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Study on the spectrum of the asymmetric quantum Rabi model

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Ph.D. Thesis

Study on the spectrum of the asymmetric quantum Rabi model

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Abstract

The quantum Rabi model is a model in quantum optics used to describe the interaction between a two-level atom and a single-level photon field. This model, described in 1963 by Jaynes and Cummings, is the fully quantized version of the original semi-classical model proposed in 1936 by Rabi. In previous years, the study of the properties of Hamiltonian of the quantum Rabi model and its energy levels (eigenvalues of the Hamiltonian) has been relegated mainly for two reasons. The first one was the belief that the quantum Rabi model was not an exactly solvable model, that is, that its energy levels could not be described analytically. The second reason is that in the parameter regime achievable at the time in experiments and applications, the quantum Rabi model could be approximated successfully by the Jaynes-Cummings model, a simpler model which is known to be exactly solvable.

Both situations changed in recent years. In 2011, Daniel Braak proved the exact-solvability of the quantum Rabi model by constructing analytical solutions and defining a transcendental function, the G-function, whose zeros determine all the spectrum (with the exception of a (possible finite) set of exceptional eigenvalues). This pioneering technique has since then been successfully applied to show the exact-solvability of several models in quantum optics. On the other hand, due to the advances in experimental physics, starting from the first decade of this century, experiments have been steadily reaching parameter regimes where the Jaynes-Cummings model becomes unsuitable for approximation and in 2014, the experiments by Maissen *et al* reached regimes where it is imperative to consider the full Hamiltonian of the quantum Rabi model. Adding to this, recently there has also been proposals for applications of the quantum Rabi model in quantum information theory and quantum computing. For these reasons, there has been a large amount of research done in theoretical and experimental physics, and, more recently, mathematics on the subject of the quantum Rabi model, its generalizations and applications.

In this thesis, we study the asymmetric quantum Rabi model, one of the generalizations of the quantum Rabi model. In this generalization, an additional non-trivial interaction term is introduced in the Hamiltonian, breaking the $\mathbb{Z}/2\mathbb{Z}$-symmetry of the quantum Rabi Hamiltonian. The presence of this symmetry in the quantum Rabi model explains the presence of crossings in the energy levels (degeneracies in the spectrum), so a priori there was no reason to expect degeneracies in the spectrum of the asymmetric version. In this work, we show that when the coefficient of the symmetry-breaking term is half-integer, degeneracies appear in the spectrum of the asymmetric quantum Rabi model. This is done by studying the properties of the constraint polynomials, polynomials appearing in certain conditions that the parameters of the model must satisfy in order to have certain eigenvalues, called Juddian eigenvalues.

The spectrum of the asymmetric quantum Rabi model is divided into different sets, an infinite set of regular eigenvalues, the zeros of the G-function and the exceptional eigenvalues, not captured as zeros of the G-function. The exceptional spectrum is further classified into Juddian and non-Juddian, according to the type of solution in the Segal-Bargmann space realization. These solutions are also described in terms of the $\mathfrak{sl}_2$ picture of the Hamiltonian in terms of irreducible representations of $\mathfrak{sl}_2$. The case for Juddian and regular eigenvalues was already known, and in this thesis we complete the picture for the non-Juddian eigenvalues. Another main result of this work is to characterize the degeneracies of the asymmetric quantum Rabi model in terms of the types of eigenvalues and the parameters. Furthermore, by carefully studying

the poles of the G-function, we define a new G-function whose zeros give the full spectrum of the asymmetric quantum Rabi model.

Finally, we present a study on continued fractions expansions of integer powers of the Napier constant e with a nice representation and good convergence properties. This study is a byproduct of the study of certain orthogonal polynomial families related to the constraint polynomials of the AQRM.

A la memoria de mis abuelos, María Márquez y Marcelino Bustos

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Notation

Acronyms

QHO	Quantum harmonic oscillator	6
QRM	Quantum Rabi model	16
AQRM	Asymmetric quantum Rabi model	16
NcHO	Non-commutative harmonic oscillator	18
OPS	Orthogonal polynomial system	70

Constants

$\hbar$	Reduced Planck constant	6
ω	Classical frequency of the QHO	6
$\sigma_x, \sigma_y, \sigma_z$	Pauli matrices	16
Δ	Half of the energy difference between the two levels of the QRM	16
g	Coupling strenght of the QRM	16
ε	Coefficient of symmetry-breaking term in AQRM	16

Mathematical notation

P, M	Position and momentum operators	6
$a^\dagger, a$	Raising and lowering operator of the QHO	7
$H_n(x)$	Hermite polynomials	8
$\mathcal{H}_\mathcal{B}$	Bargmann space	8
$SL_2(\mathbb{R}), \mathfrak{sl}_2(\mathbb{R})$	Special lineal group of real 2×2-matrices and its Lie algebra	10
$\mathcal{U}(\mathfrak{g})$	Universal enveloping algebra of the Lie algeba $\mathfrak{g}$	11
ϖ_a	Representation of $\mathfrak{sl}_2$ on the vector spaces $\mathbf{V}_i$	11
$\mathbf{F}_m$	Finite dimensional representations of $\mathfrak{sl}_2$	11
$\mathbf{D}_m^\pm$	Discrete series representations of $\mathfrak{sl}_2$	11
$\zeta_{H_{\text{Rabi}}}(s), \zeta_{H^\varepsilon_{\text{Rabi}}}(s)$	Spectral zeta function of QRM (resp. AQRM)	15

$H^{\varepsilon}_{\text{Rabi}}$	Hamiltonian of the AQRM	18
$\rho_1^{\pm}, \rho_2^{\pm}$	Exponents of system (2.4) and (2.5) at $y = 0, 1$	21
$\mathcal{K}, \tilde{\mathcal{K}}$	Second order elements of $\mathcal{U}(\mathfrak{sl}_1)$ used to capture the eigenvalue problem of AQRM	22
$G_{\varepsilon}(x; g, \Delta)$	G-function of the AQRM	24
$P_k^{(N,\varepsilon)}(x, y)$	Constraint polynomial of the AQRM	29
$c_k^{(\varepsilon)}$	$c_k^{(\varepsilon)} = k(k+\varepsilon)$	35
λ_k	$\lambda_k = k(k-1)(N-k+1)$	35
$(a)_n$	Pochhammer symbol	29
$\text{tridiag}\begin{bmatrix} a_i & b_i \\ c_i & \end{bmatrix}_{1\le i\le n}$	Tridiagonal matrix with main diagonal $\{a\}_i$, upper diagonal $\{b\}_i$ and lower diagonal $\{c\}_i$.	29
$\mathbf{e}_i$	The i-th basis vector of the standard basis of $\mathbb{R}^k$	36
$T_{\varepsilon}^{(N)}(g, \Delta)$	Constraint function for exceptional non-Juddian eigenvalues of AQRM	56
$\mathcal{G}_{\varepsilon}(x; g, \Delta)$	Generalized G-function of the AQRM	64
$\mathcal{K}_{k=1}^{\infty}(\frac{a_n}{b_n})$	The continued fraction with partial numerators a_n and partial denominators b_n	70
$Q_k^{(N,\epsilon)}(x, y)$	OPS associated to constraint polynomials	70
${}_2F_1(a, b; c; s)$	Gauss hypergeometric function	71
${}_1F_1(a; b; s)$	Confluent hypergeometric function	71
${}_2F_2(a, b; c, d; s)$	Generalized hypergeometric function	73
$\gamma(s, x)$	Incomplete gamma function	73

Introduction

The *quantum Rabi model* (QRM), originally described in [24], is the fully quantized version of the semi-classical model defined in [47] by Isidor Isaac Rabi in 1936 to describe the effect of a rapidly varying weak magnetic field on an oriented atom possessing nuclear spin. The QRM is one of the basic models in quantum optics, as it describes the simplest interaction between a two-level atom and a light field.

The Hamiltonian of the QRM is given by

$$H_{\text{Rabi}} = \omega a^\dagger a + g(a + a^\dagger)\sigma_x + \Delta\sigma_z,$$

where σ_x, σ_z are the Pauli matrices, $\omega > 0$ is the classical frequency of light field (modeled by a quantum harmonic oscillator), $2\Delta > 0$ is the energy difference of the two-level system and $g > 0$ is the interaction strength between the two system. Different combinations of the parameters of the model are classified into *parameter regimes* according to the static and dynamic properties of its energy levels and solutions (see [45] for a discussion on the different parameter regimes).

For a long time, experimental realizations of the QRM achieved parameters regimes in which the dynamic and static properties could be approximated successfully by the *Jaynes-Cummings model* [24]. The Jaynes-Cummings model was long known to be exactly solvable, and its physical properties could be compared with the experimental results. However, recent development in experimental physics [37, 65] have been able to realize parameter regimes (for instance the nonperturbative ultrastrong coupling and the deep strong coupling regimes) were the Jaynes-Cummings model (or other similar approximations) is no longer suitable to describe its physical properties. These developments, along with the prospect of applications to areas such as quantum information technologies (see [18, 50, 65]) have made the study the properties of the QRM and its spectrum a priority in physics.

Despite the simplicity of its definition, using only raising and lowering operators of a quantum harmonic oscillator and Pauli matrices, only a set of degenerate eigenvalues, known as *Juddian eigenvalues* [25], was explicitly known for a long time. It was not until 2011, when Daniel Braak, exploiting the $\mathbb{Z}/2\mathbb{Z}$-symmetry found in the Hamiltonian, was able to construct analytic solutions and describe the eigenvalues (with the exception of a (possibly finite) set of *exceptional eigenvalues*) as the zeros of a transcendental function, called G-function [5]. Since then, several extensions and generalizations of the QRM have been solved by using techniques derived of Braak's work (see e.g. [7, 13]).

The *asymmetric quantum Rabi model* (AQRM) is one of these generalizations. The Hamiltonian of the AQRM is obtained by introducing a non-trivial interaction term that breaks the $\mathbb{Z}/2\mathbb{Z}$-symmetry in the Hamiltonian of the QRM. Concretely, its Hamiltonian is given by

$$H^{\varepsilon}_{\text{Rabi}} = \omega a^\dagger a + \Delta\sigma_z + g\sigma_x(a^\dagger + a) + \varepsilon\sigma_x,$$

with $\varepsilon \in \mathbb{R}$. The absence of the $\mathbb{Z}/2\mathbb{Z}$-symmetry makes the presence of degeneracies in this model highly nontrivial, in particular there appears to be no way to define invariant subspaces (called parity subspaces in the case of the QRM) whose solutions constitute degeneracies (or crossings). Concretely, by using the symmetry found in the QRM, it is seen that $H_{\text{Rabi}} = H_{+\Delta} \oplus H_{-\Delta}$ for Hamiltonians $H_{\pm\Delta}$ acting on appropiate subspaces of the Hilbert space in which H_{Rabi} acts. Degeneracies are then found to appear between one eigenvalue of $H_{+\Delta}$ and one eigenvalue of $H_{-\Delta}$. Such a decomposition is not known for the AQRM.

Strikingly, degenerate states were discovered in numerical experiments for the case $\varepsilon = \frac{1}{2}$ by Li and Batchelor in [33]. Later, Masato Wakayama in [63] conjectured the existence of degenerate states for the general half-integer ε case in terms of divisibility of constraint polynomials and proved the conjecture for the case $\varepsilon = \frac{1}{2}$. The conjecture was recently proved affirmatively for the general case by Kazufumi Kimoto, Masato Wakayama and the author in [27]. The presence of degenerate solutions for half-integer parameter actually hints at the possibility of a hidden symmetry in the AQRM, as it has been discussed in [63, 53].

As in the case of the QRM, there is a G-function $G_\varepsilon(x; g, \Delta)$ for the AQRM that determines the *regular eigenvalues*, that is, all the eigenvalues with the exception of a set of *exceptional eigenvalues* of the form $\lambda = N \pm \varepsilon - g^2$, with $N \in \mathbb{Z}_{\geq 0}$. The exceptional eigenvalues are further classified into two types, *Juddian eigenvalues*, when the solutions of the eigenvalue problem in the Segal-Bargmann space $\mathcal{H}_{\mathcal{B}}$ can be represented by a polynomial, that is, is a quasi-exact solution, or *non-Juddian exceptional eigenvalues* when this is not the case. The presence of the Juddian eigenvalue $\lambda = N \pm \varepsilon - g^2$ is equivalent to the constraint relation

$$P_N^{(N,\pm\varepsilon)}((2g)^2, \Delta^2) = 0,$$

where $P_N^{(N,\pm\varepsilon)}(x, y)$ is a polynomial of degree N, called *constraint polynomial* (see [33] and [31] for the case of the QRM). As it is clear from the definitions, a necessary condition for two exceptional eigenvalues $\lambda_1 = N + \varepsilon - g^2$ and $\lambda_2 = M - \varepsilon - g^2$ with $N, M \in \mathbb{Z}_{\geq 0}$ and $N \neq M$, to be equal is that

$$\varepsilon = \frac{M - N}{2} = \frac{\ell}{2} \in \frac{1}{2}\mathbb{Z},$$

that is, ε must be half-integer. Since the regular eigenvalues are known to be non-degenerate (see [5] and Section 2.6 below), this is actually a necessary condition for the AQRM to have degenerate eigenvalues. Furthermore, as we show in Corollary 4.1.4, there are no degeneracies consisting of a Juddian and a non-Juddian exceptional solution. Therefore, any possible degeneracy in the spectrum of the AQRM must consist of two Juddian solutions. In terms of constraint polynomials, this is equivalent to the simultaneous satisfaction of the two constraint relations

$$P_N^{(N,\ell/2)}((2g)^2, \Delta^2) = 0 = P_{N+\ell}^{(N+\ell,-\ell/2)}((2g)^2, \Delta^2), \tag{1}$$

where $N \in \mathbb{Z}_{\geq 0}$ and $\ell \geq 0$ (for $\ell < 0$ it is enough to switch the roles of N and M in the discussion above). In addition, if all the roots of the polynomial on the left-hand side of (1) are roots of the polynomial in the right-hand side, and viceversa, then all Juddian solutions $\lambda = N + \ell/2 - g^2$ must be degenerate. Since the polynomials on

both sides are of different degrees, except in the case of $\ell = 0$ (i.e. the QRM), the relation (1) is nontrivial.

Following this argumentation, the conjecture given by Masato Wakayama in [63] is that the divisibility relation

$$P_{N+\ell}^{(N+\ell,-\ell/2)}(x,y) = A_N^{\ell}(x,y)P_N^{(N,\ell/2)}(x,y),$$

holds for $N, \ell \in \mathbb{Z}_{\geq 0}$ and that the polynomials $A_N^{\ell}(x,y)$ have no positive roots for $x, y > 0$. In other words, that any Juddian eigenvalue of the AQRM is degenerate when the parameter ε is half-integer. The proof of the conjecture in [27] was done by studying certain determinant expressions satisfied by the constraint polynomials. The proof presented in this thesis is a generalization of the said proof, in fact, we prove a stronger conjecture, also proposed in [63] (see Section 2.9).

Another important question is to determine whether exceptional solutions do, in fact, appear in the spectrum for given parameters $g, \Delta > 0$. A result of Li and Batchelor, presented in [33], gives a lower bound on the number of roots of the constraint polynomials when the parameter Δ is in certain intervals. In Section 3.5 we prove a stronger formulation of the result, giving the exact number of solutions for the same intervals. This result suffices for the case of Juddian eigenvalues.

For non-Juddian exceptional eigenvalues, we define a transcendental constraint T-function $T_{\varepsilon}^{(N)}(g,\Delta)$ such that the equation

$$T_{\varepsilon}^{(N)}(g,\Delta) = 0$$

is equivalent to the presence of the non-Juddian exceptional eigenvalue $\lambda = N + \varepsilon - g^2$. Aside from providing conditions for the existence of non-Juddian exceptional solutions, these T-functions appear, along with the constraint polynomials, in the expression of the residues of the G-function of the AQRM. By using this, we define a generalized G-function $\mathcal{G}_{\varepsilon}(x;g,\Delta)$ whose zeros determine the complete spectrum of the AQRM. In other words, it is essentially (up to a nonvanishing entire factor) the spectral determinant for the Hamiltonian of the AQRM.

The purpose of this thesis is to give a complete overview of the spectrum of the AQRM, including the complete characterization of the degeneracies in its spectrum. The thesis is intended to be a mostly self-contained exposition, however for a number of results we refer the reader to the original sources.

We begin, in Chapter 1 by giving an overview of the quantum harmonic oscillator and its raising $a^{\dagger}$ and lowering a operators and their $L^2(\mathbb{R})$ and Segal-Bargmann space $\mathcal{H}_{\mathcal{B}}$ space realizations. Furthermore, we give basic overview of the representation theory of the Lie algebra $\mathfrak{sl}_2$ and its irreducible representations.

In Chapter 2, we present a short historical review of the main research done on the QRM starting from its definition. In Section 2.2, we give a tour of the Hamiltonians of several models of quantum optics that describe the interaction between light and matter. Several of these models are generalizations of the QRM. In Section 2.3, by considering the realization as a second order pseudo-differential operator acting on $L^2(\mathbb{R})\otimes\mathbb{C}^2$ we give some of general properties of the Hamiltonian of the AQRM and its spectrum, the most important being that the spectrum consist only of the discrete set of eigenvalues. Next, in Section 2.4 we study the realization of eigenvalue problem of the Hamiltonian of the AQRM in the Segal-Bargmann

space and reduce it to a system of two linear differential equations, equivalent to a confluent Heun differential equation. Moreover, this system is captured by elements of the universal enveloping algebra of $\mathfrak{sl}_2$. In Section 2.5, we describe the classification of the eigenvalues of the AQRM into regular eigenvalues, further discussed in Section 2.6, and exceptional eigenvalues, discussed in 2.7, according to the Frobenius solutions of the system of linear differential equations of confluent Heun type. In Section 2.8, we describe how the constraint polynomials are related to the coefficients of the solutions of the differential equation system, in particular we prove the equivalence of the constraint relation with the presence of Juddian eigenvalues. In Section 2.9, we discuss the conjectures on constraint polynomials that gave the motivation for this research.

In Chapter 3, we study the constraint polynomials and its mathematical properties. Above all, we see how the "divisibility" of the conjectures follows from certain determinant expressions related to their definition by three-term recurrence relations. The positivity follows as well by the properties of the eigenvalues of the matrices involved in said determinant expressions. The conjectures are finally proved in Section 3.3. In Section 3.5, we prove the already mentioned result on the number of positive roots of constraint polynomials when one of the variables is in a given interval. In Section 3.6 we give some explicit formulas for constraint polynomials that can be used to study the constraint polynomials from the combinatorial point view.

In Chapter 4 we complete the picture of the spectrum of the AQRM, by describing the degeneracy structure using the results of the previous chapters. Notably, in Section 4.1 we characterize the degeneracy of the exceptional spectrum of the AQRM, this being sufficient to describe the degeneracy structure in the general case. In Section 4.2, we derive the aforementioned constraint T-function, that, along with the constraint polynomials, is used to study the residues of the poles of the G-function in Section 4.3. In Section 4.4 we define the generalized G-function and prove that its zeros determine the full spectrum of the AQRM. Finally, in Section 4.5 we show that exceptional solutions correspond to eigenvectors in irreducible $\mathfrak{sl}_2$-modules in the $\mathfrak{sl}_2$-picture of the eigenvalue problem of the AQRM.

As an addendum to the study of the spectrum of the AQRM, in Chapter 5 we present certain continued fraction expansions for powers of the Napier constant (or Euler's number) e^n, with $n \in \mathbb{Z}_{\geq 0}$ with good convergence properties. These continued fraction expansions appeared during the study of certain orthogonal polynomial families related to the constraint polynomials. This study is intended to give an example of the rich mathematical structure appearing in the study of the AQRM and its spectrum.

The year 2016 marked the 80 anniversary of the publication of the original paper by Rabi describing his original model, see [4] for a review of the QRM commemorating the occasion. Even after 80 years and a large amount of research (a search on arXiv.org shows more than 100 entries for quantum Rabi model and related topics since 2011), the list of mysteries and open questions concerning the quantum Rabi model is very large and is still growing. A short discussion on certain open problems is given in Chapter 6 with the hope that it motivates further research in the quantum Rabi model.

As a disclaimer, we note that some of the results of Section 2.8 and Chap-

ters 3 and 4 are (or are generalizations of) results published in [48], with Masato Wakayama, and [27], with Kazufumi Kimoto and Masato Wakayama. The results of Chapter 5 consist of previously unpublished work.

1. Preliminaries

The purpose of this chapter is to give a brief introduction of the tools and concepts to be used later in the study of the spectrum of the asymmetric quantum Rabi model.

First, we give an overview of the theory of the quantum harmonic oscillator, a model of quantum physics that is used to describe more complicated physical phenomena. Next, we introduce the Segal-Bargmann space, a Hilbert space of entire functions in which the realization of the raising and lowering operators of the harmonic oscillator have a particularly simple expression. In this Hilbert space, the eigenvalue problem of the quantum Rabi model reduces to a system of ordinary linear equations of confluent Heun type. As it is well-known, differential equations can be realized by elements of $\mathcal{U}(\mathfrak{sl}_2)$, the universal enveloping algebra of $\mathfrak{sl}_2$ via certain representations. For this reason, in the final section we introduce the basic theory of $\mathfrak{sl}_2$ representations that we use in later chapters.

1.1 The quantum harmonic oscillator

The quantum harmonic oscillator is one the simplest models in quantum mechanics. Its importance lies in that it has simple analytic solutions and that a good number of physical phenomena is modeled using coupled harmonic oscillators. For instance, the quantum Rabi models studied in this thesis are defined in terms of the the raising and lowering operators a and $a^\dagger$ that appear in the quantum harmonic oscillator.

Let $\mathcal{H}$ be a Hilbert space. Consider self-adjoint operators X and P acting on $\mathcal{H}$ satisfying the conmutation relation

$$[X, P] = i\hbar\mathbf{1},$$

and the hypothesis of the Stone-von Neumann theorem (see [17], Chapter 14). The constant $\hbar = 1.054 \times 10^{-27}$ erg $\cdot$ s $= 1.054 \times 10^{-34}$ J $\cdot$ s, is the *reduced Planck constant.*

The Hamiltonian of the one-dimensional *quantum harmonic oscillator* (QHO), or linear oscillator, is given by

$$H = \frac{1}{2}\left(\frac{P^2}{m} + kX^2\right),$$

where $m, k > 0$. The constant m is interpreted as the mass of the particle.

Introducing the constant ω, called *the classical frequency* of the oscillator, given by

$$\omega = \sqrt{\frac{k}{m}},$$

the Hamiltonian H is written as

$$H = \frac{1}{2m}\left(P^2 + (m\omega X)^2\right).$$

Next, we introduce the *raising operator* $a^\dagger$ and the *lowering operator* a, by the formulas

$$a^\dagger = \frac{m\omega X - iP}{\sqrt{2\hbar m\omega}}, \qquad a = \frac{m\omega X + iP}{\sqrt{2\hbar m\omega}}.$$

The operator $a^\dagger$ is also called *creation operator* , and correspondingly, the operator a is called *annihilation operator*. The operator $a^\dagger$ is the adjoint of a, justifying the notation.

By direct computation, we observe that

$$[a, a^\dagger] = \mathbf{1},$$

where $\mathbf{1}$ is the identity operator.

The Hamiltonian H is written in terms of the operators a and $a^\dagger$ as

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\mathbf{1}\right),$$

and therefore the study of the spectrum of the QHO is reduced to the study of the spectrum of the self-adjoint operator $a^\dagger a$. The spectrum of the operator $a^\dagger a$, and therefore of the QHO, can be described explicitly. We recall the results here and refer the reader to [17, 58, 64], for a more detailed discussion.

The following result justifies the name raising and lowering for the operators $a^\dagger$ and a, its proof is immediate from the commutation relation above.

Proposition 1.1.1. *Let ϕ be an eigenfunction of $a^\dagger a$ with eigenvalue $\lambda \in \mathbb{R}$. Then,*

$$a^\dagger a\,(a\phi) = (\lambda - 1)\phi$$
$$a^\dagger a\left(a^\dagger\phi\right) = (\lambda + 1)\phi.$$

Since a and $a^\dagger$ are adjoint operators, any eigenvalue λ of $a^\dagger a$ is non-negative, and thus by the proposition above if ϕ is an eigenfunction of $a^\dagger a$ there must be ϕ_0, a *ground state*, with $a^\dagger a\phi_0 = 0$ and $\phi = (a^\dagger)^n\phi_0$ for a non-negative integer n. In particular, λ itself is a non-negative integer.

Proposition 1.1.2. *If ϕ_0 is a unit vector with $a\phi_0 = 0$, then for $n \geq 0$, define*

$$\phi_n = (a^\dagger)^n\phi_0.$$

The following relations hold for $n \geq 0$,

$$a^\dagger a\phi_n = n\phi_n$$
$$a\phi_{n+1} = (n+1)\phi_n.$$

Furthermore, the family $\{\phi_n\}_{n\geq 0}$ is orthogonal.

Depending on the choice of Hilbert space $\mathcal{H}$, it may be the case that there are multiple independent ground states, for example in the Hilbert space $L^2(\mathbb{R}) \otimes \mathbb{C}^2$, equipped with the inner-product inherited from $L^2(\mathbb{R})$, there are two linearly independent ground states.

Finally, we make some considerations for the case of $\mathcal{H} = L^2(\mathbb{R})$. In this realization, the eigenvectors are given explicitly by the Hermite functions. Setting, for simplicity, $\hbar = m = \omega = 1$, we see that the position operator is realized by the multiplication operator

$$X = x,$$

and the momentum operator is realized by the differentiation operator

$$P = -i\frac{d}{dx}.$$

The raising and lowering operators are then given by

$$a^\dagger = \frac{1}{\sqrt{2}}\left(x - \frac{d}{dx}\right), \qquad a = \frac{1}{\sqrt{2}}\left(x + \frac{d}{dx}\right),$$

and the equation $a\phi_0 = 0$ is an ordinary differential equation of order one with general solution

$$\phi_0(x) = Ce^{-x^2/2},$$

and where the normalization condition gives immediately $C = \sqrt{\pi}$.

Proposition 1.1.3. *The ground state $\phi_0(x)$ of $a^\dagger a$ is given by*

$$\phi_0(x) = \sqrt{\pi}e^{-x^2/2},$$

and the "excited states" $\phi_n(x)$ are given by

$$\phi_n(x) = H_n(x)\phi_0(x),$$

where $H_n(x)$ is the n-th Hermite polynomial, defined by the equation

$$\frac{d^n}{dx^n}(e^{-\frac{1}{2}x^2}) = (-1)^n e^{-\frac{1}{2}x^2} H_n(x).$$

Furthermore, the family $\{\phi_n(x)\}_{\geq 0}$ is an orthonormal basis of $\mathcal{H} = L^2(\mathbb{R})$.

Therefore, in the $\mathcal{H} = L^2(\mathbb{R})$ realization, the spectrum of the QHO is

$$\mathrm{Spec}(H) = \{\hbar\omega\left(n + \frac{1}{2}\right) : n \in \mathbb{Z}_{\geq 0}\},$$

in particular, the eigenvalues (energy levels) of the QHO differ by integer multiples of the quantity $\hbar\omega$. In this thesis, we assume $\hbar = 1$ in the sequel, without loss of generality, to simplify the discussion.

1.2 The Segal-Bargmann space

In this section we give an overview of the *Segal-Bargmann space* $\mathcal{H}_\mathcal{B}$ (cf. [2]), also known as Bargmann space, Bargmann Fock space or Fock space. It is often used to study the spectrum of quantum systems, including the quantum Rabi model and related models. The space $\mathcal{H}_\mathcal{B}$ was originally defined for holomorphic functions in

$\mathbb{C}^n$, but it suffices to consider the one dimensional case for the applications presented in this work. We follow the description given in [17].

Let $\mathcal{V}(\mathbb{C})$ be the space of holomorphic functions $f : \mathbb{C} \to \mathbb{C}$. An inner-product in $\mathcal{V}(\mathbb{C})$ is defined for $f, g \in \mathcal{V}(\mathbb{C})$ by

$$(f, g)_{\mathcal{B}} = \int_{\mathbb{C}} \overline{f(z)} g(z) d\mu(z) \tag{1.1}$$

where the measure $d\mu(z)$ is given by $d\mu(z) = \frac{1}{\pi} e^{-|z|^2} dxdy$ for $z = x + iy$, and $dxdy$ is the Lebesgue measure in $\mathbb{C} \simeq \mathbb{R}^2$.

The Segal-Bargmann space $\mathcal{H}_{\mathcal{B}}$ is the space of entire functions $f : \mathbb{C} \to \mathbb{C}$ in $\mathcal{V}(\mathbb{C})$ satisfying

$$\|f\|_{\mathcal{B}} = (f, f)_{\mathcal{B}}^{1/2} = \left(\int_{\mathbb{C}} |f(z)|^2 d\mu(z) \right)^{1/2} < \infty.$$

Theorem 1.2.1 ([17] Proposition 14.15)**.** *The Segal-Bargmann space $\mathcal{H}_{\mathcal{B}}$ is a complete Hilbert space with respect to the inner product $(\cdot, \cdot)_{\mathcal{B}}$ given in* (1.1)*. In addition, the set of (holomorphic) polynomials forms a dense subspace of $\mathcal{H}_{\mathcal{B}}$.*

An important property of the space $\mathcal{H}_{\mathcal{B}}$ (see [8]) for the study of the spectrum of the quantum Rabi model is that it contains entire functions having asymptotic expansion of the form

$$e^{\alpha_1 z} z^{-\alpha_0} (c_0 + c_1 z^{-1} + c_2 z^{-2} + \cdots), \tag{1.2}$$

as $z \to \infty$. A particular case is that of normal solutions of differential equations having an unramified irregular singular point of rank 2 at infinity. This fact is important for the study of the eigensolutions of asymmetric quantum Rabi model.

The multiplication operator $Z = z$ and differentiation operator $Y = \partial_z = \frac{d}{dz}$ acting on $\mathcal{H}_{\mathcal{B}}$ satisfy the commutation relation

$$[Y, Z] = 1,$$

in other words, they satisfy the same commutation relations as the raising and lowering operators of Section 1.1. In fact, if f, g are (holomorphic) polynomials, then it holds that

$$\int_{\mathbb{C}} \overline{(f(z)} \partial_z G d\mu(z) = \int_{\mathbb{C}} \overline{zf(z)} g(z) d\mu(z).$$

In general, we have the following result.

Proposition 1.2.2. *The multiplication operator $Z = z$ is the adjoint of the differentiation operator $Y = \partial_z$ in $\mathcal{H}_{\mathcal{B}}$.*

In light of the Theorem 1.2.1 and Proposition 1.2.2, the multiplication and differentiation operators are (formally) realizations of the raising and lowering operators $a^\dagger$ and a.

Next, define the operators

$$A = \frac{1}{\sqrt{2}} (Z + Y)$$
$$B = \frac{i}{\sqrt{2}} (Z - Y).$$

The operators A and B are self-adjoint and satisfy the hypothesis of the Stone-von Neumann theorem, and thus there is a unitary map $U : \mathcal{H}_{\mathcal{B}} \to L^2(\mathbb{R})$ satisfying

$$Ue^{itA}U^{-1} = e^{itX}$$
$$Ue^{itB}U^{-1} = e^{itP}$$

where X and P are the usual position and momentum operators acting on $L^2(\mathbb{R})$. The inverse of the map U can be computed explicitly and is called the *Segal-Bargmann transform* (See [17] Theorem 14.18). This argument shows that the multiplication Z and differentiation operator Y are indeed equivalent to the raising and lowering operators introduced in Section 1.1 for the Hilbert space $L^2(\mathbb{R})$.

For the study of the spectrum of operators, the Segal-Bargmann $\mathcal{H}_{\mathcal{B}}$ has the advantage that the realization the raising and lowering operators is of lower degree (as a differential operator) than in the standard $L^2(\mathbb{R})$ realization. In addition, elements of $\mathcal{H}_{\mathcal{B}}$ are functions and not equivalence classes of functions like in $L^2(\mathbb{R})$. We refer the reader to [2, 17] for a more detailed description of the Segal-Bargmann space and to [52] for more applications to the eigenvalue problem of quantum systems.

1.3 Representation theory of $\mathfrak{sl}_2$

In this section we recall some basic representation theory of $\mathfrak{sl}_2(\mathbb{R})$ used in the next chapter to describe the $\mathfrak{sl}_2(\mathbb{R})$-picture of the eigenvalue problem of the AQRM. The reader is directed to [20, 32, 57] for the general theory of $\mathfrak{sl}_2$-representations.

Let $M_2(\mathbb{R})$ the algebra of real 2×2 matrices and $GL_2(\mathbb{R})$ be the *general linear group* of real matrices, that is, the (multiplicative) subgroup of $M_2(\mathbb{R})$ consisting of invertible real matrices. The *special linear group* $SL_2(\mathbb{R})$ is the closed subgroup of $GL_2(\mathbb{R})$ given by

$$SL_2(\mathbb{R}) = \{M \in GL_2(\mathbb{R}) \mid \det(M) = 1\}.$$

From general theory, we know that $SL_2(\mathbb{R})$ is a non-compact and semisimple connected Lie group. The Lie algebra of $SL_2(\mathbb{R})$, denoted by $\mathfrak{sl}_2$, or $\mathfrak{sl}_2(\mathbb{R})$, is given by

$$\mathfrak{sl}_2 = \{M \in M_2(\mathbb{R}) \mid \operatorname{tr}(M) = 0\},$$

is a *simple* Lie algebra. Denote by $\mathfrak{g}_{\mathbb{C}}$ the complexification of the Lie algebra $\mathfrak{g}$, then it is not difficult to verify that $(\mathfrak{sl}_2)_{\mathbb{C}}$ is $\mathfrak{sl}_2(\mathbb{C})$, the Lie algebra of $SL_2(\mathbb{C})$(c.f. [57]).

In Section 2.4, we capture the eigenvalue problem of the asymmetric quantum Rabi model, reduced to a system of two linear equations of Heun type, by an element of the universal enveloping algebra $\mathcal{U}(\mathfrak{sl}_2)$. Recall that if $\mathfrak{g}$ is a Lie algebra, define $T_0(\mathfrak{g}) = \mathbb{C}$, $T^{(n)}(\mathfrak{g}) = \mathfrak{g}^{\otimes n}$, with

$$\mathfrak{g}^{\otimes n} = \underbrace{\mathfrak{g} \otimes \mathfrak{g} \otimes \cdots \otimes \mathfrak{g}}_{n},$$

then, the tensor algebra $T(\mathfrak{g})$ is given by

$$T(\mathfrak{g}) = \bigoplus_{n=0}^{\infty} T_n(\mathfrak{g}).$$

Let J be the ideal of $T(\mathfrak{g}_{\mathbb{C}})$ generated by the elements

$$[X,Y]-(X\otimes Y-Y\otimes X)$$

with $X,Y\in\mathfrak{g}_{\mathbb{C}}$, then the *universal enveloping algebra* of $\mathfrak{g}$ is given by

$$\mathcal{U}(\mathfrak{g})=T(\mathfrak{g}_{\mathbb{C}})/J.$$

The universal property of $\mathcal{U}(\mathfrak{g})$ is that every representation of $\mathfrak{g}$ extends to a representation of $\mathcal{U}(\mathfrak{g})$(see [20], Section 1.3).

A set of *standard generators* of $\mathfrak{sl}_2$ is given by the matrices H,E and F of $\mathfrak{sl}_2(\mathbb{R})$ defined as

$$H=\begin{bmatrix}1&0\\0&-1\end{bmatrix},\quad E=\begin{bmatrix}0&1\\0&0\end{bmatrix},\quad F=\begin{bmatrix}0&0\\1&0\end{bmatrix}.$$

These generators satisfy the commutation relations

$$[H,E]=2E,\quad [H,F]=-2F,\quad [E,F]=H.$$

Next, let us introduce a representation of $\mathfrak{sl}_2$, depending on a parameter $a\in\mathbb{C}$, which is used to capture the confluent Heun differential equations in Section 2.4. The reader is directed to [63] for an extended discussion of this representation. Let $a\in\mathbb{C}$ and define the action ϖ_a of $\mathfrak{sl}_2$ on the vector spaces $\mathbf{V}_1:=y^{-\frac{1}{4}}\mathbb{C}[y,y^{-1}]$ and $\mathbf{V}_2:=y^{\frac{1}{4}}\mathbb{C}[y,y^{-1}]$ by

$$\varpi_a(H):=2y\partial_y+\frac{1}{2},\quad \varpi_a(E):=y^2\partial_y+\frac{1}{2}(a+\frac{1}{2})y,\quad \varpi_a(F):=-\partial_y+\frac{1}{2}(a-\frac{1}{2})y^{-1}$$

with $\partial_y:=\frac{d}{dy}$. It is not difficult to verify that this defines infinite dimensional representations of $\mathfrak{sl}_2$. Write $\varpi_{j,a}:=\varpi_a|_{\mathbf{V}_j}$ and put $e_{1,n}:=y^{n-\frac{1}{4}}$ and $e_{2,n}:=y^{n+\frac{1}{4}}$. Then we have

$$\begin{cases}\varpi_{1,a}(H)e_{1,n}=2ne_{1,n},\\ \varpi_{1,a}(E)e_{1,n}=\big(n+\dfrac{a}{2}\big)e_{1,n+1},\\ \varpi_{1,a}(F)e_{1,n}=\big(-n+\dfrac{a}{2}\big)e_{1,n-1},\end{cases}\qquad \begin{cases}\varpi_{2,a}(H)e_{2,n}=(2n+1)e_{2,n},\\ \varpi_{2,a}(E)e_{2,n}=\big(n+\dfrac{a+1}{2}\big)e_{2,n+1},\\ \varpi_{2,a}(F)e_{2,n}=\big(-n+\dfrac{a-1}{2}\big)e_{2,n-1}.\end{cases}$$

When $a\notin 2\mathbb{Z}$ (resp. $a\notin 2\mathbb{Z}-1$) the representation $(\varpi_{1,a},\mathbf{V}_1)$ (resp. $(\varpi_{2,a},\mathbf{V}_2)$) is an irreducible representation, called *principal series*. Note that there is an equivalence between $\varpi_{j,a}$ and $\varpi_{j,2-a}$ under the same condition.

For a non-negative integer m, define subspaces $\mathbf{D}^{\pm}_{2m},\mathbf{F}_{2m-1}$ of $\mathbf{V}_{1,2m}(=\mathbf{V}_1)$, and $\mathbf{D}^{\pm}_{2m+1},\mathbf{F}_{2m}$ of $\mathbf{V}_{2,2m+1}(=\mathbf{V}_2)$ respectively by

$$\mathbf{D}^{\pm}_{2m}:=\bigoplus_{n\geq m}\mathbb{C}\cdot e_{1,\pm n},\quad \mathbf{F}_{2m-1}:=\bigoplus_{-m+1\leq n\leq m-1}\mathbb{C}\cdot e_{1,n},$$

$$\mathbf{D}^{-}_{2m+1}:=\bigoplus_{n\geq m+1}\mathbb{C}\cdot e_{2,-n},\quad \mathbf{D}^{+}_{2m+1}:=\bigoplus_{n\geq m}\mathbb{C}\cdot e_{2,n},\quad \mathbf{F}_{2m}:=\bigoplus_{-m\leq n\leq m-1}\mathbb{C}\cdot e_{2,n}.$$

The spaces $\mathbf{D}^{\pm}_{2m}$ (resp. $\mathbf{D}^{\pm}_{2m+1}$) are invariant under the action $\varpi_{1,2m}(X)$, (resp. $\varpi_{2,2m+1}(X)$), $(X\in\mathfrak{sl}_2)$, and define irreducible representations (having lowest and

highest weight vector respectively) known to be equivalent to (holomorphic and anti-holomorphic) *discrete series* for $m > 0$ of $\mathfrak{sl}_2(\mathbb{R})$. The irreducible representation $\mathbf{D}_1^{\pm}$ are the *(infinitesimal version of) limit of discrete series* of $\mathfrak{sl}_2(\mathbb{R})$ (see e.g. [20, 32]). Moreover, the finite dimensional space $\mathbf{F}_m$ ($\dim_{\mathbb{C}} \mathbf{F}_m = m$), is invariant and defines irreducible representation of $\mathfrak{sl}_2$ for $a = 2 - 2m$ when $j = 1$ and $a = 1 - 2m$ when $j = 2$, respectively. We remark here that the finite dimensional representations $\mathbf{F}_m$ are not unitarizable.

The following result describes the irreducible decompositions of $(\varpi_a, \mathbf{V}_{j,a})$ ($a = m \equiv j-1 \mod 2$) for $m \in \mathbb{Z}_{\geq 0}$ and $j = 1, 2$. In particular, it gives the relation between the finite representations $\mathbf{F}_m$ and the invariant submodules $\mathbf{D}_m^{\pm}$.

Lemma 1.3.1. *Let $m \in \mathbb{Z}_{\geq 0}$.*

1. *The subspaces $\mathbf{D}_{2m}^{\pm}$ are irreducible submodules of $\mathbf{V}_{1,2m}$ under the action $\varpi_{1,2m}$ and $\mathbf{F}_{2m-1}$ is an irreducible submodule of $\mathbf{V}_{1,2-2m}$ under $\varpi_{1,2-2m}$. In the former case, the finite dimensional irreducible representation $\mathbf{F}_{2m-1}$ can be obtained as the subquotient as $\mathbf{V}_{1,2m}/\mathbf{D}_{2m}^{-} \oplus \mathbf{D}_{2m}^{+} \cong \mathbf{F}_{2m-1}$. In the latter case, the discrete series $\mathbf{D}_{2m}^{\pm}$ can be realized as the irreducible components of the subquotient representation as $\mathbf{V}_{1,2-2m}/\mathbf{F}_{2m-1} \cong \mathbf{D}_{2m}^{-} \oplus \mathbf{D}_{2m}^{+}$.*
2. *The subspaces $\mathbf{D}_{2m+1}^{\pm}$ are irreducible submodule of $\mathbf{V}_{2,2m+1}$ under the action $\varpi_{2,2m+1}$ and $\mathbf{F}_{2m}$ is an irreducible submodule of $\mathbf{V}_{2,1-2m}$ under $\varpi_{2,1-2m}$. In the former case, the finite dimensional irreducible representation $\mathbf{F}_{2m}$ can be obtained as the subquotient as $\mathbf{V}_{2,2m+1}/\mathbf{D}_{2m+1}^{-} \oplus \mathbf{D}_{2m+1}^{+} \cong \mathbf{F}_{2m}$, while in the latter case, the discrete series $\mathbf{D}_{2m+1}^{\pm}$ can be realized as the irreducible components of the subquotient representation as $\mathbf{V}_{2,1-2m}/\mathbf{F}_{2m} \cong \mathbf{D}_{2m+1}^{-} \oplus \mathbf{D}_{2m+1}^{+}$.*
3. *The space $\mathbf{V}_{2,1}$ is decomposed as the irreducible sum: $\mathbf{V}_{2,1} = \mathbf{D}_1^{-} \oplus \mathbf{D}_1^{+}$.*

Moreover, the spaces of irreducible submodules $\mathbf{D}_m^{\pm}(\subset \mathbf{V}_{j,m})$, $\mathbf{F}_m(\subset \mathbf{V}_{j,1-m})$ and the direct sum $\mathbf{D}_m^{+} \oplus \mathbf{D}_m^{-}(\subset \mathbf{V}_{j,m})$ above are the only non-trivial invariant subspaces of $\mathbf{V}_{j,m}$ for $j = 1$ (resp. $j = 2$) when m is even (resp. odd) under the action of $\mathcal{U}(\mathfrak{sl}_2)$, the universal enveloping algebra of $\mathfrak{sl}_2$. □

In Section 4.5, we make use of the isomorphism described in the proposition above to describe how certain solutions of the eigenvalue problem of the quantum Rabi model determine elements in irreducible submodules of $\mathfrak{sl}_2(\mathbb{R})$.

2. The asymmetric quantum Rabi model

This chapter is an introduction to the study of the quantum Rabi model and its generalization, the asymmetric quantum Rabi model.

First, in Section 2.1 we give a short historical note on the research done on the quantum Rabi model and its spectrum, including experimental realizations. In Section 2.2 we give a tour of the Hamiltonians of various models describing the interaction of light and matter, including the quantum Rabi model and different generalizations. After that, in Section 2.3 we focus on the asymmetric quantum Rabi model and give some general properties of its Hamiltonian when considered as an operator acting in $L^2(\mathbb{R}) \otimes \mathbb{C}^2$.

In Section 2.4, by using the Segal-Bargmann $\mathcal{H}_{\mathcal{B}}$ space realization we see that the eigenvalue problem of the AQRM reduces to a set of two linear ordinary differential equations of confluent Heun type and how they can be captured in the $\mathfrak{sl}_2$-representation picture. Next, in Section 2.5, we give the classification of the spectrum of the AQRM according to the type of the solutions of the aforementioned system. In particular, there is a regular spectrum governed by the zeros of a G-function, described in Section 2.6. The remaining eigenvalues of the AQRM are called exceptional, these appear from certain solutions of the differential equation system where the difference of the exponents are integer. These solutions are studied in Section 2.7, where we see that there can be polynomial solutions, called Juddian solutions, and non-polynomial, called non-Juddian exceptional solutions.

The Juddian solutions are determined by the roots of certain polynomials, called constraint polynomials. In Section 2.8, we see how these polynomials are related to the coefficients of the solutions of the differential equation system. Finally, in Section 2.9 we describe, in terms of constraint polynomials, the conjectures on the degeneracy of the Juddian solutions of the AQRM, proposed by Masato Wakayama in [63]. In Chapter 3 we prove these conjectures, and in Chapter 4 complete the degeneracy picture of the asymmetric quantum Rabi model.

2.1 A brief history of the quantum Rabi model

In this section we give a short historical review on the research on the QRM relevant to the studies in the present thesis. It is important to note that due to the amount of research done on the QRM, any such list is necessarily incomplete. For more information on the experimental realizations and parameter regimes of the QRM, we refer the reader to [45, 51] (see also the discussion on Section 6.3)

In 1936, Isidor Isaac Rabi introduced in [47] a model to discuss the effect of a rapidly varying weak magnetic field on an oriented atom possessing nuclear spin.

This model is the semi-classical version of the model which is now known as the quantum Rabi model. In 1944, Rabi would go on to receive the Nobel Prize in Physics for the discovery of nuclear magnetic resonances.

In 1963, E.T. Jaynes and F.W. Cummings considered in [24] the fully quantized version of the quantum Rabi model for the case where the rotating-wave approximation applies, that is, were the model now known as the the Jaynes-Cummings model successfully approximates the QRM.

In 1979, Judd described in [25] the presence of quasi-exact solutions which are now known as Juddian eigenvalues.

In 1987, Kuś showed in [31] the degeneracy of the Juddian eigenvalues and proved that there are at least $n-k$ degenerate Juddian points for each value of n for Δ/ω satisfying $k < \Delta/\omega < k+1$.

In 2007, Gleyzes, Kuhr, Guerlin, Bernu, Delèglise, Hoff, Brune, Raimond and Haroche in [16] realized the QRM experimentally in the *strong coupling regime* using a single atom in the context of cavity in microwave cavity quantum electrodynamics experiments. In this regime, the model can be successfully approximated by the Jaynes-Cummings model.

In 2009, Anappara, De Liberato, Tredicucci, Ciuti, Biasiol, Sorba and Beltram in [1] reported signatures of the QRM of the *perturbative ultrastrong coupling regime* in a quantum-well intersubband microcavity. In this case, the Jaynes-Cummings model is not suitable to approximate the properties of the energy levels of the QRM, however it can still be approximated by the Bloch-Siegert Hamiltonian.

In 2011, Daniel Braak constructed in [3] analytical solutions of the QRM and gave conditions for existence by showing the existence of a transcendental function whose zeros exactly describe the eigenvalues of the QRM. He also conjectured that the spacing between two consecutive eigenvalues of the QRM is always less than or equal to 2 and gave a (conjectural) description on the number of eigenvalues in intervals $[n, n+1)$ for $n \in \mathbb{Z}_{\geq 0}$. In the same paper, he defined the AQRM (under the name of generalized QRM) and extended his results on solvability to it.

In 2012, M. Hirokawa and F. Hiroshima proved in [19] that the ground state of the quantum Rabi model is non-degenerate.

In 2012, Chen, Wang, He, Liu and Wang reformulated Braak's result in [9] using the Bogoliubov transform avoiding the use of Segal-Bargmann space methods.

In 2013, Zhong, Xie, Batchelor and Lee showed in [67] the existence of analytic solutions using confluent Heun functions. This method is equivalent to the G-function approach.

In 2013, A.J. Maciejewski and M. Przybylska and T. Stachowiak showed in [36] the existence of non-Juddian exceptional eigenvalues numerically and gave conditions for their presence in terms of the confluent Heun functions. The existence of non-Juddian exceptional solutions has not been considered before the publication of this work.

In 2014, Masato Wakayama proved in [61] (see also [62]) that the eigenvalue problem of the quantum Rabi model can be captured by a second order element $\mathcal{R} \in \mathcal{U}(\mathfrak{sl}_2)$ via a confluent process. The element $\mathcal{R} \in \mathcal{U}(\mathfrak{sl}_2)$ is associated to the eigenvalue problem of the non-commutative harmonic oscillator via certain representation, the reader is refered also to [39] for more information.

In 2014, M. Wakayama and T. Yamasaki showed in [60] the existence of a second order element $\mathbb{K} \in \mathcal{U}(\mathfrak{sl}_2)$ that realizes the eigenvalue problem of the quantum Rabi model via a representation (described in Section 1.3). This is $\mathfrak{sl}_2$-representation picture of the QRM.

In 2014, Maissen, Scalari, Valmorra, Beck, Fais, Cibella, Leoni, Reichl, Charpentier and Wegscheider in [37] successfully realized experimentally the QRM in the *nonperturbartive ultrastrong coupling regime* using metallic and superconducting complementary split-ring resonators coupled to the cyclotron transition of two-dimensional electron gases. In this coupling regime, the Jaynes-Cummings model, or other approximations like the Bloch-Siegert Hamiltonian, are not appropriate to study the energy levels of the QRM.

In 2015, Li and Batchelor in [33] made the striking numerically discovery of degenerate Juddian points in the spectrum of AQRM for the parameter $\varepsilon = \frac{1}{2}$. Furthermore, they explicitly defined the constraint polynomials for the Juddian solutions and extended some of Kuś results on constraint polynomials (see Section 3.5 for discussion on this result).

In 2015, Pedernales, Lizuain, Felicetti, Romero, Lamata and Solano proposed in [44] a method to simulate the quantum Rabi model in all parameter regimes by means of detuned bichromatic sideband excitations of a single trapped ion. In particular, this proposal permits the simulation of the QRM in the ultrastrong and deep strong couplings regimes using current setups.

In 2016, Shingo Sugiyama proved in [55] that the spectral zeta function of the QRM

$$\zeta_{H_{\mathrm{Rabi}}}(s) = \sum_{\lambda \in \mathrm{Spec}(H_{\mathrm{Rabi}})} \frac{1}{\lambda^s}$$

can be extended meromorphically to the complex plane with a single pole at $s = 1$. In addition, he showed that

$$N_H(T) \sim 2T$$

as $T \to \infty$, where $N_H(T)$ is the number of eigenvalues smaller than $T \in \mathbb{R}$. Asymptotics for the spectrum of the type $N_H(T) \sim 2T$ are in general called Weyl laws. This result supports Braak's conjecture on the distribution of eigenvalues of the QRM.

In 2017, Masato Wakayama proved in [63] the existence of degenerate Juddian states for the case $\varepsilon = \frac{1}{2}$ and conjectured the result for general half-integer $\varepsilon = \ell/2 \in \frac{1}{2}\mathbb{Z}$ in terms of divisibility of constraint polynomials. In addition, he described how the regular solutions and Juddian solutions can be captured in elements of irreducible representations in the $\mathfrak{sl}_2$-representation picture of the AQRM.

In 2017, Yoshihara, Fuse, Ashhab, Kakuyanagi, Saito and Semba in [65] successfully achieved the *deep strong coupling regime* experimentally between a flux qubit and an LC oscillator. The authors expect that using this method the QRM can be realized in this parameter regime.

2.2 Matter and light interaction models

In this section we described several quantum models describing the interaction between light and matter. In general, the Hamiltonian of the models are given in the

following general form

$$\boxed{H = \underbrace{H_M}_{\text{atom}} + \underbrace{H_L}_{\text{light}} + \underbrace{H_I}_{\text{interaction terms}}}$$

where the Hamiltonian H_M corresponds to the two-level atom (or in general a two-level system), expressed by Pauli matrices σ_x, σ_y and σ_z

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

the Hamiltonian H_L corresponds to a photon field, described by the raising and lowering operators $a^\dagger, a$ of the QHO and, the interaction terms between the two systems, with Hamiltonian H_I. For a more detailed introduction to the study of these models, we refer the reader to [8].

The first category of models we describe are those where a number of two-level atoms are interacting with a single level photon field in a cavity. The main representative of these models is the quantum Rabi model, and the remaining models can be regarded as generalizations. As we discussed in Section 1.1, the Hamiltonians of these models are operators acting in a Hilbert space $\mathcal{H}\otimes\mathbb{C}^{2M}$, where $\mathcal{H}$ is a Hilbert space satisfying the hypothesis of the Stone-von Neumann theorem, with raising and lowering operators $a^\dagger$ and a, and M is the number of two-level atoms.

The *quantum Rabi model*(QRM) is often called the simplest model in quantum optics describing the interaction between light and matter. It describes the interaction between a two-level atom and a single level photon field. Its Hamiltonian H_{Rabi} is given by

$$H_{\text{Rabi}} = \omega a^\dagger a + g(a + a^\dagger)\sigma_x + \Delta\sigma_z,$$

where $\omega > 0$ is the frequency of photon field in the cavity (essentially a QHO), $2\Delta > 0$ is the energy difference of the two-level system and $g > 0$ is the interaction strength. The QRM has a $\mathbb{Z}/2\mathbb{Z}$-symmetry, at the level of the Hamiltonian it amounts to the existence of a parity operator $\Pi = -\sigma_z(-1)^{a^\dagger a}$ satisfying $[\Pi, H_{\text{Rabi}}] = 0$ and with eigenvalues $p = \pm 1$ (c.f. [45]).

The main topic of study of this thesis, the *asymmetric quantum Rabi model* (AQRM), is a direct generalization of the QRM, defined by the Hamiltonian

$$H^{\varepsilon}_{\text{Rabi}} = H_{\text{Rabi}} + \epsilon\sigma_x,$$

where $\epsilon \in \mathbb{R}$. The AQRM has been also referred to as generalized, biased or driven QRM (see, e.g. [5, 33, 45]). We remark that the QRM is considered to be an integrable model, but this is not the case for the AQRM. We direct the reader to [5] for the discussion on integrability of these models.

The presence of the term $\epsilon\sigma_x$ breaks the $\mathbb{Z}/2\mathbb{Z}$-symmetry of the QRM, however a symmetry can be found by embedding the system into a larger system or by studying the Segal-Bargmann space realization of the system. We discuss this symmetry in Section 2.4 and Section 2.6 below.

The quantum Rabi model can be generalized for M two-level atoms interacting with a single level photon field with frequency $\omega > 0$. The Hamiltonian is defined

as an operator acting on $\mathcal{H} \otimes \mathbb{C}^{2M}$ and we denote by $\sigma_x^{(j)}, \sigma_z^{(j)}$ the Pauli matrices acting in the j-th atom. Concretely, the matrix $\sigma_x^{(j)}$ is given by

$$\sigma_x^{(j)} = I_2 \otimes \cdots \otimes I_2 \otimes \sigma_x \otimes I_2 \otimes \cdots \otimes I_2,$$

where σ_x, the usual Pauli matrix, is at the j-th position. The matrix I_2 is the 2×2 identity matrix. The definition of σ_z^j is completely analogous.

The Hamiltonian of the *M-atom model* H_{Ma} is

$$H_{Ma} = \omega a^\dagger a + \sum_{i=1}^{M} \Delta_j \sigma_z^{(j)} + \sum_{j=1}^{M} g_j (a + a^\dagger) \sigma_x^{(j)}.$$

where the parameters $(2\Delta_1, 2\Delta_2, \ldots, 2\Delta_M) \in (\mathbb{R}_{\geq 0})^M$ and $(g_1, g_2, \ldots, g_M) \in (\mathbb{R}_{\geq 0})^M$ are the difference in levels and coupling strengths between each of the two-level atoms and the photon field, respectively. Clearly, we have $H_{1a} = H^0_{\text{Rabi}}$.

Note that these models receive different names in accordance to certain conditions met by the parameters, for instance, if $\Delta_i = \frac{1}{2}\Delta > 0$ for all $i = 1, 2, \ldots, M$ the model is called *Dicke model* (see for instance [7] for the case $M = 3$).

We can also introduce the *asymmetric M-atom model* in the natural way. The Hamiltonian is given by

$$H^{\varepsilon}_{Ma} = H_M + \sum_{j=1}^{M} \varepsilon_j \sigma_x^{(j)},$$

for $(\varepsilon_1, \varepsilon_2, \cdots, \varepsilon_M) \in \mathbb{R}^M$. Similarly to the one two-level atom model, the introduction of the additional term breaks the symmetries in the Hamiltonian H_{Ma}.

The following models are used to approximate the QRM and its generalizations described above. The main advantage of these models is that they are solvable and, therefore their spectrum is explicitly known.

The *Jaynes-Cummings model* is the model with Hamiltonian

$$H_{\text{JC}} = \omega a^\dagger a + g(\sigma^+ a + \sigma^- a^\dagger) + \Delta \sigma_z,$$

where $\sigma^\pm = (\sigma_x \pm i\sigma_y)/2$. Notice that the QRM can be written as

$$H_{\text{Rabi}} = \omega a^\dagger a + g(\sigma^- a^\dagger + \sigma^+ a) + g(\sigma^+ a^\dagger + \sigma^- a) + \Delta \sigma_z,$$

the term $g(\sigma^- a^\dagger + \sigma^+ a)$ is called the *rotating term* and $g(\sigma^+ a^\dagger + \sigma^- a)$ the *counter-rotating term*. From this point of view, the Jaynes-Cummings model is called the *rotating wave approximation* (RWA) of the QRM (see [24]) since it is obtained disregarding the counter rotating terms from the QRM. This model has a continuous $U(1)$-symmetry in contrast to the discrete $\mathbb{Z}/2\mathbb{Z}$-symmetry of the quantum Rabi model. The symmetry amounts to the existence of a conserved quantity (operator) $N = a^\dagger a + \sigma^+ \sigma^-$ with $[H_{\text{JC}}, N] = 0$. Due to its symmetry the Jaynes-Cummings model is super-integrable and there is a explicit description of the eigenvalues of the Hamiltonian.

The generalization of the Jaynes-Cummings model for M two-level atoms is the *Tavis-Cummings model* (see [56]). Its Hamiltonian is given by

$$H_{TV} = \omega a^\dagger a + \sum_{i=1}^{M} \Delta_j \sigma_z^{(j)} + \sum_{j=1}^{M} g(\sigma_+^{(j)} a + \sigma_-^{(j)} a^\dagger),$$

where $\sigma_{\pm}^{(j)}$ are defined in a manner analogous to $\sigma_x^{(j)}$. The Tavis-Cummings model is integrable via Bethe ansatz methods and, like the Jaynes-Cummings model, has a precise description of its eigenvalues.

We conclude this section by listing certain models related to the QRM, but having a different structure in the Hamiltonian or in the spectral structure.

The *two-photon quantum Rabi model*, is the model with Hamiltonian given by

$$H_{TP} = \omega a^\dagger a + g((a)^2 + (a^\dagger)^2)\sigma_x + \Delta\sigma_z.$$

The spectrum of this model behaves very differently than the QRM under the changes of parameters. In particular, it exhibits a spectral collapse phenomena (c.f. [12]). Note that in the same way it is possible to formally define *M-photon quantum Rabi model*, however it is known that these models are ill-defined for $M \geq 3$.

The *quantum Rabi-Stark model* is a model describing an experiment where the single-level photon in a cavity is subject to two auxiliary laser beams. Its Hamiltonian is given by

$$H_{RS} = H^0_{\text{Rabi}} + \gamma\sigma_z a^\dagger a.$$

Note that, compared to the QRM, the interaction includes the nonlinear term $a^\dagger a$. Its spectrum has been studied by adapting a method similar to the one used in the QRM (see [13]).

The last model that we describe in this section is not a generalization of the QRM. The *non-commutative harmonic oscillator*(NcHO), defined by Parmeggiani and Wakayama[42] in 2001, is the model with the Hamiltonian (acting on $L^2(\mathbb{R}) \otimes \mathbb{C}^2$) given by

$$Q = \begin{bmatrix} \alpha & 0 \\ 0 & \beta \end{bmatrix} \left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 \right) + \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \left(x\frac{d}{dx} + \frac{1}{2} \right),$$

for real parameters α, β. It is a formal model (it does not correspond to known physical phenomena) but a mysterious relation with the QRM has been found through a confluent process (c.f. [62]). The reader is refered to [43, 40] for an extensive introduction to the theory of the NcHO and to [41] for a review of recent research on the topic.

2.3 General properties of the asymmetric quantum Rabi model

The asymmetric quantum Rabi model (AQRM), already introduced in Section 2.2, is the main topic of study of this thesis. In this section we give some of its basic properties of the Hamiltonian as a linear operator acting on $L^2(\mathbb{R}) \otimes \mathbb{C}^2$.

Recall that the Hamiltonian $H^\varepsilon_{\text{Rabi}}$ of the AQRM is given by

$$H^\varepsilon_{\text{Rabi}} = \omega a^\dagger a + \Delta\sigma_z + g\sigma_x(a^\dagger + a) + \varepsilon\sigma_x, \tag{2.1}$$

where $a^\dagger$ and a are the raising and lowering operators, 2Δ is the energy difference between the two levels, g denotes the coupling strength between the two-level atom and single-mode photon field with frequency ω (subsequently, we set $\omega = 1$ without loss of generality) and ε is a real parameter.

In the $L^2(\mathbb{R}) \otimes \mathbb{C}^2$ realization, it is clear that $H^{\varepsilon}_{\text{Rabi}}$ is a unbounded, closed and symmetric operator. In particular, it can be regarded as a elliptic global pseudo-differential operator of order 2 in the sense described in Chapter 3 of [40]. Then, using the results on the spectral properties of global pseudo-differential operators given in Section 3.3 of [40] one can prove the following result.

Proposition 2.3.1 (Prop. 2.1-2.3 of [55])**.** *The operator $H^{\varepsilon}_{\text{Rabi}}$ is self-adjoint. In addition, the spectrum of $H^{\varepsilon}_{\text{Rabi}}$ consist only of the (discrete) set of eigenvalues of $H^{\varepsilon}_{\text{Rabi}}$, that is, the continuous and residual spectra are empty.*

We remark that since the matrices involved in the AQRM are constant, self-adjointness in the $L^2(\mathbb{R})$ realization can also be shown by using the Kato-Rellich theorem (see Theorems 9.37 and 9.38 of [17]).

In the previous sections (for instance, in Section 2.2 above), we purposedly omitted the discussion on the domain of the operator $H^{\varepsilon}_{\text{Rabi}}$ as we were discussion in terms of an abstract Hilbert space with raising and lowering operators $a^{\dagger}$ and a satisfying the hypothesis of the Stone-von Neumann theorem. In the $L^2(\mathbb{R}) \otimes \mathbb{C}^2$ realization, it can be shown that

$$\mathcal{D}(H^{\varepsilon}_{\text{Rabi}}) = B^2(\mathbb{R}) \otimes \mathbb{C}^2,$$

where $B^2(\mathbb{R})$ is a Shubin-Sobolev space, dense and compactly embedded in $L^2(\mathbb{R})$. The reader is direct to [55] for a complete discussion for the case of the QRM.

Finally, following the proof of Proposition 2.2 of [55], it is easy to see the eigenvalues are bounded below, that is, there is finite ground state eigenvalue.

Proposition 2.3.2. *The eigenvalues λ of $H^{\varepsilon}_{\text{Rabi}}$ satisfy*

$$\lambda \geq -g^2 - \Delta - 2|\varepsilon|.$$

The facts above suffice to begin the study of the spectrum of the AQRM and its degeneracy. Note that starting from Section 2.4 below, we use the Segal-Bargmann space realization of the Hamiltonian $H^{\varepsilon}_{\text{Rabi}}$.

2.4 The confluent Heun and $\mathfrak{sl}_2$-representation theoretic pictures of the AQRM

In this section we study the eigenvalue problem of $H^{\varepsilon}_{\text{Rabi}}$ in the Segal-Bargmann space $\mathcal{H}_{\mathcal{B}}$ introduced in Section 1.2 and see how it is formulated as a system of linear differential equations of confluent Heun type. In this form, it can be realized as the image of an element of the universal enveloping algebra $\mathcal{U}(\mathfrak{sl}_2)$ under the representation discussed in Section 1.3.

The Hamiltonian $H^{\varepsilon}_{\text{Rabi}}$, realized as an operator acting on $\mathcal{H}_{\mathcal{B}} \otimes \mathbb{C}^2$, corresponds to the operator

$$\tilde{H}^{\varepsilon}_{\text{Rabi}} := \begin{bmatrix} z\partial_z + \Delta & g(z+\partial_z) + \varepsilon \\ g(z+\partial_z) + \varepsilon & z\partial_z - \Delta \end{bmatrix}.$$

Then, the time-independent Schrödinger equation $H^{\varepsilon}_{\text{Rabi}}\varphi = \lambda\varphi\,(\lambda \in \mathbb{R})$ is equivalent to the system of first order differential equations

$$\tilde{H}^{\varepsilon}_{\text{Rabi}}\psi = \lambda\psi, \quad \psi = \begin{bmatrix}\psi_1(z)\\ \psi_2(z)\end{bmatrix},$$

where eigenfunctions of $H^{\varepsilon}_{\text{Rabi}}$ associated to a given eigenvalue $\lambda \in \mathbb{R}$ correspond to solutions $\psi_i \in \mathcal{H}_{\mathcal{B}}$ $i = 1, 2$, that is $\psi \in \mathcal{H}_{\mathcal{B}} \otimes \mathbb{C}^2$.

Therefore, the eigenvalue problem of the AQRM amounts to finding entire functions $\psi_1, \psi_2 \in \mathcal{H}_{\mathcal{B}}$ and real number λ satisfying

$$\begin{cases}(z\partial_z + \Delta)\psi_1 + (g(z + \partial_z) + \varepsilon)\psi_2 = \lambda\psi_1,\\ (g(z + \partial_z) + \varepsilon)\psi_1 + (z\partial_z - \Delta)\psi_2 = \lambda\psi_2.\end{cases}$$

Now, by setting $f_{\pm} = \psi_1 \pm \psi_2$, we get

$$\begin{cases}(z + g)\dfrac{d}{dz}f_+ + (gz + \varepsilon - \lambda)f_+ + \Delta f_- = 0,\\ (z - g)\dfrac{d}{dz}f_- - (gz + \varepsilon + \lambda)f_- + \Delta f_+ = 0.\end{cases} \tag{2.2}$$

Notice that the system (2.2) has an (unramified) irregular singular point at $z = \infty$ in addition to regular singular points at $z = \pm g$ (c.f. [8]).Therefore, by the discussion in Section 1.2 (see equation (1.2)) any entire solution ψ of (2.2) is actually $\psi \in \mathcal{H}_{\mathcal{B}} \otimes \mathbb{C}^2$.

By using the substitution $\phi_{1,\pm}(z) := e^{gz} f_{\pm}(z)$ and the change of variable $y = \frac{g+z}{2g}$, we obtain

$$\begin{cases} y\dfrac{d}{dy}\phi_{1,+}(y) = (\lambda + g^2 - \varepsilon)\phi_{1,+}(y) - \Delta\phi_{1,-}(y),\\ (y-1)\dfrac{d}{dy}\phi_{1,-}(y) = (\lambda + g^2 - \varepsilon - 4g^2 + 4g^2 y + 2\varepsilon)\phi_{1,-}(y) - \Delta\phi_{1,+}(y).\end{cases} \tag{2.3}$$

Defining $a := -(\lambda + g^2 - \varepsilon)$, we get

$$\begin{cases} y\dfrac{d}{dy}\phi_{1,+}(y) = -a\phi_{1,+}(y) - \Delta\phi_{1,-}(y),\\ (y-1)\dfrac{d}{dy}\phi_{1,-}(y) = -(4g^2 - 4g^2 y + a - 2\varepsilon)\phi_{1,-}(y) - \Delta\phi_{1,+}(y).\end{cases} \tag{2.4}$$

Similarly, by applying the substitutions $\phi_{2,\pm}(z) := e^{-gz} f_{\pm}(z)$ and $\bar{y} = \frac{g-z}{2g}$ to the system (2.2), we get

$$\begin{cases}(\bar{y}-1)\dfrac{d}{d\bar{y}}\phi_{2,+}(\bar{y}) = -(4g^2 - 4g^2\bar{y} + a)\phi_{2,+}(\bar{y}) - \Delta\phi_{2,-}(\bar{y}),\\ \bar{y}\dfrac{d}{d\bar{y}}\phi_{2,-}(\bar{y}) = -(a - 2\varepsilon)\phi_{2,-}(\bar{y}) - \Delta\phi_{2,+}(\bar{y}).\end{cases} \tag{2.5}$$

Note that $a - 2\varepsilon = -(\lambda + g^2 + \varepsilon)$. This system gives another (possible) solution $(\phi_{2,+}(\bar{y}), \phi_{2,-}(\bar{y}))$ to the eigenvalue problem. Notice also that $\bar{y} = 1 - y$, where y is the variable used in (2.4). Note that by applying the substitution $y \to \bar{y} = 1 - y$

and $\varepsilon \to -\varepsilon$ to (2.4) we obtain (2.5) (up to labeling of the equations). In particular, the application of this transformation to a solution furnishes another solution of the eigenvalues problem, this is the manifestation of the $\mathbb{Z}/2\mathbb{Z}$-symmetry that was mentioned in Section 2.2. This symmetry is essential to the verification of the analyticity of the solutions on the complex plane.

The finite singularities of system (2.4) and (2.5) at $y = 0$ and $y = 1$ are regular. The exponents of the equation system can be obtained by standard computation, and are shown in Table 2.1 for reference.

Table 2.1: Exponents of systems (2.4) and (2.5).

	$\phi_{1,-}(y)$	$\phi_{1,+}(y)$	$\phi_{2,-}(1-y)$	$\phi_{2,+}(1-y)$
$y = 0$	$0, -a+1$	$0, -a$	$0, -a+1$	$0, -a$
$y = 1$	$0, -a+2\varepsilon$	$0, -a+2\varepsilon+1$	$0, -a+2\varepsilon$	$0, -a+2\varepsilon+1$

We remark here that due to the presence of finite singularities, solutions of (2.4) (or (2.5)) are not to be automatically assumed to correspond to solutions of the eigenvalue problem of the AQRM. In other words, it is imperative to verify the analyticity of the solutions in the complex plane. The verification for solutions with $\lambda \neq N \pm \varepsilon - g^2$, for $N \in \mathbb{Z}_{\geq 0}$ leads to the study of G-functions (see Section 2.6 below). In the case $\lambda = N \pm \varepsilon - g^2$, the solutions are either polynomial (see Section 2.7) or power series, in the former case the solutions are immediately entire, In the later case this leads to the study of the T-function (see Section 4.1). Note that when solutions are not polynomial we need to consider solutions of both systems in order to have analyticity.

For the case $\varepsilon \neq \ell/2 \in \frac{1}{2}\mathbb{Z}$, it is known that the regular solutions are non-degenerate (see [5]). In general, since the linearly independent solutions of the confluent Heun system (2.4) (resp. (2.5)) are at most two, the foregoing discussion shows that the multiplicity of the eigenvalues is in general at most 2 (see also Corollary 4.1.4).

The representation theoretical picture of the AQRM

In this section by using the representation of a particular element of the universal enveloping algebra $\mathcal{U}(\mathfrak{sl}_2)$ we capture the confluent Heun differential equations corresponding to the eigenvalue problem of AQRM in the Bargmann space, that is, the second order differential equations corresponding to systems (2.4) and (2.5). Let $(\alpha, \beta, \gamma, C) \in \mathbb{R}^4$. Define a second order element $\mathbb{K} = \mathbb{K}(\alpha, \beta, \gamma; C) \in \mathcal{U}(\mathfrak{sl}_2)$ and a constant $\lambda_a = \lambda_a(\alpha, \beta, \gamma)$ depending on the representation ϖ_a as follows:

$$\begin{aligned}\mathbb{K}(\alpha, \beta, \gamma; C) :=& \left[\frac{1}{2}H - E + \alpha\right](F + \beta) + \gamma\left[H - \frac{1}{2}\right] + C,\\ \lambda_a(\alpha, \beta, \gamma) :=& \beta\left(\frac{1}{2}a + \alpha\right) + \gamma\left(a - \frac{1}{2}\right).\end{aligned}$$

By the elementary identity $y^{-\frac{1}{2}(a-\frac{1}{2})}\, y\partial_y\, y^{\frac{1}{2}(a-\frac{1}{2})} = y\partial_y + \frac{1}{2}(a - \frac{1}{2})$, we obtain the following lemma.

Lemma 2.4.1 ([63, 60])**.** *We have the following expression.*

$$\frac{y^{-\frac{1}{2}(a-\frac{1}{2})}\varpi_a(\mathbb{K}(\alpha,\beta,\gamma;C))y^{\frac{1}{2}(a-\frac{1}{2})}}{y(y-1)}$$
$$=\frac{d^2}{dy^2}+\Big\{-\beta+\frac{\frac{1}{2}a+\alpha}{y}+\frac{\frac{1}{2}a+2\gamma-\alpha}{y-1}\Big\}\frac{d}{dy}+\frac{-a\beta y+\lambda_a(\alpha,\beta,\gamma)+C}{y(y-1)}.$$

Now, by choosing suitable parameters $(\alpha,\beta,\gamma;C)$ we define from $\mathbb{K}=\mathbb{K}(\alpha,\beta,\gamma;C)$ two second order elements $\mathcal{K}$ and $\tilde{\mathcal{K}}\in\mathcal{U}(\mathfrak{sl}_2)$ that capture the eigenvalue problem of the Hamiltonian $H^{\varepsilon}_{\text{Rabi}}$ of the AQRM. In the following proposition, $\mathcal{H}^{\varepsilon}_1$ is the second order differential operator (confluent Heun ODE [14, 54]) corresponding to the solution $\phi_{1,+}$ in the system (2.3). Similarly, $\mathcal{H}^{\varepsilon}_2$ is the second order differential operator (confluent Heun ODE) corresponding to $\phi_{2,+}$ of (2.5).

Proposition 2.4.2. *Let λ be an eigenvalue of $H^{\varepsilon}_{\text{Rabi}}$. Set $a=-(\lambda+g^2-\varepsilon)$, $a'=a-2\varepsilon+1$ and $\mu=(\lambda+g^2)^2-4g^2(\lambda+g^2)-\Delta^2$.*

1. *Define*

$$\mathcal{K}:=\mathbb{K}\Big(1+\frac{a}{2},4g^2,\frac{a'}{2};\mu+4\varepsilon g^2-\varepsilon^2\Big)\in\mathcal{U}(\mathfrak{sl}_2),$$
$$\Lambda_a:=\lambda_a\Big(1-\frac{a}{2},4g^2,\frac{a'}{2}\Big).$$

Then

$$y(y-1)\mathcal{H}^{\varepsilon}_1(\lambda)=y^{-\frac{1}{2}(a-\frac{1}{2})}(\varpi_a(\mathcal{K})-\Lambda_a)y^{\frac{1}{2}(a-\frac{1}{2})}. \tag{2.6}$$

2. *Define*

$$\tilde{\mathcal{K}}:=\mathbb{K}\Big(-1+\frac{a'}{2},4g^2,\frac{a}{2};\mu-4\varepsilon g^2-\varepsilon^2\Big)\in\mathcal{U}(\mathfrak{sl}_2),$$
$$\tilde{\Lambda}_{a'}:=\lambda_{a'}\Big(-1+\frac{a'}{2},4g^2,\frac{a}{2}\Big).$$

Then

$$y(y-1)\mathcal{H}^{\varepsilon}_2(\lambda)=y^{-\frac{1}{2}(a'-\frac{1}{2})}(\varpi_{a'}(\tilde{\mathcal{K}})-\tilde{\Lambda}_{a'})y^{\frac{1}{2}(a'-\frac{1}{2})}. \tag{2.7}$$

In Section 4.5, we use this realization of the eigenvalue problem of the AQRM to describe the solutions in terms of irreducible representations of $\mathfrak{sl}_2$.

2.5 The spectrum of the AQRM

Recall from Proposition 2.3.1 that the continuous and residual spectrum of the $H^{\varepsilon}_{\text{Rabi}}$ is empty, so the spectrum consists only of a discrete set of eigenvalues. In this section we introduce the classification of the spectrum of the AQRM based on the study of the solutions of the confluent Heun picture of the ARQM given in Section 2.4 above.

Let $\lambda\in\mathbb{R}$ is an eigenvalue of $H^{\varepsilon}_{\text{Rabi}}$, then

1. if there is an integer $\mathbb{N}\in\mathbb{Z}$ such that $\lambda=N\pm\varepsilon-g^2$, λ is called *exceptional eigenvalue*,

2. if λ is not an exceptional eigenvalue, we say that λ is a *regular eigenvalue.*

If λ is a regular (resp. exceptional) eigenvalue, then the associated eigenfunction is also called regular (resp. exceptional) eigenfunctions (or solutions).

There is finer classification of the exceptional eigenvalues. If λ is an exceptional eigenvalue, and the solution of the system (2.4) consists of polynomial functions (that is, terminating power series) the solutions (resp. the eigenvalue) is called *Juddian* . Otherwise, we say it is a *non-Juddian exceptional eigenvalue.*

Historically, the first eigenvalues of QRM to be described were the Juddian eigenvalues, studied by Judd in [25] and Kuś in [31]. Concretely, Kuś showed the presence of degenerate eigenvalues of the form $\lambda = N - g^2$ in the spectrum of the QRM, subject to a polynomial equation. We discuss the generalization of the polynomial condition for the AQRM in Section 2.8. The existence of non-Juddian exceptional eigenvalues in the QRM was first discovered numerically by Maciejewski, Przybylska and Stachowiak[36].

In 2011, Daniel Braak described the regular spectrum of the AQRM analytically. This is done by defining a G-function that gives the conditions for a regular solution of system (2.4) to be entire, then all the zeros of said function (all other parameters being fixed) correspond to the regular spectrum of the AQRM. We give a sketch of the argument in Section 2.6.

To finish this section, from the confluent Heun picture, we give an important property of the spectrum of the AQRM.

Proposition 2.5.1. *The spectrum of the Hamiltonian $H^{\varepsilon}_{\text{Rabi}}$ of AQRM depends only on $|\varepsilon|$. In other words, the spectrum of Hamiltonian $H^{-\varepsilon}_{\text{Rabi}}$ coincides with that of $H^{\varepsilon}_{\text{Rabi}}$.*

Proof. It follows also from the comparison of the two systems of differential equations (2.4) and (2.5) under the application of the transformation $\varepsilon \to -\varepsilon$. □

2.6 Regular spectrum and the G-function of the AQRM

In this section we begin the description of the solutions of (2.4) corresponding to solutions of the eigenvalue problem of the AQRM. If $a = -(\lambda + g^2 - \varepsilon)$ is not an integer, by Table 2.1 the difference between the exponents in (2.4) is not an integer. In particular, around the singularity $y = 0$ the Frobenius solution is

$$\phi_{1,-}(y) = y^b \sum_{n=0}^{\infty} K_n y^n,$$

where $b \in \{\rho_1^-, \rho_2^-\}$ is one of the exponents of the system. In order for the solution to be entire the only option is to take the exponent $\rho_1^- = 0$. Integration of the first equation of (2.17) gives

$$\phi_{1,+}(y) = -\Delta \sum_{n=0}^{\infty} \frac{K_n}{n+a} y^n,$$

with constant $c \in \mathbb{C}$. Moreover, we can get recurrence relations to determine the coefficients K_n. However, as we mentioned before in Section 2.4 above, to show

that this solution is a solution of the eigenvalue problem of AQRM, it is necessary to prove that the solution is entire. The conditions are given by the G-function of Braak. For consistency with the existing literature, we describe the G-function with the original notation.

Definition 2.6.1. *The G-function for the Hamiltonian $H^{\varepsilon}_{\mathrm{Rabi}}$ is defined as*

$$G_{\varepsilon}(x;g,\Delta) := \Delta^2 \bar{R}^{+}(x;g,\Delta,\varepsilon)\bar{R}^{-}(x;g,\Delta,\varepsilon) - R^{+}(x;g,\Delta,\varepsilon)R^{-}(x;g,\Delta,\varepsilon)$$

where

$$R^{\pm}(x;g,\Delta,\varepsilon) = \sum_{n=0}^{\infty} K_n^{\pm}(x) g^n \quad \text{and} \quad \bar{R}^{\pm}(x;g,\Delta,\varepsilon) = \sum_{n=0}^{\infty} \frac{K_n^{\pm}(x)}{x-n\pm\varepsilon} g^n, \tag{2.8}$$

whenever $x \mp \varepsilon \notin \mathbb{Z}_{\geq 0}$, respectively. For $n \in \mathbb{Z}_{\geq 0}$, define the functions $f_n^{\pm} = f_n^{\pm}(x,g,\Delta,\varepsilon)$ by

$$f_n^{\pm}(x,g,\Delta,\varepsilon) = 2g + \frac{1}{2g}\Big(n - x \pm \varepsilon + \frac{\Delta^2}{x-n\pm\varepsilon}\Big), \tag{2.9}$$

then, the coefficients $K_n^{\pm}(x) = K_n^{\pm}(x,g,\Delta,\varepsilon)$ are given by the recurrence relation

$$nK_n^{\pm}(x) = f_{n-1}^{\pm}(x,g,\Delta,\varepsilon)K_{n-1}^{\pm}(x) - K_{n-2}^{\pm}(x) \quad (n \geq 1) \tag{2.10}$$

with initial condition $K_{-1}^{\pm} = 0$ and $K_0^{\pm} = 1$.

It is well-known (e.g. [5, 6, 45]) that for fixed parameters $\{g,\Delta,\varepsilon\}$ the zeros x_n of $G_{\varepsilon}(x;g,\Delta)$ correspond to regular eigenvalues $\lambda_n = x_n - g^2$ of $H^{\varepsilon}_{\mathrm{Rabi}}$. We sketch the proof next, following the argument of Braak in [6]. The eigenvalue equation for $H^{\varepsilon}_{\mathrm{Rabi}}$, that is (2.2), is equivalent via embedding to the system of differential equations given by

$$\frac{d}{dz}\Psi(z) = A(z)\Psi(z), \tag{2.11}$$

where

$$A(z) = \begin{bmatrix} \frac{\lambda-\varepsilon-gz}{z+g} & 0 & 0 & \frac{-\Delta}{z+g} \\ 0 & \frac{\lambda+\varepsilon-gz}{z+g} & \frac{-\Delta}{z+g} & 0 \\ 0 & \frac{-\Delta}{z-g} & \frac{\lambda-\varepsilon+gz}{z-g} & 0 \\ \frac{-\Delta}{z-g} & 0 & 0 & \frac{\lambda+\varepsilon+gz}{z-g} \end{bmatrix}, \tag{2.12}$$

for the vector valued function

$$\Psi(z) := {}^t(\psi_1(z), \psi_2(z), \bar{\psi}_1(z), \bar{\psi}_2(z)).$$

The functions $\psi_i, \bar{\psi}_i$ are essentially the solutions to system (2.2) and a transformation (similar to the case of (2.4) and (2.5)). The system (2.11) has a $\mathbb{Z}/2\mathbb{Z}$-symmetry: if $\psi(z)$ is a solution then

$$\Phi(z) := {}^t(\bar{\psi}_1(-z), \bar{\psi}_2(-z), \psi_1(-z), \psi_2(-z)),$$

is also a solution of (2.11). Notice that if the solution $\Psi(z)$ is expanded in power series around the critical point $-g$ (resp. $\Phi(z)$ is expanded around the critical point g) with convergence radius of $2g$, then in any (ordinary) point z_0 in the common

domain of convergence of $\phi(z)$ and $\psi(z)$ and the solutions are linearly dependent we must necessarily have $\Psi(z_0) = c\Phi(z_0)$ for some constant $c \in C$. Moreover, the solution is actually holomorphically continued to the whole complex plane. As we have discussed before, this is enough for the solution $\Psi(z_0)$ to be an element of the Segal-Bargmann space and thus a solutions to the eigenvalue problem of the AQRM. Let z_0 be as described above, then the equation $\Psi(z_0) = c\Phi(z_0)$ yields

$$\begin{cases} e^{-gz_0}\sum_{n=0}^{\infty}\frac{\Delta K_n^-}{x-\epsilon-n}(z_0+g)^n = c\,e^{gz_0}\sum_{n=0}^{\infty}K_n^+(z_0-g)^n, \\ e^{gz_0}\sum_{n=0}^{\infty}K_n^-(z_0+g)^n = c\,e^{-gz_0}\sum_{n=0}^{\infty}\frac{\Delta K_n^+}{x+\epsilon-n}(z_0+g)^n, \\ e^{gz_0}\sum_{n=0}^{\infty}\frac{\Delta K_n^-}{x-\epsilon-n}(z_0-g)^n = c\,e^{-gz_0}\sum_{n=0}^{\infty}K_n^+(z_0+g)^n, \\ e^{-gz_0}\sum_{n=0}^{\infty}K_n^-(z_0+g)^n = c\,e^{gz_0}\sum_{n=0}^{\infty}\frac{\Delta K_n^+}{x+\epsilon-n}(z_0-g)^n, \end{cases} \tag{2.13}$$

For $z_0 = 0$, it is obvious that the first and third (resp. second and forth) equations are equivalent, and the system reduces to

$$\begin{cases} \sum_{n=0}^{\infty}\left[cK_n^+ - \frac{\Delta K_n^-}{x-\epsilon-n}\right]g^n = 0 \\ \sum_{n=0}^{\infty}\left[K_n^- - \frac{c\Delta K_n^+}{x-\epsilon-n}\right]g^n = 0 \end{cases} \tag{2.14}$$

for some non-zero constant c. By eliminating the constant c we obtain the equation

$$G_\varepsilon(x; g, \Delta) = 0,$$

justifying the definition of the G-function. Likewise, starting from a zero of the G-function it is possible to construct the entire solution corresponding to the zero, proving the claim. We refer the reader to the already cited literature for further details.

Remark 2.6.2. We remark that in the case of the QRM (i.e. $\varepsilon = 0$), we have $G_0(x; g, \Delta) = G_+(x) \cdot G_-(x)$, $G_\pm(x)$ being the G-functions corresponding to the parity defined as

$$G_\pm(x) = \sum_{n=0}^{\infty} K_n(x)\Big(1 \mp \frac{\Delta}{x-n}\Big)g^n,$$

where $K_n(x) = K_n^\pm(x, g, \Delta, 0)$ [5]. Note also that there are no degeneracies within each parity subspace, that is there are no common zeros of $G_+(x)$ and $G_-(x)$.

The following result is obvious from the definitions and the equality

$$K_n^\pm(x, g, \Delta, -\varepsilon) = K_n^\mp(x, g, \Delta, \varepsilon), \tag{2.15}$$

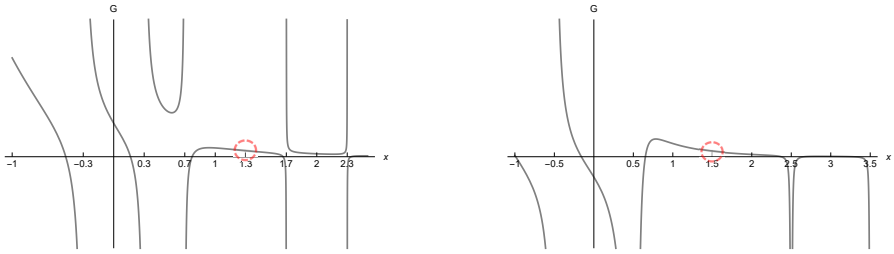
obtained by direct computation.

Lemma 2.6.3. *The G-functions of $H_{\text{Rabi}}^{\varepsilon}$ coincides with that of $H_{\text{Rabi}}^{-\varepsilon}$:*

$$G_\varepsilon(x; g, \Delta) = G_{-\varepsilon}(x; g, \Delta). \tag{2.16}$$

In other words, the regular spectrum of $H_{\text{Rabi}}^{\varepsilon}$ depends only on $|\varepsilon|$. □

We conclude this section by showing in Figure 2.1 the graphs of $G_\varepsilon(x; g, \Delta)$, as a function of x, for different values of Δ and g. As we have discussed in this section, the zeros of the function $G_\varepsilon(x; g, \Delta)$, represented in the figures by the crossings of the graph of $G_\varepsilon(x; g, \Delta)$ with the horizontal line $y = 0$, correspond to regular eigenvalues of the AQRM for the given parameters g and Δ. Furthermore, we notice that for certain parameters the poles at $x = N \pm \varepsilon$, $N \in \mathbb{Z}_{\geq 0}$, of the G-function vanish, as shown in Figure 2.1(a) and Figure 2.1(b). In Chapter 4 we will see that this is related to the presence of exceptional eigenvalues in the spectrum of the AQRM. The analysis of the poles and the characterization of the vanishing, or lifting, of poles is done in Section 4.3, after we have given a precise description of the exceptional eigenvalues.



(a) $\varepsilon = 0.3, g \approx 0.5809, \Delta = 1/2$ (b) $\varepsilon = 0.5, g = 0.5, \Delta = 1$

Figure 2.1: Plot of $G_\varepsilon(x; g, \Delta)$ for fixed g and Δ, corresponding to roots of constraint polynomials $P_N^{(N,\varepsilon)}((2g)^2, \Delta^2)$. Notice the vanishing of the poles (indicated with red circles) at $x = N + \varepsilon$ for $N = 1$ in (a) and (b).

2.7 Exceptional spectrum and exceptional solutions

In this section we study the exceptional solutions of the AQRM. Recall that an eigenvalue λ of $H^\varepsilon_{\text{Rabi}}$ is called exceptional if there is an integer $N \in \mathbb{Z}_{\geq 0}$ such that $\lambda = N \pm \varepsilon - g^2$. For the case $\lambda = N + \varepsilon - g^2$, this corresponds to taking $-a = (\lambda + g^2 - \varepsilon) = N \in \mathbb{Z}_{\geq 0}$. The system (2.4) of differential equations is then given by

$$\begin{cases} y\dfrac{d}{dy}\phi_{1,+}(y) = N\phi_{1,+}(y) - \Delta\phi_{1,-}(y) \\ (y-1)\dfrac{d}{dy}\phi_{1,-}(y) = (N - 4g^2 + 4g^2 y + 2\varepsilon)\phi_{1,-}(y) - \Delta\phi_{1,+}(y). \end{cases} \tag{2.17}$$

The exponents of $\phi_{1,-}$ at $y = 0$ are $\rho_1^- = 0, \rho_2^- = N + 1$. Likewise, the exponents of $\phi_{1,+}$ at $y = 0$ are $\rho_1^+ = 0, \rho_2^+ = N$. Since the difference between the exponents is a positive integer, the local analytic solutions may develop a logarithmic branch-cut at $y = 0$.

The case $\lambda = N - \varepsilon - g^2$ corresponds to taking $-a = (\lambda + g^2 - \varepsilon) = N - 2\varepsilon$. The system (2.5) is then equivalent to system (2.17) under the transformations $y \to \bar{y} = 1 - y$ and $\varepsilon \to -\varepsilon$. Due to this, in this section and in the remainder of the chapter we consider only the case $\lambda = N + \varepsilon - g^2$ without loss of generality.

Solutions corresponding to the smallest exponent

The local Frobenius solution corresponding to the smallest exponent $\rho_1^- = 0$ has the form

$$\phi_{1,-}(y)(=\phi_{1,-}(y;\varepsilon)) = \sum_{n=0}^{\infty} K_n^{(N,\varepsilon)} y^n, \tag{2.18}$$

where $K_0^{(N,\varepsilon)} \neq 0$ and $K_n^{(N,\varepsilon)} = K_n^{(N,\varepsilon)}(g,\Delta)$. Integration of the first equation of (2.17) gives

$$\phi_{1,+}(y)\ (=\phi_{1,+}(y;\varepsilon)) = cy^N - \Delta \sum_{n\neq N}^{\infty} \frac{K_n^{(N,\varepsilon)}}{n-N} y^n - \Delta K_N^{(N,\varepsilon)} y^N \log y, \tag{2.19}$$

with constant $c \in \mathbb{C}$. A necessary condition for $\phi_{1,+}(y)$ to be an element of the Segal-Bargmann space $\mathcal{H}_{\mathcal{B}}$ is that $\phi_{1,+}(y)$ is an entire function, forcing $K_N^{(N,\varepsilon)} = 0$ to make the logarithmic term vanish. Suppose $\phi_{1,+}(y) \in \mathcal{H}_{\mathcal{B}}$, then by using the second equation of (2.17) we obtain the recurrence relation for the coefficients

$$(n+1)K_{n+1}^{(N,\varepsilon)} + \left(N - n - (2g)^2 + \frac{\Delta^2}{n-N} + 2\varepsilon\right) K_n^{(N,\varepsilon)} + (2g)^2 K_{n-1}^{(N,\varepsilon)} = 0, \tag{2.20}$$

valid for $n \neq N$. This recurrence relation clearly shows the dependence of the coefficients $K_n^{(N,\varepsilon)} = K_n^{(N,\varepsilon)}(g,\Delta)$ on the parameters of the system. Additionally, for $n = N$, by the second equation of (2.17), we have

$$\Delta c = (2g)^2 K_{N-1}^{(N,\varepsilon)} + (N+1)K_{N+1}^{(N,\varepsilon)}. \tag{2.21}$$

Setting $c = (2g)^2 K_{N-1}^{(N,\varepsilon)}/\Delta$ makes $K_{N+1}^{(N,\varepsilon)}$ vanish, and then, by repeated use of the recurrence (2.20), we see that for all positive integers k the coefficients $K_{N+k}^{(N,\varepsilon)}$ also vanish. Thus, the solutions of (2.17) given by

$$\begin{aligned} \phi_{1,-}(y) &= \sum_{n=0}^{N-1} K_n^{(N,\varepsilon)} y^n, \\ \phi_{1,+}(y) &= \frac{4g^2 K_{N-1}^{(N,\varepsilon)}}{\Delta} y^N - \Delta \sum_{n=0}^{N-1} \frac{K_n^{(N,\varepsilon)}}{n-N} y^n, \end{aligned} \tag{2.22}$$

are polynomial solutions. Since polynomials solutions are entire, these solutions, called *Juddian solutions*, Judd solutions or Juddian points, are automatically solutions of the eigenvalue problem of the AQRM.

Conversely, note that given the condition

$$K_N^{(N,\varepsilon)} = 0,$$

we can always construct solutions of the type given above. This is the key observation for the study of Juddian solutions.

To finish this subsection, we make a note on Juddian solutions in light of the already described symmetry in the solutions of the AQRM (between (2.4) and (2.5)). If $\varepsilon \notin \frac{1}{2}\mathbb{Z}$, then, upon applying $y \to 1-y$ and $\varepsilon \to -\varepsilon$, to (2.17), we obtain a system

of equations where the difference between the exponents is not an integer, and thus the solution should correspond to a regular solution. However, as we discussed on Section 2.6, such solution cannot be entire (entireness requires the use of solutions to both systems for the G-function), and therefore the Juddian solution in this case is non-degenerate. On the other hand, in the case of $\varepsilon = \frac{1}{2}\mathbb{Z}$ there may a case of a doubly degenerate Juddian solution, we further discuss this case in Section 2.9.

Solutions corresponding to the largest exponent

The largest exponent of $\phi_{1,-}$ at $y = 0$ is $\rho_2^- = N + 1$, therefore it follows then that there is a local Frobenius solution analytic at $y = 0$ of the form

$$\phi_{1,-}(y)(= \phi_{1,-}(y;\varepsilon)) = \sum_{n=N+1}^{\infty} \bar{K}_n^{(N,\varepsilon)} y^n, \tag{2.23}$$

where $\bar{K}_{N+1}^{(N,\varepsilon)} \neq 0$ and $\bar{K}_n^{(N,\varepsilon)} = \bar{K}_n^{(N,\varepsilon)}(g, \Delta)$. Integration of the first equation of (2.17) gives

$$\phi_{1,+}(y)(= \phi_{1,+}(y;\varepsilon)) = cy^N - \Delta \sum_{n=N+1}^{\infty} \frac{\bar{K}_n^{(N,\varepsilon)}}{n-N} y^n, \tag{2.24}$$

with constant $c \in \mathbb{C}$. The second equation of (2.17) gives the recurrence relation

$$(n+1)\bar{K}_{n+1}^{(N,\varepsilon)} + \Big(N - n - (2g)^2 + \frac{\Delta^2}{n-N} + 2\varepsilon\Big)\bar{K}_n^{(N,\varepsilon)} + (2g)^2 \bar{K}_{n-1}^{(N,\varepsilon)} = 0, \tag{2.25}$$

for $n \geq N + 1$ with initial conditions $\bar{K}_{N+1}^{(N,\varepsilon)} = 1$ and $\bar{K}_N^{(N,\varepsilon)} = 0$. Furthermore, we also have the condition

$$(N+1)\bar{K}_{N+1}^{(N,\varepsilon)} = (N+1) = c\Delta,$$

which determines value of the constant $c = (N+1)/\Delta$. Notice that the radius of convergence of each series above equals 1 from the defining recurrence relation (2.25).

Summarizing, the solutions for the largest exponent are of the form

$$\begin{aligned} \phi_{1,-}(y) &= \sum_{n=N+1}^{\infty} \bar{K}_n^{(N,\varepsilon)} y^n \\ \phi_{1,+}(y) &= \frac{(N+1)}{\Delta} y^N - \Delta \sum_{n=N+1}^{\infty} \frac{\bar{K}_n^{(N,\varepsilon)}}{n-N} y^n, \end{aligned} \tag{2.26}$$

when these solutions correspond to solutions of the eigenvalue problem of AQRM, these are called *non-Juddian exceptional solutions*.

As in the case of the regular spectrum, it is necessary to verify the analyticity of the solution in the complex plane. We do this by defining a T-function for non-Juddian exceptional eigenvalues in Section 4.2.

2.8 Exceptional solutions and constraint polynomials

In 2.7 we discussed how the Juddian eigenvalues, exceptional solutions corresponding to the smaller exponent, are determined by the condition $K_N^{(N,\varepsilon)} = 0$. The coefficient $K_N^{(N,\varepsilon)}$ is in general a rational function on its parameters g and Δ. Thus, it is convenient to introduce a polynomial that has the same zeros as $K_N^{(N,\varepsilon)}$, this polynomial is the constraint polynomial $P_N^{(N,\varepsilon)}(x,y)$ of the AQRM.

Definition 2.8.1. *Let $N \in \mathbb{Z}_{\geq 0}$. The polynomials $P_k^{(N,\varepsilon)}(x,y)$ of degree k are defined recursively by*

$$\begin{aligned}
&P_0^{(N,\varepsilon)}(x,y) = 1,\\
&P_1^{(N,\varepsilon)}(x,y) = x + y - 1 - 2\varepsilon,\\
&P_k^{(N,\varepsilon)}(x,y) = (kx + y - k(k+2\varepsilon))P_{k-1}^{(N,\varepsilon)}(x,y) - k(k-1)(N-k+1)xP_{k-2}^{(N,\varepsilon)}(x,y).
\end{aligned}$$

In order to work with polynomials satisfying a three term recurrence relation, we introduce some notations here. For a tridiagonal matrix we write

$$\operatorname{tridiag}\begin{bmatrix} a_i & b_i \\ c_i & \end{bmatrix}_{1\leq i\leq n} := \begin{bmatrix} a_1 & b_1 & 0 & 0 & \cdots & 0 \\ c_1 & a_2 & b_2 & 0 & \cdots & 0 \\ 0 & c_2 & a_3 & b_3 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 0 & c_{n-2} & a_{n-1} & b_{n-1} \\ 0 & \cdots & 0 & 0 & c_{n-1} & a_n \end{bmatrix}.$$

The symbol $(a)_n$ denotes the Pochhammer symbol, or raising factorial, that is,

$$(a)_n := a(a+1)\cdots(a+n-1) = \frac{\Gamma(a+n)}{\Gamma(a)}$$

for $a \in \mathbb{C}$ and a non-negative integer n.

Recall that the determinant J_n of a tridiagonal matrix

$$J_n = \det \operatorname{tridiag}\begin{bmatrix} a_i & b_i \\ c_i & \end{bmatrix}_{1\leq i\leq n}$$

is called *continuant* (see [38]). It satisfies the three-term recurrence relation

$$J_n = a_n J_{n-1} - b_{n-1}c_{n-1}J_{n-2}, \tag{2.27}$$

with initial condition $J_{-1} = 0, J_0 = 1$. As a consequence of this, notice that the continuant equivalence

$$\det \operatorname{tridiag}\begin{bmatrix} a_i & b_i \\ c_i & \end{bmatrix}_{1\leq i\leq n} = \det \operatorname{tridiag}\begin{bmatrix} a_i & b_i' \\ c_i' & \end{bmatrix}_{1\leq i\leq n} \tag{2.28}$$

holds whenever $b_i c_i = b_i' c_i'$ for all $i = 1, 2, \cdots, n-1$, since the continuants on both sides of the equation define the same recurrence relations with the same initial conditions.

The next result allows to work using constraint polynomials in the study of the Juddian eigenvalues of the AQRM.

Proposition 2.8.2 ([27]). *Let $N \in \mathbb{Z}_{\geq 0}$ and fix $\Delta > 0$. Then, the zeros g of $K_N^{(N,\varepsilon)} = K_N^{(N,\varepsilon)}(g,\Delta)$ defined by (2.20) and $P_N^{(N,\varepsilon)}((2g)^2,\Delta^2)$ coincide. In particular, if g is a zero of $P_N^{(N,\varepsilon)}((2g)^2,\Delta^2)$, then $\lambda = N+\varepsilon-g^2$ is an exceptional eigenvalue with corresponding Juddian solution given by $\phi_{1,+}(y)$ and $\phi_{1,-}(y)$ in (2.22).*

Proof. By multiplying $K_n^{(N,\varepsilon)}$ by $(K_0^{(N,\varepsilon)})^{-1}$ for all $n \in \mathbb{Z}_{\geq 0}$, we can assume that $K_0^{(N,\varepsilon)} = 1$. Then, we can rewrite the recurrence relation for the coefficients $K_n^{(N,\varepsilon)}$ as

$$K_n^{(N,\varepsilon)} = \frac{1}{n}\left((2g)^2 + \frac{\Delta^2}{N-n+1} + n - 1 - N - 2\varepsilon\right)K_{n-1}^{(N,\varepsilon)} - \frac{1}{n}(2g)^2 K_{n-2}^{(N,\varepsilon)},$$

for $n \leq N$. We easily see that $K_N^{(N,\varepsilon)}$ has the determinant expression

$$K_N^{(N,\varepsilon)} = \det \operatorname{tridiag}\begin{bmatrix} \frac{1}{N-i+1}((2g)^2 + \frac{\Delta^2}{i} - i - 2\varepsilon) & \frac{2g}{N-i+1} \\ 2g & \end{bmatrix}_{1\leq i\leq N}.$$

Next, for $i = 1,2,\ldots,N$, factor $\frac{1}{i(N+1-i)}$ from the i-th row in the determinant to get the expression of $K_N^{(N,\varepsilon)}$ as

$$\frac{1}{(N!)^2}\det \operatorname{tridiag}\begin{bmatrix} i(2g)^2 + \Delta^2 - i^2 - 2i\varepsilon & 2ig \\ (2N-1-i)g & \end{bmatrix}_{1\leq i\leq N}.$$

The recurrence relation corresponding to this continuant is the same as the recurrence relation of Definition 2.8.1 for the constraint polynomials $P_k^{(N,\varepsilon)}((2g)^2,\Delta^2)$, including the initial conditions. Thus

$$K_N^{(N,\varepsilon)}(N+\varepsilon; g,\Delta,\varepsilon) = \frac{1}{(N!)^2}P_N^{(N,\varepsilon)}((2g)^2,\Delta^2),$$

completing the proof. □

Remark 2.8.3. We note that there are different ways to prove that the constraint relation

$$P_N^{(N,\varepsilon)}((2g)^2,\Delta^2) = 0$$

gives rise to Juddian solutions. We refer the reader to [33, 63] for other arguments.

In order to describe the behavior of the G-function at the poles in Section 4.3, we need to prove a relation between the coefficients of the G-function and the constraint polynomials in the following lemma. The proof can be done in the same manner as Proposition 2.8.2.

Lemma 2.8.4 ([27]). *Let $N \in \mathbb{Z}_{\geq 0}$. Then the following relation hold for $g > 0$.*

$$(N!)^2(2g)^N K_N^-(N+\varepsilon; g,\Delta,\varepsilon) = P_N^{(N,\varepsilon)}((2g)^2,\Delta^2), \tag{2.29}$$

In addition, if $\varepsilon = \ell/2\,(\ell \in \mathbb{Z})$, it also holds that

$$((N+\ell)!)^2(2g)^{N+\ell}K_{N+\ell}^+(N+\ell/2; g,\Delta,\ell/2) = P_{N+\ell}^{(N+\ell,-\ell/2)}((2g)^2,\Delta^2).$$

To finish this section, we give some generalizations of Lemma 2.8.4. First, we note a simple but important relation between the coefficients $K_n^-(N+\varepsilon;g,\Delta,\varepsilon)$ and $K_n^-(n+\varepsilon;g,\Delta,\varepsilon)$ of the G-functions and the corresponding relation between constraint polynomials.

Lemma 2.8.5. *For $N,n\in\mathbb{Z}_{\geq 0}$ with $n\leq N$, then*

$$K_n^-(N+\varepsilon;g,\Delta,\varepsilon)=K_n^-(n+\varepsilon;g,\Delta,\varepsilon)+q_0(g,\Delta,\varepsilon,n,N),$$

where $(2g)^n q_0(g,\Delta,\varepsilon,n,N)\in\mathbb{Z}[g,\Delta,\varepsilon,n,N]$ and $q_0(g,\Delta,\varepsilon,N,N)=q_0(g,\Delta,\varepsilon,n,n)=0$. Moreover,

$$P_k^{(N,\varepsilon)}(x,y)=P_k^{(k,\varepsilon)}(x,y)+\bar{q}_0(g,\Delta,\varepsilon,n,N),$$

where $\bar{q}_0(g,\Delta,\varepsilon,n,N)\in\mathbb{Z}[g,\Delta,\varepsilon,n,N]$ and $\bar{q}_0(g,\Delta,\varepsilon,N,N)=\bar{q}_0(g,\Delta,\varepsilon,n,n)=0$.

Proof. We give the proof for the polynomials $P_k^{(N,\varepsilon)}(x,y)$ as the proof for the coefficients $K_n^-(N+\varepsilon;g,\Delta,\varepsilon)$ is done in a completely analogous way. In the determinant expression (3.1) for $P_k^{(N,\varepsilon)}(x,y)$, in each term $\lambda_i=i(i-1)(N-i+1)$, we write $N=k+(N-k)$ and then factor out the terms including $N-k$ by the multilinearity of the determinant. This gives the result. □

For $n\leq N$, consider the polynomials $P_k^{(N,n,\varepsilon)}(x,y)$ defined by the three-term recurrence relation

$$\begin{aligned}P_k^{(N,n,\varepsilon)}(x,y)=&((N-n+k)x+y-(N-n+k)^2-2(N-n+k)\varepsilon)P_{k-1}^{(N,n,\varepsilon)}(x,y)\\&-(N-n+k)(N-n+k-1)(n-k+1)xP_{k-2}^{(N,n,\varepsilon)},\end{aligned}\tag{2.30}$$

with initial conditions $P_0^{(N,n,\varepsilon)}(x,y)=1$ and $P_1^{(N,n,\varepsilon)}(x,y)=(N-n+1)x+y-(N-n+1)^2-2(N-n+1)\varepsilon$. Note that setting $n=N$ gives $P_k^{(N,N,\varepsilon)}(x,y)=P_k^{(N,\varepsilon)}(x,y)$.

Lemma 2.8.6. *For $N,n\in\mathbb{Z}_{\geq 0}$ with $n\leq N$, we have*

$$n!(N-n+1)_n(2g)^nK_n^-(N+\varepsilon;g,\Delta,\varepsilon)=P_n^{(N,n,\varepsilon)}((2g)^2,\Delta^2).$$

Moreover, it holds that

$$n!(N-n+1)_n(2g)^nK_n^-(N+\varepsilon;g,\Delta,\varepsilon)=P_n^{(n,\varepsilon)}((2g)^2,\Delta^2)+q_1(x,y;N,n,\varepsilon),$$

with $q_1(x,y;N,n,\varepsilon)\in\mathbb{Z}[x,y,N,n,\varepsilon]$ such that $q_1(x,y;N,N,\varepsilon)=q_1(x,y;n,n,\varepsilon)=0$.

Proof. The proof of the first claim follows in the same way as Lemma 2.8.4. For the second claim it is enough to factor out the elements containing $N-n$ from the determinant associated to the three-term recurrence relation (2.30). □

From Lemmas 2.8.5 and 2.8.6, we immediately have the following Corollary.

Corollary 2.8.7. *For $N,n\in\mathbb{Z}_{\geq 0}$ with $n\leq N$, we have*

$$P_n^{(N,\varepsilon)}((2g)^2,\Delta^2)=(n!)^2(2g)^kK_n^-(N+\varepsilon;g,\Delta,\varepsilon)+q_2(g^2,\Delta^2,n,N),$$

where $q_2(g^2,\Delta^2,n,N)\in\mathbb{Z}[g^2,\Delta^2,N,n,\varepsilon]$ such that $q_2(g^2,\Delta^2,n,n)=q_2(g^2,\Delta^2,N,N)=0$.

Furthermore, we have

$$P_n^{(N,\varepsilon)}((2g)^2,\Delta^2)=(n!)^2(2g)^kK_n^-(n+\varepsilon;g,\Delta,\varepsilon)+\bar{q}_2(g^2,\Delta^2,n,N),$$

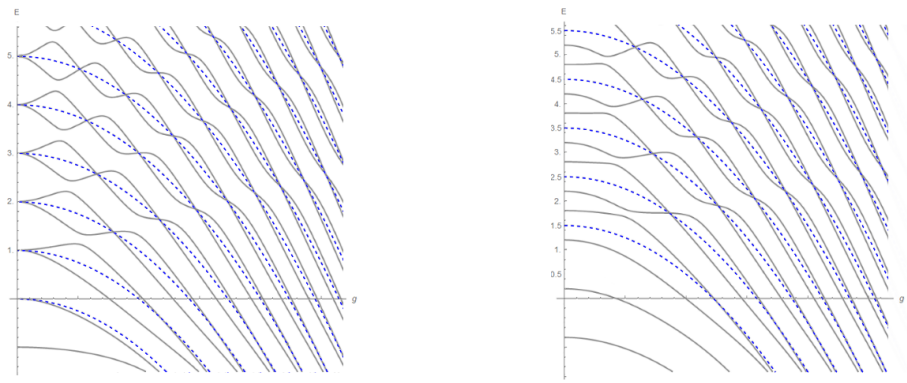
with $\bar{q}_2(g^2,\Delta^2,n,N)$ satisfying the same properties as $q_2(g^2,\Delta^2,n,N)$

2.9 Degeneracy of Juddian eigenvalues of the AQRM

In this section we return to the discussion of degeneracy of exceptional solutions in the AQRM, starting with a numerical experiment to illustrate the situation.

In Figure 2.2, we show the spectral graphs for fixed $\Delta = 1$ and $\varepsilon = 0, \frac{3}{2}$. In the graphs, the blue dashed lines represent the exceptional energy curves $y = i + \ell/2 - g^2$ for $i \in \mathbb{Z}_{\geq 0}$, any crossings of these curves with the spectral curves correspond to exceptional eigenvalues.

The crossings of the eigenvalue curves in the exceptional points correspond to degenerate solutions, we will see later that, in fact, these degenerate solutions are of Juddian type. Notice also the non-degenerate exceptional points in the curves, in turn we will see that these points correspond to non-Juddian exceptional eigenvalues.



(a) $\varepsilon = 0$ (b) $\varepsilon = 1.5$

Figure 2.2: Spectral curves for the case of $\Delta = 1$ for the cases $\varepsilon \in \{0, 1.5\}$ for $0 \leq g \leq 2.7$ and energy (E) $-1.5 \leq E \leq 5.5$.

The degeneracy of Juddian eigenvalues in the AQRM was first observed numerically by Li and Batchelor in [33] for the case $\varepsilon = \frac{1}{2}$. In general, the presence of degenerate Juddian solutions in terms of constraint polynomials was formulated by Masato Wakayama in [63].

Conjecture 2.9.1 ([63]). *For $\ell, N \in \mathbb{Z}_{\geq 0}$, there exists a polynomial $A_N^\ell(x,y) \in \mathbb{Z}[x,y]$ such that*

$$\boxed{P_{N+\ell}^{(N+\ell,-\ell/2)}(x,y) = A_N^\ell(x,y) P_N^{(N,\ell/2)}(x,y).} \tag{2.31}$$

Moreover, the polynomial $A_N^\ell(x,y)$ is positive for any $x, y > 0$. □

If Conjecture 2.9.1 holds and the parameters $g, \Delta > 0$ satisfy $P_N^{(N,\ell/2)}((2g)^2, \Delta^2) = 0$, the exceptional eigenvalue $\lambda = N + \ell/2 - g^2 (= (N+\ell) - \ell/2 - g^2)$ of $H_{\text{Rabi}}^{\ell/2}$ is degenerate.

In order to complete the argument, it is necessary to prove that the associated solutions are linearly independent. For the case $0 \neq \varepsilon \in \frac{1}{2}\mathbb{Z}$ this is trivial, since the associated solution (2.22) are polynomials of different degree N and $N + \ell$.

The case $\varepsilon = 0$ was originally proved in [31] by Kuś by direct verification. For an elegant argument using the representation theoretical picture of the solutions, see Proposition 6.6 of [63].

The condition $A_N^\ell(x,y) > 0$ of Conjecture 2.9.1 ensures that for $N \in \mathbb{Z}_{\geq 0}$ there are no non-degenerate exceptional eigenvalues $\lambda = N + \ell/2 - g^2$ corresponding to Juddian solutions (see Corollary 4.1.3 below).

Using the results in Section 2.8, we can interpret the divisibility of constraint polynomials in terms of the coefficients of the G-function.

Corollary 2.9.2 (Assuming Conjecture 2.9.1)**.** *For $N, \ell \in \mathbb{Z}_{\geq 0}$, we have*

$$K_{N+\ell}^+(N+\ell/2; g, \Delta, \ell/2) = \left(\frac{N!}{(N+\ell)!}\right)^2 (2g)^{-\ell} A_N^\ell((2g)^2, \Delta^2) K_N^-(N+\varepsilon; g, \Delta, \varepsilon),$$

In the same paper, Masato Wakayama also proposed the following more general conjecture.

Conjecture 2.9.3. *For $\ell \in \mathbb{Z}_{\geq 0}$, there exist polynomials $A_k^{(N,\ell/2)}(x,y) \in \mathbb{Z}[x,y]$ and $B_k^{(N,\ell/2)}(x,y) \in \mathbb{Z}[x,y]$ $(k = 0, 1, \ldots, N)$ such that*

$$\boxed{P_{k+\ell}^{(N+\ell,-\ell/2)}(x,y) = A_k^{(N,\ell/2)}(x,y) P_k^{(N,\ell/2)}(x,y) + B_k^{(N,\ell/2)}(x,y),} \tag{2.32}$$

with $B_N^{(N,\ell/2)}(x,y) = B_0^{(N,\ell/2)}(x,y) = 0$. Moreover, the polynomials $A_k^{(N,\ell/2)}(x,y)$ are positive for any $x, y > 0$.

Clearly, Conjecture 2.9.3 implies Conjecture 2.9.1. The proof of Conjecture 2.9.1 was given by Kazufumi Kimoto, Masato Wakayama and the author in [27]. In Chapter 3 we give a proof of Conjecture 2.9.1 by proving Conjecture 2.9.3 using a related method.

In addition, by applying the identities of Section 2.8 to Conjecture 3.2.3, we get the divisibility conditions for the coefficients of the G-function.

Corollary 2.9.4 (Assuming Conjecture 2.9.3)**.** *For $N, \ell, n \in \mathbb{Z}_{\geq 0}$, we have*

$$K_{n+\ell}^+(N+\ell/2; g, \Delta, \ell/2) = \left(\frac{n!}{(n+\ell)!}\right)^2 (2g)^{-\ell} A_n^{(N,\ell/2)}((2g)^2, \Delta^2) K_n^-(N+\varepsilon; g, \Delta, \varepsilon) + q(g^2, \Delta^2, n, N),$$

with $q(g^2, \Delta^2, n, N) \in \mathbb{Z}[g^2, \Delta^2, N, n, \varepsilon]$ such that $q(g^2, \Delta^2, n, n) = q(g^2, \Delta^2, N, N) = 0$.

Note that by Lemma 2.8.5 we can replace $K_{n+\ell}^+(N+\ell/2; g, \Delta, \ell/2)$ (resp. $K_n^-(N+\varepsilon; g, \Delta, \varepsilon)$) in the left-hand side (resp. right-hand side) with $K_{n+\ell}^+(n+\ell/2; g, \Delta, \ell/2)$ (resp. $K_n^-(n+\varepsilon; g, \Delta, \varepsilon)$) and obtain a similar identity.

3. Constraint polynomials

In this chapter, we study the properties of the constraint polynomials and their defining families from a strictly mathematical point of view. The main objective of this section is to prove Conjecture 2.9.3. This is done in two parts. First, in Section 3.2 we show the existence of the polynomial $A_k^{(\ell)}(x,y)$ by showing that $P_k^{(N,\ell/2)}(x,y)$ divides $P_{k+\ell}^{(N+\ell,-\ell/2)}(x,y)$ modulo $N-k$ (under an appropiate interpretation) as polynomials in $\mathbb{Z}[x,y]$. This method gives an explicit determinant expression for the polynomial $A_k^{(N,\ell/2)}(x,y)$. The proof is completed in Section 3.3 by studying the eigenvalues of the matrices involved in the determinant expressions for $A_k^{(N,\ell/2)}(x,y)$.

In Section 3.5, we give an estimate on the number of positive roots of constraint polynomials when one of the variables is in a given interval, this is done by using certain interlacing properties of the roots of the constraint polynomials studied in Section 3.4. Finally, in Section 3.6 we give an explicit formula for constraint polynomials that can be used for the combinatorial study of its coefficients (see for example [48]). The results of this chapter generalize the results first given in [27] to prove Conjecture 2.9.1.

In this section, bold font is reserved for matrices and vectors, subscript denotes the dimensions of the square matrices and the superscript denotes dependence on parameters. Moreover, N always denotes a nonnegative integer and $\varepsilon \in \mathbb{R}_{\geq 0}$.

3.1 Determinant expressions for constraint and related polynomials

In this section we give determinant expressions for constraint polynomials and their defining families. It is well-known that orthogonal polynomials can be expressed as determinants of tridiagonal matrices. Those determinant expressions are derived from the fact that orthogonal polynomials satisfy three-term recurrence relations. It is not difficult to verify that the polynomials $\{P_k^{(N,\varepsilon)}(x,y)\}_{k\geq 0}$ do not constitute families of orthogonal polynomials with respect to either of their variables (see Section 5.1 for a related construction of orthogonal polynomials). Nevertheless, since they are defined by three-term recurrence relations we can derive determinant expressions using the same methods. We direct the reader to [10] or [26] for an introduction for the case of orthogonal polynomials.

Recall from Section 2.8 the definition of the constraint polynomials.

Definition 3.1.1. *Let $N \in \mathbb{Z}_{\geq 0}$. The polynomials $P_k^{(N,\varepsilon)}(x,y)$ of degree k are defined*

recursively by

$$
\begin{aligned}
&P_0^{(N,\varepsilon)}(x,y) = 1,\\
&P_1^{(N,\varepsilon)}(x,y) = x + y - 1 - 2\varepsilon,\\
&P_k^{(N,\varepsilon)}(x,y) = (kx + y - k(k+2\varepsilon))P_{k-1}^{(N,\varepsilon)}(x,y) - k(k-1)(N-k+1)xP_{k-2}^{(N,\varepsilon)}(x,y).
\end{aligned}
$$

Example 3.1.2. For $k = 2, 3$, the first few polynomials are

$$
\begin{aligned}
P_2^{(N,\varepsilon)}(x,y) &= 2x^2 + 3xy + y^2 - 2(N + 2(1+2\varepsilon))x - (5+6\varepsilon)y + 2(1+2\varepsilon)(2+2\varepsilon),\\
P_3^{(N,\varepsilon)}(x,y) &= 6x^3 + 11x^2y + 6xy^2 + y^3 - 6(2N + 3(1+2\varepsilon))x^2\\
&\quad - 2(4N + 17 + 22\varepsilon)xy - 2(7+6\varepsilon)y^2 + 6(2N + 3(1+2\varepsilon))(2+2\varepsilon)x\\
&\quad + (49 + 4\varepsilon(24 + 11\varepsilon))y - 6(1+2\varepsilon)(2+2\varepsilon)(3+2\varepsilon).
\end{aligned}
$$

For brevity, we set $c_k^{(\varepsilon)} = k(k+2\varepsilon)$ and $\lambda_k = k(k-1)(N-k+1)$. It is easy to see that the polynomial $P_k^{(N,\varepsilon)}(x,y)$ is the determinant of a $k \times k$ tridiagonal matrix

$$
P_k^{(N,\varepsilon)}(x,y) = \det(\mathbf{I}_k y + \mathbf{A}_k^{(N)} x + \mathbf{U}_k^{(\varepsilon)}) \tag{3.1}
$$

where $\mathbf{I}_k$ is the identity matrix of size k and

$$
\mathbf{A}_k^{(N)} = \operatorname{tridiag}\begin{bmatrix} i & 0 \\ \lambda_{i+1} & \end{bmatrix}_{1\le i\le k}, \quad \mathbf{U}_k^{(\varepsilon)} = \operatorname{tridiag}\begin{bmatrix} -c_i^{(\varepsilon)} & 1 \\ 0 & \end{bmatrix}_{1\le i\le k}.
$$

We need the following lemma.

Lemma 3.1.3. *For $1 \le k \le N$, the eigenvalues of $\mathbf{A}_k^{(N)}$ are $\{1, 2, \dots, k\}$ and the eigenvectors are given by the columns of the lower triangular matrix $\mathbf{E}_k^{(N)}$ given by*

$$
(\mathbf{E}_k^{(N)})_{i,j} = (-1)^{i-j}\binom{i}{j}\frac{(i-1)!(N-j)!}{(j-1)!(N-i)!},
$$

for $1 \le i, j \le k$.

Proof. We have to check that $(\mathbf{A}_k^{(N)}\mathbf{E}_k^{(N)})_{i,j} = j(\mathbf{E}_k^{(N)})_{i,j}$ for every i, j. By definition, we see that

$$
\begin{aligned}
(\mathbf{A}_k^{(N)}\mathbf{E}_k^{(N)})_{i,j} = j(\mathbf{E}_k^{(N)})_{i,j} &\iff (j-i)(\mathbf{E}_k^{(N)})_{i,j} = \lambda_i(\mathbf{E}_k^{(N)})_{i-1,j}\\
&\iff (j-i)\binom{i}{j} = -i\binom{i-1}{j},
\end{aligned}
$$

and the last equality is easily verified. □

In general, the polynomials $P_k^{(N,\varepsilon)}(x,y)$ can be expressed as the determinant of a tridiagonal matrix plus a rank-1 matrix.

Proposition 3.1.4. *Let $k \in \mathbb{Z}_{\ge 0}$, then*

$$
P_k^{(N,\varepsilon)} = \det\left(\mathbf{I}_k y + \mathbf{D}_k x + \mathbf{C}_k^{(N,\epsilon)} + \mathbf{e}_k{}^T\mathbf{u}\right),
$$

where $\mathbf{I}_k$ *is the identity matrix,* $\mathbf{D}_k = \operatorname{diag}(1, 2, \ldots, k)$ *and* $\mathbf{C}_k^{(N,\epsilon)}$ *is the tridiagonal matrix given by*

$$\mathbf{C}_k^{(N,\epsilon)} = \operatorname{tridiag}\begin{bmatrix} -i(2(N-i)+1+2\varepsilon) & 1 \\ i(i+1)c_{N-i}^{(\varepsilon)} & \end{bmatrix}_{1\le i\le k},$$

$\mathbf{e}_k \in \mathbb{R}^k$ *is the* k*-th standard basis vector and* $\mathbf{u} \in \mathbb{R}^k$ *is given entrywise by*

$$\mathbf{u}_j = (-1)^{k-j+2}\binom{k+1}{j}\frac{k!(N-j)!}{(j-1)!(N-k-1)!}$$

Proof. By Lemma 3.1.3, the eigenvalues of $\mathbf{A}_k^{(N)}$ are $\{1, 2, \ldots, k\}$ and the eigenvectors are given by the columns of the lower triangular matrix $\mathbf{E}_k^{(N)}$ given by

$$(\mathbf{E}_k^{(N)})_{i,j} = (-1)^{i-j}\binom{i}{j}\frac{(i-1)!(N-j)!}{(j-1)!(N-i)!}.$$

Then, it suffices to verify that

$$\mathbf{U}_k^{(\varepsilon)}\mathbf{E}_k^{(N)} = \mathbf{E}_k^{(N)}\mathbf{C}_k^{(N,\varepsilon)} + \mathbf{E}_k^{(N)}{\mathbf{e}_k}^T\mathbf{u}. \tag{3.2}$$

Note that the k-th column of $\mathbf{E}_k^{(N)}$ is $\mathbf{e}_k$, therefore the last summand reduces to ${\mathbf{e}_k}^T\mathbf{u}$. Let

$$d_{ij} = (-1)^{i-j}\binom{i}{j}\frac{(i-1)!(N-j)!}{(j-1)!(N-i)!}.$$

For $i, j \le k$, the equation

$$-c_i^{(\varepsilon)}d_{ij} + d_{i+1,j} + j(2(N-j)+1+2\varepsilon)d_{ij} - d_{i,j-1} - j(j+1)c_{N-j}^{(\varepsilon)}d_{i,j+1}, \tag{3.3}$$

by using the elementary relations

$$j(j+1)c_{N-j}^{(\varepsilon)}d_{i,j+1} = -(i-j)(N-j+2\varepsilon)d_{ij},$$

$$d_{i+1,j} - d_{i,j-1} = (i^2 + j^2 + ij - j - iN - jN)d_{ij},$$

is seen to be equal to zero. For $i, j \le k$, $d_{ij} = (\mathbf{E}_\mathbf{k}^{(\mathbf{N},\varepsilon)})_{i,j}$ and therefore (3.3) directly gives (3.2) for $1 \le j \le k$ and $1 \le i \le k-1$. For $i = k$, formula (3.3) reads

$$(\mathbf{U}_k^{(\varepsilon)}\mathbf{E}_k^{(N)} - \mathbf{E}_k^{(N)}\mathbf{C}_k^{(N,\varepsilon)})_{k,j} = -d_{k+1,j},$$

and the right-hand side is equal to the i-th entry of $\mathbf{u}$, as desired. □

Note that when $k = N$, by the definition of the entries, the vector $\mathbf{u}$ is equal to the zero vector, and the proposition above reduces to Proposition 4.2 of [27].

Corollary 3.1.5. *Let* $k \in \mathbb{Z}_{\ge 0}$*, then*

$$P_k^{(N,\varepsilon)}(x, y) = \det\left(\mathbf{I}_k y + \mathbf{D}_k x + \mathbf{C}_k^{(N,\epsilon)}\right) + Q_k^{(N,\varepsilon)}(x, y),$$

for a polynomial $Q_k^{(N,\varepsilon)} \in \mathbb{R}[x, y]$ *with* $Q_N^{(N,\varepsilon)}(x, y) = 0$.

Proof. It well-known that if $\mathbf{A}$ is a square matrix, then

$$\det(\mathbf{A} + \mathbf{v}^T\mathbf{u}) = \det(\mathbf{A}) + {}^T\mathbf{v}\,\mathrm{adj}(\mathbf{A})\mathbf{u},$$

where $\mathrm{adj}(A)$ is the adjugate matrix, the transpose of the matrix of cofactors of A. Applying this result along with Proposition 3.1.4, we get the determinant expression. Furthermore, we see that

$$Q_k^{(N,\varepsilon)}(x,y) = {}^T\mathbf{e}_k\,\mathrm{adj}\left(\mathbf{I}_k y + \mathbf{D}_k x + \mathbf{C}_k^{(N,\epsilon)}\right)\mathbf{u},$$

is a polynomial, since $\det\left(\mathbf{I}_k y + \mathbf{D}_k x + \mathbf{C}_k^{(N,\epsilon)}\right)$ is clearly a polynomial. As mentioned above, $\mathbf{u} = 0$ when $N = k$, and thus the second claim follows. □

We prove the divisibility part of Conjecture 2.9.3 in Section 3.2. In the remaining of this section we show some special properties of the constraint polynomials (the case $k = N$).

Corollary 3.1.6. *Let $N \in \mathbb{Z}_{\geq 0}$. We have*

$$P_N^{(N,\varepsilon)}(x,y) = \det\left(\mathbf{I}_N y + \mathbf{D}_N x + \mathbf{S}_N^{(N,\varepsilon)}\right),$$

where $\mathbf{D}_N$ is the diagonal matrix of Proposition 3.1.4 and $\mathbf{S}_N^{(N,\varepsilon)}$ is the symmetric matrix given by

$$\mathbf{S}_N^{(N,\varepsilon)} = \mathrm{tridiag}\begin{bmatrix} -i(2(N-i)+1+2\varepsilon) & \sqrt{i(i+1)c_{N-i}^{(\varepsilon)}} \\ \sqrt{i(i+1)c_{N-i}^{(\varepsilon)}} & \end{bmatrix}_{1\leq i\leq N}.$$

Proof. Consider the case $k = N$ in Proposition 3.1.4. Notice that the matrices $\mathbf{I}_N y + \mathbf{D}_N x + \mathbf{C}_N^{(N,\varepsilon)}$ and $\mathbf{I}_N y + \mathbf{D}_N x + \mathbf{S}_N^{(N,\varepsilon)}$ are tridiagonal. Then, it is clear by the continuant equivalence (2.28) that the determinants of the matrices are equal, establishing the result. □

As a corollary to the discussion on the determinant expression (3.1) we have the following result used in Section 3.3 to prove the positivity of the polynomial $A_N^{\ell}(x,y)$.

Corollary 3.1.7. *For $x \geq 0$, $\varepsilon \in \mathbb{R}$ and $N, k \in \mathbb{Z}_{\geq 0}$, all the roots of $P_k^{(N,\varepsilon)}(x,y)$ with respect to y are real.*

Proof. When $x \geq 0$, using the continuant equivalence (2.28) on the determinant expression (3.1) of $P_k^{(N,\varepsilon)}(x,y)$ we can find an equivalent expression $\det(\mathbf{I}_k y - \mathbf{V}_k(x))$ for a real symmetric matrix $\mathbf{V}_k(x)$. Since the roots of $P_k^{(N,\varepsilon)}(x,y)$ with respect to y are the eigenvalues of the real symmetric matrix $\mathbf{V}_k(x)$, the result follows immediately. □

In the case of the constraint polynomials $P_N^{(N,\varepsilon)}(x,y)$, the determinant expression of Corollary 3.1.6 gives the following result of similar type, used for the estimation of positive roots of constraint polynomials in Section 3.5.

Theorem 3.1.8. *Let $N \in \mathbb{Z}_{\geq 0}$ and $\varepsilon > -1/2$. Then, for fixed $x \in \mathbb{R}$ (resp. $y \in \mathbb{R}$), all the roots of $P_N^{(N,\varepsilon)}(x,y)$ with respect to y (resp. x) are real.*

Proof. Upon setting $x = \alpha \in \mathbb{R}$, the zeros of $P_N^{(N,\varepsilon)}(\alpha, y)$ are the eigenvalues of the matrix $-(\mathbf{D}_N\alpha + \mathbf{S}_N^{(N,\varepsilon)})$. For $\varepsilon > -1/2$, the matrix is real symmetric, so the eigenvalues, therefore the zeros, are real. The case of $y = \beta \in \mathbb{R}$ is completely analogous since $P_N^{(N,\varepsilon)}(x,\beta) = \det \mathbf{D}_N \det(\mathbf{I}_N x + \mathbf{D}_N^{-1}\beta + \mathbf{D}_N^{-1/2}\mathbf{S}_N^{(N,\varepsilon)}\mathbf{D}_N^{-1/2})$. □

The next example shows that we should not expect a determinant expression of the type of Corollary 3.1.6 for general $P_k^{(N,\varepsilon)}(x,y)$ with $k \neq N$.

Example 3.1.9. For a fixed y, the roots of the polynomial

$$P_2^{(6,0)}(x,y) = 2x^2 + y^2 - 16x + 3xy - 5y + 4,$$

are given by

$$\frac{1}{4}\left(16 - 3y \pm \sqrt{y^2 - 56y + 224}\right).$$

Clearly, this polynomial may have non-real roots for general $y \in \mathbb{R}$.

3.2 Divisibility of constraint and related polynomials

When the parameter ϵ is half-integer, i.e. $\varepsilon = \ell/2 \in \frac{1}{2}\mathbb{Z}$, we have special divisibility properties for the polynomials $P_k^{(N,\varepsilon)}(x,y)$. In this section, using these properties we prove the divisibility part of Conjecture 2.9.3.

Proposition 3.2.1. *Let $\ell, k \in \mathbb{Z}_{\geq 0}$, then*

$$P_{k+\ell}^{(N+\ell,-\frac{\ell+N-k}{2})}(x,y) = \bar{A}_k^{(N,\ell)}(x,y) P_k^{(N,\frac{\ell+N-k}{2})}(x,y) + \bar{B}_k^{(N,\ell)}(x,y)$$

with $\bar{B}_N^{(N,\ell)}(x,y) = 0$. Moreover, the polynomial $\bar{A}_k^{(N,\ell)}(x,y)$ is given by

$$\bar{A}_k^{(N,\ell)}(x,y) = \frac{(k+\ell)!}{k!} \det \operatorname{tridiag} \begin{bmatrix} x + \frac{y}{k+i} + 2i - 1 + k - N - \ell & 1 \\ & c_{-i}^{(\frac{N+\ell-k}{2})} \end{bmatrix}_{1 \leq i \leq \ell}.$$

By taking N to be a variable, this result, along with Theorem 3.2.3 below, can be interpreted as divisibility modulo $N - k$, that is,

$$P_{k+\ell}^{(N+\ell,-\frac{\ell+N-k}{2})}(x,y) \equiv \bar{A}_k^{(N,\ell)}(x,y) P_k^{(N,\frac{\ell+N-k}{2})}(x,y) \pmod{N-k}.$$

To simplify the proofs we make this assumption in the remaining of this section.

Proof. We begin with the determinant expression of Corollary 3.1.5 for $P_{k+\ell}^{(N+\ell,-\frac{\ell+N-k}{2})}(x,y)$, that is

$$P_{k+\ell}^{(N+\ell,-\frac{\ell+N-k}{2})}(x,y) = \det\left(\mathbf{I}_{k+\ell}y + \mathbf{D}_{k+\ell}x + \mathbf{C}_{k+\ell}^{(N+\ell,-\frac{\ell+N-k}{2})}\right) + q_{k+\ell}(x,y),$$

where $q_{k+\ell}(x,y)$ is a polynomial divisible by $N-k$. The tridiagonal matrix $\mathbf{C}_{k+\ell}^{(N+\ell,-\frac{\ell+N-k}{2})}$ is given by

$$\mathbf{C}_{k+\ell}^{(N+\ell,-\frac{\ell+N-k}{2})} = \operatorname{tridiag}\begin{bmatrix} -i(-2i+1+\ell+N+k) & 1 \\ i(i+1)(N+\ell-i)(k-i) & \end{bmatrix}_{1\le i\le k+\ell}.$$

Note that when $i=k$, the off-diagonal element $i(i+1)(N+\ell-i)(k-i)$ vanishes and $\det\left(\mathbf{I}_{k+\ell}y+\mathbf{D}_{k+\ell}x+\mathbf{C}_{k+\ell}^{(N+\ell,-\frac{\ell+N-k}{2})}\right)$ can be computed as the product of the determinant of a $k\times k$ matrix and the determinant of a $\ell\times\ell$ matrix.

Let us first consider the determinant of the $\ell\times\ell$-matrix factor. It is given by

$$\det\operatorname{tridiag}\begin{bmatrix} y+(k+i)x-(k+i)(-2(k+i)+1+\ell+N+k) & 1 \\ (k+i)(k+i+1)(N+\ell-k-i)(-i) & \end{bmatrix}_{1\le i\le \ell}$$

which is easily seen to be equal to

$$\bar{A}_k^{(N,\ell)}(x,y) = \frac{(k+\ell)!}{k!}\det\operatorname{tridiag}\begin{bmatrix} x+\frac{y}{k+i}+2i-1+k-N-\ell) & 1 \\ c_{-i}^{(\frac{N+\ell-k}{2})} & \end{bmatrix}_{1\le i\le \ell}.$$

Let us denote by $q(x,y;N,\ell,k)$ the remaining factor, that is,

$$q(x,y;N,\ell,k) = \det\operatorname{tridiag}\begin{bmatrix} ix+y-i(-2i+1+\ell+N+k) & 1 \\ i(i+1)(N+\ell-i)(k-i) & \end{bmatrix}_{1\le i\le k}.$$

By Corollary 3.1.5, we have

$$P_k^{(N,\frac{\ell+N-k}{2})}(x,y)-Q_k^{(N,\frac{\ell+N-k}{2})} = \det\operatorname{tridiag}\begin{bmatrix} ix+y-i(3N-2i+1+\ell-k) & 1 \\ i(i+1)(N-i)(2N-i+\ell-k) & \end{bmatrix}_{1\le i\le k},$$

the right-hand side can be written as

$$\det\operatorname{tridiag}\begin{bmatrix} ix+y-i(-2i+1+\ell+N+k+2(N-k)) & 1 \\ i(i+1)(k-i+(N-k))(N+\ell-i+(N-k)) & \end{bmatrix}_{1\le i\le k},$$

and noticing that entrywise, the entries of the matrix of the determinant differ to those in the determinant expression of $q(x,y;N,\ell,k)$ only by factors of $N-k$, we obtain

$$q(x,y;N,\ell,k) = P_k^{(N,\frac{\ell+N-k}{2})}(x,y)+q'(x,y;N,\ell,k)$$

for a polynomial $q'(x,y;N,\ell,k)$ satisfying $q'(x,y;N,\ell,N)=0$. This completes the proof. □

The following lemma is used to obtain the main result.

Lemma 3.2.2. *Let $k\in\mathbb{Z}_{\ge 0}$ and $\delta\in\mathbb{R}$. Then, we have*

$$P_k^{(N,\varepsilon+\delta)}(x,y) = P_k^{(N,\varepsilon)}(x,y)+2\delta q_k^{(N,\varepsilon)}(x,y),$$

for some polynomial $q^{(N,\varepsilon)}(x,y)\in\mathbb{R}[x,y]$.

Proof. It is clear that $q_0^{(N,\varepsilon)}(x,y) = 0$ and $q_1^{(N,\varepsilon)}(x,y) = 1$. Then, assume that it holds for all $i \le k$ for some $k \in \mathbb{Z}_{\ge 0}$. We have,

$$\begin{aligned} P_k^{(N,\varepsilon+a)}(x,y) &= (kx + y - c_k^{(\varepsilon+a)})P_{k-1}^{(N,\varepsilon+a)}(x,y) - \lambda_k x P_{k-2}^{((N,\varepsilon+a))}(x,y) \\ &= P_k^{(N,\varepsilon)}(x,y) - 2kaP_{k-1}^{(N,\varepsilon)}(x,y) + 2a(kx + y - c_k^{(\varepsilon+a)})q_{k-1}^{(N,\varepsilon)} \\ &\quad - 2a\lambda_k x\, q_{k-2}^{(N,\varepsilon)}(x,y) \\ &= P_k^{(N,\varepsilon)}(x,y) + 2aq_k^{(N,\varepsilon)}(x,y) \end{aligned}$$

and the result follows by induction. □

Finally, we can prove the "divisibility" part of Conjecture 2.9.3.

Theorem 3.2.3. *Let $\ell, k \in \mathbb{Z}_{\ge 0}$, then*

$$P_{k+\ell}^{(N+\ell,-\frac{\ell}{2})}(x,y) = A_k^{(\ell)}(x,y)P_k^{(N,\frac{\ell}{2})}(x,y) + B_k^{(N,\ell)}(x,y)$$

with $B_N^{(N,\ell)}(x,y) = 0$. Moreover, the polynomial $A_k^{(\ell)}(x,y)$ is given by

$$A_k^{(\ell)}(x,y) = \frac{(k+\ell)!}{k!} \det \operatorname{tridiag} \begin{bmatrix} x + \frac{y}{k+i} + 2i - 1 - \ell & 1 \\ c_{-i}^{(\frac{\ell}{2})} & \end{bmatrix}_{1 \le i \le \ell}$$

Note that the polynomial $A_k^{(\ell)}(x,y)$ does not depend on the parameter N. In the sequel we use this notation for the polynomial $A_k^{(N,\ell/2)}(x,y)$ appearing in Conjecture 2.9.3.

Proof. First, by using Lemma 3.2.2 above on the polynomials at both sides of Proposition 3.2.1, it is easy to see that

$$P_{k+\ell}^{(N+\ell,-\frac{\ell}{2})}(x,y) = \bar{A}_k^{(N,\ell)}(x,y)P_k^{(N,\frac{\ell}{2})}(x,y) + \bar{C}_k^{(N,\ell)}(x,y)$$

for some polynomial $\bar{C}_k^{(N,\ell)}(x,y)$ satisfying $\bar{C}_N^{(N,\ell)}(x,y) = 0$. Note that the matrices in the determinant expressions of $\bar{A}_k^{(\ell)}(x,y)$ and $A_k^{(N,\ell)}(x,y)$ differ entrywise at most by factor of $N - k$, therefore

$$A_k^{(\ell)}(x,y) = \bar{A}_k^{(N,\ell)}(x,y) + (N-k)q^{(N,\ell)}(x,y)$$

for some polynomial $q^{(N,\ell)}(x,y) \in \mathbb{Z}[x,y]$ completing the proof. □

To complete the proof of Conjecture 2.9.3, it remains to prove that $A_k^{(\ell)}(x,y) > 0$ for $x, y > 0$. This is done in Section 3.3 below.

Example 3.2.4. ([48]) For small values of ℓ, the explicit form of $A_N^{\ell}(x,y)$ is given by

$$\begin{aligned}
A_k^1(x,y) &= (k+1)x + y,\\
A_k^2(x,y) &= (k+1)_2x^2 + \left(\sum_{i=1}^{2}(k+i)\right)xy + y(1+y),\\
A_k^3(x,y) &= (k+1)_3x^3 + \left(\sum_{i<j}^{3}(k+i)(k+j)\right)x^2y + (k+2)x(3y+4)y + y(2+y)^2,\\
A_k^4(x,y) &= (k+1)_4x^4 + \left(\sum_{i<j<k}^{4}(k+i)(k+j)(k+j)\right)x^3y\\
&\quad + \left(\sum_{i<j}^{4}(k+i)(k+j)\right)x^2y^2 + 2\left(\sum_{i<j}^{4}(k+i)(k+j) - (k+2)(k+3)\right)x^2y\\
&\quad + \left(\sum_{i=1}^{4}(k+i)\right)xy(y+2)(y+3) + y(3+y)^2(4+y).
\end{aligned}$$

3.3 Proof of the positivity of $A_N^{(\ell)}(x,y)$

In this subsection we complete the proof of Conjecture 2.9.1 by proving the positivity of the polynomial $A_k^{(\ell)}(x,y)$ for $x,y>0$. Let $k\in\mathbb{Z}_{\geq 0}$ and $\ell\in\mathbb{Z}_{>0}$ be fixed. From Theorem 3.2.3 and the continuant equivalence (2.28), we see that the polynomial $A_k^{(\ell)}(x,y)$ has the determinant expression

$$\frac{(k+\ell)!}{k!}\det(\mathbf{D}_\ell^{(k)}y + \mathbf{B}_\ell(x))$$

where $\mathbf{B}_\ell(x)$ is an matrix-valued function given by

$$\mathbf{B}_\ell(x) = \operatorname{tridiag}\begin{bmatrix} x-\ell+2i-1 & 1\\ c_{-i}^{(\ell/2)} & \end{bmatrix}_{1\leq i\leq \ell}. \tag{3.4}$$

Next, multiplying the $\frac{(k+\ell)!}{k!}$ factor into the determinant in such a way that the i-th row is multiplied by $k+i$, we obtain the expression

$$A_k^{(\ell)}(x,y) = \det(\mathbf{I}_\ell y + \mathbf{M}_\ell^{(k)}(x)) = \prod_{\lambda\in\operatorname{Spec}(\mathbf{M}_\ell^{(k)}(x))}(y+\lambda) \tag{3.5}$$

with

$$\mathbf{M}_\ell^{(k)}(x) = \operatorname{tridiag}\begin{bmatrix} (k+i)(x-\ell+2i-1) & k+i\\ (k+i+1)c_{-i}^{(\ell/2)} & \end{bmatrix}_{1\leq i\leq \ell}.$$

Thus, it suffices to show that all the eigenvalues of $\mathbf{M}_\ell^{(k)}(x)$ are positive for $x>0$ to prove that $A_k^{(\ell)}(x,y)>0$ when $x,y>0$.

First, we compute the determinant of the matrix $\mathbf{M}_\ell^{(k)}(x)$, or equivalently, the value of $A_k^{(\ell)}(x,0)$.

Lemma 3.3.1. *We have*

$$\det(\mathbf{M}_\ell^{(k)}(x)) = A_k^{(\ell)}(x,0) = \frac{(k+\ell)!}{k!}x^\ell.$$

Proof. Consider the recurrence relation

$$J_i(x) = (x+\ell+1-2i)J_{i-1}(x) + (i-1)(\ell+1-i)J_{i-2}(x),$$

with initial conditions $J_0(x) = 1$ and $J_{-1}(x) = 0$. Notice that this recurrence relation corresponds to the continuant $\det \mathbf{B}_\ell(x)$ (compare with (3.4) above) and therefore, $\frac{(k+\ell)!}{k!}J_\ell(x) = \frac{(k+\ell)!}{k!}\det \mathbf{B}_\ell(x) = \det(\mathbf{M}_\ell^{(k)}(x))$. We claim that $J_i(x) = \sum_{j=0}^i (\ell - i)_j \binom{i}{j} x^{i-j}$. Clearly, the claim holds for $J_0(x) = 1$ and $J_1(x) = x+\ell-1$. Assuming it holds for integers up to a fixed i, we have

$$\begin{aligned}
J_{i+1}(x) &= (x+\ell-1-2i)\sum_{j=0}^{i}(\ell-i)_j\binom{i}{j}x^{i-j} + i(\ell-i)\sum_{j=0}^{i-1}(\ell-i+1)_j\binom{i-1}{j}x^{i-1-j} \\
&= \sum_{j=0}^{i}(\ell-i)_j\binom{i}{j}x^{i+1-j} + (\ell-1-2i)\sum_{j=0}^{i}(\ell-i)_j\binom{i}{j}x^{i-j} \\
&\quad + i(\ell-i)\sum_{j=0}^{i-1}(\ell-i+1)_j\binom{i-1}{j}x^{i-1-j},
\end{aligned}$$

by grouping the terms in the sums we obtain

$$\begin{aligned}
&x^{i+1} + (\ell-i-1)x^i + (\ell-i-1)_{i+1} \\
&\qquad + \sum_{j=1}^{i-1}(\ell-i)_j\left((\ell-i+j)\binom{i}{j+1} + (\ell-1-2i)\binom{i}{k} + j\binom{i}{j}\right)x^{i-j}.
\end{aligned}$$

The sum on the expression above is

$$\begin{aligned}
&\sum_{j=1}^{i-1}(\ell-i)_j\binom{i}{j}\left(\frac{(\ell-i+j)(i-j)}{j+1} + \ell-1-2i+j\right)x^{i-j} \\
&\qquad = \sum_{j=1}^{i-1}(\ell-i)_j\binom{i}{j}\left(\frac{(i+1)(\ell-i-1)}{j+1}\right)x^{i-j} = \sum_{j=2}^{i}(\ell-i-1)_j\binom{i+1}{j}x^{i+1-j},
\end{aligned}$$

and the claim follows by joining the remaining terms into the sum. Finally, notice that $J_\ell(x) = \sum_{j=0}^i (0)_j\binom{\ell}{j}x^{\ell-j} = x^\ell$, as desired. □

From the lemma above, we immediately obtain the

Corollary 3.3.2. *For $N \in \mathbb{Z}_{\geq 0}$, the eigenvalue $\lambda = 0$ is in* $\mathrm{Spec}(\mathbf{M}_\ell^{(k)}(x))$ *if and only if $x = 0$.*

The next result collects some basic properties of the eigenvalues of the matrix $\mathbf{M}_\ell^{(k)}(x)$ that are used in the proof of the positivity of $A_k^{(\ell)}(x,y)$.

Lemma 3.3.3. *Denote the spectrum of the matrix $\mathbf{M}_\ell^{(k)}(x)$ by* $\mathrm{Spec}(\mathbf{M}_\ell^{(k)}(x))$.

1. *For $x \geq 0$, the eigenvalues $\lambda \in \mathrm{Spec}(\mathbf{M}_\ell^{(k)}(x))$ are real.*
2. *We have $\mathrm{Spec}(\mathbf{M}_\ell^{(k)}(0)) = \{i(\ell-i) : i = 1, 2, \cdots, \ell\}$. In particular, $0 \in \mathrm{Spec}(\mathbf{M}_\ell^{(k)}(0))$ is a simple eigenvalue and any eigenvalue $\lambda \in \mathrm{Spec}(\mathbf{M}_\ell^{(k)}(0))$ satisfies $\lambda \geq 0$.*
3. *If $x' > \ell - 1$, all eigenvalues $\lambda \in \mathrm{Spec}(\mathbf{M}_\ell^{(k)}(x'))$ satisfy $\lambda > 0$.*

Proof. Note that by setting $N = k$ in Corollary 3.1.7 and the divisibility of Theorem 3.2.3, wee see that if $x \geq 0$ all the roots of $A_k^{(\ell)}(x,y)$ with respect to y are real. By definition, the same holds for the elements of $\mathrm{Spec}(\mathbf{M}_\ell^{(k)}(x))$, proving the first claim. From the defining recurrence relation, we see that $P_k^{(k,\varepsilon)}(0,y) = \prod_{i=1}^k (y - i(i+2\varepsilon))$, and by divisibility we have $A_k^{(\ell)}(0,y) = \prod_{i=1}^\ell (y - i(i-\ell))$ proving the second claim. For the third claim, notice that when $x' > \ell - 1$ all the diagonal elements of $\mathbf{M}_\ell^{(k)}(x')$ are positive. Therefore, the continuant (3.5) defines a recurrence relation with positive coefficients, so that $A_k^{(\ell)}(x',y)$ is a polynomial in y with positive coefficients and real roots. Since $y = 0$ is not a root of $A_k^{(\ell)}(x',y)$ by Corollary 3.3.2, all of the roots of $A_k^{(\ell)}(x',y)$ must be negative and the third claim follows. □

With these preparations, we come to the proof of the positivity of the polynomial $A_k^{(\ell)}(x,y)$.

Theorem 3.3.4. *With the notation of Theorem 3.2.3, $A_k^{(\ell)}(x,y) > 0$ for $x, y > 0$.*

Proof. By virtue of (3.5), it is enough to show that all the eigenvalues of $\mathbf{M}_\ell^{(k)}(x)$ are positive if $x > 0$. Notice that each eigenvalue of $\mathbf{M}_\ell^{(k)}(x)$ is a real-valued continuous function in x. Assume that there is a positive x' such that $\mathbf{M}_\ell^{(k)}(x')$ has a negative eigenvalue. Then, there also exists x'' such that $x' < x'' < \ell$ and $0 \in \mathrm{Spec}(\mathbf{M}_\ell^{(k)}(x''))$ since all eigenvalues of $\mathbf{M}_\ell^{(k)}(\ell)$ are positive by Lemma 3.3.3 (3). This contradicts to Corollary 3.3.2. □

A consequence of the positivity of $A_N^{(\ell)}(x,y)$ in Theorem 4.1.1 is that all the positive roots of the constraint polynomials $P_N^{(N,\ell/2)}(x,y)$ and $P_{N+\ell}^{(N+\ell,-\ell/2)}(x,y)$ $(N, \ell \in \mathbb{Z}_{\geq 0})$ must coincide.

Note that since $A_0^{(\ell)}(x,y) = P_\ell^{(\ell,-\ell/2)}(x,y)$ and $P_0^{(0,\ell/2)}(x,y) = 1 \neq 0$, the positivity of $A_0^{(\ell)}(x,y)$ also implies the absence of Juddian eigenvalues $\lambda = \ell/2 - g^2$ for $\ell > 0$. In fact, the positivity can be extended to a larger set of constraint polynomials $P_k^{(k,-\ell/2)}(x,y)$.

Proposition 3.3.5. *Let $\ell \in \mathbb{Z}_{>0}$ and $1 \leq k \leq \ell$. Then the constraint polynomial $P_k^{(k,-\ell/2)}(x,y)$ is positive for $x, y > 0$.*

Proof. For $1 \leq k \leq \ell$, define the $k \times k$ matrix

$$\mathbf{M}_k(x) = \mathrm{tridiag}\begin{bmatrix} x + \ell - 1 - 2(k-i) & i \\ (i+1)c_{k-i}^{(-\ell/2)} & \end{bmatrix}_{1 \leq i \leq k}$$

then $P_k^{(k,-\ell/2)}(x,y) = \det(\mathbf{I}_k y + \mathbf{M}_k(x))$ and the roots of $P_k^{(k,-\ell/2)}(x,y)$ with respect to y are the eigenvalues of the matrix $-\mathbf{M}_k(x)$. Thus, as in the case of $A_N^\ell(x,y)$, it suffices to prove that all the eigenvalues of $\mathbf{M}_k(x)$ are positive for $x > 0$.

First, we see that $\det(\mathbf{M}_k(x)) = P_k^{(k,-\ell/2)}(x,0) = k!\sum_{j=0}^k (\ell-k)_j \binom{k}{j} x^{k-j}$. Indeed, we directly verify that $\det(\mathbf{M}_k(x)) = k!J_k(x)$ where $\{J_i(x)\}_{i\geq 0}$ is the recurrence relation defined in Lemma 3.3.1. In particular, $\det(\mathbf{M}_k(x))$ is a polynomial with positive coefficients and thus it never vanishes for $x > 0$.

Next, we verify that the matrix $\mathbf{M}_k(x)$ has the properties of the matrices $\mathbf{M}_\ell^{(N)}(x)$ given in Lemma 3.3.3. From Corollary 3.1.7, it is clear that for $x \geq 0$ the eigenvalues of $\mathbf{M}_k(x)$ are real. By the definition of the constraint polynomials, it is obvious that $\mathrm{Spec}(\mathbf{M}_k(0)) = \{i(\ell-i) : i = 1,2,\cdots,k\}$, hence any eigenvalue $\lambda \in \mathrm{Spec}(\mathbf{M}_k(0))$ is non-negative. Finally, as in the proof of Lemma 3.3.3, we see that for $x' > \max(0, 2k-\ell-1)$ all eigenvalues $\lambda \in \mathrm{Spec}(\mathbf{M}_k(x'))$ satisfy $\lambda > 0$.

The proof of positivity then follows exactly as in the proof of Theorem 3.3.4. □

3.4 Interlacing of roots for constraint polynomials

When considered as polynomials in $\mathbb{R}[y][x]$, there is non-trivial interlacing among the roots of the constraint polynomials $P_N^{(N,\varepsilon)}(x,y)$. This interlacing is essential for the proof of the upper bound on the number of positive roots of the constraint polynomials in the next sections.

For $N \in \mathbb{Z}_{\geq 0}$, let

$$P_N^{(N,\varepsilon)}(x,y) = \sum_{i=0}^N a_i^{(N)}(y)x^i.$$

Noticing that $\deg(a_i^{(N)}(y)) = N-i$, the interlacing property is given in the following lemma.

Lemma 3.4.1. *Let $N \in \mathbb{Z}_{\geq 0}$ and $\varepsilon > -1/2$. Then the roots of $a_j^{(N)}(y)$ $(0 \leq j \leq N-1)$ are real. Denote the roots of $a_j^{(N)}(y)$ by $\xi_1^{(j)} \leq \xi_2^{(j)} \leq \cdots \leq \xi_{N-j}^{(j)}$. Then, for $j = 0,1,\ldots,N-2$ we have*

$$\xi_i^{(j)} < \xi_i^{(j+1)} < \xi_{i+1}^{(j)}$$

for $i = 1,2,\ldots,N-j-1$.

The constraint polynomials $P_N^{(N,\varepsilon)}(x,y)$, with $\varepsilon > -\frac{1}{2}$, belong to a special class of polynomials in two variables, the class $\mathbf{P}_2$ (see [15]). The class $\mathbf{P}_2$ is a generalization of polynomials of one variable with all real roots. A polynomial $p(x,y)$ of degree n belongs to the class $\mathbf{P}_2$ if it satisfies the following conditions:

- For any $\alpha \in \mathbb{R}$, the polynomials $p(\alpha,y)$ and $p(x,\alpha)$ have all real roots.
- Monomials of degree n in $p(x,y)$ all have positive coefficients.

Equivalently, a polynomial $p(x,y)$ is in the class $\mathbf{P}_2$ if it has a determinant expression

$$p(x,y) = \det\left(\mathbf{I}_n y + \mathbf{D}_n x + \mathbf{S}_n\right),$$

with $\mathbf{D}_n$ a diagonal matrix with positive entries and $\mathbf{S}_n$ a real symmetric matrix.

Recall the following property of polynomials of the class $\mathbf{P}_2$.

Lemma 3.4.2 (Lemma 9.63 of [15]). *Let $f(x,y) \in \mathbf{P}_2$ and set*

$$f(x,y) = f_0(x) + f_1(x)y + \cdots + f_n(x)y^n.$$

If $f(x,0)$ has all distinct roots, then all f_i have distinct roots, and the roots of f_i and f_{i+1} interlace.

Note that the lemma above tacitly implies that the roots of the polynomials f_i are real. With these preparations, we prove Lemma 3.4.1.

Proof of Lemma 3.4.1. By Corollary 3.1.6, $P_N^{(N,\varepsilon)}(x,y) \in \mathbf{P}_2$. Since $P_N^{(N,\varepsilon)}(0,y) = \prod_{i=i}^{N}(y - i(i+2\varepsilon))$, for $\varepsilon > -1/2$, the roots are different and the lemma applies, establishing the result. □

3.5 Number of positive roots of constraint polynomials

In this section we give an estimation on the number of positive roots of constraint polynomials. In particular, this result proves the existence of exceptional eigenvalues corresponding to Juddian solutions in the spectrum of the AQRM. We note that although Theorem 3.5.1 was stated for open intervals by Li and Batchelor in [34], the proof provided by the authors only gives a lower bound on the number of positive roots.

Theorem 3.5.1. *Let $\varepsilon > -\frac{1}{2}$. For each $k\,(0 \le k < N)$, there are exactly $N-k$ positive roots (in the variable x) of the constraint polynomial $P_N^{(N,\varepsilon)}(x,y)$ for y in the range*

$$k(k+2\varepsilon) \le y < (k+1)(k+1+2\varepsilon).$$

Furthermore, when $y \ge N(N+2\varepsilon)$, the polynomial $P_N^{(N,\varepsilon)}(x,y)$ has no positive roots with respect to x.

We illustrate numerically the proposition for the case $N = 6$ and $\varepsilon = 0.4$ in Figure 3.1. For fixed $\Delta > 0$ satisfying $k(k+2\varepsilon) \le \Delta^2 < (k+1)(k+1+2\varepsilon)$ $(k \in \{1,2,\ldots,N\})$, the number of points (g,Δ) with $g > 0$ in the curve $P_N^{(N,\varepsilon)}((2g)^2,\Delta^2) = 0$ is exactly $N-k$. Likewise, as it is clear in the figure, there are no points (g,Δ) in the curve with $g > 0$ and $\Delta^2 \ge N(N+2\varepsilon)$.

First, we establish a lower bound on the number of positive roots for the constraint polynomials. The following Lemma extends Li and Batchelor's result ([34], Theorem), to the case of semi-closed intervals.

Lemma 3.5.2. *Let $\varepsilon > -\frac{1}{2}$. For each $k\,(0 \le k < N)$, there are at least $N-k$ positive roots (in the variable x) of the constraint polynomial $P_N^{(N,\varepsilon)}(x,y)$ for y in the range*

$$k(k+2\varepsilon) \le y < (k+1)(k+1+2\varepsilon).$$

Remark 3.5.3. The proof is a modification to the argument given in [34] (Appendix B), which is based on the proof of Kuś for the case of the (symmetric) quantum Rabi model ([31], Section IV, Thm. 3).

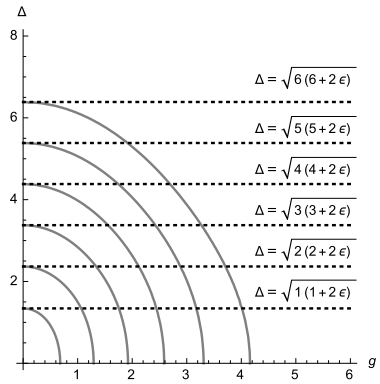


Figure 3.1: Curve $P_6^{(6,\varepsilon)}((2g)^2, \Delta^2) = 0$ with $\varepsilon = 0.4$ (for $g, \Delta > 0$)

Proof. Define the normalized polynomials $S_k^{(N,\varepsilon)}(x, y)$ by

$$S_k^{(N,\varepsilon)}(x, y) = \frac{P_k^{(N,\varepsilon)}(x, y)}{k!}.$$

Fix y and consider the polynomials $S_k^{(N,\varepsilon)}(x, y)$ as polynomials in the variable x and write $S_k^{(N,\varepsilon)}(x)$ for simplicity. Set $\alpha_i = (i(i + 2\varepsilon) - y)/i$ and $\beta_i = N - i + 1$, then the recurrence relation becomes

$$\begin{aligned} &S_0^{(N,\varepsilon)}(x) = 1, \quad S_1^{(N,\varepsilon)}(x) = x - \alpha_1 \\ &S_k^{(N,\varepsilon)}(x) = (x - \alpha_k)S_{k-1}^{(N,\varepsilon)}(x) - \beta_k x S_{k-2}^{(N,\varepsilon)}(x). \end{aligned} \tag{3.6}$$

Let $k\,(0 \le k < N)$ be fixed. If $k(k + 2\varepsilon) < y < (k + 1)(k + 1 + 2\varepsilon)$, then it is clear that $\alpha_i < 0$ for $i < k$, $\alpha_i > 0$ for $i > k$ and $\beta_i > 0$ for $0 \le i < N$. Moreover, when $y = k(k+2\varepsilon)$ we have $\alpha_k = 0$ and, from (3.6), we see that $x = 0$ is a root of all polynomials $S_{k+i}(x)$ for $i = 1, \ldots, N - k$.

For $i = 0, 1, \ldots, N - k$, set

$$\tilde{S}_{k+i}(x) = \begin{cases} S_{k+i}(x) & \text{if } y \ne k(k + 2\varepsilon) \\ (1/x)S_{k+i}(x) & \text{if } y = k(k + 2\varepsilon) \end{cases}.$$

With this modification, the proof follows as in [31]. First, notice that

$$\operatorname{sgn}(S_l^{(N,\varepsilon)}(0)) = \operatorname{sgn}((-1)^l \alpha_1 \alpha_2 \ldots, \alpha_l) = (-1)^{2l} = 1$$

for $l < k$. Similarly, $\operatorname{sgn}(S_k^{(N,\varepsilon)}(0)) = 1$ if $y \ne k(k + 2\varepsilon)$ and $\operatorname{sgn}(S_k^{(N,\varepsilon)}(0)) = 0$ if $y = k(k + 2\varepsilon)$. On the other hand, for $i = 1, \ldots, N - k$, we have

$$\operatorname{sgn}(\tilde{S}_{k+i}^{(N,\varepsilon)}(0)) = \begin{cases} \operatorname{sgn}((-1)^{k+i}\alpha_1 \ldots \alpha_{k-1}\alpha_k\alpha_{k+1} \ldots \alpha_{k+i}) = (-1)^i, & \text{if } y \ne k(k + 2\varepsilon) \\ \operatorname{sgn}((-1)^{k+i-1}\alpha_1 \ldots \alpha_{k-1}\alpha_{k+1} \ldots \alpha_{k+i}) = (-1)^i, & \text{if } y = k(k + 2\varepsilon) \end{cases}.$$

In addition, from the recurrence relation (3.6) we easily see the following

- if $S_i^{(N,\varepsilon)}(a) = 0$ for $a > 0$, then $S_{i+1}^{(N,\varepsilon)}(a)$ and $S_{i-1}^{(N,\varepsilon)}(a)$ have opposite signs,

- $S_i^{(N,\varepsilon)}(x)$ and $S_{i-1}^{(N,\varepsilon)}(x)$ cannot have the same positive root.

These remarks are easily seen to hold for the auxiliary polynomials $\tilde{S}_{k+i}(x)$ as well. Next, denote by $V(x)$ the number of change of signs of the sequence

$$\tilde{S}_N^{(N,\varepsilon)}(x), \tilde{S}_{N-1}^{(N,\varepsilon)}(x), \ldots, \tilde{S}_{k+1}^{(N,\varepsilon)}(x), S_k^{(N,\varepsilon)}(x), S_{k-1}^{(N,\varepsilon)}(x), \ldots, S_0^{(N,\varepsilon)}(x).$$

By the remarks above, variations of $V(x)$ by ± 1 occur only at zeros of $\tilde{S}_N^{(N,\varepsilon)}(x)$ or $\tilde{S}_0^{(N,\varepsilon)}(x) = 1$. At $x = 0$, the first terms of the sequence are $(-1)^{N-k-i}$ for $i = 0, \ldots, N-k-1$, then 0 if $y = k(k+2\varepsilon)$ and all the remaining terms are 1, hence $V(0) = N-k$. On the other hand, it is clear that as x tends to infinity $\operatorname{sgn}(S_i^{(N,\varepsilon)}(x)) = 1$ and $\operatorname{sgn}(\tilde{S}_{k+i}^{(N,\varepsilon)}(x)) = 1$. This proves that there are at least $N-k$ positive roots of the polynomial $\tilde{S}_N^{(N,\varepsilon)}(x)$ and the same holds for $P_N^{(N,\varepsilon)}(x)$. □

To complete the proof we give an upper bound to the number of positive roots using Descartes' rule of signs (see e.g. [26], Theorem 7.5). This result states that the number of positive roots of a polynomial does not exceed the number of the sign changes in its coefficients.

Lemma 3.5.4. *Let $\varepsilon > -\frac{1}{2}$. When $y \geq N(N+2\varepsilon)$, the polynomial $P_N^{(N,\varepsilon)}(x,y)$ has no positive roots with respect to x.*

Proof. First, using the notation of Section 3.4, we note that $y = N(N+2\varepsilon)$ is the largest root of $a_0^N(y) = P_N^{(N,\varepsilon)}(0,y)$. Then, by the interlacing of the roots of $a_i^N(y)$ ($i = 0, 1, \ldots, N-1$) of Lemma 3.4.1, all $a_i^N(y)$ must be non-negative. Thus, there are no changes of signs in the coefficients of $P_N^{(N,\varepsilon)}(x,y)$ (as a polynomial in x) and the result follows by Descartes' rule of signs. □

Lemma 3.5.5. *Let $\varepsilon > -\frac{1}{2}$. For each k $(0 \leq k < N)$, there are at most $N-k$ positive roots (in the variable x) of the constraint polynomial $P_N^{(N,\varepsilon)}(x,y)$ for y in the range*

$$k(k+2\varepsilon) \leq y < (k+1)(k+1+2\varepsilon).$$

Proof. First, note as in Lemma 3.5.4 that when $y \geq N(N+2\varepsilon)$, all the coefficients $a_i^{(N)}(y)$ of the polynomial $P_N^{(N,\varepsilon)}(x,y)$ are non-negative, with the notation of §3.4. For $(N-1)(N-1+2\varepsilon) < y < N(N+2\varepsilon)$, by Lemma 3.4.1 the sign sequence $(\operatorname{sgn} a_N^{(N)}(y)\ , \operatorname{sgn} a_{N-1}^{(N)}(y), \ldots, \operatorname{sgn} a_0^{(N)}(y))$ is given by

$$+, +, \cdots, +, -, -, \cdots, -, -,$$

that is, it consists of a subsequence $+, +, \ldots, +$ of positive signs followed by a subsequence $-, -, \ldots, -$ of negative signs. Thus, by Descartes' rule of signs we have at most $1 = N-(N-1)$ positive roots for $P_N^{(N,\varepsilon)}(x,y)$. When $y = (N-1)(N-1+2\varepsilon)$, we have $a_0^{(N)}(y) = 0$ and the sequence is the same except for a 0 at the end, so the result holds without change. Continuing this process, we see that for $(N-2)(N-2+2\varepsilon) < y < (N-1)(N-1+2\varepsilon)$, the sign sequence given by

$$+, +, \cdots, +, -, -, \cdots, -, +, +, \ldots, +$$

from where it holds that the polynomial hast at most $2 = N - (N-2)$ roots (with respect to x). We continue this process until we reach $0 < y < 1(1+2\varepsilon)$, where we have

$$+, -, +, -, \ldots, (-1)^{N-1}, (-1)^N$$

giving $N = N - 0$ roots (with respect to x) by Descartes' rule of signs. Therefore, to finish the proof we prove that the number of sign changes in the sequence $(\operatorname{sgn} a_N^{(N)}(y), \operatorname{sgn} a_{N-1}^{(N)}(y)\ , \ldots, \operatorname{sgn} a_0^{(N)}(y))$ does not vary for y satisfying $(k-1)(k-1+2\varepsilon) < y < k(k+2\varepsilon)$, and that there is exactly an additional sign change when y crosses $(k-1)(k-1+2\varepsilon)$. To see this, note that due to the interlacing of roots given in Lemma 3.4.1, the next sign change in a subsequence $+, +, \cdots, +$ (or $-, -, \cdots, -$) of contiguous coefficients with same sign must happen at right end of the subsequence. When the subsequence $+, +, \cdots, +$ (or $-, -, \cdots, -$) is at the rightmost end of the complete sign sequence $(\operatorname{sgn} a_N^{(N)}(y), \operatorname{sgn} a_{N-1}^{(N)}(y), \ldots, \operatorname{sgn} a_0^{(N)}(y))$ there is an additional sign change in the complete sequence and the sign change occurs at roots of $a_0(y)$, that is, when $y = k(k+2\varepsilon)$ for $k \in \{1, 2, \ldots, N-1\}$. In any other case there is no additional sign change. This completes the proof. □

The combination of Lemmas 3.5.2 and 3.5.5 immediately gives Theorem 3.5.1.

3.6 Explicit formulas of the constraint polynomials

In this section we give an explicit expression of the constraint polynomials, these can be used to obtain combinatorial expression for the coefficients, see for example [48] The approach we use to find the coefficients of the constrain polynomials is to compute the derivatives at all orders by differentiating the defining recurrence formula.

Proposition 3.6.1. *For $m \in \mathbb{N}$, we have*

$$\begin{aligned}\partial_x^m P_k^{(N,\ell/2)}(x,y) &= mk(\partial_x^{m-1} P_{k-1}^{(N,\ell/2)}(x,y) - (k-1)(N-k+1)\partial_x^{m-1} P_{k-2}^{(N,\ell/2)}(x,y)) \\ &\quad + (kx + y - k(k+\ell))\partial_x^m P_{k-1}^{(N,\ell/2)}(x,y) - k(k-1)(N-k+1)x\partial_x^m P_{k-2}^{(N,\ell/2)}(x,y).\end{aligned}$$

Proof. Differentiating the defining recurrence relation for $P_k^{(N,\ell/2)}$, we obtain

$$\begin{aligned}\partial_x P_k^{(N,\ell/2)}(x,y) &= k(P_{k-1}^{(N,\ell/2)}(x,y) - (k-1)(N-k+1)P_{k-2}^{(N,\ell/2)}(x,y)) \\ &\quad + (kx + y - k(k+\ell))\partial_x P_{k-1}^{(N,\ell/2)}(x,y) - k(k-1)(N-k+1)x\partial_x P_{k-2}^{(N,\ell/2)}(x,y).\end{aligned}$$

Repeating this process m times gives the result. □

To find the coefficients of the constraint polynomials, it is enough to consider the constant term of the polynomials given by the partial derivatives, in other words, the case $x = 0$.

Corollary 3.6.2. *For $m \in \mathbb{N}$, we have*

$$\begin{aligned}&\partial_x^m P_k^{(N,\ell/2)}(0,y) \\ &= m\prod_{i=1}^{k}(y - c_i^{(\ell)}) \sum_{j=m}^{k} \frac{j(\partial_x^{m-1} P_{j-1}^{(N,\ell/2)}(0,y) - (j-1)(N-j+1)\partial_x^{m-1} P_{j-2}^{(N,\ell/2)}(0,y))}{\prod_{i=1}^{j}(y - c_j^{(\ell)})}.\end{aligned}$$

Here we use the convention that $P_{-1}^{(N,\varepsilon)}(x,y) = 0$.

Proof. The result is obtained by expanding the recurrence relation for $\partial_x^m P_k^{(N,\ell/2)}(x,y)$ in Proposition 3.6.1 and setting $x = 0$. □

These formulas can be used to recursively compute the partial derivatives of the constraint polynomials starting from $m = 1$ by computing $\partial_x^{m-1} P_{j-1}^{(N,\ell/2)}(0,y) - (j-1)(N-j+1)\partial_x^{m-1} P_{j-2}^{(N,\ell/2)}(0,y)$ for each m. For instance, it follows from Corollary 3.6.2 that

$$\partial_x P_k^{(N,\ell/2)}(0,y) = \prod_{i=1}^{k}(y - c_i^{(\ell)}) \sum_{j=1}^{k} \frac{j(y-(j-1)(N+\ell))}{(y-c_j^{(\ell)})(y-c_{j-1}^{(\ell)})}.$$

To generalize this expression, we introduce the expressions $\psi_i(j)$, with $i,j \in \mathbb{N}$, by

$$\psi_1(j) = \frac{j(y-(j-1)(N+\ell))}{(y-c_j^{(\ell)})(y-c_{j-1}^{(\ell)})},$$
$$\psi_i(j) = \frac{j}{(y-c_j^{(\ell)})}\psi_{i-1}(j-1),$$

Note that for fixed i and j, the expression is a rational function in the variable y. We extend the definition to $i,j \in \mathbb{Z}$ by setting $\psi_i(j) = 0$ whenever $i \le 0$ or $j \le 0$. With this notation, by using Corollary 3.6.2, we can directly compute

$$\partial_x^2 P_k^{(N,\ell/2)}(0,y) = \prod_{i=1}^{k}(y - c_i^{(\ell)}) \left(\sum_{j=2}^{k} \psi_2(j) + \sum_{i_1=2}^{k} \psi_1(i_1) \sum_{i_2=1}^{i_1-2} \psi_1(i_2) \right).$$

To express the general form of the derivatives of the constraint polynomials, we need a general form for sums of functions ψ_i of the kind appearing in the computation of $\partial_x^2 P_k^{(N,\ell/2)}(0,y)$ above. Fix $m \le k$, a positive integer $\alpha \le m$ and a vector $\nu = (\nu_1, \nu_2, \dots, \nu_\alpha) \in \mathbb{N}^\alpha$, with $|\nu|_1 := \nu_1 + \nu_2 + \cdots + \nu_\alpha = m$. Define the rational function $\Psi_\nu^{(m)}(k) = \Psi_\nu^{(m)}(k)(y)$ in y as

$$\Psi_\nu^{(m)}(k) = \sum_{i_1=m}^{k} \psi_{\nu_1}(i_1) \sum_{i_2=m-\nu_1}^{i_1-\nu_1-1} \psi_{\nu_2}(i_2) \cdots \sum_{i_n=m-\sum_{i=1}^{n-1}\nu_j}^{i_{n-1}-\nu_{n-1}-1} \psi_{\nu_n}(i_n) \cdots \sum_{i_\alpha=m-\sum_{i=1}^{\alpha-1}\nu_j}^{i_{\alpha-1}-\nu_{\alpha-1}-1} \psi_{\nu_\alpha}(i_\alpha).$$

By splitting the first sum in $\Psi_\nu^{(m)}(k)$, we derive an elementary identity, which is needed later in the proof of the main result of this section. Namely, for $\nu \in \mathbb{N}^\alpha$, it holds that

$$\Psi_\nu^{(m)}(k) = \psi_{\nu_1}(k)\Psi_{\nu'}^{(m-\nu_1)}(k-1-\nu_1) + \Psi_\nu^{(m)}(k-1), \tag{3.7}$$

where $\nu' \in \mathbb{N}^{\alpha-1}$ is obtained by dropping the first component ν_1 of ν. If $\nu \in \mathbb{N}^1$, we set $\Psi_{\nu'}^{(i)}(j) = 1$ for any $i,j \in \mathbb{N}$.

Summarizing the discussion above, we have the following explicit expressions of the constraint polynomials.

Theorem 3.6.3. *We have*

$$P_k^{(N,\ell/2)}(x,y) = \sum_{m=0}^{k} \prod_{i=1}^{k}(y - c_i^{(\ell)}) \left[\sum_{\alpha=1}^{m} \sum_{\substack{\nu\in\mathbb{N}^\alpha \\ |\nu|_1=m}} \Psi_\nu^{(m)}(k)(y) \right] x^m.$$

Proof. To establish the result it is enough to show, for $m \le k$, that

$$\partial_x^m P_k^{(N,\ell/2)}(0,y) = m! \prod_{i=1}^{k}(y - c_i^{(\ell)}) \left[\sum_{\alpha=1}^{m} \sum_{\substack{\nu\in\mathbb{N}^\alpha \\ |\nu|_1=m}} \Psi_\nu^{(m)}(k) \right].$$

The proof is by induction, the cases $m = 0, 1$ were already established above. Assume the identity holds for $m \in \mathbb{N}$. Computing directly from Corollary 3.6.2 and using the induction hypothesis we obtain

$$\begin{aligned}
&\partial_x^{m+1} P_k^{(N,\ell/2)}(0,y) \\
=&(m+1) \prod_{i=1}^{k}(y - c_i^{(\ell)}) \sum_{j=m+1}^{k} \frac{j(\partial_x^m P_{j-1}^{(N,\ell/2)}(0,y) - (j-1)(N-j+1)\partial_x^m P_{j-2}^{(N,\ell/2)}(0,y))}{\prod_{i=1}^{j}(y - c_j^{(\ell)})} \\
=&(m+1)! \prod_{i=1}^{k}(y - c_i^{(\ell)}) \sum_{j=m+1}^{k} \frac{1}{(y-c_j)(y-c_{j-1})} \Bigg(j(y-c_{j-1}) \sum_{\alpha=1}^{m} \sum_{\substack{\nu\in\mathbb{N}^\alpha \\ |\nu|_1=m}} \Psi_\nu^{(m)}(j-1) \\
&\qquad - j(j-1)(N-j+1) \sum_{\alpha=1}^{m} \sum_{\substack{\nu\in\mathbb{N}^\alpha \\ |\nu|_1=m}} \Psi_\nu^{(m)}(j-2) \Bigg).
\end{aligned}$$

Then, applying the identity (3.7) and factoring, we get

$$\begin{aligned}
&(m+1)! \prod_{i=1}^{k}(y - c_i^{(\ell)}) \Bigg(\sum_{\alpha=1}^{m} \sum_{\substack{\nu\in\mathbb{N}^\alpha \\ |\nu|_1=m}} \sum_{j=m+1}^{k} \frac{j}{(y-c_j)} \psi_{\nu_1}(j-1) \Psi_{\nu'}^{(m-\nu_1)}(j-2-\nu_1) \\
&\qquad + \sum_{j=m+1}^{k} \frac{j(y-(j-1)(N+\ell)}{(y-c_j)(y-c_{j-1})} \sum_{\alpha=1}^{m} \sum_{\substack{\nu\in\mathbb{N}^\alpha \\ |\nu|_1=m}} \Psi_\nu^{(m)}(j-2) \Bigg) \\
=&(m+1)! \prod_{i=1}^{k}(y - c_i^{(\ell)}) \Bigg(\sum_{\alpha=1}^{m} \sum_{\substack{\nu\in\mathbb{N}^\alpha \\ |\nu|_1=m}} \sum_{j=m+1}^{k} \psi_{\nu_1+1}(j) \Psi_{\nu'}^{(m-\nu_1)}(j-2-\nu_1) \\
&\qquad + \sum_{\alpha=1}^{m} \sum_{\substack{\nu\in\mathbb{N}^\alpha \\ |\nu|_1=m}} \sum_{j=m+1}^{k} \psi_1(j) \Psi_\nu^{(m)}(j-2) \Bigg) \\
=&(m+1)! \prod_{i=1}^{k}(y - c_i^{(\ell)}) \Bigg(\sum_{\alpha=1}^{m} \sum_{\substack{\nu\in\mathbb{N}^\alpha \\ |\nu|_1=m+1 \\ \nu_1\neq 1}} \Psi_\nu^{(m+1)}(k) + \sum_{\alpha=2}^{m+1} \sum_{\substack{\nu\in\mathbb{N}^\alpha \\ |\nu|_1=m+1 \\ \nu_1=1}} \Psi_\nu^{(m+1)}(k) \Bigg) \\
=&(m+1)! \prod_{i=1}^{k}(y - c_i^{(\ell)}) \sum_{\alpha=1}^{m+1} \sum_{\substack{\nu\in\mathbb{N}^\alpha \\ |\nu|_1=m+1}} \Psi_\nu^{(m+1)}(k).
\end{aligned}$$

Hence the desired result follows. □

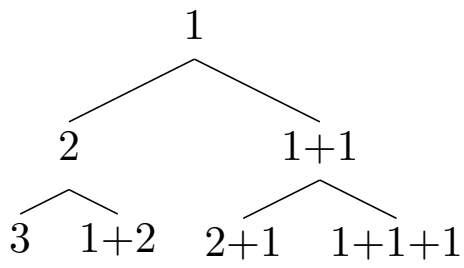


Figure 3.2: Compositions for $n = 1, 2, 3$.

Remark 3.6.4. The vectors $\nu \in \mathbb{N}^\alpha$ with $|\nu|_1 = m$ in the sum $\Psi_\nu^{(m)}(k)$ represent the *compositions* (ordered partitions) of the integer m that consist of α elements. For instance, for the case $m = 2$ above, there are only two compositions, $\{2, 1+1\}$. These are precisely the indices of the functions ψ_i involved in the sums in the expression for $\partial_x^2 P_k^{(N,\ell/2)}(0, y)$. In fact, the use of identity (3.7) in the proof of Theorem 3.6.3 resembles the way of constructing compositions of a number n starting with the compositions of $n - 1$. Suppose $a_1 + a_2 + \ldots + a_k$ is a composition of $n - 1$, then we construct two compositions $(a_1 + 1) + a_2 + \ldots + a_k$ and $1 + a_1 + a_2 + \ldots + a_k$ of n. It is easy to verify that this algorithm produces all compositions of n. For $n = 1, 2, 3$ we illustrate the algorithm as a tree in Figure 3.2.

4. The spectrum of the AQRM

In this chapter, we apply the results of Chapter 3 to complete the picture of the spectrum of the AQRM. For instance, in Section 4.1 we describe the degeneracy structure of the exceptional spectrum of the AQRM, since the regular spectrum is non-degenerate, this is enough to characterize the degeneracy for the general case.

In Section 4.2, we define a T-function that gives a constraint condition for non-Juddian exceptional eigenvalues in the same way that the G-function controls the regular eigenvalues. This function, along with the constraint polynomials, is used to study the residues of the poles of the G-function in Section 4.3. In Section 4.4 we define a generalized G-function in such a way that its zeros determine the full spectrum of the AQRM.

Finally, in Section 4.5 we show how exceptional solutions are captured in irreducible $\mathfrak{sl}_2$-modules, following the study of the representation theoretical picture of the AQRM, started in in Section 2.4.

4.1 Structure of the exceptional spectrum

The statement of Conjecture 2.9.1, now proved by virtue of 3.2.3 and 3.3.4, is now reformulated in terms of the parameters g, Δ of the AQRM.

Theorem 4.1.1. *For $\ell, N \in \mathbb{Z}_{\geq 0}$, there exists a polynomial $A_N^\ell(x,y) \in \mathbb{Z}[x,y]$ such that*

$$P_{N+\ell}^{(N+\ell,-\ell/2)}((2g)^2,\Delta^2) = A_N^\ell((2g)^2,\Delta^2)P_N^{(N,\ell/2)}((2g)^2,\Delta^2). \tag{4.1}$$

for $g, \Delta > 0$. Moreover, the polynomial $A_N^\ell(x,y)$ is positive for any $x, y > 0$. □

For the remaining Juddian eigenvalues not covered in Theorem 4.1.1 above, we have the following result.

Corollary 4.1.2. *For $\ell \in \mathbb{Z}_{>0}$ and $0 \leq k \leq \ell$ there are no Juddian eigenvalues $\lambda = k - \ell/2 - g^2$ in $H_{\text{Rabi}}^{\ell/2}$.*

Proof. The case $k = \ell$ was already proved in the discussion above and the case $k = 0$ is trivial since $P_0^{(0,-\ell/2)}((2g)^2,\Delta^2) = 1 \neq 0$. For $1 \leq k < \ell$, if $\lambda = k - \ell/2 - g^2$ is a Juddian eigenvalue then $P_k^{(k,-\ell/2)}((2g)^2,\Delta^2) = 0$ for some parameters $g, \Delta > 0$. This is a contradiction to Proposition 3.3.5. Note that in this case there is no possibility of a contribution of Juddian eigenvalues by roots of constraint polynomials $P_N^{(N,\ell/2)}((2g)^2,\Delta^2)$ as this would necessarily require $N = k - \ell < 0$. □

In Proposition 5.8 of [63], it is shown that the roots of the constraint polynomials $P_N^{(N,\varepsilon)}(x,y)$ are simple. In particular, this implies that for $\varepsilon \notin \frac{1}{2}\mathbb{Z}$, there are no degenerate exceptional eigenvalues consisting of two Juddian solutions.

Since the multiplicity of the eigenvalues is at most two, as a corollary of Theorem 4.1.1 and Corollary 4.1.2, we have the following result.

Corollary 4.1.3. *If $x = (2g)^2$ is a root of the equation $P_N^{(N,\ell/2)}(x, \Delta^2) = 0$, then the (Juddian) eigenvalue $\lambda = N + \ell/2 - g^2$ must be a degenerate exceptional eigenvalue. In fact, the multiplicity of the exceptional eigenvalue λ is exactly 2 and the two linearly independent solutions are Juddian.* □

We now present the following result about the general structure on the degeneracy of the spectrum of the AQRM.

Corollary 4.1.4 ([27])**.** *The degeneracy of the spectrum of $H_{\text{Rabi}}^{\varepsilon}$ occurs only when $\varepsilon = \ell/2$ for $\ell \in \mathbb{Z}_{\geq 0}$ and $P_N^{(N,\ell/2)}((2g)^2, \Delta^2) = 0$. In particular, any non-Juddian exceptional solution is non-degenerate.*

Proof. We first consider the case $N \neq 0$. When $P_N^{(N,\varepsilon)}((2g)^2, \Delta^2) \neq 0$ if we look at the local Frobenius solutions at $y = 0$, then there is always a local solution containing a log-term as seen in Section 2.7 (see Proposition 2.8.2), so the solutions corresponding to the smaller exponent cannot be components of the eigenfunction. Then, the solution corresponds to the largest exponent (i.e. non-Juddian exceptional) and this implies that the dimension of the corresponding eigenspace is at most one (cf. [5, 66]). We note that in the case $\varepsilon = \ell/2\,(\ell \in \mathbb{Z})$ there is no chance of a contribution of Juddian solution (i.e. $P_{N+\ell}^{(N+\ell,-\ell/2)}((2g)^2, \Delta^2) = 0$) by Theorem 4.1.1. Suppose next that $P_N^{(N,\varepsilon)}((2g)^2, \Delta^2) = 0$ for $\varepsilon \notin \frac{1}{2}\mathbb{Z}_{\geq 0}$. Looking at the local Frobenius solutions at $y = 1$, since the exponent different from 0 is not a non-negative integer (see Table 2.1), we observe that only the solution corresponding to the exponent 0 can give a eigensolution of $H_{\text{Rabi}}^{\varepsilon}$ so that the dimension of the eigenspace is also at most one. By Corollary 4.1.3, there is no non-Juddian exceptional eigensolution when $P_N^{(N,\ell/2)}((2g)^2, \Delta^2) = 0$ for $\ell \in \mathbb{Z}_{\geq 0}$.

On the other hand, if $N = 0$, the exponents of the system (2.17) are $\rho_1^- = 0$ and $\rho_2^- = 1$, therefore there is one holomorphic Frobenius solution and a local solution with a log-term. This implies that the corresponding eigenstate cannot be degenerate. In addition, note that if $K_0^{(N,\varepsilon)}(g, \Delta) = 0$, the log-term in the Frobenius solution with smaller exponent (2.18) vanishes making it identical to the solution (2.23) (corresponding to the larger exponent). Hence, the exceptional eigenvalue $\lambda = \pm\varepsilon - g^2$ must be non-Juddian exceptional, and thus, non-degenerate. Since $P_0^{(0,\pm\varepsilon)}((2g)^2, \Delta^2) = 1 \neq 0$ and $P_\ell^{(\ell,-\ell/2)}((2g)^2, \Delta^2) \neq 0$ for $g, \Delta > 0$ and $\ell > 0$ (cf. Proposition 3.3.5), the desired claim follows. □

Remark 4.1.5. The non-degeneracy of the ground state for the QRM was first shown in [19].

Thus, summarizing the results so far obtained in Theorem 4.1.1 with Corollary 4.1.3 and Corollary 4.1.4, we have the following result.

Theorem 4.1.6. *The spectrum of the AQRM possesses a degenerate eigenvalue if and only if the parameter ε is a half integer. Furthermore, all degenerate eigenvalues of the AQRM are Juddian.* □

4.2 A constraint function for non-Juddian exceptional eigenvalues

In this subsection, we study the condition for a solution of the system (2.4) to be a non-Juddian exceptional eigenvalues of the AQRM. As in the case of the G-function and regular solutions, we define an appropriate constraint function by studying the conditions for entireness of solutions using the symmetry between the system (2.4) and the system (2.5).

Concretely, we define a constraint T-function $T_\varepsilon^{(N)}(g,\Delta)$ that vanishes for parameters g and Δ for which $H_{\mathrm{Rabi}}^{\varepsilon}$ has the exceptional eigenvalue $\lambda = N+\varepsilon-g^2$ with non-Juddian solution (see [8] for the case of the quantum Rabi model).

In order to define the function $T_\varepsilon^{(N)}(g,\Delta)$, we first describe the local Frobenius solutions of system of differential equations (2.4) and (2.5) at the regular singular points $y = 0, 1$ (cf. Section 2.7).

Define the functions as follows:

$$\phi_{1,+}(y;\varepsilon) = \frac{(N+1)}{\Delta}y^N - \Delta\sum_{n=N+1}^{\infty}\frac{\bar{K}_n^-(N+\varepsilon;g,\Delta,\varepsilon)}{n-N}y^n, \tag{4.2}$$

$$\phi_{1,-}(y;\varepsilon) = \sum_{n=N+1}^{\infty}\bar{K}_n^-(N+\varepsilon;g,\Delta,\varepsilon)y^n, \tag{4.3}$$

with initial conditions $\bar{K}_n^-(N+\varepsilon;g,\Delta,\varepsilon) = 0\,(n \le N)$, $\bar{K}_{N+1}^-(N+\varepsilon;g,\Delta,\varepsilon) = 1$ and

$$\begin{aligned}&(n+1)\bar{K}_{n+1}^-(N+\varepsilon;g,\Delta,\varepsilon)\\ &\quad= \left(n-N+(2g)^2-2\varepsilon+\frac{\Delta^2}{N-n}\right)\bar{K}_n^-(N+\varepsilon;g,\Delta,\varepsilon)-(2g)^2\bar{K}_{n-1}^-(N+\varepsilon;g,\Delta,\varepsilon),\end{aligned}$$

for $n \ge N+1$. Then, ${}^t(\phi_{1,+}(y;\varepsilon),\phi_{1,-}(y;\varepsilon))$ is the local Frobenius solution corresponding to the largest exponent of the system (2.4) at $y = 0$.

Next, consider the solutions at $y = 1$. For the case $N+2\varepsilon \notin \mathbb{Z}_{\ge 0}$ (i.e. $\varepsilon \notin \frac{1}{2}\mathbb{Z}$ or $\varepsilon = -\ell/2\,(\ell \in \mathbb{Z}_{\ge 0})$ and $N-\ell < 0$) we define

$$\phi_{2,+}(\bar{y};-\varepsilon) = \Delta\sum_{n=0}^{\infty}\frac{\bar{K}_n^+(N+\varepsilon;g,\Delta,\varepsilon)}{N+2\varepsilon-n}\bar{y}^n, \tag{4.4}$$

$$\phi_{2,-}(\bar{y};-\varepsilon) = \sum_{n=0}^{\infty}\bar{K}_n^+(N+\varepsilon;g,\Delta,\varepsilon)\bar{y}^n, \tag{4.5}$$

with initial conditions $\bar{K}_n^+(N+\varepsilon;g,\Delta,\varepsilon) = 0\,(n < 0)$, $\bar{K}_0^+(N+\varepsilon;g,\Delta,\varepsilon) = 1$, while for the case $N+2\varepsilon \in \mathbb{Z}_{\ge 0}$ (i.e. $\varepsilon = \ell/2\,(\ell \in \mathbb{Z}_{\ge 0})$ or $\varepsilon = -\ell/2\,(\ell \in \mathbb{Z}_{\ge 0})$ and $N-\ell \ge 0$) we define

$$\phi_{2,+}(\bar{y};-\ell/2) = \frac{(N+\ell+1)}{\Delta}\bar{y}^{N+\ell} - \Delta\sum_{n=N+\ell+1}^{\infty}\frac{\bar{K}_n^+(N+\ell/2;g,\Delta,\ell/2)}{n-N-\ell}\bar{y}^n, \tag{4.6}$$

$$\phi_{2,-}(\bar{y};-\ell/2) = \sum_{n=N+\ell+1}^{\infty}\bar{K}_n^+(N+\ell/2;g,\Delta,\ell/2)\bar{y}^n, \tag{4.7}$$

with initial conditions $\bar{K}^+_n(N+\ell/2; g, \Delta, \ell/2) = 0\,(n \le N+\ell)$, $\bar{K}^+_{N+\ell+1}(N+\ell/2; g, \Delta, \ell/2) = 1$ and in both cases the coefficients satisfy

$$(n+1)\bar{K}^+_{n+1}(N+\varepsilon; g, \Delta, \varepsilon) = \left(n - N + (2g)^2 + \frac{\Delta^2}{N+2\varepsilon-n}\right)\bar{K}^+_n(N+\varepsilon; g, \Delta, \varepsilon) - (2g)^2\bar{K}^+_{n-1}(N+\varepsilon; g, \Delta, \varepsilon).$$

Then ${}^t(\phi_{2,+}(\bar{y}; -\varepsilon), \phi_{2,-}(\bar{y}; -\varepsilon))$ is the local Frobenius solution of the system (2.5) at $\bar{y} = 0$, where $\bar{y} = 1 - y$. Note also that the radius of convergence of each series above equals 1.

To define the constraint function for the non-Juddian exceptional solutions we adapt the argument used for regular eigenvalues and the G-function in Section 2.6. In particular, any solution to the eigenvalue problem of AQRM satisfies the system

$$\frac{d}{dz}\Psi(z) = A(z)\Psi(z), \tag{4.8}$$

where

$$A(z) = \begin{bmatrix} \frac{\lambda-\varepsilon-gz}{z+g} & 0 & 0 & \frac{-\Delta}{z+g} \\ 0 & \frac{\lambda+\varepsilon-gz}{z+g} & \frac{-\Delta}{z+g} & 0 \\ 0 & \frac{-\Delta}{z-g} & \frac{\lambda-\varepsilon+gz}{z-g} & 0 \\ \frac{-\Delta}{z-g} & 0 & 0 & \frac{\lambda+\varepsilon+gz}{z-g} \end{bmatrix}, \tag{4.9}$$

for the vector valued function

$$\Psi(z) := {}^t\Big(e^{-gz}\phi_{1,+}\Big(\frac{g+z}{2g}; \varepsilon\Big), e^{gz}\phi_{1,-}\Big(\frac{g-z}{2g}; \varepsilon\Big), e^{gz}\phi_{1,+}\Big(\frac{g-z}{2g}; \varepsilon\Big), e^{-gz}\phi_{1,-}\Big(\frac{g+z}{2g}; \varepsilon\Big)\Big).$$

It is not difficult to see that the function

$$\Phi(z) := {}^t\Big(e^{gz}\phi_{2,-}\Big(\frac{g-z}{2g}; -\varepsilon\Big), e^{-gz}\phi_{2,+}\Big(\frac{g+z}{2g}; -\varepsilon\Big), e^{-gz}\phi_{2,-}\Big(\frac{g+z}{2g}; -\varepsilon\Big), e^{gz}\phi_{2,+}\Big(\frac{g-z}{2g}; -\varepsilon\Big)\Big)$$

also satisfies (4.8). Hence, in order for a non-Juddian exceptional solution to exist it is necessary and sufficient that for some $z_0\,(-g < z_0 < g)$ (an ordinary point of the system), there exists a non-zero constant $c = c_N(g, \Delta, \varepsilon)$ and such that

$$\begin{cases} e^{-gz_0}\phi_{1,+}\Big(\frac{g+z_0}{2g}; \varepsilon\Big) = c\,e^{gz_0}\phi_{2,-}\Big(\frac{g-z_0}{2g}; -\varepsilon\Big), \\ e^{gz_0}\phi_{1,-}\Big(\frac{g-z_0}{2g}; \varepsilon\Big) = c\,e^{-gz_0}\phi_{2,+}\Big(\frac{g+z_0}{2g}; -\varepsilon\Big), \\ e^{gz_0}\phi_{1,+}\Big(\frac{g-z_0}{2g}; \varepsilon\Big) = c\,e^{-gz_0}\phi_{2,-}\Big(\frac{g+z_0}{2g}; -\varepsilon\Big), \\ e^{-gz_0}\phi_{1,-}\Big(\frac{g+z_0}{2g}; \varepsilon\Big) = c\,e^{gz_0}\phi_{2,+}\Big(\frac{g-z_0}{2g}; -\varepsilon\Big). \end{cases} \tag{4.10}$$

For $z_0 = 0$, it is obvious that the first and third (resp. the second and forth equations) are equivalent. Namely, the four equations reduce to the following two equations when $y = \bar{y} = \frac{1}{2}$.

$$\begin{cases} \phi_{1,-}(y; \varepsilon) = c\,\phi_{2,+}(\bar{y}; -\varepsilon) = c\,\phi_{2,+}(1-y; -\varepsilon), \\ \phi_{1,+}(y; \varepsilon) = c\,\phi_{2,-}(\bar{y}; -\varepsilon) = c\,\phi_{2,-}(1-y; -\varepsilon). \end{cases} \tag{4.11}$$

for some non-zero constant c (as can be seen by applying the substitutions $y \to \bar{y} = 1 - y$ and $\varepsilon \to -\varepsilon$ to the system (2.17)). Therefore, by setting $y = 1/2$ ($z = 0$ in the original variable, an ordinary point of the system) and eliminating the constant c in these linear relations give

$$T_\varepsilon^{(N)}(g, \Delta) = 0,$$

giving rise to the definition below.

Definition 4.2.1 ([27]). *The constraint T-function $T_\varepsilon^{(N)}(g, \Delta)$ of the AQRM is given by*

$$T_\varepsilon^{(N)}(g, \Delta) = \bar{R}^{(N,+)}(g, \Delta; \varepsilon)\bar{R}^{(N,-)}(g, \Delta; \varepsilon) - R^{(N,+)}(g, \Delta; \varepsilon)R^{(N,-)}(g, \Delta; \varepsilon), \quad (4.12)$$

with

$$\bar{R}^{(N,-)}(g, \Delta; \varepsilon) = \phi_{1,+}\Big(\frac{1}{2}; \varepsilon\Big), \qquad \bar{R}^{(N,+)}(g, \Delta; \varepsilon) = \phi_{2,+}\Big(\frac{1}{2}; -\varepsilon\Big), \quad (4.13)$$

$$R^{(N,-)}(g, \Delta; \varepsilon) = \phi_{1,-}\Big(\frac{1}{2}; \varepsilon\Big), \qquad R^{(N,+)}(g, \Delta; \varepsilon) = \phi_{2,-}\Big(\frac{1}{2}; -\varepsilon\Big). \quad (4.14)$$

Conversely, if there exists such $c = c_N(g, \Delta, \varepsilon)(\neq 0)$, $\lambda = N+\varepsilon-g^2$ is a non-Juddian exceptional eigenvalue and the corresponding functions $(\phi_{j,+}, \phi_{j,-})$ $(j = 1, 2)$ satisfy (4.11) and (4.10) (cf. [23]).

Remark 4.2.2. When $\varepsilon = 0$ we observe that

$$T_0^{(N)}(g, \Delta) = \Big(\bar{R}^{(N,+)}(g, \Delta, 0) - R^{(N,+)}(g, \Delta, 0)\Big)\Big(\bar{R}^{(N,+)}(g, \Delta, 0) + R^{(N,+)}(g, \Delta, 0)\Big)$$

since $R^{(N,+)}(g, \Delta, 0) = R^{(N,-)}(g, \Delta, 0))$ and $\bar{R}^{(N,+)}(g, \Delta, 0) = \bar{R}^{(N,-)}(g, \Delta, 0))$. It is interesting to compare this property with Remark 2.6.2 and the discussion in [8] for non-Juddian exceptional solutions of the QRM.

Remark 4.2.3. By Corollary 4.1.4, for any fixed $\Delta > 0$, there are no common zeros between the constraint polynomial $P_N^{(N,\varepsilon)}((2g)^2, \Delta^2)$ and the T-function $T_\varepsilon^{(N)}(g, \Delta)$.

In the same manner, we can define a T-function $\tilde{T}_\varepsilon^{(N)}(g, \Delta)$ that vanishes for values g, Δ corresponding to the non-Juddian exceptional eigenvalue $\lambda = N - \varepsilon - g^2$. Clearly, we have $\tilde{T}_0^{(N)}(g, \Delta) = T_0^{(N)}(g, \Delta)$, and in general it is straightforward to verify that the identity

$$\tilde{T}_\varepsilon^{(N)}(g, \Delta) = T_{-\varepsilon}^{(N)}(g, \Delta) \quad (4.15)$$

holds (up to a constant) as in the case of constraint polynomials $\tilde{P}_N^{(N,\varepsilon)}((2g)^2, \Delta^2)$ (see [63] and also [33]).

We consider the particular case of $\varepsilon = \ell/2$ $(\ell \in \mathbb{Z}_{\geq 0})$. Then, from (4.11) we have $\phi_{1,-}(y; \ell/2) = c\phi_{2,+}(1 - y; -\ell/2)$ and $\phi_{1,+}(y; \ell/2) = c\phi_{2,-}(1 - y; -\ell/2)$. This shows that the non-Juddian exceptional solution corresponding to $\lambda = (N + \ell) - \ell/2 - g^2 = N + \ell/2 - g^2$ whose existence is guaranteed by the constraint equation $T_{\ell/2}^{(N)}(g, \Delta) = 0$ (resp. $\tilde{T}_{\ell/2}^{(N+\ell)}(g, \Delta) = 0$) are identical up to a scalar multiple. Since the non-Juddian exceptional solution is non-degenerate, the compatibility of this fact, that is, that $T_{\ell/2}^{(N)}(g, \Delta)$ and $\tilde{T}_{\ell/2}^{(N+\ell)}(g, \Delta)$ have the same zero with respect to g for a fixed Δ, is confirmed by the lemma below.

Lemma 4.2.4. *For $\ell, N \in \mathbb{Z}_{\geq 0}$ we have*

$$\tilde{T}^{(N+\ell)}_{\ell/2}(g,\Delta) = T^{(N)}_{\ell/2}(g,\Delta). \tag{4.16}$$

Proof. Directly from the definitions, we have $\bar{K}^{\pm}_n(N-\ell/2; g, \Delta, -\ell/2) = \bar{K}^{\mp}_n(N+\ell/2; g, \Delta, \ell/2)$, giving

$$\begin{aligned}
\bar{R}^{(N+\ell,\pm)}(g,\Delta,-\ell/2) &= \bar{R}^{(N,\mp)}(g,\Delta,\ell/2),\\
R^{(N+\ell,\pm)}(g,\Delta,-\ell/2) &= R^{(N,\mp)}(g,\Delta,\ell/2).
\end{aligned}$$

It follows hence that

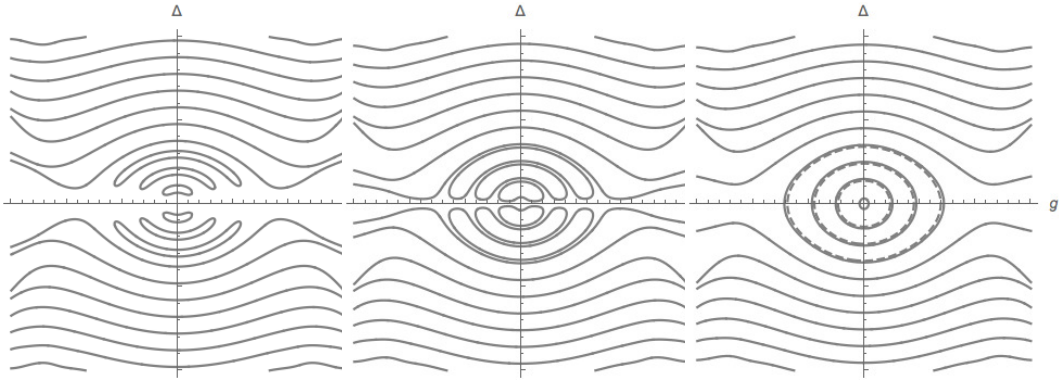
$$\begin{aligned}
\tilde{T}^{(N+\ell)}_{\ell/2}(g,\Delta) &= T^{(N+\ell)}_{-\ell/2}(g,\Delta)\\
&= \bar{R}^{(N+\ell,+)}(g,\Delta;-\ell/2)\bar{R}^{(N+\ell,-)}(g,\Delta;-\ell/2) - R^{(N+\ell,+)}(g,\Delta;-\ell/2)R^{(N+\ell,-)}(g,\Delta;-\ell/2)\\
&= \bar{R}^{(N,-)}(g,\Delta;\ell/2)\bar{R}^{(N,+)}(g,\Delta;\ell/2) - R^{(N,-)}(g,\Delta;\ell/2)R^{(N,+)}(g,\Delta;\ell/2) = T^{(N)}_{\ell/2}(g,\Delta).
\end{aligned}$$

This proves the lemma. □

By the discussion above, the condition $T^{(N)}_{\varepsilon}(g,\Delta) = 0$ (resp. $\tilde{T}^{(N)}_{\varepsilon}(g,\Delta) = 0$) can be indeed be regarded as the constraint equation for the exceptional eigenvalues $\lambda = N + \varepsilon - g^2$ (resp. $\lambda = N - \varepsilon - g^2$) with non-Juddian exceptional solutions.

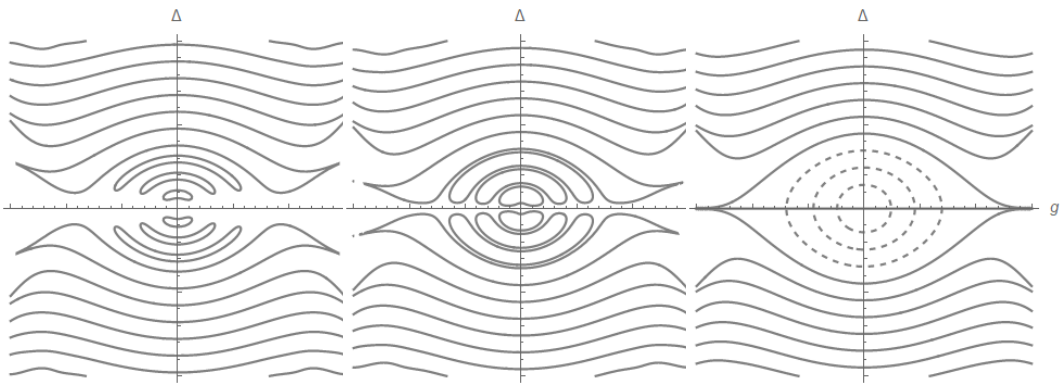
We illustrate numerically the constraint relations $P^{(N,\varepsilon)}_N((2g)^2,\Delta^2) = 0$ (for Juddian eigenvalues) and $T^{(N)}_{\varepsilon}(g,\Delta) = 0$ (for non-Juddian exceptional eigenvalues) in Figure 4.1 showing the curves in the (g,Δ)-plane defined by these relations for $\varepsilon = 0.45$ and $N = 3$. Concretely, Figures 4.1(a) and 4.1(b) depict the graph of the curve $G_\varepsilon(x,g,\Delta) = 0$ for the values $x = 3.2$ and $x = 3.4$, while Figure 4.1(c) shows the graph of the curve $T^{(3)}_{\varepsilon}(g,\Delta) = 0$ in continuous line and $P^{(3,\varepsilon)}_3((2g)^2,\Delta^2) = 0$ in dashed line. Notice that as $x \to 3.45$ adjacent closed curves near the origin in the graph of $G_\varepsilon(x,g,\Delta) = 0$ approach each other. Some of these curves join to form the closed curves (ovals) of $P^{(N,\varepsilon)}_N((2g)^2,\Delta^2) = 0$, corresponding to Juddian eigenvalues, while others form curves in the graph of $T^{(N)}_{\varepsilon}(g,\Delta) = 0$, corresponding to non-Juddian exceptional eigenvalues. Also observe that we have ovals (corresponding to non-Juddian solutions) near the origin of the graph in Figure 4.1(c), some of them very close to dashed ovals (corresponding to Juddian eigenvalues).

On the other hand, the case $\varepsilon \in \frac{1}{2}\mathbb{Z}_{\geq 0}$ is illustrated in Figure 4.2. As in the case above, Figures 4.2(a) and 4.2(b) depict the curves given by the relation $G_\varepsilon(x,g,\Delta) = 0$ for the values $x = 3.2$ and $x = 3.4$, while Figure 4.2(c) shows the graph of the curve $T^{(3)}_{\varepsilon}(g,\Delta) = 0$ ($N = 3$) in continuous line and $P^{(3,\varepsilon)}_3((2g)^2,\Delta^2) = 0$ in dashed line. Different from the case $\varepsilon \notin \frac{1}{2}\mathbb{Z}_{\geq 0}$ above, there are no continuous ovals (non-Juddian) near the origin in Figure 4.2(c). Actually, we can observe there are both dashed (Juddian) and continuous (non-Juddian) ovals when $\varepsilon = 0.45$ in Figure 4.1(c), while the continuous ovals disappear when $\varepsilon = \frac{1}{2}(\in \frac{1}{2}\mathbb{Z})$ in Figure 4.2(c) (see Corollary 4.1.3).



(a) $\varepsilon = 0.45$, $x = 3.2$ (b) $\varepsilon = 0.45$, $x = 3.4$ (c) $\varepsilon = 0.45, N = 3, x = 3.45$

Figure 4.1: Curves of constraint relations for fixed regular eigenvalues ((a),(b)) and exceptional eigenvalues ((c)) for $\varepsilon = 0.45$ for $-3 \le g \le 3$ and $-10 \le \Delta \le 10$.



(a) $\varepsilon = \frac{1}{2}$, $x = 3.2$ (b) $\varepsilon = \frac{1}{2}$, $x = 3.4$ (c) $\varepsilon = \frac{1}{2}, N = 3, x = N + \varepsilon = 3.5$

Figure 4.2: Curves of constraint relations for fixed regular eigenvalues ((a),(b)) and exceptional eigenvalues ((c), Juddian: dashed line; non-Juddian: continuous) for $\varepsilon = \frac{1}{2}$ for $-3 \le g \le 3$ and $-10 \le \Delta \le 10$.

4.3 Exceptional solutions and G-functions

In this subsection, we discuss the residues the poles and residues of the G-function.

Formally, to study the behavior of the G-function $G_\varepsilon(x; g, \Delta)$ at a point $x = N \pm \varepsilon$ $(N \in \mathbb{Z}_{\ge 0})$ we consider a sufficiently small punctured disc centered at a fixed point $x = N \pm \varepsilon$ and compute the residue of $G_\varepsilon(x; g, \Delta)$ as a function of the parameters g and Δ. According to the value of the residue for the parameters g and Δ we classify the singularity as a removable singularity or a pole. In the case of a removable singularity we consider the G-function $G_\varepsilon(x; g, \Delta)$ as a function defined at $x = N \pm \varepsilon$ for the particular parameters g and Δ. It is clear from the definition that the only singularities of $G_\varepsilon(x; g, \Delta)$ (as a function of x) appear at the points $x = N \pm \varepsilon$ $(N \in \mathbb{Z}_{\ge 0})$ and that all singularities are either removable singularities or poles. To simplify the notation, we say that a function has a pole of order $\le N$ when it has a removable singularity or a pole of order at most N.

We consider the case $\varepsilon \notin \frac{1}{2}\mathbb{Z}$ and $\varepsilon \in \frac{1}{2}\mathbb{Z}$ by separate. For the case of $\varepsilon \notin \frac{1}{2}\mathbb{Z}$,

by the defining recurrence formula (2.10), we observe that the rational functions $K_n^{\mp}(x)$, for $n \geq N+1$, have poles of order ≤ 1 at $x = N \pm \varepsilon$. Hence, $G_\varepsilon(x; g, \Delta)$ has a pole of order ≤ 1 at $x = N \pm \varepsilon$. The residue of the G-function at a point $x = N \pm \varepsilon$ is given in the following result.

Proposition 4.3.1. *Let $\varepsilon \notin \frac{1}{2}\mathbb{Z}$. Then any pole of the G-function $G_\varepsilon(x; g, \Delta)$ is simple. If $N \in \mathbb{Z}_{\geq 0}$, the residue of $G_\varepsilon(x; g, \Delta)$ at the points $x = N \pm \varepsilon$ is given by*

$$\operatorname*{Res}_{x=N\pm\varepsilon} G_\varepsilon(x; g, \Delta) = C(N)\Delta^2 P_N^{(N,\pm\varepsilon)}((2g)^2, \Delta^2) T_{\pm\varepsilon}^{(N)}(g, \Delta),$$

where $C(N) = \frac{1}{N!(N+1)!}$.

Proof. We give the proof for the case $x = N + \varepsilon$, for the case $x = N - \varepsilon$ is completely analogous. From the definition of $f_n^-(x, g, \Delta, \varepsilon)$, it is clear that $\operatorname{Res}_{x=N+\varepsilon} f_n^-(x, g, \Delta, \varepsilon) = \frac{\Delta^2}{2g}\delta_N(n)$, where $\delta_x(y)$ is the Kronecker delta function. Likewise, it is clear that $\operatorname{Res}_{x=N+\varepsilon} K_n^-(x; g, \Delta, \varepsilon) = 0$ for $0 \leq n \leq N$. For the case of $n = N$ we have

$$\begin{aligned}\operatorname*{Res}_{x=N+\varepsilon} K_{N+1}^-(x) &= \lim_{x\to N+\varepsilon}(x - N - \varepsilon)\frac{1}{N+1}\left(f_N^-(x)K_N^-(x) - K_{N-1}^-(x)\right)\\ &= \frac{1}{N+1}K_N^-(N+\varepsilon)\operatorname*{Res}_{x\to N+\varepsilon} f_N^-(x) = \frac{\Delta^2}{2g(N+1)}K_N^-(N+\varepsilon).\end{aligned}$$

Setting $a_0 = 0$, $a_1 = 1$, and

$$a_k = \frac{1}{N+k}\left(f_{N+k-1}^-(N+\varepsilon)a_{k-1} - a_{k-2}\right),$$

for $k \geq 2$, it is easy to see that $\operatorname{Res}_{x=N+\varepsilon} K_{N+k}^-(x) = \frac{\Delta^2}{2g(N+1)}K_N^-(N+\varepsilon)a_k$. Furthermore, by the same method of the proof of Proposition 2.8.2, we observe that

$$(2g)^{k-1}a_k = \bar{K}_{N+k}^-(N+\varepsilon; g, \Delta, \varepsilon),$$

for $k \geq 1$, where $\bar{K}_{N+k}^-(N+\varepsilon; g, \Delta, \varepsilon)$ are the coefficients of $\phi_{1,-}(y; \epsilon)$ in (4.3). Then, from the definition of $R^{(N,-)}(g, \Delta; \epsilon)$ we have

$$\begin{aligned}R^{(N,-)}(g, \Delta; \epsilon) = \phi_{1,-}\Big(\frac{1}{2}; \varepsilon\Big) &= \sum_{n=N+1}^{\infty}\bar{K}_n^-(N+\varepsilon; g, \Delta, \varepsilon)\Big(\frac{1}{2}\Big)^n\\ &= \Big(\frac{1}{2}\Big)^{N+1}\sum_{n=N+1}^{\infty}\bar{K}_n^-(N+\varepsilon; g, \Delta, \varepsilon)\Big(\frac{1}{2}\Big)^{n-N-1} = \Big(\frac{1}{2}\Big)^{N+1}\sum_{n=N+1}^{\infty}a_{n-N}g^{n-N-1},\end{aligned}$$

and, similarly,

$$\begin{aligned}\bar{R}^{(N,-)}(g, \Delta; \varepsilon) = \phi_{1,+}\Big(\frac{1}{2}; \varepsilon\Big) &= \frac{(N+1)}{\Delta}\Big(\frac{1}{2}\Big)^N - \Delta\sum_{n=N+1}^{\infty}\frac{\bar{K}_n^-(N+\varepsilon; g, \Delta, \varepsilon)}{n-N}\Big(\frac{1}{2}\Big)^n\\ &= \Big(\frac{1}{2}\Big)^{N+1}\Big(\frac{2(N+1)}{\Delta} - \Delta\sum_{n=N+1}^{\infty}\frac{\bar{K}_n^-(N+\varepsilon; g, \Delta, \varepsilon)}{n-N}\Big(\frac{1}{2}\Big)^{n-N-1}\Big)\\ &= \Big(\frac{1}{2}\Big)^{N+1}\Big(\frac{2(N+1)}{\Delta} - \Delta\sum_{n=N+1}^{\infty}\frac{a_{n-N}}{n-N}g^{n-N-1}\Big).\end{aligned}$$

Moreover, we recall that for $\varepsilon \notin \frac{1}{2}\mathbb{Z}$, both functions $R^+(x)$ and $\bar{R}^+(x)$ are analytic at $x = N + \varepsilon$ and

$$R^+(N+\varepsilon) = R^{(N,+)}(g,\Delta;\varepsilon), \qquad \Delta\bar{R}^+(N+\varepsilon) = \bar{R}^{(N,+)}(g,\Delta;\varepsilon).$$

With these preparations, we compute

$$\begin{aligned}
\operatorname*{Res}_{x=N+\varepsilon} R^+(x)R^-(x) &= R^+(N+\varepsilon) \operatorname*{Res}_{x=N+\varepsilon} \sum_{n=0}^{\infty} K_N^-(x)g^n \\
&= \frac{\Delta^2}{2g(N+1)} K_N^-(N+\varepsilon)R^+(N+\varepsilon) \sum_{n=N+1}^{\infty} a_{n-N}g^n \\
&= \frac{(2g)^N\Delta^2}{(N+1)} K_N^-(N+\varepsilon)R^{(N,+)}(g,\Delta;\varepsilon)R^{(N,-)}(g,\Delta;\varepsilon).
\end{aligned}$$

and, since $\operatorname{Res}_{x=N+\varepsilon} \frac{K_N^-(x)}{x-N-\varepsilon} = K_N^-(N+\varepsilon)$ holds trivially, we also obtain

$$\begin{aligned}
\operatorname*{Res}_{x=N+\varepsilon} \Delta^2\bar{R}^+(x)\bar{R}^-(x) &= \Delta^2\bar{R}^+(N+\varepsilon) \operatorname*{Res}_{x=N+\varepsilon} \sum_{n=0}^{\infty} \frac{K_N^-(x)}{x-n-\varepsilon} g^n \\
&= \Delta^2\bar{R}^+(N+\varepsilon)\Big(K_N^-(N+\varepsilon)g^N - \frac{\Delta^2}{2g(N+1)} K_N^-(N+\varepsilon) \sum_{n=N+1}^{\infty} \frac{a_{n-N}}{n-N} g^n\Big) \\
&= \frac{g^N\Delta^2}{2(N+1)} K_N^-(N+\varepsilon)(\Delta\bar{R}^+(N+\varepsilon))\Big(\frac{2(N+1)}{\Delta} - \Delta \sum_{n=N+1}^{\infty} \frac{a_{n-N}}{n-N} g^{n-N-1}\Big), \\
&= \frac{(2g)^N\Delta^2}{(N+1)} K_N^-(N+\varepsilon)\bar{R}^{(N,+)}(g,\Delta;\varepsilon)\bar{R}^{(N,-)}(g,\Delta,\varepsilon).
\end{aligned}$$

Finally, using Lemma 2.8.4 we have

$$\begin{aligned}
\operatorname*{Res}_{x=N+\varepsilon} G_\varepsilon(x;g,\Delta) &= \frac{(2g)^N\Delta^2}{(N+1)} K_N^-(N+\varepsilon)T_\varepsilon^{(N)}(g,\Delta) \\
&= \frac{\Delta^2}{N!(N+1)!} P_N^{(N,\varepsilon)}((2g)^2,\Delta^2)T_\varepsilon^{(N)}(g,\Delta),
\end{aligned}$$

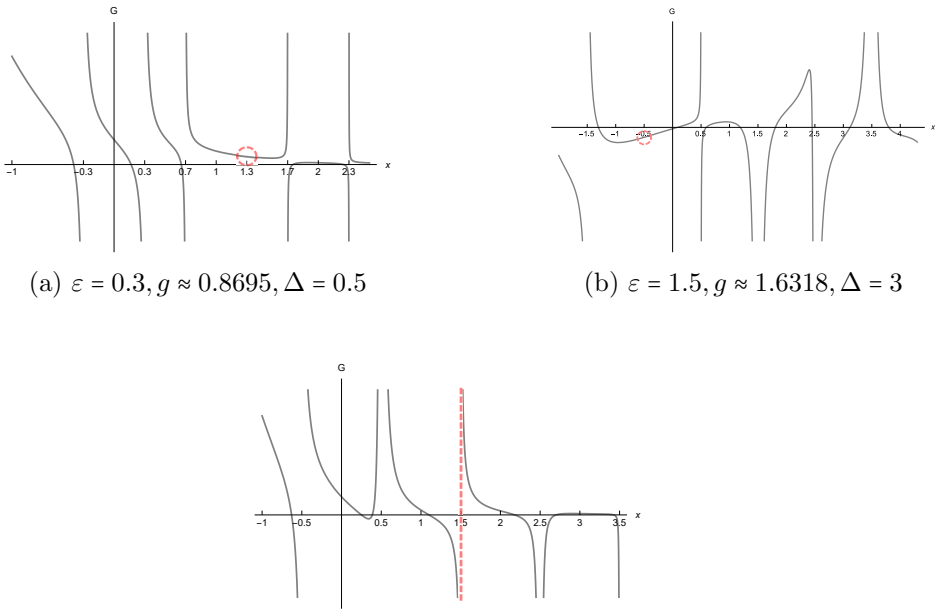
which is the desired result. □

Remark 4.3.2. We make a remark on the relation $(2g)^{k-1}a_k = \bar{K}_{N+k}^-(N+\varepsilon;g,\Delta,\epsilon)$ appearing in the proof of the proposition above. The coefficients $K_n^-(x;g,\Delta,\varepsilon)$ (and thus the numbers a_k) in the definition of the G-function $G_\varepsilon(x;g,\Delta)$ arise from the solution of the system of differential equations (2.2) by using the change of variable $y = g + z$ (instead of $y = \frac{g+z}{2g}$). The use of the change of variable $y = \frac{g+z}{2g}$ results on the system (2.4) compatible with the representation theoretical description of Proposition 2.4.2, and therefore we use the solutions arising from this system for the definition of the T-function $T_\varepsilon^{(N)}(g,\Delta)$ (see Section 2.7). We also note that it is possible to equivalently redefine the G-function $G_\varepsilon(x;g,\Delta)$ using the solutions of the system (2.4) (i.e. with the change of variable $y = \frac{g+z}{2g}$), however, we use the definition given in Section 2.6 since it is standard in the literature, including e.g., [5, 33, 45].

The proposition above completely characterizes the poles of the G-function for the case $\varepsilon \notin \frac{1}{2}\mathbb{Z}$ in terms of the exceptional spectrum of $H^{\varepsilon}_{\text{Rabi}}$. In particular, it shows that the function $G_\varepsilon(x; g, \Delta)$ is finite at points $x = N \pm \varepsilon\,(N \in \mathbb{Z}_{\geq 0})$ corresponding to non-Juddian exceptional eigenvalues $\lambda = N \pm \varepsilon - g^2$ (i.e. the parameters g and Δ are positive zeros of $T^{(N)}_\varepsilon(g, \Delta)$). This situation is illustrated in Figure 4.3(a) for the parameters $\varepsilon = 0.3, g \approx 0.8695, \Delta = 1/2$, showing the finite value of $G_{0.3}(x; g, 1/2)$ at $x = 1.3$. Here, $g \approx 0.8695$ is a root (computed numerically) of $T^{(1)}_{0.3}(g, 1/2)$. By Corollary 4.1.4, this value of g must be different to the value $g' \approx 0.5809$ in the Juddian case, which also has a finite value of $G_{0.3}(x; g', 1/2)$ at $x = 1.3$.

The following corollary justifies the claim that the exceptional eigenvalues $\lambda = N \pm \varepsilon - g^2$ vanish (or "kill") the poles of the G-function.

Corollary 4.3.3. *Suppose $\varepsilon \notin \frac{1}{2}\mathbb{Z}$ and let $N \in \mathbb{Z}_{\geq 0}$ and $\Delta > 0$ be fixed. Then, $H^{\varepsilon}_{\text{Rabi}}$ has the exceptional eigenvalue $\lambda = N \pm \varepsilon - g^2$ if and only if the G-function $G_\varepsilon(x, g, \Delta)$ does not have a pole at $x = N \pm \varepsilon$.* □



(a) $\varepsilon = 0.3, g \approx 0.8695, \Delta = 0.5$

(b) $\varepsilon = 1.5, g \approx 1.6318, \Delta = 3$

(c) $\varepsilon = 0.5, g \approx 1.3903, \Delta = 1$

Figure 4.3: Plot of $G_\varepsilon(x; g, \Delta)$ for parameters g and Δ corresponding to a non-Juddian eigenvalue $\lambda = 1 \pm \varepsilon - g^2$ (i.e. $T^{(1)}_{\pm\varepsilon}(g, \Delta) = 0$). A finite value of $G_\varepsilon(x; g, \Delta)$ at $x = 1 \pm \varepsilon$ is indicated by a red circle, while a simple pole at $x = 1 + \varepsilon$ is indicated with a red vertical line.

Next, we consider the case $\varepsilon = \ell/2\,(\ell \in \mathbb{Z}_{\geq 0})$. On the one hand, the functions $R^+(x; g, \Delta, \varepsilon)$ and $R^-(x; g, \Delta, \varepsilon)$ (resp. $\bar{R}^+(x; g, \Delta, \varepsilon)$ and $\bar{R}^-(x; g, \Delta, \varepsilon)$) have poles of order ≤ 1 at points $x = N + \ell/2\,(N \in \mathbb{Z}_{\geq 0})$. On the other hand, at points $x = N - \ell/2$ with $0 \leq N \leq \ell - 1$ only the functions $\bar{R}^+(x; g, \Delta, \varepsilon)$ and $\bar{R}^+(x; g, \Delta, \varepsilon)$ have poles of order ≤ 1. Consequently, the G-function $G_{\ell/2}(x; g, \Delta)$ has poles of order ≤ 1 at the points $x = N - \ell/2\,(0 \leq N \leq \ell - 1)$ and poles of order ≤ 2 at points $x = N + \ell/2\,(N \in \mathbb{Z}_{\geq 0})$.

Note that all possible poles of the G-function are accounted since $N = \ell + i\,(i \in \mathbb{Z}_{\geq 0})$ yields $x = N - \ell/2 = \ell + i - \ell/2 = i + \ell/2\,(i \in Z_{\geq 0})$. The residue at the poles of order ≤ 1 are given in the following proposition. The proof is identical to Proposition 4.3.1 and is therefore omitted.

Proposition 4.3.4. *Suppose $\ell > 1$ and let $1 \leq N < \ell$. Then any pole of the G-function $G_{\ell/2}(x; g, \Delta)$ at a point $x = N - \ell/2$ is simple. The residues of $G_{\ell/2}(x; g, \Delta)$ at the point $x = N - \ell/2$ is given by*

$$\operatorname*{Res}_{x=N-\ell/2} G_{\ell/2}(x; g, \Delta) = C(N)\Delta^2 P_N^{(N,-\ell/2)}((2g)^2, \Delta^2)\tilde{T}_{\ell/2}^{(N)}(g, \Delta)$$

with $C(N) = \frac{1}{N!(N+1)!}$.

Similar to the non half-integer case, the residues of $G_{\ell/2}(x; g, \Delta)$ at the points $x = N - \ell/2$ with $1 \leq N < \ell$ depend on the the constraint polynomial $P_N^{(N,-\ell/2)}((2g)^2, \Delta^2)$ and T-function $\tilde{T}_{\ell/2}^{(N)}(g, \Delta)$ for $1 \leq N < \ell$. However, by Proposition 3.3.5 $P_N^{(N,-\ell/2)}((2g)^2, \Delta^2)$ is positive for $g, \Delta > 0$, in other words, the pole vanishes (i.e. it is a removable singularity) if and only if $\tilde{T}_{\ell/2}^{(N)}(g, \Delta) = 0$, as illustrated in Figure 4.3(b).

In the following proposition we consider the remaining poles of $G_{\ell/2}(x; g, \Delta)$.

Proposition 4.3.5. *Suppose $\varepsilon = \ell/2\,(\ell \in \mathbb{Z}_{\geq 0})$ and let $N \in \mathbb{Z}_{\geq 0}$. Let*

$$G_{\ell/2}(x; g, \Delta) = \frac{A}{(x - N - \ell/2)^2} + \frac{B}{x - N - \ell/2} + H_{\ell/2}(x; \Delta, g)$$

for a function $H_{\ell/2}(x; \Delta, g)$ analytic at $x = N + \ell/2$. We have

$$A = C(N)C(N+\ell)\Delta^4 P_N^{(N,\ell/2)}((2g)^2, \Delta^2)P_{N+\ell}^{(N+\ell,-\ell/2)}((2g)^2, \Delta^2)T_{\ell/2}^{(N)}(g, \Delta)^2,$$

where $C(N)$ is defined as in Proposition 4.3.1, and

$$\begin{aligned}
B &= \operatorname*{Res}_{x=N+\ell/2} G_{\ell/2}(x; g, \Delta) \\
&= C(N)C(N+\ell)\Delta^2 P_N^{(N,\ell/2)}((2g)^2, \Delta^2) \\
&\times\Big[\frac{1}{C(N+\ell)}\Big(\bar{R}^{(N,-)}(g, \Delta, \frac{\ell}{2})(\Delta\bar{Q}^+(N + \frac{\ell}{2}; g, \Delta)) - R^{(N,-)}(g, \Delta, \frac{\ell}{2})Q^+(N + \frac{\ell}{2}; g, \Delta)\Big) \\
&+ A_N^\ell((2g)^2, \Delta^2)\frac{1}{C(N)}\Big(\bar{R}^{(N,+)}(g, \Delta, \frac{\ell}{2})(\Delta\bar{Q}^-(N + \frac{\ell}{2}; g, \Delta)) - R^{(N,+)}(g, \Delta, \frac{\ell}{2})Q^-(N + \frac{\ell}{2}; g, \Delta)\Big)\Big],
\end{aligned}$$

where $Q^+(x; g, \Delta)$ is defined by $Q^+(x; g, \Delta) = R^+(x; g, \Delta) - \frac{\operatorname{Res}_{x=N+\ell/2} R^+(x;g,\Delta)}{x-N-\ell/2}$. The functions $\bar{Q}^+(x; g, \Delta)$, $Q^-(x; g, \Delta)$ and $\bar{Q}^-(x; g, \Delta)$ are defined similarly.

Proof. To compute the term A we notice that since each of the factors $R^+(x)$ and $R^-(x)$ (resp. $\bar{R}^+(x)$ and $\bar{R}^-(x)$) can have a pole of order exactly one (simple pole) we have

$$\lim_{x\to N+\ell/2}(x - N - \ell/2)^2 R^+(x)R^-(x) = \operatorname*{Res}_{x=N+\ell/2} R^+(x) \operatorname*{Res}_{x=N+\ell/2} R^-(x),$$

and then the proof follows as in Proposition 4.3.1. The second claim follows from the basic identity

$$\operatorname*{Res}_{x=a}\left(\frac{R_1}{x-a}+A_1(x)\right)\left(\frac{R_2}{x-a}+A_2(x)\right)=R_1A_2(a)+R_2A_1(a),$$

valid for functions $A_1(x)$, $A_2(x)$ analytic at $x=a$ and $R_1,R_2\in\mathbb{C}$. □

By comparing the defining recurrence relations of $R^{\pm}(x;g,\Delta)$ and $\bar{R}^{\pm}(x;g,\Delta)$ with the residues (computed in the proof of Proposition 4.3.1) the functions $Q^-(x;g,\Delta)$, $Q^+(x;g,\Delta)$, $\bar{Q}^-(x;g,\Delta)$ and $\bar{Q}^+(x;g,\Delta)$ can also be expressed by recurrence relations. Namely, if we set $s_{-1}(x;g,\Delta)=0$, $s_0(x;g,\Delta)=1$ and

$$s_k(x;g,\Delta)=\begin{cases}\frac{1}{k}\left(f^-_{k-1}(x,g,\Delta,\varepsilon)s_{k-1}(x;g,\Delta)-s_{k-2}(x;g,\Delta)\right) & \text{if } k\neq N+1,\\ \frac{1}{N+1}\left(\left(2g+\frac{N-x-\ell/2}{2g}\right)s_N(x;g,\Delta)-s_{N-1}(x;g,\Delta)\right) & \text{if } k=N+1,\end{cases}$$

then we have

$$Q^-(x;g,\Delta)=\sum_{n=0}^{\infty}s_n(x;g,\Delta)g^n,\qquad \bar{Q}^-(x;g,\Delta)=\sum_{\substack{n\geq 0\\ n\neq N}}\frac{s_n(x;g,\Delta)}{x-n-\ell/2}g^n. \tag{4.17}$$

Similarly, setting $r_{-1}(x;g,\Delta)=0$, $r_0(x;g,\Delta)=1$ and

$$r_k(x;g,\Delta)=\begin{cases}\frac{1}{k}\left(f^+_{k-1}(x,g,\Delta,\varepsilon)r_{k-1}(x;g,\Delta)-r_{k-2}(x;g,\Delta)\right) & \text{if } k\neq N+\ell+1,\\ \frac{1}{N+\ell+1}\left(\left(2g+\frac{N-x+\ell/2}{2g}\right)r_{N+\ell}(x;g,\Delta)-r_{N+\ell-1}(x;g,\Delta)\right) & \text{if } k=N+\ell+1,\end{cases}$$

we have

$$Q^+(x;g,\Delta)=\sum_{n=0}^{\infty}r_n(x;g,\Delta)g^n,\qquad \bar{Q}^+(x;g,\Delta)=\sum_{\substack{n\geq 0\\ n\neq N+\ell}}\frac{r_n(x;g,\Delta)}{x-n+\ell/2}g^n. \tag{4.18}$$

Note that by Theorem 4.1.1, when $\lambda=N+\ell/2-g^2$ is a Juddian eigenvalue, the coefficients of the poles of $G_{\ell/2}(x;g,\Delta)$ vanish and the function $G_{\ell/2}(x;g,\Delta)$ has a finite value at $x=N+\ell/2$. However, it is possible to find numerically examples of parameters such that $G_{\ell/2}(x;g,\Delta)$ has a pole at $x=N+\ell/2$ yet $\lambda=N+\ell/2-g^2$ is a non-Juddian exceptional eigenvalue. One such example is shown in Figure 4.3(c) for the parameters $\varepsilon=1/2, g\approx 1.3903, \Delta=1$. In this case, there is a pole of $G_{1/2}(x;g,1)$ even though the parameters g and Δ correspond (numerically) to a zero of $T^{(1)}_{1/2}(g,1)$ at $x=1.5$. We remark that the pole $x=1.5$ must be simple. Indeed, in the notation of Proposition 4.3.5, since $T^{(1)}_{1/2}(g,1)=0$ the second order term A vanishes while the residue term B is non-vanishing. This is also apparent in the graph of $G_{1/2}(x;g,1)$ in Figure 4.3(c), since the lateral limits at $x=1.5$ have different signs the pole must be simple and the term B must be non-zero in a neighborhood of $x=1.5$.

The situation for the poles of the $G_{\ell/2}(x;g,\Delta)$ is summarized in the following result.

Corollary 4.3.6. *Suppose $\ell\in\mathbb{Z}_{\geq 0}$ and let $\Delta>0$ be fixed. The G-function $G_{\ell/2}(x;g,\Delta)$ has ℓ poles of order ≤ 1 at $x=N-\ell/2$ for $0\leq N<\ell$ and poles of order ≤ 2 at $x=N+\ell/2$ for $N\in\mathbb{Z}_{\geq 0}$. Moreover, for $N\in\mathbb{Z}_{\geq 0}$, we have:*

- *If $\lambda = N \pm \ell/2 - g^2$ is a Juddian eigenvalue of $H^{\ell/2}_{\text{Rabi}}$, then $x = N \pm \ell/2$ is not a pole of $G_{\ell/2}(x; g, \Delta)$.*
- *For $0 \leq N < \ell$, the function $G_{\ell/2}(x; g, \Delta)$ does not have a pole at $x = N - \ell/2$ if and only if $\lambda = N - \ell/2 - g^2$ is a non-Juddian exceptional eigenvalue of $H^{\ell/2}_{\text{Rabi}}$.*
- *If $G_{\ell/2}(x; g, \Delta)$ has a simple pole at $x = N + \ell/2$, then $\lambda = N + \ell/2 - g^2$ is a non-Juddian exceptional eigenvalue of $H^{\ell/2}_{\text{Rabi}}$.*
- *If $G_{\ell/2}(x; g, \Delta)$ has a double pole at $x = N \pm \ell/2$, then there is no exceptional eigenvalue $\lambda = N \pm \ell/2 - g^2$ of $H^{\ell/2}_{\text{Rabi}}$.*

Remark 4.3.7. In the case of the QRM (i.e. $\varepsilon = 0$), all the singularities of the G-function $G_0(x; g, \Delta)$ are of the type described in Proposition 4.3.5 (i.e. poles of order ≤ 2).

Note that is possible that non-Juddian exceptional eigenvalues corresponding to finite values of $G_{\ell/2}(x; g, \Delta)$ at points $x = N \pm \varepsilon$ are present in the spectrum. If such eigenvalues were to exist then the structure of the poles of the G-function alone would not be sufficient to completely discriminate the structure of the exceptional spectrum.

4.4 Generalized G-function and spectral determinant

In the paper of Li and Batchelor [34](p. 4), the authors define a new G-function $\mathcal{G}_\varepsilon(x; g, \Delta)$ for numerical computation of the spectrum of the AQRM. The new definition uses a divergent product to make the function $\mathcal{G}_\varepsilon(x; g, \Delta)$ vanish for all eigenvalues of AQRM, including the exceptional ones (i.e. at $x = N \pm \varepsilon$). We note that, however, it is not well-defined theoretically due to the use of the divergent product. Nevertheless, according to the following theorem, the numerical observation in [34] by taking a certain truncation of the divergent product does, in fact, works properly. To obtain a correct understanding, we use the gamma function $\Gamma(x)$ to alternatively define the new G-function $\mathcal{G}_\varepsilon(x; g, \Delta)$.

Definition 4.4.1. *The generalized G-function of the AQRM is*

$$\mathcal{G}_\varepsilon(x; g, \Delta) := G_\varepsilon(x; g, \Delta)\Gamma(\varepsilon - x)^{-1}\Gamma(-\varepsilon - x)^{-1}. \tag{4.19}$$

As a consequence of our discussion above on the poles of the G-function, we can establish the claim made in [34].

Theorem 4.4.2. *For fixed $g, \Delta > 0$, x is a zero of $\mathcal{G}_\varepsilon(x; g, \Delta)$ if and only if $\lambda = x - g^2$ is an eigenvalue of $H^{\varepsilon}_{\text{Rabi}}$.*

Proof. The statement for regular eigenvalues is clear since the factor $\Gamma(\varepsilon - x)^{-1}\Gamma(-\varepsilon - x)^{-1}$ does not contribute any further zeros in this case. Next, suppose $\varepsilon \notin \frac{1}{2}\mathbb{Z}$. Then, the point $x = N + \varepsilon$ is a simple zero of $\Gamma(\varepsilon - x)^{-1}$, therefore $\mathcal{G}_\varepsilon(N + \varepsilon; g, \Delta) = C \operatorname{Res}_{x=N+\varepsilon} G_\varepsilon(x; g, \Delta)$ for a nonzero constant $C \in \mathbb{C}$ and the result follows from Proposition 4.3.1. In the case of $\varepsilon = \ell/2\,(\ell \in \mathbb{Z}_{\geq 0})$, the result for $x = N - \ell/2$ with

$0 \le N < \ell$ follows by Proposition 4.3.4 in the same way as the case $\varepsilon \notin \frac{1}{2}\mathbb{Z}$. Similarly, notice that the double zero of $\Gamma(\ell/2-x)^{-1}\Gamma(-\ell/2-x)^{-1}$ at $x = N+\ell/2$ ($N \in \mathbb{Z}_{\ge 0}$) makes $\mathcal{G}_\varepsilon(x;g,\Delta)$ equal (up to a nonzero constant) to the coefficient A of $(x-N-\ell/2)^{-2}$ in the Laurent expansion of $G_\varepsilon(x;g,\Delta)$ at $x = N+\ell/2$ given in Proposition 4.3.5. Hence the theorem follows. □

We now recall the so-called spectral determinant of the Hamiltonian $H^\varepsilon_{\mathrm{Rabi}}$ of the AQRM. Let $\lambda_0 < \lambda_1 \le \lambda_2 \le \lambda_3 \le \lambda_4 \le \dots$ be the set of all eigenvalues of the Hamiltonian $H^\varepsilon_{\mathrm{Rabi}}$ of the AQRM. Here note that the first eigenvalue λ_0 is always simple (see the proof of Corollary 4.1.4). Then the Hurwitz-type spectral zeta function of the AQRM is defined by

$$\zeta_{H^\varepsilon_{\mathrm{Rabi}}}(s,\tau) = \sum_{i=0}^{\infty}(\tau-\lambda_i)^{-s}, \quad \mathrm{Re}(s) > 1. \tag{4.20}$$

Here we fix the log-branch by $-\pi \le \arg(\tau-\lambda_i) < \pi$. We then define the zeta regularized product (cf. [46]) over the spectrum of the AQRM as

$$\prod_{i=0}^{\infty}(\tau-\lambda_i) := \exp\Big(-\frac{d}{ds}\zeta_{H^\varepsilon_{\mathrm{Rabi}}}(s,\tau)\Big|_{s=0}\Big). \tag{4.21}$$

We can prove that $\zeta_{H^\varepsilon_{\mathrm{Rabi}}}(s,\tau)$ is holomorphic at $s=0$ by the same way as in the case of the QRM[55]. Actually, the meromorphy of $\zeta_{H^\varepsilon_{\mathrm{Rabi}}}(s,\tau)$ in the whole plane $\mathbb{C}$ follows in a similar way to the case H^0_{Rabi}. As the notation may indicate that this regularized product is an entire function possessing its zeros exactly at the eigenvalues of $H^\varepsilon_{\mathrm{Rabi}}$. Now define the spectral determinant of the AQRM $\det H^\varepsilon_{\mathrm{Rabi}}$ as

$$\det(\tau - H^\varepsilon_{\mathrm{Rabi}}) := \prod_{i=0}^{\infty}(\tau-\lambda_i). \tag{4.22}$$

The following result follows immediately from Theorem 4.4.2.

Corollary 4.4.3. *There exists an entire nonvanishing function $c(\tau;g,\Delta)$ such that*

$$\det(\tau - g^2 - H^\varepsilon_{\mathrm{Rabi}}) = c(\tau;g,\Delta)\,\mathcal{G}_\varepsilon(\tau;g,\Delta). \tag{4.23}$$

4.5 Exceptional solutions and irreducible representations of $\mathfrak{sl}_2$

The relation between polynomial solutions, or quasi-exact, solutions and representations of linear groups was observed first by Turbiner in [59] where he showed the relation of said solutions with the existence of certain finite-dimensional representations of the Lie group $SL_2(\mathbb{R})$ (or $SL_2(\mathbb{C})$). In this section, we describe how the solutions of the AQRM fit in the $\mathfrak{sl}_2$-representation picture of the AQRM (cf. §2.4). In particular, we prove that to a solution ϕ of the system (2.4), corresponding to a solution of the eigenvalue problem of the asymmetric quantum Rabi model, there is a vector v satisfying

$$\varpi_{1,a}(\mathcal{K})v = \Lambda_a v. \tag{4.24}$$

for particular parameter $a \in \mathbb{C}$. More importantly, the vector v correspond to an irreducible module (or a subquotient of irreducible modules) of $\mathfrak{sl}_2$. For the case of regular solutions, we refer the reader to [63].

Juddian eigenvalues

From the Juddian solutions we can construct an corresponding eigenvector v captured in the finite dimensional irreducible submodules $\mathbf{F}_{2m}$ (or $\mathbf{F}_{2m+1}$) of $\varpi_{j,a}$. For instance, define $v^+ := y^{-m-\frac{1}{4}}\phi_{1,+}(y)$, where

$$\phi_{1,+}(y) = \frac{4g^2 K_{2m-1}^{(N,\varepsilon)}}{\Delta} y^{2m} - \Delta \sum_{n=0}^{2m-1} \frac{K_n^{(N,\varepsilon)}}{n-2m} y^n.$$

We claim that the vector v^+ is a non-zero eigenvector corresponding to the eigenvalue problem

$$\varpi_{1,-2m}(\mathcal{K}) v_{\phi_1}^+ = \Lambda_{-2m} v_{\phi_1}^+. \tag{4.25}$$

To see this, it is enough to compute the recurrence relation satisfied by the solution of the eigenvalue problem (the computation follows like in Section 5.1 of [63]). Concretely, let $v = \sum_{n\in\mathbb{Z}} a_n e_{1,n}$ be a solution of $(\varpi_{1,-2m}(\mathcal{K}) - \Lambda_{-2m})\, v = 0$, then from the definition of the representation $\varpi_{1,-2m}$ the coefficients $\{a_n\}_{n\in\mathbb{Z}}$ must satisfy

$$\begin{aligned}(m+n+1)(m-n-1)a_{n+1} + \left((m-n)^2 - 4g^2(m-n) + 2\varepsilon(m-n) - \Delta^2\right) a_n \\ + 4g^2(m-n+1)a_{n-1} = 0.\end{aligned}$$

By shifting the index n by m, and relabeling the equation becomes

$$(2m+n+1)(n+1)a_{n+1} + \left(-n^2 - 4g^2 n + 2\varepsilon n + \Delta^2\right) a_n - 4g^2(n-1)a_{n-1} = 0. \tag{4.26}$$

Note that the coefficient of $v_{\phi_1}^+$ corresponding to the basis vector $e_{1,m+n}$ ($n \in \mathbb{Z}_{\geq 0}$) is $-\Delta K_{2m+n}^{(N,\varepsilon)})/n$, therefore by plugging these coefficients into (4.26) we get

$$(2m+n+1)\bar{K}_{2m+n+1}^{(N,\varepsilon)} + \left(-n - 4g^2 + 2\varepsilon + \frac{\Delta^2}{n}\right)\bar{K}_{2m+n}^{(N,\varepsilon)} - 4g^2 \bar{K}_{2m+n-1}^{(N,\varepsilon)} = 0,$$

which is equivalent to recurrence (2.20). This means that v^+ is an eigenvector, thus proving the claim. On the other hand, we directly note that $v^+ \in \mathbf{F}_{2m+1}$ as an irreducible submodule of $\mathbf{V}_{1,-2m}$. The remaining cases are similar, and we refer the reader to [63] for the complete description.

Non-Juddian exceptional eigenvalues

We begin with the solution corresponding to the larger exponent from §2.7. For $N = 2m$, define

$$v_{\phi_1}^+ := y^{\frac{1}{2}(a-\frac{1}{2})}\phi_{1,+}(y) = y^{-m-\frac{1}{4}}\phi_{1,+}(y) = \frac{2m+1}{\Delta}\bar{K}_{2m+1}^{(N,\varepsilon)} e_{1,m} - \Delta \sum_{n=2m+1}^{\infty} \frac{\bar{K}_n^{(N,\varepsilon)}}{n-2m} e_{1,n-m}, \tag{4.27}$$

where $\phi_{1,+}$ is the solution (2.24).

Similar to the Juddian case, we first verify that the vector $v_{\phi_1}^+$ is a non-zero eigenvector corresponding to the eigenvalue problem

$$\varpi_{1,-2m}(\mathcal{K}) v_{\phi_1}^+ = \Lambda_{-2m} v_{\phi_1}^+. \tag{4.28}$$

With the same notation as in the Juddian case, we note that the coefficient of $v^+_{\phi_1}$ corresponding to the basis vector $e_{1,m+n}$ ($n \in \mathbb{Z}_{\geq 0}$) is $-\Delta(\bar{K}^{(N,\varepsilon)}_{2m+n})/n$, and thus upong substitution in (4.26), we obtain

$$(2m+n+1)\bar{K}^{(N,\varepsilon)}_{2m+n+1} + \left(-n - 4g^2 + 2\varepsilon + \frac{\Delta^2}{n}\right)\bar{K}^{(N,\varepsilon)}_{2m+n} - 4g^2\bar{K}^{(N,\varepsilon)}_{2m+n-1} = 0,$$

which is equivalent to recurrence (2.25).

In order to identify the vector $v^+_{\phi_1}$ as a vector in an irreducible module we make use of the results of Section 1.3. There is an intertwining operator A_a between the representations $(\varpi_{1,a}, \mathbf{V}_{1,a})$, and $(\varpi_{1,2-a}, \mathbf{V}_{1,2-a})$ for $a \notin 2\mathbb{Z}$ (see [63]). The isomorphism $A_a : \mathbf{V}_{1,a} \to \mathbf{V}_{1,2-a}$ ($\mathbf{V}_{1,a} = \mathbf{V}_{1,2-a} = \mathbf{V}_1$) is explicitly given with respect to the basis $\{e_{1,n}\}_{n\in\mathbb{Z}}$) by the diagonal matrix

$$A_a = \mathrm{Diag}(\cdots, c_{-n}, \cdots, c_0, \cdots, c_n, \cdots),$$

with $c_0 \neq 0$ and

$$c_n = \left(A_a\right)_n = c_0 \prod_{k=1}^{|n|} \frac{k - \frac{a}{2}}{k - 1 + \frac{a}{2}}.$$

Recall from Lemma 1.3.1, for $a = -2m$ ($m \in \mathbb{Z}_{>0}$), there is an isomorphism

$$\mathbf{V}_{1,-2m}/\mathbf{F}_{2m+1} \simeq \mathbf{D}^-_{2(m+1)} \oplus \mathbf{D}^+_{2(m+1)} \subset \mathbf{V}_{1,2(m+1)}. \tag{4.29}$$

In fact, from the expression of the intertwiner A_a ($a \notin 2\mathbb{Z}$), we can construct the linear isomorphism $\tilde{A}_{-2m}$ of (4.29) by defining $\tilde{A}_{-2m} := \frac{1}{4\pi}\lim_{a\to -2m}\sin(2\pi a)A_a$, multiplication being elementwise. Then, as we may take $c_0 = 1$, we have

$$\left(\tilde{A}_{-2m}\right)_n = \begin{cases} (2m+1)\prod_{k=1,\,k\neq m+1}^{|n|} \frac{k+m}{k-m-1} & \text{if } |n| > m \\ 0 & \text{if } |n| \leq m. \end{cases} \tag{4.30}$$

Since $e_{1,m} \in \mathrm{Ker}\,\tilde{A}_{-2m}$, we have $\tilde{A}_{-2m}v^+_{\phi_1} \in \mathbf{D}^-_{2(m+1)} \oplus \mathbf{D}^+_{2(m+1)}$. Hence, it follows from the formula

$$\begin{aligned}\tilde{A}_{-2m}v^+_{\phi_1} &= -\Delta \sum_{n=2m+1}^{\infty} \frac{\bar{K}^{(N,\varepsilon)}_n}{n-2m}\tilde{A}_{-2m}e_{1,n-m} \\ &= -\Delta(2m+1)\sum_{n=m+1}^{\infty}\frac{\bar{K}^{(N,\varepsilon)}_{n+m}}{n-m}\prod_{k=1,\,k\neq m+1}^{n}\frac{k+m}{k-m-1}e_{1,n}\end{aligned}$$

that $\tilde{A}_{-2m}v^+_{\phi_1} \in \mathbf{D}^+_{2(m+1)}$.

By definition, if $v \in \mathbf{V}_{1,-2m}$ is a solution of $(\varpi_{1,-2m}(\mathcal{K}) - \Lambda_{-2m})v = 0$, then $\tilde{A}_{-2m}v \in \mathbf{V}_{1,2(m+1)}$ satisfies $(\varpi_{1,2(m+1)}(\mathcal{K}) - \Lambda_{-2m})\tilde{A}_{-2m}v = 0$.

The discussion above is summarized in the following theorem.

Theorem 4.5.1. *Let $N \in \mathbb{Z}_{\geq 0}$, $\Delta > 0$ and $T^{(N)}_\varepsilon(g,\Delta)$ the constraint T-function defined in §4.2. If g is a positive zero of $T^{(N)}_\varepsilon(g,\Delta)$, we have a non-degenerate non-Juddian exceptional eigenvalue $\lambda = N + \varepsilon - g^2$. Furthermore:*

- *If $N = 2m$, let $v^+_{\phi_1} \in \mathbf{V}_{1,-2m}$ be as in (4.27). Then $w := \tilde{A}_{-2m}v^+_{\phi_1}$ is a solution to the eigenproblem $(\varpi_{1,2(m+1)}(\mathcal{K}) - \Lambda_{-2m})w = 0$ and $w \in \mathbf{D}^+_{2(m+1)}$.*

- *If $N = 2m-1$, let $v^+_{\phi_1} \in \mathbf{V}_{2,1-2m}$ be as described above. Then $w := \tilde{A}_{1-2m} v^+_{\phi_1}$ is a solution of the eigenproblem $(\varpi_{2,2m+1}(\mathcal{K}) - \Lambda_{1-2m})w = 0$ and $w \in \mathbf{D}^+_{2m+1}$.*

Let $N \in \mathbb{Z}_{\geq 0}$, $\Delta > 0$ and $\tilde{T}^{(N)}_{\varepsilon}(g,\Delta)$ the constraint T-function defined in §4.2. If g is a zero of $\tilde{T}^{(N)}_{\varepsilon}(g,\Delta)$, we have a non-degenerate non-Juddian exceptional eigenvalue $\lambda = N - \varepsilon - g^2$. Furthermore:

- *If $N = 2m$, let $v^+_{\phi_2} \in \mathbf{V}_{2,1-2m}$ be as described above. Then $w := \tilde{A}_{1-2m} v^+_{\phi_2}$ is a solution to the eigenproblem $(\varpi_{2,2m+1}(\tilde{\mathcal{K}}) - \tilde{\Lambda}_{1-2m})w = 0$ and $w \in \mathbf{D}^+_{2m+1}$.*
- *If $N = 2m+1$, let $v^+_{\phi_2} \in \mathbf{V}_{1,-2m}$ be as described above. Then $w := \tilde{A}_{-2m} v^+_{\phi_2}$ is a solution of the eigenproblem $(\varpi_{1,2(m+1)}(\tilde{\mathcal{K}}) - \tilde{\Lambda}_{-2m})w = 0$ and $w \in \mathbf{D}^+_{2(m+1)}$.*

Proof. In the foregoing discussion we proved the case for $\lambda = N + \varepsilon - g^2$ and $N = 2m$. The remaining cases are proved in a similar manner, so we leave the proof of those cases to the reader (for the computations, see Section 5 of [63]). □

Remark 4.5.2. The eigenvector corresponding to the non-Juddian exceptional solutions corresponding to $N = 0$ in the proof of Corollary 4.1.4 is captured in the limit of discrete series $\mathbf{D}^+_1$.

To conclude this chapter, we summarize the relation between solutions of the QRM, constraint relations and irreducible representations of $\mathfrak{sl}_2$ in Table 4.1.

Table 4.1: Correspondence of spectrum, irreducible representations and constraint relations

Type	**Eigenvalue**[d]		**Rep. of $\mathfrak{sl}_2$**	**C**onstraint relation
Juddian[c]	$N \pm \varepsilon - g^2$	$\Leftrightarrow$	$\mathbf{F}_m$: finite dim. irred. rep.[a]	$P^{(N,\pm\varepsilon)}_N((2g)^2, \Delta^2) = 0$
Non-Juddian exceptional	$N \pm \varepsilon - g^2$	$\Leftrightarrow$	$\mathbf{D}^+_m$: irred. lowest weight rep.[b]	$T^{(N)}_{\pm\varepsilon}(g,\Delta) = 0$
Regular	$x \pm \varepsilon - g^2$	$\Leftrightarrow$	$\varpi_{j,a}$: irred. principal series	$G_\varepsilon(x; g, \Delta) = 0$

[a] Determination of m in $\mathbf{F}_m$. Case $N + \varepsilon$: $m = N + 1$. Case $N - \varepsilon$: $m = N$.
[b] Determination of m in $\mathbf{D}^+_m$ for the first component of the solution (see Theorem 4.5.1). Case $N + \varepsilon$: $m = N + 2$. Case $N - \varepsilon : m = N + 1$.
[c] Case $\varepsilon \in \frac{1}{2}\mathbb{Z}$: Non-Juddian exceptional solutions are non-degenerate. Juddian solutions are always degenerate (e.g. corresponding to the space $\mathbf{F}_m \oplus \mathbf{F}_{m+1}$ when $\varepsilon = 0$. See [63] for general $\varepsilon = \ell/2$).
[d] Constants: $N \in \mathbb{Z}_{\geq 0}$, $x \notin \mathbb{Z}_{\geq 0}$.

5. Continued fractions expansions of e^n arising from orthogonal polynomials related to the AQRM

In this chapter we present a continued fraction expansion of e that appeared in the study of constraint polynomials of the AQRM. The results in this section hold no relation to the study of the spectrum of the AQRM but are an example of the rich mathematical structure found therein that may be interesting to the general mathematical audience.

To the author's best knowledge, the continued fraction expansions of e and e^n presented here have not been published before.

5.1 A continued fraction expansion for e

In this section we present the continued fraction expansion for the Napier constant (or Euler's number)

$$\boxed{e = 3 - \cfrac{1}{4 - \cfrac{2}{5 - \cfrac{3}{6 - \cfrac{4}{7 - \cdots}}}},} \tag{5.1}$$

appearing in the study of the polynomials $P_k^{(N,\varepsilon)}(x,y)$.

Recall some well-known continued fraction expansions of e. For instance (c.f. Appendix A of [35]),

$$e = 2 + \frac{1}{1} \underset{+}{} \frac{1}{2} \underset{+}{} \frac{1}{1} \underset{+}{} \frac{1}{1} \underset{+}{} \cdots,$$
$$e = 2 + \frac{2}{2} \underset{+}{} \frac{3}{3} \underset{+}{} \frac{4}{4} \underset{+}{} \frac{5}{5} \underset{+}{} \cdots,$$
$$e = 1 + \frac{2}{1} \underset{+}{} \frac{1}{6} \underset{+}{} \frac{1}{10} \underset{+}{} \frac{1}{14} \underset{+}{} \cdots.$$

By comparing convergents, we notice that the continued fraction (5.1) is not obtained from an equivalent transformation of these continued fractions.

Denote by $C_n = P_n/Q_n$ the n-th convergent of (5.1). Notice that since the partial numerators are negative, all the convergents are monotonically decreasing. The first convergents are given by

$$C_0 = 3, \quad C_1 = \frac{11}{4}, \quad C_2 = \frac{49}{18}, \quad C_3 = \frac{87}{32}, \quad C_4 = \frac{1631}{600}, \quad C_5 = \frac{11743}{4320}.$$

The difference between two successive convergents is

$$C_1 - C_0 = \frac{-1}{4}, \quad C_2 - C_1 = \frac{-1}{36}, \quad C_3 - C_2 = \frac{-1}{784}, \quad C_4 - C_3 = \frac{-1}{2400}, \dots$$

In general (see Proposition 5.3.4), the absolute value of the numerators of the differences is 1, similar to the case of regular continued fractions.

The convergence of the continued fraction is faster than the regular continued fraction. In fact, in Corollary 5.3.5, we see that

$$|e - C_k| = O\left(\frac{1}{k!(k+1)^2(k+2)^2)}\right).$$

The continued fraction expansion (5.1) for e can be extended to a continued fraction for positive integer powers e^n and similar properties hold in this general case. In Section 5.2, we explain how the continued fraction expansion (5.1) appears in relation with the study of constraint polynomials of the AQRM. In Section 5.3 we establish the above results in general and relate the result to a continued fraction expansion of the incomplete gama function.

The notation $\mathcal{K}_{k=1}^{\infty}(\frac{a_n}{b_n})$ stands for the continued fraction with partial numerators a_n and partial denominators b_n.

5.2 Motivation: Orthogonal polynomials related to the AQRM

In this section, we consider a set of orthogonal polynomials related to the polynomials $P_k^{(N,\varepsilon)}(x,y)$ appearing in the study of the degeneracy of the eigenvalues of the AQRM.

By setting $k = N+1$ in Definition 2.8.1, we see at once that $P_N^{(N,\epsilon)}(x,y)$ divides $P_{N+1}^{(N,\epsilon)}(x,y)$ and, in general, $P_{N+k}^{(N,\epsilon)}(x,y)$ for $k \in \mathbb{N}$. Thus, for a fixed $N \in \mathbb{N}$, we define the polynomials

$$Q_k^{(N,\epsilon)}(x,y) = \frac{P_{N+k}^{(N,\epsilon)}(x,y)}{P_N^{(N,\epsilon)}(x,y)}.$$

These polynomials satisfy, by definition, the recurrence relation

$$\begin{aligned} Q_k^{(N,\epsilon)}(y) = (y + (N+k)(x - (N+k) - 2\epsilon))Q_{k-1}^{(N,\epsilon)}(y) - \\ + (N+k)(N+k-1)(k-1)(-x)Q_{k-2}^{(N,\epsilon)}(y) \end{aligned}$$

for $k \geq 1$, with initial conditions $Q_{-1}^{(N,\epsilon)}(y) = 0$ and $Q_0^{(N,\epsilon)}(y) = 1$.

By Favard's theorem, for a fixed $x < 0$, the set $\{Q_k^{(N,\epsilon)}\}$ form a system of orthogonal polynomials (OPS) with respect to y. The associated moment functional of the OPS is denoted by $\mathcal{L}$. We note that the moment functional depends on the parameters N, ϵ, x but we omit them from the notation for simplicity.

Let

$$\begin{aligned} \lambda_1 &= 1 \\ \lambda_k &= (N+k)(N+k-1)(k-1)(-x) \\ c_k &= (N+k)(-x + (N+k) + 2\epsilon), \end{aligned}$$

then, we have

$$\mathcal{L}[1] = 1, \qquad \mathcal{L}[Q_m^{(N,\epsilon)} Q_n^{(N,\epsilon)}] = 0,$$
$$\mathcal{L}[(Q_k^{(N,\epsilon)})^2] = (1)_k (N+2)_k (N+1)_k (-x)^k$$

for $m \neq n$. In fact, it is not difficult to see that

$$f(t) = {}_2F_1(N+2, N+1; 1; -xt)$$

is an exponential generating function for

$$\frac{\mathcal{L}[(Q_k^{(N,\epsilon)})^2]}{(k!)^2}.$$

For $\ell \in \mathbb{N}$, the relation

$$A_N^\ell(x,y) = \sum_{j=0}^{\ell} \binom{\ell}{j} \frac{(N+\ell)!(N+\ell+1)!}{(N+j)!(N+j+1)!} Q_j^{(N,\ell/2)}(x,y), \tag{5.2}$$

holds (see [27], Remark 7.2). This is the Fourier expansion of the polynomials $A_N^\ell(x,y)$ in terms of the basis $\{Q_k^{(N,\ell)}\}_{k\geq 0}$.

From general theory (see e.g. [10]) we know that the polynomials $Q_k^{(N,\epsilon)}(y)$ are the denominators of the convergents $C_n(y)$ of the continued fraction

$$\cfrac{\lambda_1}{y - c_1 - \cfrac{\lambda_2}{y - c_2 - \cfrac{\lambda_3}{y - c_3 - \cfrac{\lambda_4}{y - c_4 - \cdots}}}}.$$

In addition, it is interesting to study the analytic function $F(x,y,N,\epsilon)$ obtained as the limit of the convergentes $\lim_{n\to\infty} C_n(y)$. In general, this is complicated problem, however for the case $y = 0$ we can obtain an expression of this functions using elementary methods.

For $y = 0$, the function $F(x,y,N,\epsilon)$ is given by

$$F(x,0,N,\epsilon) = \cfrac{1}{-(N+1)(N+1+2\epsilon-x)) - \cfrac{2(N+1)(N+2)(-x)}{-(N+2)(N+2+2\epsilon-x) - \dots}},$$

applying the equivalent transformation given by the sequence $\beta_i = -\frac{1}{N+i}$, we obtain

$$F(x,0,N,\epsilon) = \frac{1}{(N+1)(-x)} \mathop{\mathcal{K}}_{k=1}^{\infty} \left(\frac{kx}{N+k+2\epsilon-x} \right).$$

Proposition 5.2.1. *For $x \neq 0$ and $-(N+2\epsilon) \notin \mathbb{N}_0$, we have*

$$F(x,0,N,\epsilon) = \frac{1}{(N+1)(-x)}\left(x - (N+2\epsilon) + \frac{N+2\epsilon}{{}_1F_1(1;N+1+2\epsilon;x)}\right),$$

and, when $-(N+2\epsilon) \notin \mathbb{N}_0$, we have

$$F(x,0,N,\epsilon) = \frac{x-(N+2\epsilon)}{(N+1)(-x)},$$

Proof. Note that when $-(N+2\epsilon) \notin \mathbb{N}_0$, the continued fraction (T-fraction) expansion of ${}_1F_1(1;N+1+2\epsilon;x)$ (see [11]) is given by

$${}_1F_1(1;N+1+2\epsilon;x) = \frac{N+2\varepsilon}{N+2\varepsilon-x} + \mathop{\mathcal{K}}_{k=1}^{\infty}\left(\frac{kx}{N+k+2\epsilon-x}\right),$$

from where the claim follows. For the case $-(N+2\epsilon) = n \in \mathbb{N}_0$, the result follows by fixing N and x and using the Riemann continuation theorem for $F(x,0,N,\epsilon)$ at the removable singularity $N+1+2\epsilon = \frac{n-N-1}{2}$ in the expression above. □

As a corollary of the proposition, we have the following continued fraction identitiy.

Corollary 5.2.2. *For $n \in \mathbb{N}_0$, we have*

$$\mathop{\mathcal{K}}_{k=1}^{\infty}\left(\frac{kx}{k-n-x}\right) = x+n$$

Example 5.2.3. We have the following special values

$$F(-1,0,0,0) = \frac{1}{2}(\coth(\frac{1}{2})-3),$$
$$F(-1,0,1,0) = -1 + \frac{e}{2(e-1)}$$

In particular, we have

$$\boxed{F(-1,0,2,0) = \frac{1}{3}\mathop{\mathcal{K}}_{k=1}^{\infty}\left(\frac{-k}{k+3}\right) = \frac{e-3}{3},}$$

which is equivalent to (5.1).

5.3 The continued fraction expansion

In this section we prove the convergence of the generalization of the continued fraction expansion (5.1) and provide an estimate for its convergence speed.

Theorem 5.3.1. *For $n \in \mathbb{N}$ we have*

$$e^n = \sum_{k=0}^{n-1}\frac{n^k}{k!} + \frac{n^{n-1}}{(n-1)!}\left(1+n+\mathop{\mathcal{K}}_{k=1}^{\infty}\left(\frac{-n(k+n-1)}{k+2n+1}\right)\right)$$

To prove the theorem we construct a tail sequence using an associated recurrence relation and then use the Waadeland tail theorem (See chapter 2 of [35]) to establish the convergence. We make use of some lemmas to prove this result.

Lemma 5.3.2. *For a fixed $n \in \mathbb{N}$, the recurrence relation*

$$X_k = (k+2n+2)X_{k-1} - n(k+n)X_{k-2},$$

has the solution

$$X_k = (k+2)\Gamma(k+n+2),$$

for $k \geq 1$.

Proof. We directly verify, the right-hand is equal to

$$\begin{aligned}
&(k+2n+2)(k+1)\Gamma(k+n+1) - n(k+n)k\Gamma(k+n) \\
&\qquad = \Gamma(k+n+1)\left((k+2n+2)(k+1) - nk\right) \\
&\qquad = \Gamma(k+n+1)(k+n+1)(k+2) \\
&\qquad = (k+2)\Gamma(k+n+2),
\end{aligned}$$

which is equal to X_k, as desired. □

The next lemma is used for the evaluation of a hypergeometric function that appears in in the computation of the limit by Waadeland's Tail Theorem. We recall the definition of the incomplete gamma function $\gamma(s,x)$, namely

$$\gamma(s,x) := \int_0^x t^{s-1}e^{-t}dt,$$

as it is used in the lemma and in the remainder of the chapter.

Lemma 5.3.3. *The formula*

$${}_2F_2(1,1;3,z+2;z) = \frac{2(z+1)}{z^2}\left(1+z-\frac{\gamma(z,z)}{z^{z-1}e^{-z}}\right),$$

is valid for z in the cut plane $z \in \{z \in \mathbb{C} : |\arg(s)| < \pi\}$. In particular, for $n \in \mathbb{N}$ we have

$${}_2F_2(1,1;3,n+2;n) = \frac{2(n+1)}{n^2}\left(1+n-\frac{(n-1)!}{n^{n-1}}\left(e^n - \sum_{k=0}^{n-1}\frac{n^k}{k!}\right)\right).$$

Proof. Using the Euler's integral transform two times to the hypergeometric function, we get

$$\begin{aligned}
{}_2F_2(1,1;3,z+2;z) &= (z+1)\int_0^1 (1-t)^z {}_1F_1(1;3;tz)\,dt \\
&= 2(z+1)\int_0^1 (1-t)^z \int_0^1 (1-s)e^{stz}dsdt \\
&= \frac{2(z+1)}{n^2}\int_0^1 \frac{(1-t)^z}{t^2}\left(e^{zt} - zt - 1\right)dt,
\end{aligned}$$

then, by partial integration, we obtain

$$\frac{2(z+1)}{z}\int_0^1 (1-t)^{z-1}\left(1+z-e^{zt}\right)dt = \frac{2(z+1)}{z}\left(\frac{1+z}{z} - \int_0^1 (1-t)^{z-1}e^{zt}dt\right). \quad (5.3)$$

A change of variable $s = 1-t$ gives the first statement of the lemma

$$\frac{2(z+1)}{z}\left(\frac{1+z}{z} - \frac{e^z}{z^z}\int_0^z s^{z-1}e^{-s}dt\right) = \frac{2(z+1)}{z}\left(\frac{1+z}{z} - \frac{e^z}{z^z}\gamma(z,z)\right).$$

For the second statement, recall the expression for the residue term R_n of the n-th order Taylor's expansion of $f(x) = e^x$ around $x = 0$, evaluated at n,

$$R_n = \frac{n^n}{(n-1)!}\int_0^1 (1-t)^{n-1}e^{nt}dt = e^n - \sum_{k=0}^{n-1}\frac{n^k}{k!}.$$

Using this expression in (5.3) gives the desired expression

$$\frac{2(n+1)}{n^2}\left(1+n-\frac{(n-1)!}{n^{n-1}}\left(e^n - \sum_{k=0}^{n-1}\frac{n^k}{k!}\right)\right).$$

□

Next, we present the proof of Theorem 5.3.1.

Proof of Theorem 5.3.1. We obtain the result by computing the value of the shifted continued fraction $\mathcal{K}_{k=1}^{\infty}(\frac{-n(k+n)}{k+2n+2})$. By Lemma 5.3.2, a tail sequence $\{t_k\}$ for the continued fraction is given by

$$t_k = -\frac{(k+n+1)(k+2)}{k+1}, \qquad t_0 = -2(n+1).$$

The partial sum associated with the continued fraction in Waadeland's theorem is

$$\Sigma_l = \sum_{k=0}^{l}\frac{(1)_k(1)_k}{(3)_k(n+2)_k}\frac{l^k}{k!}.$$

Taking the limit and using Lemma 5.3.3 we get

$$\Sigma_\infty = {}_2F_2(1,1;3,n+2;n) = \frac{2(n+1)}{n^2}\left(1+n-\frac{(n-1)!}{n^{n-1}}\left(e^n - \sum_{k=0}^{n-1}\frac{n^k}{k!}\right).\right).$$

It follows that the continued fraction $\mathcal{K}_{k=1}^{\infty}\left(\frac{-n(k+n)}{k+2n+2}\right)$ converges to a finite value f_1 given by

$$f_1 = -2(1+n)\left(1-\frac{1}{\Sigma_\infty}\right).$$

Clearly, $\mathcal{K}_{k=1}^{\infty}\left(\frac{-n(k+n-1)}{k+2n+1}\right)$ is also convergent and

$$\begin{aligned}\mathop{\mathcal{K}}_{k=1}^{\infty}\left(\frac{-n(k+n-1)}{k+2n+1}\right) &= \frac{-n^2}{2(1+n)-2(n+1)(1-\frac{1}{\Sigma_\infty})} = \frac{-n^2}{2(1+n)}\Sigma_\infty \\ &= \frac{(n-1)!}{n^{n-1}}\left(e^n - \sum_{k=0}^{n-1}\frac{n^k}{k!}\right) - (1+n).\end{aligned}$$

The result follows immediately. □

Next, we establish the explicit expression of the difference between successive convergents and the estimate of the rate of convergence.

Proposition 5.3.4. *Let $C_k = P_k/Q_k$ be the convergents of the continued fraction expansion of e^n given in Theorem 5.3.1. We have*

$$C_k - C_{k-1} = -\frac{n^{n+k+1}}{(n-1)!(n)_{k+1}(k+1)k}$$

In particular, n divides the numerator of $C_k - C_{k-1}$.

Proof. From the Euler-Wallis identities, it holds that

$$\frac{P_k}{Q_k} - \frac{P_{k-1}}{Q_{k-1}} = \frac{(-1)^{k-1}a_1a_2\dots a_k}{Q_kQ_{k-1}} \times \frac{n^{n-1}}{(n-1)!} = -\frac{n^{n+k-1}(n)_k}{(n-1)!Q_kQ_{k-1}}, \tag{5.4}$$

with $a_k = -n(k+n-1)$. The denominators Q_k satisfy the recurrence relation $Q_k = (k+2n+1)Q_{k-1} - n(k+n-1)Q_{k-2}$, with initial condition $Q_{-1} = 0, Q_0 = 1$, and it can easily be verified that a solution is given by $Q_k = (1/n)(k+1)(n)_{k+1}$. Replacing this expression in (5.4) gives the result. □

The curious property mentioned in the introduction on the convergents of (5.1) is just a special case of the fact that in the continued fraction expansion of e^n, the difference between two successive convergents is divisible by n. The estimate on the rate of convergence follows immediately.

Corollary 5.3.5. *Let $C_k = P_k/Q_k$ be the convergents of the continued fraction expansion of e^n given in Theorem 5.3.1. We have*

$$|e^n - C_k| = O\left(\frac{n^{k+1}}{(k+1)(k+2)(n)_{k+2}}\right).$$

Remark 5.3.6. Here, we would like to point out the reason of using the shifted continued fraction in the proof of Theorem 5.3.1. In this case, using the original continued fraction we obtain a tail sequence given by the associated recurrence relation (as in the proof of Proposition 5.3.4). However, the initial value of the tail sequence is $t_0 = -b_1$ so the sequence does not satisfy the hypothesis of Waadeland's theorem. On the other hand, a direct approach by finding a solution of the recurrence relation for the numerators P_k is considerably more complicated.

5.4 An extension

The proof of Theorem 5.3.1 suggest that the continued fraction expansion of e^n is just a special case of a more general result. First, it is clear that Lemma 5.3.2 still holds when we replace n with $z \in \mathbb{C} - \{0, -1, -2, \dots\}$.

Theorem 5.4.1. *For $z \in \{z \in \mathbb{C} : |\arg(z)| < \pi\}$, we have*

$$\frac{\gamma(z,z)}{z^{z-1}e^{-z}} = 1 + z + \mathop{\mathcal{K}}_{k=1}^{\infty}\left(\frac{-z(k+z-1)}{k+2z+1}\right),$$

pointwise and uniformly in compacts.

Proof. As mentioned above, it is clear that both lemmas and the proof of the theorem hold for z in the indicated cut plane, so it only remains to prove the uniform convergence in compacts. Suppose D is compact domain in the cut plane, next suppose $M \in \mathbb{R}_{>0}$ is such that

$$|\frac{z^2}{2(z+1)}| \leq M,$$

for all $z \in D$. Let $f_n(z)$ denote the convergents of the continued fraction and $f(z)$ the pointwise limit, we have

$$|f(z) - f_n(z)| \leq M|\Sigma_\infty(z) - \Sigma_n(z)|,$$

where $\Sigma_n(z)$ and $\Sigma_\infty(z)$ are defined as in the proof of Theorem 5.3.1. The uniform convergence then follows from that of the hypergeometric series. □

Remark 5.4.2. For $z \in \{z \in \mathbb{C} : |\arg(z)| < \pi\}$ and $n \in \mathbb{N}$, it holds that

$$\begin{aligned} {}_1F_1(1; z+1; z) &= 1 + z + \mathop{\mathcal{K}}_{k=1}^{\infty} \left(\frac{-z(k+z-1)}{k+2z+1} \right) \\ \int_0^1 (1-t)^{n-1} e^{tn} dt &= \frac{1}{n} \left(1 + n + \mathop{\mathcal{K}}_{k=1}^{\infty} \left(\frac{-n(k+n-1)}{k+2n+1} \right) \right). \end{aligned}$$

It would seem at first glance that the continued fraction expansion of Theorem 5.3.1 could be extended to a continued fraction for arbitrary powers of e. However, by the proof of the theorem and from Theorem 5.4.1 we see that the expansion is *accidental* in the sense that it arises from special values of the incomplete gamma function $\gamma(x, s)$.

6. Future research

In this chapter we describe certain open questions related to the study of the QRM (and AQRM) and its spectrum. We remark that the list of open questions is not comprehensive and it is influenced by the author's interests and motivations.

6.1 A finer classification of the non-Juddian eigenvalues of the AQRM

In Section 4.3, we showed that the constraint polynomials and constraint T-functions appear in the residues of the poles of the G-function (see Propositions 4.3.1, 4.3.4 and 4.3.5). Using this fact, we proved that the zeros of the generalized G-function $\mathcal{G}_\varepsilon(x;g,\Delta)$ completely determine the spectrum of the AQRM in Theorem 4.4.2.

In the case of $\varepsilon = \frac{\ell}{2} \in \mathbb{Z}$, there is a possibility of non-Juddian exceptional eigenvalues corresponding to finite values of $G_{\ell/2}(x;g,\Delta)$ at points $x = N \pm \varepsilon$. The presence of such non-Juddian exceptional eigenvalues could give a finer classification of the exceptional spectrum of the AQRM.

Defining the function

$$B_\ell^N(g,\Delta) = \frac{1}{C(N)}\left(\bar{R}^{(N,+)}(g,\Delta,\frac{\ell}{2})(\Delta\bar{Q}^-(N+\frac{\ell}{2};g,\Delta)) - R^{(N,+)}(g,\Delta,\frac{\ell}{2})Q^-(N+\frac{\ell}{2};g,\Delta)\right),$$

then, by Proposition 4.3.5 and the proof of Lemma 4.2.4, if $T_{\ell/2}^{(N)}(g,\Delta) = 0$ the vanishing of the residue $\mathrm{Res}_{x=N+\ell/2}\, G_{\ell/2}(x;g,\Delta)$ is equivalent to the equation

$$B_{-\ell}^{N+\ell}(g,\Delta) + A_N^\ell((2g)^2,\Delta^2)B_\ell^N(g,\Delta) = 0. \tag{6.1}$$

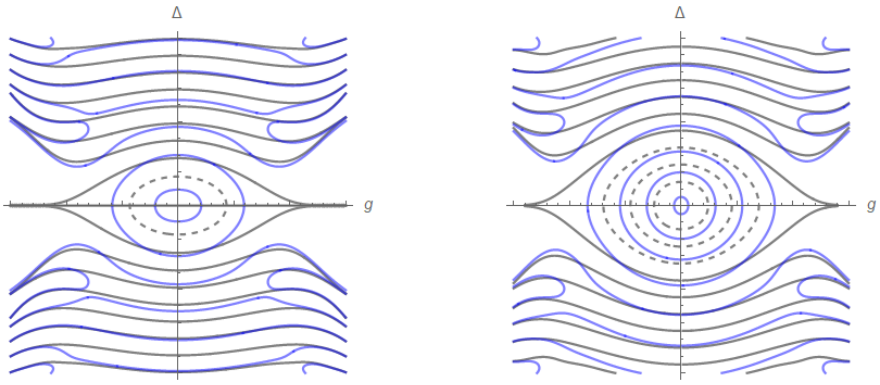
Notice the similarity of this equation with the conjectures on the divisibility of constraint polynomials, including the presence of the quotient polynomial $A_N^\ell((2g)^2,\Delta^2)$ (c.f. Section 2.9).

Problem 6.1.1. With the notation of Proposition 4.3.5,

- Are there non-Juddian exceptional eigenvalues $\lambda = N \pm \ell/2 - g^2$ corresponding to finite values of G-function $G_{\ell/2}(x;g,\Delta)$ at the point $x = N \pm \ell/2$? If the answer is affirmative, what are the properties of these non-Juddian exceptional eigenvalues?

- In case the first question is affirmative. Is it possible to characterize these solutions in terms of the constraint function $T_{\ell/2}^{(N)}(g,\Delta)$ and the polynomials $A_N^\ell((2g)^2,\Delta^2)$?

Next, we present the graphs in the (g, Δ)-plane of the curves defined by the residue vanishing condition (6.1) and the constraint conditions for exceptional eigenvalues in Figure 6.1. In the graphs, we show the curve given by $T_{\ell/2}^{(N)}(g, \Delta) = 0$ in continuous gray lines, the curve given by $P_N^{(N,\ell/2)}((2g)^2, \Delta^2) = 0$ in dashed gray lines and the residue vanishing condition (6.1) in blue lines. Figure 6.1(a) shows the case $N = 1$ and $\ell = 2$ while Figure 6.1(b) depicts the case $N = 3$ and $\ell = 1$. Notice that in both cases there appears to be intersections in the vanishing condition (6.1) and the constraint relation $T_{\ell/2}^{(N)}(g, \Delta) = 0$, in other words, there are non-Juddian exceptional eigenvalues which kill the corresponding (double) poles of the G-function $G_{\ell/2}(x; g, \Delta)$. While further investigation including numerical experiments is needed, the observations made on the numerical graphs shown in Figure 6.1 provide actually evidence for the affirmative answer of the problem above. In addition, from Figure 6.1, we notice there are apparently no intersections between the curves of the Juddian constraint conditions and the curves of the vanishing condition (6.1). Further numerical experimentations we have done so far support that this observation may be true in general.



(a) $N = 1$, $\ell = 2$ (b) $N = 3$, $\ell = 1$

Figure 6.1: Plot of constraint relations $T_{\ell/2}^{(N)}(g, \Delta) = 0$ (gray), $P_N^{(N,\ell/2)}((2g)^2, \Delta^2) = 0$ (dashed gray) and residue vanishing condition (6.1) (blue).

6.2 Special values of the spectral zeta function of the QRM

As mentioned Section 2.1 the spectral zeta function of the QRM, given by

$$\zeta_{H_{\text{Rabi}}}(s) = \sum_{\lambda \in \text{Spec}(H_{\text{Rabi}})} \frac{1}{\lambda^s},$$

has been shown to extend meromorphically to the complex plane with a simple pole at $s = 1$(see [55]).

One of the most fascinating topics in the study of spectral zeta functions are the special values, that is, the values $\zeta_{H_{\text{Rabi}}}(s)$ at positive integer values

$$\zeta_{H_{\text{Rabi}}}(2), \zeta_{H_{\text{Rabi}}}(3), \zeta_{H_{\text{Rabi}}}(4), \zeta_{H_{\text{Rabi}}}(5), \cdots.$$

For instance, for the case of the non-commutative harmonic oscillator (NcHO), the special values have interesting number theoretical properties, with relation with Apéry-like number, elliptic curves, modular forms and Eichler integrals (see [22, 28, 30, 29]). As we remarked in Section 2.1, there is a relation in the representation theoretical picture of the NcHO and the QRM via a confluent process, so there is an expectation that some of these arithmetical properties may also appear in the study of the special values of the spectral zeta function of the QRM. Informally speaking, it may also give a relation between number theory and a model occurring naturally in physical phenomena.

The special values of the spectral zeta function $\zeta_{H_{\mathrm{Rabi}}}(s)$ can be computed (see [21] for the case of the NcHO), for $n \geq 2$, as

$$\zeta_{H_{\mathrm{Rabi}}}(n) = \int_0^\infty dt \int_{-\infty}^\infty \cdots \int_{-\infty}^\infty dx dx_1 dx_2 \cdots dx_{n-1} \operatorname{tr} K_{\mathrm{Rabi}}(t,x,x_1) K_{\mathrm{Rabi}}(t,x_1,x_2) \cdots K_{\mathrm{Rabi}}(t,x_{n-1},x),$$

where $K_{\mathrm{Rabi}}(t,x,y)$ is the *heat kernel* of the QRM. The heat kernel of the QRM is the integral kernel of the fundamental solution of the heat equation

$$\left(H_{\mathrm{Rabi}} + \frac{d}{dt}\right) f = 0$$

of the QRM, that is, the integral kernel of the operator $e^{-tH_{\mathrm{Rabi}}}$. We note that the heat kernel is related to the *partition function* $Z_{\mathrm{Rabi}}(\beta)$ of the QRM, defined as

$$Z_{\mathrm{Rabi}}(\beta) := \mathrm{Tr}[e^{-t\beta H_{\mathrm{Rabi}}}] = \sum_{\mu \epsilon \mathrm{Spec}(H_{\mathrm{Rabi}}} e^{-\beta E(\mu)},$$

this function is of fundamental importance in statistical mechanics for the description of the properties of the system at thermal equilibrium. From this point of view, it becomes clear that the computation of the heat kernel of the QRM is of great importance to physics (statistical physics) and mathematics (special values of the spectral zeta function). This relation is made clear by the expression

$$\zeta_{H_{\mathrm{Rabi}}}(s) = \frac{1}{\Gamma(s)} \int_0^\infty t^{s-1} Z_{\mathrm{Rabi}}(t) dt,$$

obtained via a Mellin transform.

We note that the method used for computing special values of the NcHO in [21] cannot be applied here. Indeed, recalling the expression of the Hamiltonian Q of the NcHO

$$Q = \begin{bmatrix} \alpha & 0 \\ 0 & \beta \end{bmatrix} \left(-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}x^2 \right) + \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \left(x\frac{d}{dx} + \frac{1}{2} \right).$$

we observe that the operator is defined in terms of two non-commutative matrices

$$\mathbf{A} = \begin{bmatrix} \alpha & 0 \\ 0 & \beta \end{bmatrix}, \qquad \mathbf{J} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},$$

making the computation of the heat kernel a nontrivial task. However, by setting $Q' = \mathbf{A}^{-1/2} Q \mathbf{A}^{-1/2}$, it is shown that there is an explicit expression for the heat

kernel of the operator Q'. Since for the computation of the special values of the spectral zeta function it is enough to consider the matrix trace of the expression of the iterated heat kernel, the expression for the heat kernel of Q' suffices for the computation.

On the other hand, observe that the Hamiltonian of the QRM

$$H_{\text{Rabi}} = a^\dagger a + g(a + a^\dagger)\sigma_x + \Delta\sigma_z,$$

is defined in terms of two matrices

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \qquad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

in addition to the identity matrix. Since the three matrices are not simultaneously "diagonalizable" in the way that the matrices $\mathbf{A}$ and $\mathbf{J}$ are in the case of the NcHO, this excludes the possibility of using the technique described in [21].

One strategy for computing the heat kernel of the QRM to write the Hamiltonian as

$$H_{\text{Rabi}} = (a^\dagger + g\sigma_x)(a + g\sigma_x) + \Delta\sigma_z - g^2 = b^\dagger b - g^2 + \Delta\sigma_z,$$

with $[b, b^\dagger] = \mathbf{I}_2$ and noticing that $b, b^\dagger$ can be considered to be raising and lowering operators of a *displaced quantum Harmonic oscillator*. We note that care should be taken since the operators b and $b^\dagger$ do not commute with σ_z. Using this expression it is possible to consider the computation of the heat kernel by using the Krato-Trotter product formula (see [17]). The computation is very complicated and involves, for example, certain nontrivial combinatorial problems. It is well-known that the spectral zeta function of the quantum Harmonic oscillator is essentially the Riemann zeta function, so we anticipate that the spectral zeta function of the QRM and its special values will have a rich arithmetic structure. The author of this thesis is preparing a paper with Masato Wakayama on this topic [49].

6.3 Characterization of coupling regimes of the QRM

In Section 2.1, we mentioned the concept of coupling regimes of QRM in the context of experimental realizations of the quantum Rabi model. The coupling regimes are defined in terms of the parameters g, Δ of the Hamiltonian. Generally accepted (see [45]) coupling regimes are

- decoupling regime: $2\Delta \ll g \ll \omega$,
- JC regime: $g \ll \omega, 2\Delta$, and $|\omega - 2\Delta| \ll |\omega + 2\Delta|$,
- anti JC regime: $g \ll \omega, 2\Delta$, and $|\omega - 2\Delta| \gg |\omega + 2\Delta|$,
- intermediate regime: $2\Delta \sim g \ll \omega$,
- two-fold dispersive regime: $g < \omega, 2\Delta, |\omega - 2\Delta|, |\omega + 2\Delta|$,
- ultrastrong coupling regime: $0.1 < g < \omega$,
- deep strong coupling regime: $g > \omega$.

The regimes are defined according to different observed properties of the QRM for the different choices of parameters, including properties of the energy levels (spectrum), dynamics and whether the model is approximable by simpler models (like the Jaynes-Cummings models). However, as remarked in [51], the characterization of the coupling regimes is not universally agreed and there is a need for a more specific criterion. In the same paper, the authors give a new proposal for characterization on the coupling regimes of the QRM that depends not only in the parameters of the system but also on the energy levels of the system. This new classification is based on the study of approximate solutions of eigenvalue problem of the QRM (see Sections 2.6 and 2.7) and therefore it is deeply related to the spectrum of the system.

For instance, in this proposal the *perturbative ultrastrong coupling regime*(pUSC) roughly corresponds to combinations of parameters g, ω, Δ and eigenvalues λ lying to the left of the first Juddian solution in the spectral curve graph (for example Figure 2.2). The *perturbative deep strong coupling regime*(pDSC) is similarly defined by the combination of parameters g, ω, Δ and eigenvalues λ lying past a boundary curve (in the $(\lambda - g/w)$-plane) past the last Juddian solution. The *nonperturbative ultrastrong-deep strong coupling regime* (npUSC-DSC) would then correspond to the remaining region in the $(\lambda - g/w)$-plane. This classification has the advantage of giving precise differentiation between the coupling regimes, based on observations made by the authors on the statical and dynamical properties of the QRM in these regimes.

The existence of such a classification also allows the possibility of a more concrete mathematical study of said static and dynamical properties that under the classical characterization of the coupling regimes was not achievable. In particular, a relation to the study of constraint polynomials is expected due to the fact that the boundary between the pUSC and npUSC-DSC regime is defined in terms of the Juddian points of the QRM.

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