Exact Solution of the Rabi Hamiltonian by Known Functions?

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It is conjectured that the component wave functions of the Rabi Hamiltonian in Bargmann's Hilbert space are terminating series of spheroidal wave functions and generalized spheroidal wave functions of Leitner and Meixner. Numerical calculations strongly support the conjecture.

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The Rabi Hamiltonian has isolated exact solutions for particular values of the interaction constant.[1] In Bargmann's Hilbert space of analytical functions[2-4] the component wave functions are, in this case, terminating series of elementary transcendental functions.[1,5-7] This property is due to similarities in the pole structure of the differential equations defining the expansion functions and the differential equations of the component wave functions for the particular values of the interaction constant. We asked ourselves whether this observation could be a guide to more complicated but possibly known expansion functions, which allow for terminating expansions of the wave functions in the general case. By applying these principles (and a fair amount of intuition) we have in fact been able to guess the expansion functions and the expansion. We are, however, unable to produce a mathematical proof. However, we have a vast amount of numerical evidence, which, without any exception, supports our conjecture.

The Rabi Hamiltonian in Bargmann's method[1,4] is a linear first-order matrix differential operator,

$$H=\xi\, d/d\xi+\tfrac{1}{2}+(\tfrac{1}{2}+2\delta)\sigma_z+\sqrt{2}\kappa(\xi+d/d\xi)(\sigma_{(+)}+\sigma_{(-)}), \tag{1}$$

whose eigenvalues λ_i in the excited state i ($i=0,1,2\ldots$) are determined by the requirement that the up and down components of the wave functions

$$\psi_i^{(m)}\rangle=(\xi/\sqrt{2})^{m+1/2}\phi_i^{(m)}(\xi)|\uparrow\rangle+(\xi/\sqrt{2})^{-m+1/2}f_i^{(m)}(\xi)|\downarrow\rangle \tag{2}$$

($m=\pm\frac{1}{2}$) belong to the space of entire functions. We introduce a new independent variable $z=\frac{1}{2}\xi^2$, insert (1) and (2) in the Schrödinger equation, and collect the spin-up and -down components. We then obtain the following system of differential equations:

$$z\frac{d}{dz}\phi_i^{(m)}(z)-(\epsilon_i-\delta-\tfrac{1}{2}\{m+\tfrac{1}{2}\})\phi_i^{(m)}(z)+\kappa\left[(z^{-m+1/2}-\tfrac{1}{2}\{m-\tfrac{1}{2}\}z^{-m+1/2})f_i^{(m)}(z)+z^{+m+1/2}\frac{d}{dz}f_i^{(m)}(z)\right]=0, \tag{3}$$

$$\kappa\left[(z^{m+1/2}+\tfrac{1}{2}\{m+\tfrac{1}{2}\}z^{m-1/2})\phi_i^{(m)}(z)+z^{m+1/2}\frac{d}{dz}\phi_i^{(m)}(z)\right]+z\frac{d}{dz}f_i^{(m)}(z)-(\epsilon_i+\delta+\tfrac{1}{2}\{m+\tfrac{1}{2}\})f_i^{(m)}(z)=0. \tag{4}$$

Here

$$\lambda_i=2\epsilon_i+1=v_i+\tfrac{1}{2}-2\kappa^2 \tag{5}$$

and v_i is the baseline parameter introduced by Judd.[8] For $m=-\frac{1}{2}$ Eqs. (3) and (4) are identical with (2.28) and (2.29), for $m=+\frac{1}{2}$ with (2.28a) and (2.29a), of Ref. 1. Equations (3) and (4) have an irregular singularity at infinity and two regular singularities at $z=\kappa^2$ (exponents 0 and v_i) and $z=0$ (exponents 0 and $-\frac{1}{2}$). Therefore, this singularity is elementary in Ince's classification.[9]

The conjecture is that the functions $\phi_i^{(m)}(z)$, $f_i^{(m)}(z)$ can be expanded in $i+4$ solutions $w_2^{(3)}(\bar{j},\bar{v};\Lambda;z)$ of a second-order differential equation with the same location and character of the singular points. The differential equation is given by

$$\frac{d^2}{dz^2}w_2^{(3)}(z)+\left[\frac{\bar{j}+1}{z}+\frac{1-\bar{v}}{z-\kappa^2}\right]\frac{d}{dz}w_2^{(3)}(z)+\left[-\frac{\kappa^2}{z}+\frac{\Lambda}{z(z-\kappa^2)}\right]w_2^{(3)}(z)=0, \tag{6}$$

where the parameter dependence of the functions is suppressed. The function $w_2^{(3)}(\bar{j},\bar{v};\Lambda;z)$ has first been treated by Lambe and Ward[10,11]; the transformed function $\psi(\eta)\eta^{\bar{j}+1/2}(1-\eta^2)^{-\bar{v}/2}w_2^{(3)}(\bar{j},\bar{v};\Lambda;\kappa^2\eta)$, $\kappa^2\eta^2=z$, is a generalized spheroidal wave function (Leitner and Meixner[12]). For $\bar{j}=-\frac{1}{2}$ the regular singularity $z=0$ becomes elementary and $\psi(\eta)$ reduces to a spheroidal wave function.[13-18] As we shall see [Eq. (16)], all but one of the expansion functions are of the simpler type. We call the solutions of (6) the natural expansion functions for the solutions of (3) and (4). We are now going to study the relevant properties of the natural expansion functions, in particular their eigenvalues Λ_n, which show a simple κ^2 and v dependence.

We expand the function $w_2^{(3)}(\bar{j},\bar{v};\Lambda;z)$ in series:

$$w_2^{(3)}(\bar{j},\bar{v};\Lambda;z)=\sum_{n=0}\frac{C_n(\bar{j},\bar{v};\Lambda)}{n!\kappa^{4n}}w_2^{(2)}(\bar{j}-n;z), \tag{7}$$

$$w_2^{(2)}(\bar{j}-n;z)=(\kappa^2z)^{-(\bar{j}-n)/2}I_{-\bar{j}+n}(2\kappa z^{1/2}) \tag{8}$$

$$=(\kappa^2z)^{-(\bar{j}-n)}\sum_{k=0}\frac{(\kappa^2z)^k}{\Gamma(k+1)\Gamma(-\bar{j}+n+k+1)}. \tag{9}$$

Insertion of (7) in (6) leads to the recurrence relations

$$-C_{n+1}(\bar{j};\bar{v};\Lambda)+C_n(\bar{j},\bar{v},\Lambda)\{(n-\bar{j})(n+1-\bar{v})+\Lambda\}+C_{n-1}(\bar{j},\bar{v};\Lambda)\kappa^4n(n-\bar{v})=0, \tag{10}$$

which can be turned into the form

$$\frac{C_n(\bar{j};\bar{v};\Lambda)}{C_{n-1}(\bar{j},\bar{v};\Lambda)}=\frac{-\kappa^4n(n-\bar{v})W_n}{(n-\bar{j})(n+1-\bar{v})+\Lambda}. \tag{11}$$

Here W_n is a continued fraction given by

$$W_n=1/(1+a_nW_{n+1}), \tag{12}$$

$$a_n=\frac{\kappa^4(n+1)(n+1-\bar{v})}{[(n-\bar{j})(n+1-\bar{v})+\Lambda][(n+1-\bar{j})(n+2-\bar{v})+\Lambda]}. \tag{13}$$

Equation (11) determines the eigenvalues Λ_n; see the dotted curves in Fig. 1. For $\kappa^2<1$ very good approximations $\Lambda_n^{(0)}$ are obtained by putting the wavy bracket in Eq. (10) equal to zero. One has

$$\Lambda_n^{(0)}=-(n-\bar{j})(n+1-\bar{v}), \tag{14}$$

which explains the labeling in Fig. 1.

For all integer values of $\bar{v}$, terminating expansions (7) can be found. E.g., for $\bar{v}=1$ and W_1 finite, $C_1(\bar{j},1;\Lambda)=0$ from (11) and $\Lambda=0$ from (10) for $n=0$. For $\bar{v}=2$ and W_2 finite, $W_1=1$ from (12) and (13), and $C_2(j,2;\Lambda)=0$ from (11) for $n=2$. Furthermore, from (11) for $n=1$ one has $C_1(\bar{j},2;\Lambda)=\kappa^4\Lambda^{-1}C_0(\bar{j},2;\Lambda)$ and Eq. (10) for $n=0$ gives $C_1(\bar{j},2;\Lambda)=+(\bar{j}+\Lambda)C_0(\bar{j},2;\Lambda)$. Equating the two expressions leads to

$$\Lambda(\Lambda+\bar{j})-\kappa^4=0, \tag{15}$$

whose two roots determine the eigenvalues for which the series (7) terminates. Similarly for $\bar{v}=N$, Nth-order equations for Λ can be derived whose roots correspond to expansions (7) for which $C_N=C_{N+1}=0$; see full circles in Fig. 1. These expansions are isolated exact solutions of (6) of the type discovered by Judd[8] in simple Jahn-Teller systems.

In the following we concentrate on $\phi_i^{(-1/2)}(z)$, Eqs.

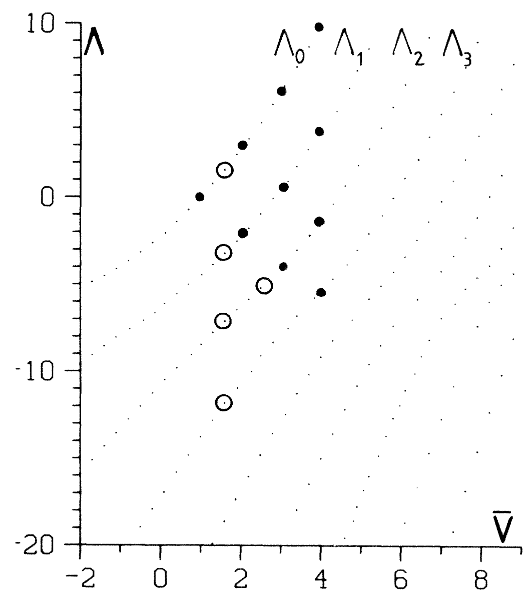

FIG. 1. The eigenvalues Λ_n of (10) vs $\bar{v}$ for $\kappa^2=2.503\,081\,502\,222\,39$, $\bar{j}=-\frac{1}{2}$ (dotted curves): full circles, eigenvalues for terminating series (7); open circles, eigenvalues for the first five expansion functions in (16); $i=2$ (second excited state).

TABLE I. The expansion coefficients x_l and eigenvalues Λ_l in expansion (16) for $\delta=1.5$, $\kappa^2=2.503\,081\,50$, $v=1.589$, second excited state $i=2$.

l	x_l	Λ_l
0	$-6.075\,128\,781\,792\,735\,94\times10^{-4}$	1.565 573 499 507 168 75
1	$-2.648\,951\,778\,561\,378\,54\times10^{-1}$	−3.237 791 500 337 626 82
2	$1.312\,615\,681\,928\,325\,04\times10^{-1}$	−7.152 321 825 278 410 63
3	$-1.894\,432\,120\,916\,318\,14\times10^{-6}$	−11.881 057 781 130 561 0
4	1.134 243 017 003 605 53	−5.017 451 414 696 186 40
5	$-2.191\,049\,502\,676\,856\,64\times10^{-3}$	−8.025 333 560 521 037 38

(3) and (4). According to the conjecture the function $\phi_i^{(-1/2)}(z)$ is a terminating series of $i+4$ natural expansion functions whose first $i+3$ are spheroidal wave functions:

$$\phi_i^{(-1/2)}(z)=\sum_{l=0}^{i+1}x_l w_2^{(3)}(-\tfrac{1}{2},v;\Lambda_l;z)+x_{i+2}w_2^{(3)}(-\tfrac{1}{2},v+1;\Lambda_i;z)+x_{i+3}w_2^{(3)}(-\tfrac{3}{2},v;\Lambda_i;z). \tag{16}$$

The choice of the natural expansion functions is indicated in Fig. 1 for $i=2$, $v_i=1.589$. In order to test the conjecture we expand $\phi_i^{(-1/2)}(z)$ *also* in $w_2^{(2)}(-\frac{1}{2}-n;z)$,

$$\phi_i^{(-1/2)}(z)=\sum_{n=0}^{\infty}\frac{A_n}{n!\kappa^{4n}}w_2^{(2)}(-\tfrac{1}{2}-n;z). \tag{17}$$

From (3) and (4) we obtain a three-term recurrence relation for A_n

$$-A_{n+1}+A_n\{(n+\tfrac{1}{2})(n+1-v)+L(n)\}+A_{n-1}\kappa^4\{n(n-1-v)R(n)\}=0, \tag{18}$$

$$L(n)=-\tfrac{1}{2}(1-v)-\kappa^2(1+v)+(v/2-\tfrac{3}{4}+\delta)(v/2-\tfrac{3}{4}-\delta)-\kappa^4(v/2+\tfrac{3}{4}+\delta)O(n), \tag{19}$$

$$R(n)=O(n)+1, \tag{20}$$

$$O(n)=\frac{\{v/2-n+\delta-\frac{3}{4}\}\{v/2+\delta+\frac{3}{4}\}+\kappa^2(n+1)}{\{v/2-n+1+\delta-\frac{3}{4}\}\{v/2+\delta+\frac{3}{4}\}+\kappa^2 n}-1. \tag{21}$$

Note that $O(n)$ does not depend strongly on n, and $\lim_{n\to\infty}O(n)\to0$. The similarity between the recurrence relations (18) and (10) is obvious; this is a consequence of the similarities in the pole structure of (3) *cum* (4) and (6). From (16) we have the following relation between the expansion coefficients:

$$A_n=\sum_{l=0}^{i+1}x_lC_n(-\tfrac{1}{2},v;\Lambda_l)+x_{i+2}C_n(-\tfrac{1}{2},v+1;\Lambda_i)+x_{i+3}C_{n-1}(-\tfrac{3}{2},v;\Lambda_i)n\kappa^4, \tag{22}$$

where Λ_l,Λ_i are eigenvalues of (6) referring to the parameters in front of them. Now we insert (22) in (18) and take proper care of (10). By this a lot of the n dependence in the coefficients of A_n,A_{n-1} drops out and we obtain a system of equations for x_l:

$$\sum_{l=0}^{i+3}x_l\Gamma_n^{(l)}=0,\quad n=0,1,2,\ldots. \tag{23}$$

The lengthy expressions for $\Gamma_n^{(l)}$ will not be reproduced here; they can be easily obtained from (18)–(22). We just mention that $\Gamma_n^{(l)}$ still contains Λ_l, $C_n(\bar{j},v;\Lambda_l)$, and $C_{n-1}(\bar{j},v;\Lambda_l)$.

We take the first $i+4$ equations (23), fix δ and v, and put the determinant equal to zero. This determines κ^2 [and, at the same time, Λ_l and $C_n(\bar{j},v,\Lambda_l)$]. The equations are then solved for x_l (see Table I). We check that the coefficients x_l also satisfy the rest of the equations (23). Finally we use Eq. (22) to calculate the expansion coefficients A_n of (17). On the other hand, we calculate κ^2 and A_n directly from (18)–(21). Here the conjecture (16) is not used. The calculation

TABLE II. The interaction constant κ^2 as function of v for second excited state $i=2$, $\delta=-1.5$.

v	κ^2
2.056	0.250 015 286 404 49|
1.804	0.500 023 440 100 82|
1.648	0.749 870 230 364 32|
1.553	0.999 800 377 249 4|8
1.501	1.254 569 917 844 27|
1.483	1.518 216 153 290 67
1.514	1.997 814 294 505 60|
1.589	2.503 081 502 222 39|
1.663	3.000 101 177 393 3|5

TABLE III. The coefficients of the expansion (17) and check of Eq. (22) for $\upsilon = 1.589$, $\kappa^2 = 2.503\,081\,502\,223\,9$, second excited state $i = 2$.

n	$\Lambda_n / n!\kappa^{4n}$
0	1.000 000 000 000 00|
1	−1.061 132 370 282 02|
2	4.111 760 376 202 40| × 10^{-1}
3	−5.824 865 074 499 56| × 10^{-2}
4	9.109 051 532 773 71| × 10^{-3}
5	−1.285 734 025 421 21| × 10^{-3}
6	1.617 913 072 702 69| × 10^{-4}
7	−1.824 747 125 652 3|2 × 10^{-5}
8	1.859 547 610 631 1|9 × 10^{-6}
9	−1.725 955 133 195 5|7 × 10^{-7}
10	1.469 602 081 418 0|4 × 10^{-8}
11	−1.155 269 107 016|96 × 10^{-9}
12	8.431 575 990 59|711 × 10^{-11}
13	−5.741 338 893 177|65 × 10^{-12}
14	3.663 391 065 709|51 × 10^{-13}
15	−2.198 839 714 723|83 × 10^{-14}
16	1.245 770 002 720|64 × 10^{-15}
17	−6.682 756 299 512|77 × 10^{-17}
18	3.403 719 564 601|61 × 10^{-18}
19	−1.650 155 474 485|12 × 10^{-19}
20	7.632 418 800 69|515 × 10^{-21}

is by standard continued-fraction technique.

The entries in Tables II and III are the results of *this* calculation which are accurate to fourteen decimal places. The vertical bars indicate the position up to which there is agreement between the results of the two methods. This and a lot of further data show that the conjecture must be true: The solutions of the Rabi Hamiltonian in Bargmann's Hilbert space can be expanded in $i+4$ natural expansion functions. The first $i+3$ expansion functions are related to spheroidal wave functions, while the last is related to the generalized spheroidal wave functions of Leitner and Meixner. All our calculations have been done for low-lying excited states $i \leq 2$. Numerical work by Graham and Höhnerbach[19] and numerical and analytical work by Klenner, Weis, and Doucha[20] indicate that the highly excited states might be simpler than expected. The recent discovery of a scaling law[21] in the large-i limit points in the same direction.

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