The quantization of the Rabi Hamiltonian

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Abstract
The Rabi Hamiltonian addresses the proverbial paradigmatic case of a two-level fermionic system coupled to a single bosonic mode. It is expressed by a system of two coupled first-order differential equations in the complex field, which may be rewritten in a canonical form under the Birkhoff transformation. The transformation gives rise to leapfrog recurrence relations, from which the eigenvalues and eigenvectors could be obtained. The interesting feature of this approach is that it generates integer quantum numbers, which rationalize the spectrum by relating the solutions to the Juddian baselines. The relationship with Braak’s integrability claim (Braak 2011 Phys. Rev. Lett. 107 100401) is discussed.

Keywords: Rabi Hamiltonian, Bargmann mapping, quasi-exact solutions

Introduction
The Rabi Hamiltonian describes the coupling of a two-level fermion system with a single bosonic mode. In spite of its extreme simplicity, it shows up in an incredible range of applications, and moreover continues to stimulate further theoretical work. In the focus point of much of the recent theoretical developments is the integrability claim by Braak [1]. Braak derived a transcendental function, the zeros of which correspond to the energy spectrum of the Rabi Model. Each level is characterized by two quantum numbers, consisting of a two-valued parity label distinguishing symmetric and anti-symmetric states, and an integer, counting the nodes of the transcendental function. States with the same parity do not show level crossings. For this reason the two quantum numbers together provide a unique labeling of each individual state of the system, which therefore is said to be quantum integrable. So far the integer quantum number remains a mere counting number, with no apparent relation to the nature of the corresponding quantum state. In the present study we consider a further transformation
of the Rabi Hamiltonian to a canonical form, which gives rise to a quantization condition expressed in integer numbers.

**The model system**

The model system consists of two fermion states, coupled to a single harmonic oscillator. It is a two-parameter system: the fermion level splitting is parametrized as $2\Delta$ and the linear vibronic coupling parameter is represented by $g$. The oscillator quantum $\hbar \omega$ is taken as the unit of energy. This Hamiltonian is a universal key which fits to an amazing set of locks both in physics and in chemistry. It is at the core of the Holstein polaron model [2] and of the vibronic theory of chemical reactions. It describes an adiabatic potential energy surface consisting of a two-well potential with an avoided crossing, as shown in figure 1. This surface represents the prototype of an elementary chemical reaction proceeding along a single reaction coordinate. It lies at the basis of electron transfer reactions [3] and of exciton transfer in the Fulton–Gouterman dimer model in spectroscopy [4].

The potential surface has a reflection symmetry in the displacement coordinate. This property plays an important role in the quantization of the Rabi Hamiltonian. The localized electronic states in the separate wells will be denoted as $|1\rangle$ and $|2\rangle$. The level splitting acts as a constant off-diagonal coupling term between the localized states:

$$H_{12} = \Delta (|1\rangle \langle 2| + |2\rangle \langle 1|).$$

(1)
Further developments have been considered where a bias between the two wells is introduced, but we will limit ourselves here to the simplest symmetric case. The Hamiltonian can be written in a matrix form, acting in the space $|1\rangle, |2\rangle$:

$$\mathcal{H} - \frac{1}{2} \equiv \begin{pmatrix} a^d a + g(a^d + a) & \Delta \\ \Delta & a^d a - g(a^d + a) \end{pmatrix}.$$  \hspace{1cm} (2)

The corresponding vibronic wavefunction is a combination of the fermion states with coefficients that are functions of the boson excitations. The solution of the corresponding Schrödinger equation can be obtained by expanding the coefficients in the boson space. The further treatment depends on the choice of the oscillator basis set: either centered in the coordinate origin or displaced towards the minimum of the well. Here we will recapitulate the existing treatments and discuss their respective merits.

**Central basis set**

A straightforward basis set consists of the unperturbed oscillator functions, centered in the coordinate origin:

$$|n\rangle = \frac{1}{\sqrt{n!}} (a^d)^n |0\rangle.$$  \hspace{1cm} (3)

The reflection symmetry, $\hat{\sigma}$, will affect both the boson and the fermion parts as follows:

$$\hat{\sigma}(a^d) = - a^d$$  
$$\hat{\sigma}(a) = - a$$  
$$\hat{\sigma}|1\rangle = |2\rangle$$  
$$\hat{\sigma}|2\rangle = |1\rangle.$$  \hspace{1cm} (4)

Since the reflection plane is a binary symmetry element it has two representations: a symmetric and an anti-symmetric one, hence one has:

$$\hat{\sigma} |\Psi\rangle = \pm |\Psi\rangle.$$  \hspace{1cm} (5)

As a result the Ansatz for the symmetric and anti-symmetric eigenfunctions becomes:

$$|\Psi_+\rangle = \sum_{n=0}^{\infty} c_n \frac{1}{\sqrt{n!}} (a^d)^n |0\rangle \times \frac{1}{\sqrt{2}} \{ |1\rangle + (-1)^n |2\rangle \}$$  
$$|\Psi_-\rangle = \sum_{n=0}^{\infty} c_n \frac{1}{\sqrt{n!}} (a^d)^n |0\rangle \times \frac{1}{\sqrt{2}} \{ |1\rangle - (-1)^n |2\rangle \}.$$  \hspace{1cm} (6)

The corresponding Hamiltonian matrices are:

$$\mathbb{H}_\pm - \frac{1}{2} = \begin{pmatrix} \pm \Delta & g & 0 & 0 & 0 & \ldots \\ g & 1 \mp \Delta & \sqrt{2} g & 0 & 0 & \ldots \\ 0 & \sqrt{2} g & 2 \pm \Delta & \sqrt{3} g & 0 & \ldots \\ 0 & 0 & \sqrt{3} g & 3 \mp \Delta & \sqrt{4} g & \ldots \\ 0 & 0 & 0 & \sqrt{4} g & 4 \pm \Delta & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots & \ldots \end{pmatrix}.$$  \hspace{1cm} (7)
The roots can then be obtained by straightforward diagonalization of the truncated matrices. Convergence is rather slow since the increase of the diagonal elements is offset by the simultaneous increase of the off-diagonal elements. Note that a sign change of $\Delta$ leads to a switch of symmetric and anti-symmetric solutions. A continued fractions approach to the solution was first presented by Swain [5]. Its analyticity has been discussed by several authors [6–8].

**Displaced oscillator states**

An alternative basis set makes use of displaced oscillator states which localize the oscillator in one of the wells. This is the basis set used by Braak in the framework of the Bargmann–Fock mapping. Later on Chen et al rederived Braak’s results in the Schrödinger representation [9]. In the latter setting $|n\rangle_A$ denotes the oscillator state displaced to the well on the left, and $\hat{D}(g)$ is the displacement operator:

$$
A^i = a^i + g \\
|n\rangle_A = \frac{1}{\sqrt{n!}}(A^i)|0\rangle_A \\
|0\rangle_A = \hat{D}(g)|0\rangle = \exp(-\frac{g^2}{2})\exp(-ga^i)|0\rangle.
$$

(8)

In the formalism of Chen et al [9] the wavefunction is expressed in the displaced oscillator states as:

$$
|\Psi\rangle_A = \sum_{n=0}^{\infty} \left( \sqrt{n!} e_n|n\rangle_A|1\rangle + \sqrt{n!} f_n|n\rangle_A|2\rangle \right).
$$

(9)

The action of the Hamiltonian on this wavefunction finally leads to the following defining relations for the coefficients:

$$
0 = e_m + \frac{f_m}{m - g^2 - E} \\
0 = \Delta e_m + (m + 3g^2 - E)f_m - 2g(m + 1)f_{m+1} - 2g(m - 1)f_{m-1}
$$

(10)

from which one may derive the three-term recurrence in the $f$-coefficients:

$$
f_{n+1} = \frac{1}{n + 1} \Omega_n f_n + \frac{1}{n + 1} f_{n-1} = 0
$$

(11)

with:

$$
\Omega_n = \frac{1}{2g} \left( n + 3g^2 - E - \frac{\Delta^2}{n - g^2 - E} \right).
$$

(12)

In this treatment the zero-point energy of $\frac{1}{2}\hbar\omega$ is incorporated into the $E$ variable. The series starts off at $f_0$, which we can fix to unity; then one has:

$$
f_0 \equiv 1 \\
f_1 = \Omega_0 \\
f_2 = \frac{1}{2} (\Omega_0 \Omega_1 - 1) \ etc.
$$

(13)

The recurrence may be rewritten as:

4
Let $t$ be defined as the limiting value of the ratio between consecutive coefficients:

\[
    t = \lim_{n \to \infty} \frac{f_{n+1}}{f_n}.
\]

The roots of the corresponding characteristic Poincaré polynomial [10] are then given by:

\[
    \tau_1 = 0, \quad \tau_2 = \frac{1}{2g}.
\]

The zero root corresponds to the *minimal* solution, which is square integrable, while the upper root is the *dominant* solution which converges to a finite non-zero value. The solution of the recurrence relations should be aiming at finding the minimal solution which is the only one that satisfies the quantization condition. Moroz has argued that it is possible to obtain the eigenenergies by truncating the recurrence for sufficiently high $n$, and requiring the series to start at $f_0 = 1$ [11, 12]. The difference between the fixed value from $f_0$ and the initial value of the truncated recurrence relation is then Moroz’ transcendental function, $F_0$, which reproduces the eigenenergies. This function is shown in figure 2.

There is no guarantee though that this truncation will always lead to the minimal solution. Moreover so far no use was made of the reflection symmetry, which commutes with the Hamiltonian. As argued by Braak [8] both aspects are related since the reflection symmetry can be used to construct a new transcendental function which will always lead to the minimal solution. Applying $\hat{\sigma}$ to the oscillator functions maps the displacement from one well to the other. Let the oscillator basis functions in the well to the right be represented as $|n\rangle_0$. One then has:

---

*Figure 2.* Plot of Moroz’ $F_0(E + g^2)$ in the interval $[-1, 5]$ for $g = 0.7$ and $\Delta = 0.4$. 

\[
    \frac{f_{n+1}}{f_n} = \frac{1}{n+1} \Omega_n + \frac{1}{n+1} \frac{f_{n-1}}{f_n} = 0. 
\]
The reflection of $|\Psi_A\rangle$ then is given by:

$$|\Psi_B\rangle = \sum_{n=0}^{\infty} (\sqrt{n+1} (-1)^n |n\rangle_B + \sqrt{n+1} (-1)^n e_n |n\rangle_B) = |\Psi\rangle_A.$$  

Since the exact wavefunction must have reflection symmetry and has to be single-valued, one has:

$$|\Psi\rangle_A = \pm |\Psi\rangle_B.$$  

Repeating now the derivation of the recurrence relations finally leads to a new transcendental function, $G_\sigma(E)$, originally proposed by Braak [1], that has the eigenvalues as roots:

$$G_\sigma(E) = \sum_{n=0}^{\infty} g^n f_n(E) \left[ 1 \pm \frac{\Delta}{n - g^2 - E} \right].$$  

Here the $\pm$ sign refers to symmetric versus anti-symmetric solutions respectively. This function is displayed in figure 3.

**The Birkhoff transformation**

We now continue the treatment in the Bargmann–Fock mapping. In this mapping [13] the creation and annihilation operators are replaced by a complex variable $z$, and its derivative respectively: $a^\dagger \rightarrow z$, $a \rightarrow \frac{dz}{dz}$. The requirement that both operators remain each others adjoint is taken into account by defining the inner product of two functions as follows:

$$\langle f | g \rangle = \frac{1}{\pi} \int \overline{f(z)} g(z) \exp(-z \bar{z}) dx dy, \quad z = x + iy.$$  

**Figure 3.** Braak’s transcendental function $G_\sigma(E + \sigma^2)$. Red and blue lines represent the symmetric and anti-symmetric roots resp. in the interval $[-1.5]$ for $\sigma = 0.7$ and $\Delta = 0.4$. 

The reflection of $|\Psi\rangle_A$ then is given by:

$$|\Psi\rangle_B = \sum_{n=0}^{\infty} (\sqrt{n+1} (-1)^n |n\rangle_B + \sqrt{n+1} (-1)^n e_n |n\rangle_B).$$  

Here the $\pm$ sign refers to symmetric versus anti-symmetric solutions respectively. This function is displayed in figure 3.
As a result the Schrödinger equation is transformed into a set of two coupled first-order differential equations in $z$.

\[
\frac{d}{dz}f_1 = \frac{E - gz}{z + g} f_1 - \frac{\Delta}{z + g} f_2,
\]

\[
\frac{d}{dz}f_2 = -\frac{\Delta}{z - g} f_1 + \frac{E + gz}{z - g} f_2.
\]

(22)

Note that the reflection symmetry, $(z) \leftrightarrow (-z)$, for this set of equations is preserved:

\[
f(z) = \begin{pmatrix} f_1(z) \\ f_2(z) \end{pmatrix} = \pm \begin{pmatrix} f_1(-z) \\ f_2(-z) \end{pmatrix}
\]

(23)

The set of equations has two finite singular points at $z = \pm g$. Reik et al have studied analytic solutions taking this pole structure explicitly into account [14]. The two linear equations in the Bargmann representation are then transformed into a single second-order equation, which has been studied in general by Maciejewski et al [15] In the case of the Rabi Hamiltonian this leads to a transcendental function which can be expressed in terms of the confluent Heun functions [16]. Here we follow an alternative treatment [17] based on the Birkhoff transformation [18]. It provides a method to coalesce the singular points to the origin. For a precise formulation of this transformation we refer to the book by Ince [19]. As has been noted by Gantmacher [20], there are restrictions on the applicability of this theorem. We are interested in local solutions, which correspond to the quantized states, and show convergence at infinity, while formal solutions generally diverge. Let us first rewrite the equations in a more general way as:

\[
\frac{d}{dz}f_1 = p_{11}(z)f_1 + p_{12}(z)f_2
\]

\[
\frac{d}{dz}f_2 = p_{21}(z)f_1 + p_{22}(z)f_2
\]

(24)

or,

\[
\frac{d}{dz}f = p f.
\]

(25)

Outside the circle $|z| = g$ the $p_{ij}$-coefficients can be expanded in a Laurent series

\[
p_{ij} = \sum_{k=-\infty}^{q} p_{ij}^{(k)} z^k, \quad p_{ij}^{(k)} \in \mathbb{C}.
\]

(26)

Here $q + 1$ is the rank of the singular point at infinity. For the Rabi Hamiltonian the rank is equal to 1, hence $q = 0$. The corresponding series expansions are as follows:

\[
p_{11}(z) = \frac{E - gz}{z + g}
\]

\[
= -g + \frac{E + g^2}{z} - \frac{g(E + g^2)}{z^2} + \frac{g^3(E + g^2)}{z^3} - \frac{g^4(E + g^2)}{z^4} + O\left(\frac{1}{z^5}\right)
\]

\[
p_{12}(z) = \frac{\Delta}{z + g}
\]

\[
= -\frac{\Delta}{z} + \frac{g\Delta}{z^2} - \frac{g^2\Delta}{z^3} + \frac{g^3\Delta}{z^4} - O\left(\frac{1}{z^5}\right)
\]

\[
p_{21}(z) = -\frac{\Delta}{z - g} = -p_{12}(-z)
\]

\[
p_{22}(z) = \frac{E + gz}{z - g} = -p_{11}(-z).
\]

(27)
Now assume a linear transformation of the form:

\[ \mathbf{f} = a \mathbf{F} \]  

(28)

where the transformation coefficients \( a_{ij}(z) \) are analytic at infinity and reduce at infinity to the unit matrix:

\[ a_{ij}(z) = \sum_{k=0}^{\infty} \frac{a_{ij}^{(k)}}{z^k}, \quad a_{ij}^{(k)} \in \mathbb{C}. \]  

(29)

This matrix transformation contains all the finite singularities of the initial system. In view of the symmetry of this matrix we adopt a simplified notation as:

\[ \sum_{k=0}^{\infty} a_k z^k \]  

(30)

with: \( a_0 = 1 \) and \( b_0 = 0 \). By combining these expressions the original set of equations can be turned into a transformed system, which is called the canonical form or Birkhoff-transform:

\[ z \frac{d}{dz} \mathbf{F} = P \mathbf{F}. \]  

(31)

The coefficients of this canonical system are related to the original coefficients by the following matrix transformation:

\[ \frac{1}{z} \mathbf{A} \mathbf{P} = \mathbf{P} \mathbf{A} - \frac{d}{dz} \mathbf{A}. \]  

(32)

Now according to the Birkhoff theorem the \( P_{ij} \) coefficients of the transformed equation will be polynomials of a degree that does not exceed the rank of the original equation. They can thus be easily obtained from the previous equation by collecting the terms in \( 1/z^k \) with \( k = 0,1 \). The results are:

\[ P_{11}(z) = E + g^2 - gz \]
\[ P_{12}(z) = -\Delta - 2gb_1 \]
\[ P_{21}(z) = P_{12}(-z) \]
\[ P_{22}(z) = P_{11}(-z). \]  

(33)

These are indeed polynomials of rank not higher than 1. Note that these terms contain the expansion coefficient \( b_1 \) as a kind of gauge potential, which will have to be fixed by the quantization conditions. The canonical form of the Rabi equation thus reads:

\[ z \frac{d}{dz} F_1 = (E + g^2 - gz)F_1 + (-\Delta - 2gb_1)F_2 \]
\[ z \frac{d}{dz} F_2 = (-\Delta - 2gb_1)F_1 + (E + g^2 + gz)F_2. \]  

(34)

The original and transformed system share the same reflection symmetry:
where the plus and minus sign denote symmetric and anti-symmetric solutions respectively. By eliminating $F_2$ the canonical set may be transformed into a second-order differential equation in $F_1$:

$$z^2 F''_1(z) + z([1 - 2(E + g^2)]F'_1(z) + [(E + g^2)^2 - A^2 + g z - g^2 z^2]F_1) = 0.$$  

(36)

Here we have introduced $A$ to denote the gauge factor: 

$$A = \Delta + 2gb_1.$$  

(37)

By applying the Frobenius method we obtain as the roots of the indicial equation:

$$\rho_{\pm} = E + g^2 \pm A.$$  

(38)

The differential equation can be reduced to the Kummer equation, which is solved by the confluent hypergeometric functions $\text{F}(a, b; z)$. The general solution reads:

$$F_1(z) = C_1 \exp(gz) \text{F}(1 + A, 1 + 2A; -2gz) z^{E + g^2 + A}$$

$$+ C_2 \exp(gz) \text{F}(1 - A, 1 - 2A; -2gz) z^{E + g^2 - A}.$$  

(39)

While this solution for $\lvert z \rvert \to \infty$ belongs to the Bargmann–Fock space, the function can only be single-valued if it is entire, this means that at least one of the roots of the indicial equation should be a non-negative integer. This provides an additional quantum condition which allows to fix the gauge factor and determines the spectrum of the Rabi Hamiltonian.

Quantization of indicial roots

As indicated previously [17], the solutions of the Rabi Hamiltonian can be classified on the basis of the roots of the indicial equation. The physical requirement that the solution should belong to the Bargmann–Fock space implies the simple quantization condition that one of the roots of the indicial equation should be a non-negative integer. This criterion gives rise to different classes of solutions:

1. If $E + g^2$ is neither an integer nor a half integer, then only one of the roots can be integer. Indeed, suppose that both roots are integer, then one has:

$$\rho_+ + \rho_- = 2(E + g^2) \in \mathbb{Z}$$  

(40)

which is contrary to the starting assumption. Hence in this case the solution of the second-order differential equation will be one-dimensional, i.e. either $C_1$ or $C_2$ must be zero, depending on which of the roots is taken to be a non-negative integer.

2. If $E + g^2$ is half-integer, then $A$ also must be half-integer. Nonetheless the solution still remains one-dimensional, since one of the functional parameters, $1 + 2A$ or $1 - 2A$, is a negative integer or zero, and the corresponding Kummer function is not defined.

3. If $E + g^2$ is integer and the gauge factor $A = 0$, the two first-order differential equations are uncoupled and the corresponding eigenspace is two-dimensional. These correspond to the Juddian exact solutions [21–23] where the symmetric and anti-symmetric states cross, as was explained previously. The $b_1$ coefficient in this case is given by:
\[ b_1 = -\frac{\Delta}{2g}. \]  

(41)

Note that for the solutions to be entire \( E + g^2 \) must be non-negative, which would imply that its lowest value could be zero. However for \( A = 0 \) the value of \( b_1 \) cannot be zero, and as a result the first Juddian eigenvalue is found at \( E + g^2 = 1 \) [17].

4. Finally it is possible that both \( E + g^2 \) and \( A \) are both taken to be integer. In this case at least one of the solutions will be analytic. Below we present a rare example of this case.

Except for the sporadic crossing points, the solutions of the Rabi Hamiltonian will belong to the first class. In this case the requirement that one of the roots of the indicial equation should be a non-negative integer number is of paramount importance since it introduces a simple quantum number to characterize the solution space. In fact there are two possibilities:

\[ \rho_+ = 0, 1, 2, ... \]  

(42)

or:

\[ \rho_- = 0, 1, 2, ... \]  

(43)

These two possibilities distinguish between symmetric and anti-symmetric solutions. This can be shown as follows. Take \( \rho_+ = k \), with \( k = 0, 1, 2, ... \). Then as explained before \( \rho_- \) cannot be an integer, and the solution is one-dimensional of the following type:

\[ F(z) = \exp(gz) F_1(1 + A, 1 + 2A; -2gz) z^{E+g^2+A}. \]  

(44)

By inserting this into the set of differential equations we may obtain \( F_2(z) \):

\[ F_2(z) = \frac{1}{A} (1 - 2gz) F_1(z) - \frac{1 + A}{A} \exp(gz) F_1(2 + A, 1 + 2A; -2gz) z^{E+g^2+A}. \]  

(45)

Using the appropriate recursion formulas for the hypergeometric functions, one can easily demonstrate:

\[ F_2(z) = (-1)^{k+1} F_1(-z). \]  

(46)

Hence if \( k \) is even, the quantization of \( \rho_+ \) will lead to anti-symmetric solutions, while odd \( k \) values will generate the symmetric solutions. On the other hand imposing the quantization condition for \( \rho_- \) leads to the opposite rule, since in this case:

\[ F_2(z) = (-1)^k F_1(-z). \]  

(47)

**Results**

In the previous treatment [17] it was shown that the expressions do generate the Juddian exact solutions, but no general recurrence relations could be derived, and hence most of the solution space remained uncharted territory. We have now been able to find these defining recurrence relations, and to generate from them the full spectrum.

**Recurrence and series expansion**

In addition to the quantization of \( \rho \) also the expansion coefficients in the Laurent series are constrained by the requirement that the solution of the initial system should belong to the Bargmann–Fock space. The recurrence relationships which determine these coefficients
are more involved than in Braak’s case since we now have two interrelated recurrence relations. The series expansion of equation (30) for the $a_{11}$ matrix element yields expressions for the $a$-coefficients, from $n = 1$ onwards:

$$a_n = \frac{1}{n} \left[-(\Delta + 2gb) b_n + (-1)^n \Delta \sum_{\nu=1}^{n} g^{n-\nu} b_\nu + (E + g^2) \sum_{\nu=1}^{n} (-1)^{\nu+1} g^{\nu} a_{n-\nu} \right].$$  \hfill (48)

By combining $na_n + g(n-1)a_{n-1}$ one then obtains the first four-term recursion relation, which generates $a_n$ from $a_{n-1}$ and $b_n, b_{n-1}$ coefficients:

$$na_n = (E + g^2 - n + 1) g a_{n-1} - [2gb + \Delta [1 + (-1)^{n+1}]] b_n - g(\Delta + 2gb) b_{n-1}.$$  \hfill (49)

Starting from $n = 2$ the $b_n$ coefficients are given by:

$$2gb_n = (n-1)b_{n-1} + (\Delta + 2gb) a_{n-1} + (-1)^n \Delta \sum_{\nu=0}^{n-2} g^{n-1-\nu} a_\nu,$$

$$+(E + g^2) \sum_{\nu=1}^{n-2} (-1)^{n-\nu} g^{n-1-\nu} b_\nu.$$  \hfill (50)

Again by combining $2gb_n + 2g^2 b_{n-1}$ one obtains the second five-term recursion relation, which generates $b_n$ from the previous $a_{n-1}, a_{n-2}, b_{n-1}$, and $b_{n-2}$ coefficients.

$$2gb_n = g(\Delta + 2gb) a_{n-2} + [2gb + \Delta [1 + (-1)^{n}]] a_{n-1} +$$

$$+ g [n-2 - (E + g^2)] b_{n-2} + (n-1 - 2g^2) b_{n-1}.$$  \hfill (51)

Consecutive coefficients are thus obtained by leapfrogging the recurrence relations from $b_1$ onwards:

$$b_1 \rightarrow a_1 \rightarrow b_2 \rightarrow a_2 \rightarrow b_3 \rightarrow ...$$

The eigenvalue equation

Everything is now in place to obtain the eigenvalue equation. Again it is based on limiting the recurrent series at either end. At the lower end of the series the zeroth-order parameters are fixed by the limiting unit matrix, and the first-order $b_1$ coefficient is quantized by the requirement on the $\rho$ parameter. One thus chooses a value of $k$ and the plus or minus root of the indicial equation. This is sufficient to start the recurrence:

$$a_0 = 1$$

$$b_0 = 0$$

$$b_1 = \frac{k - (E + g^2) + \Delta}{2g}.$$  \hfill (52)

From this input onwards all higher-order coefficients are generated by the leapfrog recurrence relations. For a fixed integer $k$ and a choice of the parity sign of the roots, the only remaining variable in which all coefficients will be expressed is the energy. To determine then the energy we follow the same argument as before and require that the series terminate at the high end, i.e. we require:

$$\lim_{n \rightarrow \infty} b_n (E + g^2) = 0.$$  \hfill (53)
Alternatively one could also terminate the series at $a_n$, yielding the same results. The $b_n$ or $a_n$ coefficient is a polynomial in $E + g^2$, the roots of which again will determine the eigenvalues. This is a new kind of transcendental function. It is determined by three choices: $\rho_+$ versus $\rho_-$, the value of $k$, and the value of $n$. Concerning this last choice, in figures 4 and 5 we plot the functions $b_n(E + g^2)$ for $n = 5, 6, 7, 8$, and $k = 0, 1$ for anti-symmetric and symmetric roots respectively. These functions clearly resemble Kummer-type polynomials themselves [24]. It is remarkable that even for small $n$ values the previous results of Moroz [11] and Braak [1] are easily recovered. However truncating the series at higher $n$-value will lead to sharper warping of the functions and hence more accurate eigenvalues. For convenience the lower eigenvalues are listed in table 1. In the next two figures we take $b_8 = 0$, and $\rho_+ = k$, with even (figure 6) and odd (figure 7) values for $k$; in this way one recovers the anti-symmetric and symmetric eigenenergies respectively. Most importantly as the figures show, different $k$ values reproduce the same spectrum, but with higher $k$-values the higher energy roots can be obtained more accurately. In figure 6 it is noted that for $k = 6$ a peculiar non-physical root appears at $E + g^2 = -0.111 577$. This is probably due to a numerical instability and disappears for higher $n$-values. We will return to the issue of non-physical roots in the next section.

**Discussion**

**The quantum number $k$**

When solving the Birkhoff equation an integer number $k$ naturally appears which we may associate with the quantum number that was used by Braak to label states of the same reflection symmetry. Let us study this number into more detail. It relates to the energy as:

$$ k = E + g^2 \pm A. $$
The gauge parameter $A$ is seen to measure the distance between the actual eigenenergy and the Juddian baselines, $E_k$. These baselines are straight decreasing lines in an $\{E, g^2\}$ plot, defined by:

$$E_k = k - g^2.$$  \hspace{1cm} (55)

In the limit of strong coupling, the surface consists of two deep wells with the same energy, and hence becomes a nearly degenerate boson spectrum, which in the limit coincides with the Juddian baselines. Reflection symmetry adaptation yields for each baseline one symmetric and one anti-symmetric state. Above this limit the appearance of the $A$ parameter makes it possible to associate a given eigenenergy with a Juddian baseline. So in a sense the baselines acts as ‘attractors’ for the eigenenergy. However this association is not uniquely defined, since as was shown in figures 6 and 7, different $k$-values can lead to the same eigenenergies. For the association to be more strict one should have a closer look at the eigenfunctions themselves. It seems always to be the case that the $a_n$ and $b_n$ coefficients show the fastest convergence when the $k$ value corresponds to the index of the nearby Juddian baseline. Increasing the value of $k$ for the same eigenenergy will simply increase $A$ by the same integer, and thus increase the rank of the Kummer function [24]. Since the eigenfunction should not change, this increase is countered by a concomitant shift in the $a_n$ and $b_n$ coefficients, putting more weights on

**Figure 5.** Plot of the transcendental function $b_n(E + g^2)$ for $n = 5$ (green), $n = 6$ (brown), $n = 7$ (purple), $n = 8$ (blue). The $k$-value is set to one, and the $\rho_\ast$ root is chosen. The roots correspond to the symmetric eigenvalues.

**Table 1.** Eigenenergies $E + g^2$ for $\Delta = 0.4$ and $g = 0.7$ ($b_9 = 0$).

| Symmetric | Anti-symmetric |
|-----------|----------------|
| +0.062956 | −0.217805      |
| +1.163604 | +0.86095       |
| +1.85076  | +2.12701       |
| +3.03523  | +2.9567        |
| +4.0569   | +3.95113       |

The gauge parameter $A$ is seen to measure the distance between the actual eigenenergy and the Juddian baselines, $E_k$. These baselines are straight decreasing lines in an $\{E, g^2\}$ plot, defined by:

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coefficients with larger $n$ and thus reducing the rate of convergence. The fact that different values of $k$ can still give rise to the same overall eigenfunctions is an outcome from the ‘contiguity’ relations of the confluent hypergeometric functions. In short a given eigenstate should always be labeled by the quantum number $k$ which corresponds to the smallest distance $A$ between the actual eigenenergy and the $E_k$ Juddian baseline.

As already indicated in the discussion of the Birkhoff gauge potential, integer and half-integer values of $A$ constitute special points in the solution space. When $A$ is zero (case 3), the

Figure 6. Plot of the transcendental function $b_k(E + g^2)$ for $n = 8$, based on the expression for $\rho_\pm$ with different even $k$-values: $k = 0$ (blue), $k = 2$ (purple), $k = 4$ (brown), $k = 6$ (green). The roots correspond to eigenenergies of anti-symmetric states.

Figure 7. Plot of the transcendental function $b_k(E + g^2)$ for $n = 8$, based on the expression for $\rho_\pm$ with different odd $k$-values: $k = 1$ (blue), $k = 3$ (purple), $k = 5$ (brown). The roots correspond to eigenenergies of symmetric states.
state will cross the \( k \)th Juddian baseline. It is observed that such a crossing always involves pairs of states of opposite parity which cross simultaneously in opposite directions, as is indicated in figure 8(a). Consider a symmetric state which is approaching the baseline \( E + g^2 = k \). Its energy is given by:
\[
E_+ = -g k A \lim_{A \to 0}.
\] (56)

There will then be a complimentary anti-symmetric solution with the same \( k \)-value which is approaching the baseline from the opposite side, as:
\[
E_- = g k A \lim_{A \to 0}.
\] (57)

As \( A \) becomes zero both roots will cross simultaneously and thus become degenerate. At this point the fermion states are uncoupled. Since both solutions will approach the baseline from opposite sides, they will not alter the number of eigenstates in between two baselines: if one eigenstate leaves this region another one will enter at the same time. Note that this rule only applies when \( A \) is zero. If it is a non-zero integer, only one of the \( \rho_\pm \) roots could be analytic, and thus cross the baseline without having a counterpart crossing in the opposite direction. These are the so-called non-Juddian crossings, which correspond to case 4. We will discuss this case below.

The case of half-integer values of \( E + g^2 \) (case 2), is represented in figure 8(b). Suppose a root \( \rho \) is approaching the halfway line in between the baselines \( E + g^2 = k \) and \( E + g^2 = k + 1 \) from below. Further assume that \( k \) is even, so this will be a symmetric state. Its energy is given by:
\[
E_+ = g k A \lim_{A \to 1/2}.
\] (58)
Simultaneously there will be a $\rho$ root belonging to $k + 1$ which is approaching this line from above. Since $k + 1$ is now odd, and we take the $\rho$ root, this state will be symmetric too. Its energy is given by:

$$E' + g^2 = k + 1 - \lim_{A \to 1/2} A.$$  (59)

These expressions suggest that the two states of the same parity will cross midway, but, as indicated in case 2, for $A$ half integer, one of the Kummer solutions does not exist, and hence there can’t be two degenerate states at a half-way crossing point. This implies that the crossing will be avoided, at least if both states are analytic. The halfway lines thus act as a separatrix in between the Juddian baselines. Although pairs of levels of the same parity seem to intersect the half-way lines at a common crossing point, they in fact repel each other, as detailed calculations by Maciejewski et al have pointed out [16].

Taken together the two rules for integer and half-integer $E + g^2$ roots, lead to a regular distribution of roots through the eigenvalue spectrum, as was observed by Braak. However, as we have indicated, these rules do not cover all possibilities, since the case considered in figure 8(a) requires that both states involved be analytic.

**Analyticity**

Quantum mechanics requires that the eigenfunctions should belong to the Bargmann–Fock space, which is the set of all entire functions with a finite norm. This criterion should apply to the solutions $f_1(z)$ and $f_2(z)$ of the original Hamiltonian equations. It certainly applies to the $F_1(z)$ and $F_2(z)$ solutions of the canonical equations. The Kummer series $F(a, b; z)$ is absolutely convergent for all values of the parameters, except for $b = 0, -1, -2,...$ where it has simple poles. It is furthermore single-valued and differentiable for all values of $z$, real or complex. For $a = -n$, with $n = 0, -1, -2,...$, it becomes a finite polynomial of degree $n$. With $k$ a non-negative integer the solutions are moreover entire. However the fact that the solutions of the canonical equations are within the Bargmann–Fock space, does not necessarily imply that the actual eigenfunctions of the original equation are too. Indeed it is found that for the low-energy end of the spectrum one may obtain roots of the transcendental equation which are non-physical. In figure 9 we show in detail the lower roots of the $b_{20}$ polynomial for $k = 0, 2, 4$. The lower one of these is consistently reproduced, but it is not a physical eigenstate, as it is below the lowest physical state of the Bargmann equation. The unphysical character of this state is not due to divergence of the $b_n$ coefficients, since they converge in the same way as the eigenvectors of the physical states. So where is it coming from? It turns out that the unphysical solutions are not entire. This can easily be demonstrated by tracing back these states to the origin where the coupling parameter $g$ is turned off.

For $g = 0$ the original Bargmann equations reduce to:

$$\frac{d}{dz} f_1 = \frac{E}{z} f_1 - \frac{\Delta}{z} f_2$$

$$\frac{d}{dz} f_2 = -\frac{\Delta}{z} f_1 + \frac{E}{z} f_2.$$  (60)

These equations give rise to two harmonic oscillator series. For $\Delta > 0$, the lower series is based on an anti-symmetric vacuum state at $E = -\Delta$, with eigenfunctions:

$$f_1 = z^{E+\Delta}$$

$$f_2 = -z^{E+\Delta}.$$  (61)
Analyticity requires $E + \Delta$ to be a nonnegative integer, hence:

$$E = k - \Delta \quad \text{with } k = 0, 1, 2, ...$$  \hfill (62)

The upper series is based on a symmetric vacuum state at $E = +\Delta$, with eigenfunctions:

$$f_1 = z^{E-\Delta}, \quad f_2 = z^{E-\Delta}.$$  \hfill (63)

and:

$$E = k + \Delta \quad \text{with } k = 0, 1, 2, ...$$  \hfill (64)

By gradually reducing $g$ to zero, we may correlate the states adiabatically to the oscillator levels in the origin. The lowest antisymmetric physical state, considered in figure 9 with $E + g^2 = -0.2178$, converges to $E = -0.4$ when the vibronic coupling vanishes. This corresponds to $E = -\Delta$, as expressed in equation (62), with $k = 0$. The unphysical state however, at $E = g^2 = -0.3526$, connects to $E = -0.6$, which corresponds to $E = -1 + \Delta$ in equation (64), with $k = -1$. Hence in this case $k$ is negative, and as a result the state is not entire, and cannot belong to the physical spectrum.

We show this in figure 10 for a more extreme case with large splitting, which was already simulated by Reik [25]. It is characterized by $\Delta = 1.5$, which corresponds to $\delta = \frac{1}{\Delta}$ in Reik’s notation. The unphysical state is an anti-symmetric A-state, indicated by a dashed line. At zero coupling this state is found at $E = 0.5$. In figure 8(c) we show a close-up of this spectral
These states are indicated by solid lines in figure 8(c). The dashed line, representing the unphysical state, lies below the symmetric vacuum state, and has energy $E = k + \Delta$, with $k = -1$. Hence clearly this state is not entire and thus does not belong to the physical spectrum. This requirement is thus more strict than the indicial equation of the Birkhoff canonical form. Nevertheless this unphysical state plays an interesting role in the spectrum. As can be seen from figure 10, it crosses the first Juddian baseline at $E + g^2 = 1$ at precisely the same point where an entire physical solution with opposite parity is crossing in the opposite sense. So this is an example of only one root with integer $E + g^2$. According to the treatment by Kus and Lewenstein [23] the crossing point with the first baseline is determined by the condition $4g^2 + \Delta^2 = 1$. Now since $\Delta > 1$, this condition cannot be met for real values of $g$, and hence there is no pairwise crossing of physical states. A similar lonely crossing is observed at the second baseline $E + g^2 = 2$. Here the condition reads:

$$32g^4 - 32g^2 + 12g^2\Delta^2 - 5\Delta^2 + \Delta^4 + 4 = 0. \quad (65)$$

The solutions for $\Delta = 1.5$ are: $g^2 = 0.1689$ and $-0.0126$. We have to reject the negative solution, and as a result only one pairwise crossing is expected on this baseline, at $g^2 = 0.411$. The second crossing shown in figure 10 involves only one physical state, but is nicely accompanied by a reverse crossing by an unphysical partner.
Conclusions

According to Maciejewski et al [16], and contrary to Braak’s integrability claim, quantum integrability should anyhow require another commuting operator, besides of the parity operation. By transforming the Rabi equations into their canonical form an interesting new perspective is opened on this simplest case of boson-fermion coupling. Introduction of quantization in this scheme is based on the association of the Rabi eigenvalues with the strict quantization of the displaced harmonic oscillator. The quantum numbers of this displaced oscillator correspond to the integer indices of the Juddian baselines. The canonical equations introduce a gauge potential which measures the distance between the actual eigenenergy and the integer quantum numbers of the Juddian baselines. In this way they realize an association between the Rabi Hamiltonian and the displaced oscillator. Admittedly, this association is based on the additional requirement that the gauge potential should be minimal, but at least this gauge criterion provides a way to replace mere counting numbers by ‘effective’ quantum numbers. The analysis further draws attention to the fact that eigenvalues should be characterized as spectral functions in a global $(\Delta, g)$ parameter space, rather than discrete points for a fixed parameter set. As we have argued in a previous paper [26] the canonical equation for the Jahn–Teller Hamiltonian is identical to the Rabi case. In a forthcoming publication we will report the results of an analogous treatment on the Jahn–Teller case.

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