modèle de Jaynes-Cummings (l'approximation de l'onde tournant) et proposent les corrections des valeurs propres. Les auteurs de [60] évoquent les difficultés à maîtriser une matrice infinie et proposent de regarder un petit bloc dans l'espoir d'obtenir des approximations correctes. Dans notre travail, on développe la théorie de perturbations quasi-dégénérées de Schrieffer-Wolff pour calculer les coefficients de la série perturbative et donner des estimations explicites d'erreurs. De plus, on détermine la taille minimale du bloc pour récupérer un coefficient donné de la série perturbative. Il apparaît que les coefficients proposés dans [60] ne sont pas corrects car le bloc est trop petit.

Notre premier résultat dans cette partie concerne les perturbations d'une valeur propre simple de  $D$ . Pour cela, on fixe  $k \in \mathbb{N}^*$  et suppose que

$$d_k \neq d_i \text{ pour } i \in \mathbb{N}^* \setminus \{k\}. \quad (2.2)$$

Puisque  $\sigma(J(g) - (d + gb)I) = \sigma(J(g)) - (d + gb)$ , notre analyse de  $J(g)$  peut être réduite à une analyse de  $J(g) - (d + gb)I$  et en particulier, on peut utiliser  $d = d_k$ ,  $b = b'_k$ . Ainsi, sans aucune perte de la généralité, on peut supposer que  $d_k = b'_k = 0$ . De plus, on note

$$\beta_i := |b_{i-1}| + |b_i| + |b'_i| \quad (2.3)$$

et on introduit

$$0 < \rho < \inf_{i \neq k} \frac{|d_i|}{\beta_i + \beta_k}. \quad (2.4)$$

On suppose également que **(H1)**-**(H3)** sont vérifiées et  $\rho \leq \rho_0$ . On montre les résultats suivants :

- (i) Si  $-\rho < g < \rho$  alors l'intervalle  $[-\beta_k \rho, \beta_k \rho]$  contient exactement une valeur propre de  $J(g)$ ,

$$[-\beta_k \rho, \beta_k \rho] \cap \sigma(J(g)) = \{\lambda_k(J(g))\}. \quad (2.5)$$

(ii) La valeur  $\lambda_k(J(g))$  est simple et  $g \rightarrow \lambda_k(J(g))$  est analytique réelle, c'est-à-dire

$$\lambda_k(J(g)) = \sum_{\nu=1}^{\infty} c_{k,\nu} g^\nu \text{ si } -\rho < g < \rho. \quad (2.6)$$

(iii) Les coefficients dans (2.6) satisfont aux estimations  $|c_{k,\nu}| \leq \beta_k \rho^{1-\nu}$  et on a

$$\left| \lambda_k(J(g)) - \sum_{1 \leq \nu \leq N} c_{k,\nu} g^\nu \right| \leq \frac{\beta_k |g|^{N+1}}{(\rho - |g|) \rho^{N-1}} \text{ si } -\rho < g < \rho. \quad (2.7)$$

(iv) Si  $b'_j = 0$  pour tout  $j \in \mathbb{N}^*$ , alors  $c_{k,\nu} = 0$  lorsque  $\nu$  est impair et (2.6) est vérifié avec

$$c_{k,2} = -\frac{b_k^2}{d_{k+1}} - \frac{b_{k-1}^2}{d_{k-1}} \quad (2.8)$$

$$c_{k,4} = \frac{b_k^4}{d_{k+1}^3} + \frac{b_{k-1}^4}{d_{k-1}^3} + \frac{b_k^2 b_{k-1}^2}{d_{k-1}^2 d_{k+1}} + \frac{b_k^2 b_{k-1}^2}{d_{k+1}^2 d_{k-1}} - \frac{b_k^2 b_{k+1}^2}{d_{k+1}^2 d_{k+2}} - \frac{b_{k-1}^2 b_{k-2}^2}{d_{k-1}^2 d_{k-2}}. \quad (2.9)$$

(v) Dans le cas général, on a

$$\lambda_k(J(g)) = c_{2,k}(g) g^2 + c_{4,k}(g) g^4 + O(g^6), \quad (2.10)$$

où  $c_{2,k}(g)$  et  $c_{4,k}(g)$  sont donnés en utilisant  $d_i + gb'_i$  au lieu de  $d_i$  dans (2.8)-(2.9).

Notre deuxième résultat dans cette partie concerne les perturbations d'une valeur propre double de  $D$ . Pour cela, on fixe  $k \in \mathbb{N}^*$  et suppose que

$$d_{k+1} = d_k \neq d_j \text{ pour } j \in \mathbb{N}^* \setminus \{k, k+1\}. \quad (2.11)$$

Sans perte de la généralité, on remplace  $J(g)$  par  $J(g) - (d + gb)I$  avec  $d = d_k$ ,  $b = (b'_k + b'_{k+1})/2$  et on suppose que

$$d_{k+1} = d_k = 0 \text{ et } b'_{k+1} = -b'_k. \quad (2.12)$$

On introduit les quantités

$$\mu_k := (b_k^2 + b_k'^2)^{1/2}, \quad (2.13)$$

$$\beta'_{k-1} := |b_{k-2}| + |b'_{k-1}|, \quad (2.14)$$

$$\beta'_{k+2} := |b_{k+2}| + |b'_{k+2}|, \quad (2.15)$$

$$\gamma_k := 3 \max\{|b_{k-1}|, |b_{k+1}|\} + 2 \max\{\mu_k, \beta'_{k-1}, \beta'_{k+2}\}, \quad (2.16)$$

$$\gamma'_k := \max \left\{ \left| \frac{b_{k-1}}{d_{k-1}} \right|, \left| \frac{b_{k+1}}{d_{k+2}} \right| \right\} \quad (2.17)$$

et

$$\beta'_i := |b_{i-1}| + |b_i| + |b'_i| \text{ si } i \notin [k-1, k+2]. \quad (2.18)$$



On suppose que **(H1)**-**(H3)** sont vérifiées et  $0 < \rho \leq \rho_0$  satisfait aux conditions

$$\rho \leq \inf_{i \notin \{k, k+1\}} \frac{|d_i|}{2(\beta'_i + \mu_k)}, \quad (2.19)$$

$$4\rho\mu_k \leq \inf_{i \notin \{k, k+1\}} |d_i|, \quad (2.20)$$

$$\rho \gamma_k \gamma'_k e^{2\rho\gamma'_k} < \mu_k, \quad (2.21)$$

où  $\mu_k, \gamma_k, \gamma'_k, \beta'_i$  sont donnés par (2.13)-(2.18). On montre les résultats suivants :

(i) Si  $-\rho < g < \rho$  et  $g \neq 0$ , alors

$$[-2\mu_k\rho, 2\mu_k\rho] \cap \sigma(J(g)) = \{\lambda_k(J(g)), \lambda_{k+1}(J(g))\}, \quad (2.22)$$

où les valeurs propres  $\lambda_k(J(g)), \lambda_{k+1}(J(g))$  sont simples et vérifient

$$\begin{cases} \lambda_k(J(g)) < 0 < \lambda_{k+1}(J(g)) \text{ if } g > 0, \\ \lambda_{k+1}(J(g)) < 0 < \lambda_k(J(g)) \text{ if } g < 0 \end{cases} \quad (2.23)$$

(ii) Si  $j = 0, 1$  et  $\mu_{k+1} := -\mu_k$ , alors on a

$$\lambda_{k+j}(J(g)) = -\mu_{k+j}g + \sum_{\nu=2}^{\infty} c_{k+j,\nu}g^\nu \text{ si } -\rho < g < \rho. \quad (2.24)$$

(iii) Les coefficients dans (2.24) satisfont aux estimations  $|c_{k+j,\nu}| \leq \mu_k\rho^{1-\nu}$  pour  $j = 0, 1$  et

$$\left| \lambda_{k+j}(J(g)) + \mu_{k+j}g - \sum_{2 \leq \nu \leq N} c_{k+j,\nu}g^\nu \right| \leq \frac{\mu_k|g|^{N+1}}{(\rho - |g|)\rho^{N-1}} \text{ si } -\rho < g < \rho. \quad (2.25)$$

Ensuite, on désigne

$$d_i^0(g) := d_i + gb'_i \text{ pour } i \in \mathbb{N}^*, \quad (2.26)$$

$$b_k^1(g) := b'_k + g \frac{b_{k-1}^2}{d_k^0(g) - d_{k-1}^0(g)}, \quad (2.27)$$

$$b_{k+1}^1(g) := b'_{k+1} + g \frac{b_{k+1}^2}{d_{k+1}^0(g) - d_{k+2}^0(g)}, \quad (2.28)$$

$$\widehat{b}_k^1(g) := b_k \left( 1 - \frac{g^2 b_{k-1}^2}{2(d_k^0(g) - d_{k-1}^0(g))^2} - \frac{g^2 b_{k+1}^2}{2(d_{k+1}^0(g) - d_{k+2}^0(g))^2} \right) \quad (2.29)$$

et on introduit la matrice

$$B_k^1(g) := \begin{pmatrix} b_k^1(g) & \widehat{b}_k^1(g) \\ \widehat{b}_k^1(g) & b_{k+1}^1(g) \end{pmatrix}. \quad (2.30)$$

Pour  $j = 0, 1$ , on désigne par  $\lambda_{k+j}^1(g)$  la valeur propre de  $B_k^1(g)$  qui vérifie

$$\lambda_{k+j}^1(g) \xrightarrow{g \rightarrow 0} -\mu_{k+j}.$$

On montre que

(iv) Pour  $j = 0, 1$ , on a

$$\lambda_{k+j}(J(g)) = g \lambda_{k+j}^1(g) + O(g^4). \quad (2.31)$$

(v) Si  $b'_k = 0$ , alors l'estimation (2.31) implique

$$\lambda_{k+j}(J(g)) = -\mu_{k+j}g - g^2 \left( \frac{b_{k-1}^2}{2d_{k-1}} + \frac{b_{k+1}^2}{2d_{k+2}} \right) + O(g^3) \quad (2.32)$$

où  $j = 0, 1$ , et  $\mu_{k+1} := -\mu_k$ .

En plus, on donne la formule détaillée de  $\lambda_{k+j}(J(g))$  avec l'estimation d'erreur  $O(g^6)$ .

Une autre partie de la thèse est consacrée à l'étude asymptotique de grandes valeurs propres. L'étude du comportement asymptotique des grandes valeurs propres de différents modèles de Rabi a été mentionné dans de nombreuses recherches physiques (voir par exemple [50], [86], [109], [134]), mais l'analyse mathématique de cette question a été initiée par E. A. Yanovich dans [123], [124], [135], et A. Boutet de Monvel, S. Naboko, L. O. Silva dans [27], [28] et a été poursuivie par A. Boutet de Monvel et Zielinski dans [31], [34], [30], [33] et elle fait l'objet de cette thèse.

Le modèle quantique de Rabi comporte le paramètre réel  $\Delta$  qui est la différence entre deux niveaux d'énergie et il s'avère que les valeurs propres peuvent être exprimées explicitement seulement dans le cas  $\Delta = 0$ . On considère donc le cas général comme une perturbation du cas  $\Delta = 0$ .

Dans cette thèse, nous considérons le modèle de Rabi quantique asymétrique décrit dans [61]. On l'appelle le QRM avec un biais statique fini ou le modèle de Rabi quantique asymétrique (AQRM). Ce modèle contient un terme supplémentaire  $\frac{1}{2}\epsilon\sigma_x$ , où  $\sigma_x$  est la matrice de Pauli et  $\epsilon$  est un paramètre appelé le biais statique du modèle. Il attire l'attention en relation avec des expériences récentes de couplage ultra-fort par des circuits supraconducteurs [133, 82]. En fait, les expériences avec un faisceau laser dans la cavité concerne le QRM avec un force de couplage  $g \sim 10^{-6}$ , tandis que des expériences avec des circuits qubits peuvent atteindre la valeur  $g \sim 10^{-1}$  et le biais statique  $\epsilon$  apparaît en raison de l'effet tunnel entre les deux états courants [61]. Dans l'absence de biais  $\epsilon$ , l'AQRM se réduit au modèle quantique de Rabi. Ce modèle a été étudié dans plusieurs travaux (voir par exemple [14], [20], [88] et [133]). Notre but est de donner le comportement asymptotique de grandes valeurs propres pour ce modèle, c'est-à-dire pour l'hamiltonien défini par

$$I_{\mathbb{C}^2} \otimes \hat{a}^\dagger \hat{a} + \frac{1}{2}(\Delta\sigma_z + \epsilon\sigma_x) \otimes I_{\ell^2(\mathbb{N})} + g\sigma_x \otimes (\hat{a} + \hat{a}^\dagger), \quad (2.33)$$

où  $\Delta$ ,  $\epsilon$  et  $g$  sont des paramètres réels. Ce problème a été étudié dans le cas où  $\epsilon = 0$  par E. A. Yanovich (Tur) dans [135] (voir aussi [124]) où l'estimation d'erreur obtenue est  $O(n^{-\frac{1}{16}})$  et plus tard ce résultat a été amélioré dans [34] qui donne la formule asymptotique

à trois termes pour les grandes valeurs propres. Dans le cas  $\epsilon \neq 0$  l'opérateur ne peut plus être décomposé en somme directe des opérateurs définis par des matrices tridiagonales et le comportement asymptotique de grandes valeurs propres n'a pas été étudié quand  $\epsilon \neq 0$ .

On démontre que le spectre de l'opérateur est discret et formé de deux suites de valeurs propres. On obtient la formule asymptotique pour la  $n$ -ième valeur propre avec l'estimation de l'erreur  $O(n^{-1/2} \ln n)$  lorsque  $n$  tend vers l'infini. Le principal outil utilisé est la méthode de quasi-similitude des opérateurs de J. Janas, S. Naboko [75] et E. A. Yanovich (Tur) [135]. Il s'avère que le problème peut être réduit à un problème analogue pour une perturbation compacte d'un opérateur diagonal obtenu par la diagonalisation du modèle quand  $\Delta = 0$ . L'approche est basée sur une approximation de vecteurs propres dans le cas  $\Delta = 0$ . Pour obtenir cette approximation, nous utilisons l'espace  $l^2(\mathbb{Z})$ . L'avantage de l'espace  $l^2(\mathbb{Z})$  réside dans la possibilité d'utiliser les séries de Fourier et étudier le cas  $\Delta = 0$  à l'aide des opérateurs pseudodifférentiels à coefficients périodiques. L'approximation de vecteurs propres est alors construite à l'aide des opérateurs du type de Fourier.

Plus précisément, on a montré que le spectre de l'opérateur (2.33) se compose de deux suites  $(E_m^-)_{m \in \mathbb{N}}$ ,  $(E_m^+)_{m \in \mathbb{N}}$ , qui vérifient la formule asymptotique

$$E_m^\pm = m - g^2 \pm \frac{1}{2} \epsilon + O(m^{-1/4}) \text{ quand } m \rightarrow \infty \quad (2.34)$$

Notre résultat est nouveau pour le modèle de Rabi asymétrique à un photon c'est-à-dire pour le cas où  $\epsilon \in \mathbb{R} \setminus \{0\}$ . L'estimation (2.34) est un résultat crucial que nous utilisons pour améliorer l'estimation (2.34). On prouve que l'hypothèse  $\epsilon \notin \mathbb{Z}$  implique la formule asymptotique

$$E_m^\pm = m - g^2 \pm \frac{1}{2} \epsilon + O(m^{-1/2} \ln m) \text{ quand } m \rightarrow \infty$$

et on prouve que dans le cas  $l_0 := \epsilon \in \mathbb{N}$  on a la formule asymptotique à trois termes

$$E_{i+l_0}^- = i + \frac{1}{2} l_0 - g^2 - |\mathbf{r}_i| + O(i^{-1/2} \ln i) \text{ quand } i \rightarrow \infty \quad (2.35)$$

$$E_i^+ = i + \frac{1}{2} l_0 - g^2 + |\mathbf{r}_i| + O(i^{-1/2} \ln i) \text{ quand } i \rightarrow \infty \quad (2.36)$$

avec

$$\mathbf{r}_i := i^{-1/4} \frac{\Delta}{2\sqrt{2\pi g}} \cos\left(4g\sqrt{i} - \frac{\pi}{4} - l_0 \frac{\pi}{2}\right). \quad (2.37)$$

Dans le cas  $\epsilon \in \mathbb{Z}$  la formule asymptotique comporte un terme oscillant d'ordre  $n^{-1/4}$ . L'expression de ce terme vient de l'application de la méthode de la phase stationnaire. Dans le cas  $\epsilon \notin \mathbb{Z}$  ce terme n'apparaît pas et pour cette raison il est raisonnable de dire que  $\epsilon \notin \mathbb{Z}$  donne lieu à un modèle non résonnant, pendant que le cas  $\epsilon \in \mathbb{Z}$  donne lieu à un modèle résonnant.

Dans cette thèse, on étudie aussi le modèle de Rabi asymétrique à deux photons, c'est-à-dire pour l'hamiltonien défini sur  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$  par

$$I_{\mathbb{C}^2} \otimes \hat{a}^\dagger \hat{a} + \frac{1}{2} (\Delta \sigma_z + \epsilon \sigma_x) \otimes I_{\ell^2(\mathbb{N})} + g \sigma_x \otimes (\hat{a}^2 + (\hat{a}^\dagger)^2), \quad (2.38)$$

où  $\Delta$ ,  $\epsilon$  et  $g$  sont des paramètres réels. Dans ce modèle, l'interaction est médiée par l'échange de deux photons et le biais statique  $\epsilon$  n'est pas nécessairement nul.

En supposant que  $0 < g < \frac{1}{2}$ , on montre que l'opérateur (2.38) est auto-adjoint dans  $\mathbb{C}^2 \otimes \ell^2(\mathbb{N})$ , son spectre est discret et se compose de deux suites des valeurs propres  $(E_{-1,m})_{m \in \mathbb{N}}$ ,  $(E_{1,m})_{m \in \mathbb{N}}$  qui vérifient la formule asymptotique

$$E_{\nu,m} = \beta m + \beta_\nu + O(m^{-1/2}), \quad \nu = \pm 1 \text{ quand } m \rightarrow \infty \quad (2.39)$$

où

$$\beta := \sqrt{1 - 4g^2}, \quad (2.40)$$

$$\beta_\nu = \frac{1}{2}(\beta - 1) + \nu \frac{\epsilon}{2} \text{ pour } \nu = \pm 1. \quad (2.41)$$

Pour obtenir ce résultat on a utilisé l'idée de [33] où ce problème avec  $\epsilon = 0$  a été étudié et le comportement de grandes valeurs propres a été obtenu avec l'estimation de l'erreur  $O(n^{-1/3})$ . Cependant nous rencontrons une différence majeure par rapport à [33] : dans le cas où  $\epsilon$  est un multiple de  $\beta$  on doit surmonter une difficulté supplémentaire due au fait que dans le cas où  $\Delta = 0$  l'opérateur (2.38) a des valeurs propres doubles qui ne peuvent pas être découplées lorsque  $\epsilon \neq 0$ .

On utilise une approximation de l'hamiltonien à deux photons avec  $\Delta = 0$  par un opérateur similaire à un opérateur différentiel du premier ordre sur le cercle afin que ses vecteurs propres puissent être exprimés explicitement. Dans le cas de l'hamiltonien à un photon donné par (2.33) avec  $\Delta = 0$ , une idée pareille donne un opérateur pseudo-différentiel d'ordre 1/2 et il faut construire une approximation de ses vecteurs propres.

Pour ce modèle, on retrouve la situation où on doit considérer une perturbation de valeurs propres doubles quand  $\epsilon$  est un multiple de  $\beta = \sqrt{1 - 4g^2}$  et dans ce cas la formule asymptotique comporte un terme oscillant d'ordre  $n^{-1/2}$ . Dans le cas où  $\epsilon/\beta$  n'est pas entier, le terme d'ordre  $n^{-1/2}$  n'apparaît pas. Ainsi, comme avant, on peut parler d'un modèle résonnant quand  $\epsilon/\beta \in \mathbb{Z}$  et d'un modèle résonnant dans le cas  $\epsilon/\beta \in \mathbb{Z}$ .

Plus précisément, en supposant que  $0 < g < \frac{1}{2}$  et  $\epsilon/\beta \notin \mathbb{Z}$ , on prouve que les valeurs propres  $(E_{-1,m})_{m \in \mathbb{N}}$ ,  $(E_{1,m})_{m \in \mathbb{N}}$  de l'opérateur (2.38), vérifient la formule asymptotique

$$E_{\nu,m} = \beta m + \beta_\nu + O(m^{-1} \ln m), \quad \nu = \pm 1 \text{ quand } m \rightarrow \infty$$

avec  $\beta_\nu = \beta_0 + \nu\epsilon/2$ .

Et en supposant que  $0 < g < \frac{1}{2}$  et  $l_0 = \epsilon/\beta \in \mathbb{N}$ , on montre que  $(\lambda_n(\mathbf{H}))_{n=1}^\infty$ , la suite des valeurs propres de l'opérateur (2.38) disposées dans l'ordre croissant et répétées selon leurs multiplicité, peut être exprimée comme la réunion des suites  $(E_m^-)_{m \in \mathbb{N}}$  et  $(E_m^+)_{m \in \mathbb{N}}$ , définies de manière suivante

$$E_n^- = \lambda_n(\mathbf{H}) \text{ for } n = 0, \dots, l_0,$$

$$E_{i+l_0}^- = \lambda_{2i+l_0}(\mathbf{H}) \text{ for } i \in \mathbb{N},$$

$$E_i^+ = \lambda_{2i+1+l_0}(\mathbf{H}) \text{ for } i \in \mathbb{N}.$$

De plus on a les formules asymptotiques suivantes

$$E_{i+l_0}^- = \beta i + \beta_0 + \frac{1}{2}\epsilon - |\mathbf{r}_i| + O(i^{-1} \ln i) \text{ quand } i \rightarrow \infty \quad (2.42)$$

$$E_i^+ = \beta i + \beta_0 + \frac{1}{2}\epsilon + |\mathbf{r}_i| + O(i^{-1} \ln i) \text{ quand } i \rightarrow \infty \quad (2.43)$$

avec

$$\begin{aligned} \beta &:= \sqrt{1 - 4g^2}, & \beta_0 &:= \frac{1}{2}(\beta - 1), \\ \mathbf{r}_i &:= 0 \text{ si } l_0 \text{ est impair} \\ \mathbf{r}_i &:= i^{1/2} \frac{\Delta}{2} \sqrt{\frac{\beta}{\pi g}} \cos\left((2\alpha - \frac{\pi}{2})(i + l_0) + (1 - l_0)\alpha\right) \text{ si } l_0 \text{ est pair} \end{aligned} \quad (2.44)$$

où

$$\alpha = \arctan \sqrt{\frac{1 - 2g}{1 + 2g}}. \quad (2.45)$$

Dans le cas du QRM à deux photons avec le biais  $l_0 = \epsilon = 0$  on obtient les formules asymptotiques

$$E_m^\pm = \beta m + \beta_0 \pm |\mathbf{r}_m| + O(m^{-1} \ln m) \text{ quand } m \rightarrow \infty \quad (2.46)$$

qui peuvent être considérées comme la généralisation de l'approximation de l'onde tournant (GRWA) pour ce modèle. Compte tenu du fait que  $\mathbf{r}_m$  est un terme oscillant dont l'amplitude est d'ordre  $m^{-1/2}$ , on voit que l'exposant  $-\frac{1}{2}$  dans l'estimation (2.39) est optimal.

Notre amélioration est basée sur l'estimation (2.39) et elle est obtenue par une approche qui est une adaptation de la théorie des perturbations de Schrieffer-Wolff [57].

**Mots clés :** spectre discret, valeurs propres, asymptotiques, matrices infinies, opérateur auto-adjoint, modèle de Rabi

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# Estimations du spectre discret des opérateurs définis par des matrices infinies non-bornées et le modèle quantique de Rabi

## Résumé

Le modèle quantique de Rabi, décrivant les interactions entre un système à deux niveaux et un mode du champ quantique, est considéré comme un modèle fondamental dans l'optique quantique, l'électrodynamique de circuits, l'étude de qubits supraconducteurs etc. L'objectif de cette thèse est une étude des valeurs propres des opérateurs auto adjoints définis par le modèle quantique de Rabi. Une partie de la thèse est consacrée à l'étude asymptotique des grandes valeurs propres pour le modèle quantique de Rabi avec un paramètre supplémentaire  $\epsilon$ , appelé le biais du modèle. On décrit le comportement asymptotique de la  $n$ -ième valeur propre avec l'erreur  $O(n^{-1/2} \ln n)$  lorsque  $n$  tend vers l'infini. Il s'avère que certaines valeurs de  $\epsilon$  présentent une difficulté supplémentaire due au fait que l'on doit considérer une perturbation de valeurs propres doubles et dans ce cas la formule asymptotique comporte un terme oscillant d'ordre  $n^{-1/4}$ . Ces résultats sont nouveaux dans le cas  $\epsilon \neq 0$ . On obtient aussi des résultats analogues pour le modèle de Rabi à deux photons. L'estimation d'erreur  $O(n^{-1} \ln n)$  pour ce modèle est nouveau même dans le cas  $\epsilon = 0$  et la formule asymptotique à trois termes peut être considérée comme une généralisation de l'approximation de l'onde tournant pour le modèle de Rabi à deux photons. Une autre partie de la thèse est consacrée à la théorie des perturbations pour une classe des opérateurs définis dans l'espace de Hilbert des suites de carré sommable par des matrices tridiagonales non bornées. Afin d'étudier la qualité de l'approximation du modèle de Rabi par le modèle de Jaynes-Cummings (l'approximation de l'onde tournant) on s'intéresse au comportement des valeurs propres en fonction du paramètre de couplage dans le cas de la perturbation des valeurs propres doubles. Grâce à un développement de la théorie de perturbations quasi-dégénérées de Schrieffer-Wolff, on obtient des estimations explicites du rayon de convergence de la série perturbative et des estimations d'erreur.

**Mots clés :** spectre discret, valeurs propres, asymptotiques, matrices infinies, opérateur auto-adjoint, modèle de Rabi

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## Estimates of discrete spectrum of operators defined by unbounded infinite matrices and the quantum Rabi model

### Abstract

The quantum Rabi model, which describes the interactions between a two-level system and a single-mode quantum field, is considered as a fundamental model in quantum optics, circuits quantum dynamics, analysis of superconducting qubits etc. The aim of this thesis is to study eigenvalues of self-adjoint operators defined by the quantum Rabi model. The first part of the thesis is devoted to the asymptotic analysis of large eigenvalues of the quantum Rabi model with an additional parameter  $\epsilon$ , called the bias of the model. We give the asymptotic behavior of the  $n$ -th eigenvalue with error of the form  $O(n^{-1/2} \ln n)$  as  $n$  tends to infinity. It appears that some values of  $\epsilon$  present an additional difficulty due to the fact that one must consider the perturbations of double eigenvalues and, in this case, the asymptotic formula contains an oscillating term of order  $n^{-1/4}$ . These results are new in the case  $\epsilon \neq 0$ . We also obtain analogue results for the two-photon quantum Rabi model. The error estimate  $O(n^{-1} \ln n)$  for this model is new even in the case  $\epsilon = 0$  and the three-term asymptotic formula can be considered as a generalized rotating wave approximation for the two-photon quantum Rabi model. Another part of the thesis is devoted to the perturbation theory for operators defined in the Hilbert space of square summable sequences by means of tridiagonal unbounded matrices. In order to study the quality of the approximation of the quantum Rabi model by the Jaynes-Cummings model (the rotating wave approximation), we are interested in the dependence of the eigenvalues on the coupling constant in the case of perturbations of double eigenvalues. Thanks to a development of the Schrieffer-Wolff theory of quasi-degenerate perturbations, we obtain explicit estimates of the convergence radius of the perturbation series and explicit error estimates.

**Keywords :** discrete spectrum, eigenvalues, asymptotics, infinite matrices, self-adjoint operator, Rabi model