Note on the Analytical Solution of the Rabi Model

D. Braak

EP VI and Center for Electronic Correlations and Magnetism,
University of Augsburg, 86135 Augsburg, Germany
(Dated: November 23, 2012)

It is shown that a recent critique (arXiv:1210.1130 and arXiv:1211.4639) concerning the analytical solution of the Rabi model is unfounded.

PACS numbers: 03.65.Ge,02.30.Ik,42.50.Pq

It was demonstrated in [1] that the spectrum of the quantum Rabi Hamiltonian ($\omega = \hbar = 1, g > 0$),

$$ H_R = a^\dagger a + g\sigma_z(a + a^\dagger) + \Delta \sigma_z, \quad (1) $$

consists of two parts, the regular spectrum with energy eigenvalues $E_{\pm}^R + g^2 \notin \mathbb{N}$ and the exceptional spectrum (Juddian solutions) with $E_{\pm}^{sc} + g^2 \in \mathbb{N}$, which may occur for special values of the model parameters $g$ and $\Delta$. The index $\pm$ denotes the parity of the regular eigenstate belonging to $E_{\pm}^R$. The exceptional states (if they are present) are all doubly degenerate with respect to parity. The parity invariance of the model ($H_R$ commutes with $e^{\pm i\sigma_z \phi}$) is instrumental to derive the function $G_{\pm}(x)$,

$$ G_{\pm}(x) = \sum_{n=0}^{\infty} K_n(x) \left( 1 \mp \frac{\Delta}{x - n} \right) g^n, \quad (2) $$

where the $K_n(x)$ are known functions of $g, \Delta$ and $x$. $G_{+}(x)$ ($G_{-}(x)$) determines the regular spectrum of (1) in the subspace with positive (negative) parity, because $G_{\pm}(x_{\pm}^\pm)$ $= 0$ for real $x_{\pm}^\pm$ if and only if $E_{\pm}^R + g^2 = x_{\pm}^\pm$.

Maciejewski et al. argue in [2] that this result is invalid because some of the real zeroes of $G_{\pm}(x)$ may not correspond to eigenvalues of (1). The authors of [2] do not dispute the fact that all points of the regular spectrum correspond to zeroes of (2), but suspect that not all those zeroes are physical. I shall now prove that this is not the case.

It is sufficient to confine the discussion to fixed (positive) parity (negative parity is obtained by replacing $\Delta$ with $-\Delta$ in the subsequent formulæ). The subspace $H_+$ with positive parity is isomorphic to $B$, the Bargmann space of analytic functions (see [1]) and the derivation of [2] starts with the following system of coupled differential equations for the wave function $\psi(z)$, which solves the Schrödinger equation $H_+ \psi(z) = E \psi(z)$ in $H_+$,

$$ (z + g) \frac{d}{dz} \phi_1(z) + (gz - E) \phi_1(z) + \Delta \phi_2(z) = 0 \quad (3a) $$

$$ (z - g) \frac{d}{dz} \phi_2(z) - (gz + E) \phi_2(z) + \Delta \phi_1(z) = 0. \quad (3b) $$

Here we have used the notation $\psi(z) = \phi_1(z), \psi(-z) = \phi_2(z)$. This system corresponds to a linear homogeneous differential equation of the first order for the vector-valued function $\Psi(z) = (\phi_1(z), \phi_2(z))^T$,

$$ \frac{d}{dz} \begin{pmatrix} \phi_1(z) \\ \phi_2(z) \end{pmatrix} = \begin{pmatrix} \frac{E - g^2}{z - g} & \frac{-\Delta}{z - g} \\ \frac{-\Delta}{z + g} & \frac{E + g^2}{z + g} \end{pmatrix} \begin{pmatrix} \phi_1(z) \\ \phi_2(z) \end{pmatrix}. \quad (4) $$

(4) has regular singular points at $z = \pm g$ and an irregular singular point (of rank 1) at infinity. Now it follows from the symmetry of this equation under the reflection $z \rightarrow -z$ that the function $\Phi(z) = (\phi_2(-z), \phi_1(-z))^T$ satisfies (4) as well. $\phi_{1,2}(z)$ have power series expansions around $z = -g$,

$$ \phi_1(z) = e^{-g^2} \sum_{n=0}^{\infty} K_n(x)(z + g)^n, \quad (5a) $$

$$ \phi_2(z) = e^{-g^2} \sum_{n=0}^{\infty} K_n(x)(z + g)^n. \quad (5b) $$

where $x$ denotes the spectral parameter $x = E + g^2$. It follows that $\Psi(z)$ is analytic in an open disk $D_1$ with radius $2g$ centered at $z = -g$. Likewise, $\Phi(z)$ is analytic in a disk $D_2$ with the same radius centered at $z = g$. All points in $D_0 = D_1 \cap D_2$ are ordinary points of (4). It means that if $\Psi(z_0) = \Phi(z_0)$ for any $z_0 \in D_0$, $\Psi(z)$ and $\Phi(z)$ coincide for all $z \in D_0$. But this entails that $\phi_1(z) = \psi(z)$ is analytic in the whole complex plane because then $\phi_2(-z)$ is its analytic continuation beyond the radius of convergence of (5a), comprising the second regular singular point of (4) at $z = g$. It follows that the conditions

$$ \phi_1(z_0) = \phi_2(-z_0) \quad (6a) $$

$$ \phi_2(z_0) = \phi_1(-z_0) \quad (6b) $$

for any $z_0 \in D_0$ are necessary and sufficient for $\psi(z)$ to be an element of the Bargmann space; the spectral parameter $x$, determined by (6a) (6b), corresponds therefore to an energy eigenvalue. Now (6a) is equivalent to (6b) if $z_0 = 0 \in D_0$, from which the expression for $G_{\pm}(x)$ given in Eq. (2) follows immediately. This completes the proof sketched in [4]. In a comment [5] to the first version of this note, Maciejewski et al. still doubt the validity of the proof by invoking a standard theorem of complex analysis which says that a function holomorphic in a bounded,
connected region $D$ of $\mathbb{C}$ vanishes identically if it vanishes at a denumerable infinity of points within $D$. This theorem has nothing to do with the present problem. Here we use the following elementary result [3] from the theory of linear differential equations:

Theorem: Let the vector-valued function $f(z)$ satisfy a linear homogeneous differential equation of the first order which has only ordinary points in the connected complex domain $D$. If $f(z)$ vanishes at some point $z_0 \in D$, it vanishes everywhere in $D$.

The condition $f(z_0) = \Phi(z_0) - \Psi(z_0) = 0$ corresponds to (6a) and (6b), and both are equivalent for $z_0 = 0 \in D_0$. If (6a) is satisfied at $z_0 = 0$, (6b) is satisfied as well and the vector $f(0)$ vanishes. This is enough to conclude that $\Phi(z) = \Psi(z)$ throughout $D_0$. It is not necessary that one of the components of $f(z)$ vanishes at two distinct points (see below), but both components must vanish at one point. This is equivalent to the condition $f(z_0) = f'(z_0) = 0$ if the scalar $f(z)$ satisfies a second order differential equation, as the components of $f(z)$ do.

For $z_0 \neq 0$, Eqs. (6a) and (6b) are not equivalent and it becomes possible to have a solution to (6a), while (6b) is not satisfied. This was discovered numerically in [2] for real $z_0$. Clearly, no unphysical solutions were obtained for $z_0 = 0$, but this is not a “lucky” accident as the authors of [2] believe, who checked the zeroes of $G_x(x)$ for $x$ up to 30.

The same argument applies to the generalized Rabi model with broken $\mathbb{Z}_2$-symmetry. Its Hamiltonian reads,

$$H_\epsilon = a^\dagger a + g\sigma_x(a + a^\dagger) + \epsilon\sigma_x + \Delta\sigma_z. \quad (7)$$

As was shown in [4], the eigenvalue equation for $H_\epsilon$ is equivalent via integrable embedding to the following differential equation for the vector-valued function $\Psi(z) = (\phi_1(z), \phi_2(z), \phi_1(z), \phi_2(z))^T$,

$$\frac{d}{dz}\Psi(z) = A(z)\Psi(z), \quad (8)$$

with the coefficient matrix,

$$A(z) = \begin{pmatrix} \frac{E_0 - i + g}{z + g} & \frac{E_0 + i - g}{z - g} & \frac{\Delta}{z + g} & \frac{\Delta}{z - g} \\ 0 & \frac{E_0 + i - g}{z + g} & \frac{\Delta}{z - g} & 0 \\ 0 & \frac{\Delta}{z + g} & \frac{E_0 + i + g}{z - g} & \frac{\Delta}{z - g} \\ \frac{-\Delta}{z - g} & 0 & 0 & \frac{E_0 + i + g}{z - g} \end{pmatrix}. \quad (9)$$

[8] has the same singularity structure as [4] and regions $D_0, D_1, D_2$ can be defined as in the symmetric case. Due to the embedding, Eq. [8] has again a $\mathbb{Z}_2$-symmetry, which entails that with $\Psi(z)$ also the function $\Phi(z) = (\phi_1(-z), \phi_2(-z), \phi_1(-z), \phi_2(-z))^T$ satisfies [8]. After expansion of $\Psi(z)$ in powers of $z$ around the regular singular point $-g$, the condition $\Psi(z_0) = \Phi(z_0)$ for $z_0 \in D_0$ leads to the following set of equations,

$$e^{-gz_0} \sum_{n=0}^{\infty} \frac{\Delta K^+_{n}}{x + \epsilon - n}(z_0 + g)^n = ce^{gz_0} \sum_{n=0}^{\infty} K^+_{n}(g - z_0)^n, \quad (10a)$$

$$e^{-gz_0} \sum_{n=0}^{\infty} \frac{\Delta K^-_{n}}{x + \epsilon - n}(z_0 + g)^n = e^{gz_0} \sum_{n=0}^{\infty} K^-_{n}(g - z_0)^n, \quad (10b)$$

$$e^{-gz_0} \sum_{n=0}^{\infty} K^+_{n}(z_0 + g)^n = e^{gz_0} \sum_{n=0}^{\infty} \frac{\Delta K^-_{n}}{x + \epsilon - n}(g - z_0)^n, \quad (10c)$$

$$e^{-gz_0} \sum_{n=0}^{\infty} K^-_{n}(z_0 + g)^n = ce^{gz_0} \sum_{n=0}^{\infty} \frac{\Delta K^+_{n}}{x + \epsilon - n}(g - z_0)^n, \quad (10d)$$

with an unknown constant $c$. The $K^\pm_n$ are known functions of $g, \Delta$ and $x = E + g^2$. For $z_0 = 0$ it is obvious that (10a) is equivalent to (10c) and (10b) to (10d). We are left with the two equations,

$$\sum_{n=0}^{\infty} \left[ cK^+_{n} - \frac{\Delta}{x - \epsilon - n}K^+_{n} \right] g^n = 0 \quad (11a)$$

$$\sum_{n=0}^{\infty} \left[ K^-_{n} - \frac{c\Delta}{x + \epsilon - n}K^-_{n} \right] g^n = 0. \quad (11b)$$

Eliminating $c$ from Eqs. (11), we obtain the $G$-function for the generalized Rabi model [1],

$$G_\epsilon(x) = \Delta^2 R^+(x)\bar{R}^-(x) - R^+(x)\bar{R}^- (x) \quad (12)$$

with

$$R^\pm (x) = \sum_{n=0}^{\infty} K^\pm_n(x)g^n \quad (13a)$$

$$\bar{R}^\pm (x) = \sum_{n=0}^{\infty} \frac{K^\pm_n(x)}{x - n \pm \epsilon} g^n. \quad (13b)$$

The reflection symmetry of the extended model allows to reduce the number of conditions as in the manifestly symmetric case. Therefore, the function $W(x, g, \Delta, \epsilon)$ derived in [3] has exactly the same real zeroes as $G_\epsilon(x)$ and yields the same spectrum as seen in Fig. 5 of [2]. However, the proposed method is an interesting generalization of the approach introduced in [1] which could be applicable to cases where embedding into a symmetric model is not possible.

Regarding the numerical computation of the spectrum of the quantum Rabi model [1], it may be advantageous to define a generalized $G$-function $G_\pm(x; z)$ by

$$G_\pm(x; z) = \phi_2(-z) - \phi_1(z). \quad (14)$$

The vanishing of $G_\pm(x; z_0)$ for $z_0 \in D_0$ corresponds to [4a]. Interestingly, this condition is sufficient to determine the spectrum if $\Im(z_0) \neq 0$. To see this, we note
that the conditions (6) correspond to a two-point boundary value problem for $G_\pm(x;z)$ in the complex plane, namely $G_\pm(x;z_0) = G_\pm(x; -z_0) = 0$. Because $G_\pm(x;z)$ satisfies a linear homogeneous differential equation of the second order, which is obtained from Eq. [4] by eliminating $\phi_2(z)$, this boundary value problem is incompatible [7] and has only the solution $G_\pm(x;z) = 0$. Let $G_\pm^j(x;z)$ for $j = 1, 2$ denote two linearly independent solutions of the differential equation satisfied by $G_\pm(x;z)$ (Eq. (11) in [2]). Let us assume that $G_\pm(x;z_0) = 0$ for $z_0 \in D_0$. Clearly, $G_\pm(x;z_0^*) = 0$ as well. But because the coefficients of the power series of $G_\pm(x;z)$ in $z$ are real (see Eq. (5)), we have $G_\pm(x;z_0^*) = 0$, i.e. $G_\pm(x;z)$ vanishes at $z_0$ and $z_0^*$. This is again an incompatible two-point boundary value problem if $\Im(z_0) \neq 0$, because $G_\pm^1(x;z_0)G_\pm^2(x;z_0^*) \neq G_\pm^1(x;z_0^*)G_\pm^2(x;z_0)$ for almost all $z_0 \in D_0$. It does not preclude isolated points $z_0 \in D_0$ which yield non-trivial solutions to $G_\pm(x;z_0) = G_\pm(x;z_0^*) = 0$. In [3] the following statement is made: "The key observation is that the function in question satisfies a second order linear homogeneous equation so that we only need to make it equal to zero at two distinct points." This is obviously incorrect in general; $\sin(z)$ satisfies the linear homogeneous second order equation $f''(z) = -f(z)$ and vanishes at many distinct points without being identically zero: $\sin(z)$ solves the two-point boundary value problem $f(z_1) = f(z_2) = 0$ e.g. for $z_1 = 0$, $z_2 = \pi$. However, in the present case it is not required that $G_\pm(x;z)$ vanishes at two points in $D_0$ but that both components of $f(z) = (G_\pm(x;z), -G_\pm(x;-z))^T$ vanish at a single point $z_0 \in D_0$. Because $0 \in D_0$, the condition $G_\pm(x;0) = 0$ is necessary and sufficient for $x - g^2$ to be an eigenvalue of $H_R$. Maciejewski et al. write: "Numerical work seems to suggest that the condition at zero is somehow distinguished, ..." The reason for this distinction is a simple mathematical fact explained above in great detail.

Whereas isolated solutions of $G_\pm(x;z_0) = G_\pm(x;z_0^*) = 0$ may exist for some $z_0 \in D_0$, it cannot happen for $z_0 \in iR$, because then $z_0 = -z_0^*$ and $G_\pm(x;z_0) = 0$ is equivalent to [5a, 6b]. This is the interesting case from a numerical point of view, as it allows to overcome instabilities in the computation of $G_\pm(x;z)$ for large $x$. It is remarkable that $G_\pm(x;z_0)$ has zeroes in $x$ at the correct values even when $z_0 \in iR$ is outside $D_0$. The nonzero values of $G_\pm(x;z_0)$ depend then on the order at which the defining series [5a] and [6b] are truncated, but the position of $x_0^\pm_n$ with $G_\pm(x_0^\pm_n; z_0) = 0$ converges to the correct value $E_0^\pm + g^2$ for the following reason: The functions $\phi_1(z_0)$ and $\phi_2(z_0)$ are holomorphic in $C$ exactly at $x_n^\pm$, which entails a convergent series expansion in $z$ at this point, even for $z \notin D_0$. In Fig. 1 the real and imaginary part of $G_\pm(x;5i)$ is shown for $x \approx 71$. $z_0$ is outside $D_0$ but the joint zero of $\Re(G_\pm(x;5i))$ and $\Im(G_\pm(x;5i))$ allows to determine the energy eigenvalue $E_{71}^+ = 70.00462935$ to high precision, even though the series defining $G_\pm(x;5i)$

does not converge for $x \notin \{ x_0^\pm \}$.

We conclude that the $z_0$ which may yield unphysical zeroes of $G_\pm(x;z_0)$ are likely confined to the set $R \cap D_0 \setminus \{0\}$. This set is of measure zero within $D_0$ [8]. In any case, its presence does not invalidate the results of [1], which are based on the function $G_\pm(x)$ in Eq. (2) and not on the generalized function $G_\pm(x;z)$ for real $z \neq 0$, which is the subject of criticism in [2]. The authors of [2] neither correct nor extend the findings of [1] in these two cases, the only examples for which [2] presents explicit calculations. Nevertheless, Maciejewski et al. have correctly pointed out a gap in the derivation of $G_\pm(x)$ [4], giving me the opportunity to close it.

[1] D. Braak, Phys. Rev. Lett. 107, 100401 (2011).
[2] A.J. Maciejewski, M. Przybylska, and T. Stachowiak, arXiv:1210.1130
[3] E.L. Ince, Ordinary Differential Equations, Dover, N.Y. (1956), p. 357.
[4] Online supplement to Ref. [3].
[5] A.J. Maciejewski, M. Przybylska, and T. Stachowiak, arXiv:1211.4639
[6] E.A. Coddington and R. Carlson, Linear Ordinary Differential Equations, SIAM, Philadelphia (1997), p. 26.
[7] see [2], Chap. IX.
[8] This conclusion is not affected by the possibility that the two-point boundary value problem $G_\pm(z_0) = G_\pm(z_0^*) = 0$ has non-trivial solutions for isolated points $z_0 \notin R \cup iR$. 

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{fig1.png}
\caption{Real and imaginary part of $G_\pm(x,5i)$ for $g = 1$ and $\Delta = 0.7$ in the vicinity of $x = 71$.}
\end{figure}