Continued fractions and the Rabi model

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Abstract

Techniques based on continued fractions to numerically compute the spectrum of the quantum Rabi model are reviewed. They are of two essentially different types. In the first case, the spectral condition is implemented using a representation in the infinite-dimensional Bargmann space of analytic functions. This approach is shown to approximate the correct spectrum of the full model if the continued fraction is truncated at sufficiently high order. In the second case, one considers the limit of a sequence of models defined in finite-dimensional state spaces. In contrast to the first, the second approach is ambiguous and can be justified only through recourse to the analyticity argument from the first method.

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1. Introduction

The fully quantized Rabi model \([1, 2]\) constitutes probably the simplest strongly coupled quantum system with an infinite-dimensional Hilbert space. It is described by the Hamiltonian \((\hbar = 1)\)

\[
H_R = \omega a^\dagger a + g \sigma_x(a + a^\dagger) + \Delta \sigma_z.
\]  

\((1)\)

\(H_R\) possesses a \(\mathbb{Z}_2\)-symmetry which renders it integrable [3], although the associated two invariant subspaces (parity chains) are each infinite-dimensional themselves. The regular spectrum of \((1)\) is determined in each parity chain by the zeros of a transcendental function \(G_\pm(x)\), which can be expressed through confluent Heun functions [4]. \(G_\pm(x)\) has poles at integer multiples of \(\omega\), which allows us to obtain results on the distribution of eigenvalues and the location of degeneracies which are related to the quasi-exact (exceptional) spectrum [3]. The approach based on the symmetry of the model leads in this way to a unified picture of all spectral properties.

Independent from the qualitative understanding of the physics governing the quantum Rabi model is the question whether the analytical solution could invalidate the widely used
numerical determination of the spectrum through exact diagonalization on a truncated state space or the equivalent continued fraction techniques [5–12]. There has been recent confusion on this point [13, 14], and this paper intends to clarify the situation regarding the methods based on continued fractions. These fall into two classes, which we denote with A and B.

2. Method A

One considers the full model, i.e. the state space is assumed to be infinite dimensional, $\mathcal{H} = L^2(\mathbb{R}) \otimes \mathbb{C}^2$. Work in this direction goes back to the seminal paper by Schweber [5]. He used the isomorphism between $L^2(\mathbb{R})$ and the Bargmann space $\mathcal{B}$ of analytic functions [15] to obtain a differential equation for the spin-up component of the eigenfunction with energy $E$,

$$\psi_E(z) = e^{-g/\omega} \sum_{n=-\infty}^{\infty} K_n(E) \left( z + \frac{g}{\omega} \right)^n,$$

leading to a linear three-term recurrence relation for the coefficients $K_n(E)$,

$$nK_n = f_{n-1}(E)K_{n-1} - K_{n-2},$$

with

$$f_n(E) = \frac{2g}{\omega} + \frac{1}{2g} \left( n\omega - x(E) + \frac{\Delta^2}{x(E) - n\omega} \right)$$

and $x(E) = E + g^2/\omega$. The same equation results if the $\mathbb{Z}_2$-invariance is used to project the Hamiltonian to one of its invariant subspaces with fixed parity [3]. Each of the parity chains $\mathcal{H}_\pm$ is isomorphic to $\mathcal{B}$ [3] and we set $\mathcal{H} = \mathcal{H}_+ = \mathcal{B}$ in the following, confining the discussion to positive parity. The energy eigenvalues $E_n, n = 0, 1, 2, \ldots,$ of $H_B$ are determined by imposing on $\psi_E(z)$ the condition to be an element of $\mathcal{B}$, henceforth called the ‘spectral condition’. This condition consists of two parts: the first is the familiar normalizability, $|\psi_E(z)| < \infty$, where $| \cdot |$ denotes the norm in $\mathcal{B}$. Because the differential equation for $\psi_E(z)$ in (2) has an irregular singular point of rank 1 at infinity [16], $\psi_E(z) \sim e^{cz}z^\nu(c_0 + c_1/z + \cdots)$ with complex constants $c, \rho, c_0, c_1$ [17]. As $\mathcal{B}$ contains all functions growing like $e^{cz}$ for $|z| \to \infty$, $\psi_E(z)$ fulfills the first part of the spectral condition for any real $E$. The second part demands $\psi_E(z)$ to be analytic everywhere in $\mathbb{C}$, and it is this second part which fixes the discrete set $\{ E_n | n \in \mathbb{N}\}$, the spectrum of $H_B$. The differential equation for $\psi_E(z)$ has two regular singular points at $z = \pm g/\omega$, and $\psi_E(z)$ will be analytic in $\mathbb{C}$ if it is analytic at both of these points. $\psi_E(z)$ is expanded in (2) around $z = -g/\omega$ and is analytic there if $K_0 = 0$ for $n \leq -1$. This leads to the initial condition for the recurrence (3): $K_0 = 1$ and $K_1(E) = f_0(E)$. It still yields no equation for $E$, which is obtained by demanding analyticity at the second singular point $z = g/\omega$. From the Poincaré analysis of (3) it follows that there are two possibilities for the limiting behavior of the $K_n(E)$: $K_{n+1}(E)/K_n(E) \to \omega/(2g)$ or $K_{n+1}(E)/K_n(E) \to 0$. The latter behavior corresponds to the unique minimal solution $\{K_n^{\text{min}}\}_{n \in \mathbb{N}}$ of (3) with the initial condition $K_0 = 1$.\footnote{One assumes here that the minimal solution has $K_0 \neq 0$, which does not follow from (3). It is therefore not clear a priori that $K_n^{\text{min}}$ is related for all $E$ to the continued fraction (5), which means that the convergence of (7) has to be proven independently.}

Note that $K_1^{\text{min}}$ is determined in terms of $\{ f_1(E), f_2(E), \ldots \}$ for any $E$ and does not depend on $f_0(E)$ [18, 19]. All other solutions $\{K_n\}_{n \in \mathbb{N}}$ of (3) are dominant, i.e. $\lim_{n \to \infty} K_n^{\text{min}}/K_n = 0$. In general, $K_1^{\text{min}}(E) \neq f_0(E)$, but for $E \in \{ E_0, E_1, \ldots \}$ one has $K_n^{\text{min}}(E_n) = f_0(E_n)$. This condition determines the spectrum because only then $\psi_E(z)$ is analytic at both $-g/\omega$ and $g/\omega$ and therefore in all of $\mathbb{C}$. Analyticity at $-g/\omega$ fixes $K_1 = f_0(E)$ and analyticity at $g/\omega$ enforces an infinite radius of convergence of expansion (2), which would be finite ($R = 2g/\omega$) for any
dominant solution with $K_{n+1}(E)/K_n(E) \to \omega/(2g)$. Only the minimal solution yields $R = \infty$; therefore, $K_1(E) = K_{\text{min}}^0(E) = f_0(E)$, which is the sought after equation for $E$.

To compute the minimal solution of (3), Schweber proceeds to represent the quotient $K_1(E)/K_0$ through the infinite continued fraction

$$\frac{K_1(E)}{K_0} = f_0(E) = 1|f_1(E) - 2|f_2(E) - 3|f_3(E) - \cdots.$$  \hspace{1cm} (5)

As pointed out in [3], this equation amounts to a tautology if the formal expression on its right-hand side is not augmented with a prescription for the asymptotics of the tail $\xi_n(E)$ in

$$F_{\infty}(E) = 1|f_1(E) - 2|f_2(E) - 3|f_3(E) - \cdots = 1|f_1(E) - 2|f_2(E) - \cdots (N - 1)|F_{N-1}(E) = \xi_n(E).$$  \hspace{1cm} (6)

Fortunately, the standard definition of an infinite continued fraction $F_{\infty}(E)$ as the limit (if it exists) of a sequence of finite continued fractions $F_n(E)$,

$$F_{\infty}(E) = \lim_{n \to \infty} (1|f_1(E) - 2|f_2(E) - \cdots n|f_n(E)) = \lim_{n \to \infty} F_n(E),$$  \hspace{1cm} (7)

yields the correct prescription. The reason is that the limit (7) exists in the case of the asymptotic behavior

$$\lim_{n \to \infty} \frac{\xi_n(E)}{f_{n-1}(E)} = 0,$$  \hspace{1cm} (8)

but because $\xi_n = n\xi_n/E_{n-1}$ and $f_n \sim n\omega/(2g)$ for large $n$, this can only happen if $\lim_{n \to \infty} K_n(E)/K_{n-1}(E) = 0$, which characterizes the minimal solution. Pincherle’s theorem, which connects minimal solutions with $K_0 \neq 0$ to continued fractions, is a simple consequence of the uniqueness of $[K_{\text{min}}^0]$ [18]. In other words, the continued fraction (7) is a short-hand notation for the minimal solution $K_{\text{min}}^0(E)/K_0$ of the recurrence (3), which is defined for arbitrary $E$. Schweber has proven the (pointwise) convergence of (7) using a corollary of Pringsheim’s main theorem [20, 21]. However, in contrast to power series expansions, the actual value of (7) can only be obtained by checking the convergence numerically for each $E$ separately, by computing a set of $F_n(E)$ with large enough $n$. It is not possible to deduce from the smallness of the tail

$$\xi_n(E) = n|f_n(E) - (n + 1)|f_{n+1}(E) - \cdots$$  \hspace{1cm} (9)

the value of $F_{\infty}(E)$ for given $F_{n-1}(E)$ to a prescribed accuracy because the continued fraction itself may diverge while $\xi_n$ stays finite\textsuperscript{2}. Therefore, the actual computation concerns always some $F_n(E)$ with finite $N$. It is easy to see that the equation $f_0(E) = F_0(E)$ is just the spectral condition for the Hamiltonian $H_N = \hat{P}_N H_R \hat{P}_N$, where $\hat{P}_N$ denotes the projector onto the finite-dimensional Hilbert space $H_N$, spanned by functions of the form

$$\phi_n(z) = e^{-\omega z} (z + \frac{g}{\omega})^n, \hspace{1cm} n = 0, 1, 2, \ldots N.$$  \hspace{1cm} (10)

If $\psi_E(z) = \sum_{n=0}^{\infty} K_n \phi_n(z)$ satisfies formally $\langle H_R - E \rangle \psi_E(z) = 0$, then it follows

$$\sum_{n=0}^{\infty} K_n H_R \phi_n = \sum_{n=0}^{\infty} [(2g f_n(E) + E)K_n - 2g(n + 1)K_{n+1} + K_{n-1}]\phi_n,$$  \hspace{1cm} (11)

\textsuperscript{2} See the discussion on pp 38–40 in [21].
because of (3). Obviously, $F_0H_P\phi_{N+1} = 0$, which entails that the coefficient of $\phi_0$ in (11) becomes $(2g f_3(E) + E)K_N - 2gK_{N-1}$, which means $K_{N+1} = 0$, i.e. the recurrence (3) is cut-off at $K_N$. Now (3) together with the initial condition $K_1 = f_0(E)$ and additionally $K_{N+1} = 0$ is equivalent to an equation involving a finite continued fraction,

$$f_0(E) = 1 | f_1(E) - 2 | f_2(E) - 3 | f_3(E) - \cdots | f_N(E) = F_N(E),$$

and provides therefore the spectral condition in the space $\mathcal{H}_N$.

Note that this space does not correspond to the span of a finite subset of Fock states $\{z^n, n = 0, \ldots, N\}$ as the truncated spaces $\mathcal{H}^{(N)}$ used in method B, but all elements of $\mathcal{H}_N$ can be approximated to arbitrary precision by elements of $\mathcal{H}^{(N)}$ for sufficiently large $N$ (see below). Each solution $E_n^N$ of (12) approximates some solution $E_n$ of $F_N(E) = f_0(E)$ to precision $\varepsilon$ if $N > N(n, \varepsilon)$. The latter property follows from the fact that the convergence of the tail $\xi_2(E)$ depends on the value of $E$ being smaller than a certain upper bound depending on $N$ (see [5] or equation (24) below). The solution $E_n^N$ of (12) must be smaller than this bound for $F_N(E_n^N)$ to be a good approximation of $F_\infty(E_n^N)$. However, for each finite $E_n$ being a solution of the exact equation $f_0(E) = F_\infty(E)$, there is an $N(E_n)$ such that for all $N > N(E_n)$ the function $F_N(E_n)$ approximates $F_\infty(E_n)$ to a given precision and $E_n \approx E_n^N$ will be thus close to the solution $E_n^N$ of (12).

One may formalize this statement as follows. The domain of the operators $H_N$ is extended to $\mathcal{H}$ by setting $H_N\phi_m = 0$ for $m \geq N + 1$. Then, the spectrum $\sigma(H_R) = \{E_n\}_{n \in \mathbb{N}}$ of the operator $H_R$ is the limit of the spectra $\sigma(H_N) = \{E_n^N\}_{n \in \mathbb{N}}$ in the sense that there exists a number $M(N)$, unbounded in $N$, such that

$$\lim_{N \to \infty} \max_{N \leq n < M(N)} | E_n^N - E_n | = 0.$$  

The spectral condition on $\mathcal{H}_N$ provides an approximation to the spectrum of the full model precisely because it approximates the exact condition of analyticity in the Bargmann space. It follows that the continued fraction approach initiated by Schweber and pursued by several authors [7–11] can be used to obtain the spectrum of the quantum Rabi model to arbitrary precision. The method does not use the $\mathbb{Z}_2$-symmetry of $H_R$ as the Bargmann condition is implemented via (5). Indeed, (5) only depends on $\Delta^2$ and does not discern the two parity chains, which is the reason why the relation of isolated (Juddian) solutions at $x(E) = \mu_0$ to level crossings, i.e. reducible representations of $\mathbb{Z}_2$, appears to be accidental within the Schweber approach [22]. The infinite continued fraction $F_\infty(E)$ is completely opaque to an analysis of its general behavior as a function of $E$: $F_\infty(E)$ is the formal quotient of two functions,

$$F_\infty(E) = \lim_{n \to \infty} \frac{A_n(E)}{B_n(E)},$$

where $A_n$ and $B_n$ both satisfy the recurrence relation

$$C_n = f_0(E)C_{n-1} - nC_{n-2}, \quad n \geq 2$$

and $A_0 = 0, A_{-1} = 1, B_0 = 1, B_{-1} = 0$. Only the quotients of $A_n$ and $B_n$ are well defined for $n \to \infty$. Therefore, the location of zeros and poles of $F_\infty(E) - f_0(E)$ cannot be read off from the behavior of the numerator or denominator in the limit $n \to \infty$, in contrast to the function $G_\pm(x)$, whose pole structure is known and leads to simple rules for the distribution of eigenvalues. Method A can be used to calculate the spectrum of the Rabi model to any desired accuracy, but provides no insight beyond direct numerically exact diagonalization in a finite-dimensional state space with dimension $N + 1$, if (5) is truncated at the order $N$. 

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3. Method B

This approach goes back to Swain [6]. It is based on a three-term recurrence relation for the determinants of tridiagonal matrices. Because the quotient of two such determinants can be interpreted as a matrix element of the resolvent of $H_R^{(N)}$, if defined on a truncated Hilbert space, $\mathcal{H}_t^{(N)} = \mathbb{C}^{N+1} \otimes \mathbb{C}^2$, one may write this matrix element as a finite continued fraction. By repeating Swain’s calculation, the authors of recent work [12, 14] tie the ‘solvability’ of the Rabi model to his representation of the resolvent. It is further claimed in [14] that this representation, which is defined in $\mathcal{H}_t^{(N)}$ only, has a well-defined limit $N \to \infty$ at least for $g^2 < \omega$ and in this way provides an exact solution of the Rabi model without making use of the analyticity condition employed by method A. This claim is based on the belief that the operator $H_R$, defined on an infinite-dimensional Hilbert space, can be approximated by the sequence of finite-dimensional matrices $H_R^{(N)}$, which is incorrect because $H_R$ is not compact [23]. Nevertheless, the full spectrum of $H_R$ can be obtained by method B as well—but this is entirely due to the equivalence of the spaces $\mathcal{H}_t^{(N)}$ to the spaces $\mathcal{H}_t \otimes \mathbb{C}^2$ from method A—and rests therefore again on the Bargmann criterion, as shown in the following.

There are several equivalent formulations of Swain’s approach [6, 12, 14, 24]. In its simplest form [12], one considers the Hamiltonian in each parity chain separately, where it corresponds to a tridiagonal matrix. Define the parity chain $\mathcal{H}_\pm = \text{span}\{|n, \pm (-1)^n\rangle\}_{n \in \mathbb{N}_0}$ with $|n, 1\rangle = |n\rangle \otimes |\uparrow\rangle$ and $|n, -1\rangle = |n\rangle \otimes |\downarrow\rangle$. The Fock states $|n\rangle$ are eigenstates of $a^\dagger a$: $a^\dagger a |n\rangle = n |n\rangle$. $\mathcal{H}_\pm$ is isomorphic to $L^2(\mathbb{R})$, i.e., to the span of Fock states $|n\rangle$ for $n \in \mathbb{N}_0$. To define the finite-dimensional approximants $H_{\pm}^{(N)}$ to $H_\pm$ in $\mathcal{H}_\pm$, one uses projection operators $\hat{P}_{\pm}^{(N)}$ projects onto $\mathcal{H}_\pm^{(N)} = \text{span}\{|n, \pm (-1)^n\rangle\}_{0 \leq n \leq N}$. The truncated parity chain $\mathcal{H}_\pm^{(N)}$ is then isomorphic to $\mathbb{C}^{N+1}$ and the truncated Hamiltonian in $\mathcal{H}_\pm^{(N)}$ reads $\hat{H}_{\pm}^{(N)} = \hat{P}_{\pm}^{(N)} H_\pm \hat{P}_{\pm}^{(N)}$. $\hat{H}_{\pm}^{(N)}$ assumes the tridiagonal form

$$
\hat{H}_{\pm}^{(N)} = M_0^{\pm} = 
\begin{pmatrix}
\frac{b_0}{\sqrt{a_1}} & \sqrt{a_1} & 0 & \cdots \\
\sqrt{a_1} & \frac{b_1}{\sqrt{a_2}} & \sqrt{a_2} & \ddots \\
0 & \sqrt{a_2} & \ddots & \ddots \\
\ddots & \ddots & \ddots & \sqrt{a_{N-1}} \\
& \sqrt{a_{N-1}} & \sqrt{a_N} & \frac{b_N}{b_N^{\pm}}
\end{pmatrix},
$$

(16)

with

$$
b_j^{\pm} = j \omega \pm (-1)^j \sqrt{\Delta}, \quad a_j = j g^2, \quad j = 0, 1, \ldots, N.
$$

(17)

To derive a recurrence relation for $\det M_0^{\pm}$, define matrices $M_j^{\pm}$ by deleting the first $j$ rows and columns from $M_0^{\pm}$. Then it follows

$$
\det M_j^{\pm} = b_j^{\pm} \det M_{j-1}^{\pm} - a_{j+1} \det M_{j+2}^{\pm}
$$

(18)

for $j = 0, \ldots, N$, setting $\det M_{N+1}^{\pm} = 1$ and $\det M_{N+2}^{\pm} = 0$. This three-term recurrence can be turned into a nonlinear two-term recurrence for $G_j^{\pm} = \det M_{j+1}^{\pm} / \det M_j^{\pm}$,

$$
G_j^{\pm} = \frac{1}{b_j^{\pm} - a_{j+1} G_{j+1}^{\pm}}.
$$

(19)

To compute the resolvent of $\hat{H}_{\pm}^{(N)}$, we set $M_0^{\pm} = E - \hat{H}_{\pm}^{(N)}$ and find for $G_0^{\pm}(E) = \langle 0, \pm 1 | (E - \hat{H}_{\pm}^{(N)})^{-1} | 0, \pm 1 \rangle$ a representation in terms of a finite continued fraction

$$
G_0^{\pm}(E) = 1 | b_0^{\pm}(E) - a_1 | b_1^{\pm}(E) - a_2 | b_2^{\pm}(E) - \cdots - a_N | b_N^{\pm}(E),
$$

(20)

5
where the \( b_j^\pm (E) \), \( \alpha_j \) are now defined as
\[
b_j^\pm (E) = E - j \omega \mp (-1)^j \Delta, \quad \alpha_j = j g^2, \quad j = 0, 1, \ldots, N.
\] (21)

We drop the parity index from now on and write \( G_0^{(N)} (E) \) for expression (20). \( G_0^{(N)} (E) = \det M_1 / \det M_0 \) has poles at the eigenvalues of \( H^{(N)} \), provided that the pole (a zero of \( \det(E - H^{(N)}) \) at \( E_n \)) is not lifted by a zero of \( \det M_1 \), which could occur if \( (0, \pm 1) \psi_n = 0 \) for the eigenstate \( |\psi_n \rangle \). This does not happen in this case because all \( \alpha_j \) are nonzero. Nevertheless, the numerical evaluation of (20) is compromised by the rapid decay of the overlap \( (0, \pm 1) \psi_n \) with growing \( n \). It becomes apparent in figure 1 of [14], where the peaks of the spectral density are very small already for \( n = 9, 10 \).

Method B presumes that the poles of \( \lim_{N \to \infty} G_0^{(N)} \) give the spectrum of the truncated Rabi model if \( G_0^\infty (E) = \lim_{N \to \infty} G_0^{(N)} \) can be shown to exist for any real \( E \). To prove this, Ziegler [14] invokes the main theorem of Pringsheim [21], which states that the sequence of finite continued fractions
\[
F_N = \alpha_1 |\beta_1| - \alpha_2 |\beta_2| - \alpha_3 |\beta_3| - \cdots - \alpha_N |\beta_N
\] (22)
converges for \( N \to \infty \) to a value \( F \) with \( |F| \leq 1 \) if \( |\beta_j| \geq |\alpha_j| + 1 \) for all \( j = 1, 2, \ldots \). If \( \alpha_j, \beta_j \) would be dimensionless, then this theorem could be used to compute the tail \( \xi_n \) of \( G_0^\infty \):
\[
\xi_n (E) = \alpha_n |b_n - a_{n+1} b_{n+1} + \cdots
\] (23)
for sufficiently large \( n \) and fixed \( E \), because \( |b_j| \sim j \omega \) and \( |\alpha_j| \sim j g^2 \) for \( j \geq n \gg 1 \) such that \( |b_j| \geq |\alpha_j| + 1 \) for all \( j \geq n \), provided \( g^2 < \omega \). The convergence of \( \xi_n (E) \) then ensures the convergence of the full continued fraction \( G_0^\infty (E) \) in the generalized sense, which is sufficient to conclude that the distribution of the poles of \( G_0^\infty (E) \) is well defined.

To obtain dimensionless quantities, \( g \) and \( \Delta \) in (1) are scaled with \( \omega \); \( \tilde{g} = g / \omega \) and \( \tilde{\Delta} = \Delta / \omega \). \( \tilde{\omega} = 1 \). The condition \( \tilde{g}^2 < \omega \) turns into \( \tilde{g}^2 < 1 \) or \( |g| < \omega \). This condition seems to invalidate the proof for the deep strong coupling regime \( |g| \gg \omega \), which is of current interest [25]. But Ziegler [14] does not rescale the Hamiltonian and obtains instead of \( |g| < \omega \) the meaningless expression \( \tilde{g}^2 < \omega \), which compares quantities of different dimension. However, it is easy to correct this mistake by using the following generalization of Pringsheim’s theorem for dimensionful quantities which lifts at the same time the restriction \( |g| < \omega \).

**Theorem.** Consider the continued fractions (22) and assume for the dimension \( [F_N] \) of \( F_N \), the relations \([\beta_j] = [\beta_1] \) and \([\alpha_j] = [F_N^2] \). If \( \prod_{j=1}^n |\alpha_j| \) is unbounded in \( n \) and the inequalities \( |\beta_j| \geq |\alpha_j| / c + c \) hold for all \( j \geq 1 \) and some constant \( c \) with dimension \([c] = [\beta_1] \), then \( \lim_{n \to \infty} F_N = F \) exists and \([F] \leq c \).

The theorem is applicable to the tail \( \xi_n (E) \) of \( G_0^\infty (E) \). Moreover, the possibility of choosing \( c \) freely leads to the following lower bound for \( n \):
\[
n \geq |E| + |\Delta| \omega + \frac{2 \tilde{g}^2}{\omega^2} \left( 1 + \sqrt{1 + \frac{|E| + |\Delta| \omega}{\tilde{g}^2}} \right).
\] (24)

In this way, the convergence of \( G_0^\infty (E) \) can be proven for arbitrary model parameters. (An alternative would be to apply the corollary used by Schweber3.)

I shall now demonstrate that this proof of convergence is not sufficient to show that \( \lim_{N \to \infty} G_0^{(N)} (E) \) is related to the spectrum of the full Rabi model for fixed parity. The reason is the intrinsic ambiguity in the definition of the finite-dimensional approximants to \( H_R \). If

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3 This generalization does not appear in the literature, but it is easily obtained by modifying the proof of the main theorem [21].

4 Theorem 2.22 in [21].
If one sets matrix elements of \( \lim_{\sigma(N) \to \infty} H^{(N)} \) in the norm topology and \( \sigma(H^{(N)}) \) would converge toward \( \sigma(H_R) \) in the sense defined in (13) because the sets \( [E_n^{(N)}] \) and \( [E_n] \) would satisfy the even stronger condition
\[
\lim_{N \to \infty} \sup_{n \in \mathbb{N}_0} |E_n^{(N)} - E_n| = 0.
\]
(25)

But \( H_R \) is unbounded in \( \mathcal{H} \) and therefore is not the limit of any sequence of finite-dimensional operators. Even if the sequence of truncated state spaces \( \{\mathcal{H}^{(N)}\}_{N \in \mathbb{N}} \) could be determined in a unique way (which is not the case), the approximating operators \( H^{(N)} \) need not to be the \( H^{(N)} = \hat{P}^{(N)} H_R \hat{P}^{(N)} \), used in method B. The projection \( \hat{P}^{(N)} \) affects only the states \( |N\rangle \) and \( |N+1\rangle \) because it is equivalent to setting \( \langle N| H_R |N+1\rangle = |g| \sqrt{N+1} \) to zero. But as these matrix elements grow as \( \sqrt{N} \) for \( N \to \infty \), it is not clear whether the spectra \( \sigma(H^{(N)}) \) converge to \( \sigma(H_R) \), even if they do converge to a limit. One could think of other modifications of the matrix elements of \( H_R \) between states with high energy and claim that these are also admissible truncation prescriptions. A similar ambiguity is well-known from quantum field theory: the regularization scheme needed to make the perturbative expressions finite by truncating the ultra-violet modes is not uniquely definable. One has to prove that the resulting (renormalized) expressions are independent from the choice of cut-off. In our case, the task is to show that the spectra of a sequence of finite-dimensional Hamiltonians \( \{H^{(N)}\} \) converge to \( \sigma(H_R) \), and to this end one would have to prove that this limit does not depend on the modification of \( H_R \) in the high-energy region which is used to define the approximants \( H^{(N)} \).

The formal condition reads as follows.

If the elements of two sequences of operators \( \{H^{(N)}\} \) and \( \{\hat{H}^{(N)}\} \) are defined on the spaces \( \mathcal{H}^{(N)} \) for \( N = 0, 1, \ldots \) with \( \mathcal{H}^{(0)} \subset \mathcal{H}^{(1)} \subset \cdots L^2(\mathbb{R}) \) and \( H^{(N)} = \hat{H}^{(N)} = H_R \) if projected onto \( \mathcal{H}^{(N-1)} \), then the limit of the spectra of both sequences as defined in (13) must coincide:
\[
\lim_{N \to \infty} \sigma(H^{(N)}) = \lim_{N \to \infty} \sigma(\hat{H}^{(N)}).
\]

This is obviously necessary (albeit not sufficient) to justify the claim that \( \sigma(H^{(N)}) \) converges to the unique \( \sigma(H_R) \), if \( H_R \) is not compact and the \( H^{(N)} \) do not converge to it in the operator sense, but it is violated in the present case. One may define a cut-off prescription for \( H^{(N)} \) which affects only the states \( |N-1\rangle, |N\rangle \) and \( |N+1\rangle \) but produces a (fictitious) pole in \( G_0^{(N)}(E) \) at an arbitrary value \( E_0 \). Consider expression (20) for \( G_0 \), which reads
\[
G_0(E) = \frac{1}{|b_0(E) - a_1|} |b_1(E) - a_2| |b_2(E) \cdots a_{N-1}| |b_{N-1} - a_N| G_N(E)
\]
(26)
as follows from (19). The standard cut-off using the projection \( \hat{P}^{(N)} \) sets \( G_N(E) = 1/|b_N(E)| \). But \( G_N(E) \) can also be determined from below by a recurrence relation equivalent to (19),
\[
G_{j+1}(E) = \frac{b_j(E)}{a_{j+1}} - \frac{1}{a_{j+1} G_j(E)}.
\]
(27)

If one sets \( G_0(E_0) = \infty \), corresponding to a pole of \( G_0(E) \) at \( E_0 \), the recurrence (27) with the initial condition \( G_1(E_0) = b_0(E_0)/a_1 \) yields a \( G_N(E_0) \) which will tend to the value \( -\omega/\sqrt{g^2} \) for \( N \to \infty \). The matrix element \( \langle N|\hat{H}^{(N)}|N\rangle \) of the truncated Hamiltonian \( \hat{H}^{(N)} \) is defined by
\[
\langle N|\hat{H}^{(N)}|N\rangle = \hat{H}_{N,N}^{(N)} = E_0 - \frac{1}{G_N(E_0)}.
\]
(28)
For all \( i, j \neq (N, N) \), \( \hat{H}_{ij}^{(N)} = \hat{H}_{ji}^{(N)} \). But the ensuing \( \hat{G}_0^{(N)}(E) \) will have a pole at \( E_0 \), although only a single-matrix element was changed and therefore \( \hat{P}^{(N-1)} \hat{H}^{(N)} \hat{P}^{(N-1)} = \hat{P}^{(N-1)} H_R \hat{P}^{(N-1)} \). The same result follows if one sets \( \hat{H}_{N,N}^{(N)} = E_0 - N/G_N(E_0) \) and modifies at the same time \( \hat{H}_{N-1,N}^{(N)} = gN \), which does not yield a low-energy state a priori if \( G_N + \omega/\sqrt{g^2} \) tends slower to zero than \( 1/N \). It is therefore possible to define a sequence of Hamiltonians \( \{\hat{H}^{(N)}\} \) with

5 Theorem VI.13 in [23].
eigenvalues which are not close to the elements of the spectrum of the untruncated Rabi model, but differ from $H^{(N)}$ in at most three matrix elements and coincide with $H_R$ on $\mathcal{H}^{(N-1)}$. Neither $\{\tilde{H}^{(N)}\}$ nor $\{H^{(N)}\}$ converge to $H_R$ in norm topology because $H_R$ is unbounded. This entails that no independent criterion exists to select the ‘correct’ sequence $\{\tilde{H}^{(N)}\}$ apart from the convergence of the spectrum in the sense of (13) to some set $\{\varepsilon_n\}_{n\in\mathbb{N}}$. However, the spectra of the sequence $\{H^{(N)}\}$ converge as well, if $H_{R,N}, \tilde{H}^{(N)}_{N,N}$ are appropriate functions of $N$. The problem cannot be solved by the consideration of resolvents instead of the Hamiltonians. $H_R$ has a compact resolvent, whereas the resolvents of the finite-range operators $H^{(N)}$ and $\tilde{H}^{(N)}$ are bounded but not compact and do not converge to $(z - H_R)^{-1}$ in the norm topology. Even if one could prove that only $\{H^{(N)}\}$ and not $\{\tilde{H}^{(N)}\}$ converges to $H_R$ in the strong resolvent sense, it would be insufficient to determine $\sigma(H_R)$ unambiguously.  

The standard cut-off prescription leads indeed to the correct spectrum of the full model as the comparison with the analytical solution [3] shows. But this prescription is only valid because the finite approximants $H_N$ obtained by method A are the projections $P_N H_R P_N$ and thus correspond to the standard cut-off of the model in the finite-dimensional state spaces $\mathcal{H}_N$ as shown above. These spaces are not generated by the first $N + 1$ Fock states as the $\mathcal{H}^{(N)}$ but are sufficiently close to them for large $N$ because the coherent factor $e^{-\varepsilon_0/\omega}$ appearing in the $\psi(z;N)$ has a convergent expansion in Fock states. The isomorphism $\hat{I}$ between $\mathcal{B}$ and $L^2(\mathbb{R})$ maps the function $z^N/\sqrt{n!}$ onto $|n\rangle$; it follows that for any vector $|\psi_N\rangle \in \hat{I}(\mathcal{H}_N) \subset L^2(\mathbb{R})$ and its projection $|\psi'_N\rangle$ onto $\mathcal{H}^{(N)}$, we have

$$\lim_{N \to \infty} \langle \psi_N - \psi'_N | \psi_N - \psi'_N \rangle = 0. \tag{29}$$

Therefore, $\hat{P}_N H_R \hat{P}_N - \hat{P}^{(N)} H_R \hat{P}^{(N)}$ tends to zero in the norm topology for $N \to \infty$. We may conclude that method B yields the spectrum of the Rabi model in the limit $N \to \infty$ precisely because the finite-dimensional approximants $H_N$ of method A are the correct ones. Method B cannot be justified independently from method A.  

Apart from the implicit dependence on method A, method B shares with it the same problems: the expressions derived from continued fractions do not allow for qualitative analysis because the singularities of neither $F_\infty(E)$ nor $1/G^2_\infty(E)$ are known, which would be necessary to infer the distribution of the eigenvalues of $H_R$. Moreover, the position and nature of spectral degeneracies cannot be obtained from those functions, as exemplified in [14], where the following is said on level crossings. ‘The individual matrix elements $g, h$ avoid level crossing due to parity conservation, since eigenstates of consecutive eigenvalues have different parity’. However, $g$ and $h$ correspond to the subspaces with even and odd parities, respectively; parity does not change within each subspace. The idea that alternating parity forbids level crossing between consecutive eigenvalues is erroneous, because the converse is true [3]. If applied to the full Hilbert space, Ziegler’s statement is wrong as well: energetically neighboring states do not have always different parity. Finally, the fact that the degeneracies (of states with different parity) occur only if $E + g^2/\omega$ is an integer multiple of $\omega$ can be deduced neither with method A nor with method B.

4. Conclusions

We conclude that both methods A and B yield correct approximations for the spectrum of the quantum Rabi model and are equivalent to numerically exact diagonalization in finite-dimensional Hilbert spaces of sufficient large dimension. Diagonalization on a truncated state

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6 Theorem VIII.24 in [23].

7 While an independent justification cannot be excluded in principle, it seems likely that it will involve sophisticated mathematical arguments, which, to the best of my knowledge, have not been presented yet.
space has been used for many years as a tool to obtain numerically exact results which were subsequently compared to a variety of analytical approximations (see e.g. [26]) without questioning its correctness, although the Hamiltonian $H_R$ is not the limit of a sequence of finite-dimensional operators. The soundness of the approach was taken for granted because of the numerical convergence of the results, which is equivalent to the convergence of the corresponding continued fraction. The pointwise convergence of the latter has been established by Schweber [5] for method A and by Durst et al [24] for method B. In the case of method A, this convergence is equivalent to the analyticity condition for the untruncated model and therefore sufficient to prove the numerical identity with the exact spectrum for large enough $N$. In contrast to method A, the convergence of the continued fraction says nothing about the spectrum of the full model within the framework of method B. The sequence of approximating Hamiltonians $H^{(N)}$ is not uniquely determined and the spectral convergence alone is not sufficient to prove a connection with $H_R$. But because the cut-off scheme employed by method B is equivalent (for large $N$) to the sequence of finite-dimensional approximants $H_N$ from method A, it yields the (numerically) exact spectrum in the limit $N \to \infty$ as well. It owes this to the validity of method A. In contrast to the claim made in [14], method B cannot be considered as an independent way to obtain the correct spectrum of $H_R$.

In this way, the use of continued fractions and (equivalently) numerically exact diagonalization can be rigorously justified in the case of the Rabi model. The key to the proof is Bargmann’s analyticity condition for functions as elements of an infinite-dimensional Hilbert space. Whether this equivalence with the analytical solution can be extended to more complicated systems or breaks down in some cases [27] should be the subject of future study.

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References

[1] Rabi I I 1936 Phys. Rev. 49 324
Rabi I I 1937 Phys. Rev. 51 652

[2] Jaynes E T and Cummings F W 1963 Proc. IEEE 51 89

[3] Braak D 2011 Phys. Rev. Lett. 107 100401

[4] Ronveaux A and Arscott F M 1995 Heun’s Differential Equations (Oxford: Oxford University Press)

[5] Schweber S 1967 Ann. Phys., NY 41 205

[6] Swain S 1973 J. Phys. A: Math. Nucl. Gen. 6 192
Swain S 1973 J. Phys. A: Math. Nucl. Gen. 6 1919

[7] Stenholm S 1981 Opt. Commun. 36 75

[8] Reik H G, Nusser H and Amarante Ribeiro L A 1982 J. Phys. A: Math. Gen. 15 3491

[9] Kleinr N, Weiss J and Doucha M 1986 J. Phys. C: Solid State Phys. 19 4673

[10] Reik H G and Doucha M 1986 Phys. Rev. Lett. 57 787

[11] Szopa M, Mys G and Ceulemans A 1996 J. Math. Phys. 37 5402

[12] Moolekamp F 2012 arXiv:1201.3843

[13] Moroz A 2012 Europhys. Lett. 100 60010

[14] Ziegler K 2012 J. Phys. A: Math. Theor. 45 452001

[15] Bargmann V 1961 Commun. Pure Appl. Math. 14 187

[16] Braak D 2013 Ann. Phys. (Berlin) 525 1.23

[17] Ince E L 1956 Ordinary Differential Equations (New York: Dover)

[18] Gautschi W 1967 SIAM Rev. 9 24

[19] Erdelyi A et al 1955 Higher Transcendental Functions vol 3 (New York: McGraw-Hill)

[20] Wall H 1973 Analytic Theory of Continued Fractions (New York: Chelsea)

[21] Perron O 1957 Die Lehre von den Kettenbrüchen vol 2 (Stuttgart: Teubner)
[22] Kuś M and Lewenstein M 1986 J. Phys A: Math. Gen. 19 305
[23] Reed M and Simon B 1980 Methods of Modern Mathematical Physics vol 1 (San Diego, CA: Academic)
[24] Durst C, Sigmund E, Reineker P and Scheuing A 1986 J. Phys. C: Solid State Phys. 19 2701
[25] Casanova J, Romero G, Lizuain I, García-Ripoll J J and Solano E 2010 Phys. Rev. Lett. 105 263603
[26] Irish E K 2007 Phys. Rev. Lett. 99 173601
[27] Travěnec I 2012 Phys. Rev. A 85 043805