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2002 J. Phys. A: Math. Gen. 35 9425

(http://iopscience.iop.org/0305-4470/35/44/311)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **35** (2002) 9425–9430 PII: S0305-4470(02)36704-0

# Quasi exact solution of the Rabi Hamiltonian

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Received 8 May 2002
Published 22 October 2002
Online at stacks.iop.org/JPhysA/35/9425

**Abstract**

A method is suggested to obtain the quasi exact solution of the Rabi Hamiltonian. It is conceptually simple and can be easily extended to other systems. The analytical expressions are obtained for eigenstates and eigenvalues in terms of orthogonal polynomials. It is also demonstrated that the Rabi system, in a particular case, coincides with the quasi exactly solvable Pöschl–Teller potential.

PACS numbers: 03.65.Ge, 02.30.Gp

## 1. Introduction

Considerable attention has been paid over the years to the solution of the Rabi and Jahn–Teller (JT) Hamiltonians [1–3]. The $E \otimes \epsilon$ JT problems have been solved by Judd when certain relations between the parameters of the Hamiltonian were invoked [2]. Such solutions are known as Juddian isolated exact solutions. The problem has been studied in the Bargmann–Fock space by Reik *et al* [4] and its canonical form has been obtained by Szopa *et al* [5]. It has been proved [6, 7] that the Rabi Hamiltonians, i.e. $E \otimes \beta$ JT and $E \otimes \epsilon$ JT systems, are mathematically identical. Moreover, it is possible to generalize the method for a wider class of Jahn–Teller systems.

In quantum mechanics there exist potentials for which it is possible to find a finite number of exact eigenvalues and associated eigenfunctions in the closed form. These systems are said to be quasi exactly solvable (QES). The connection of quasi exact solvability with conformal quantum field theories in solid-state physics has been described recently [8]. In this paper we take a new look at the solution of the Rabi Hamiltonian through the method of quasi exact solvability.

One of the methods for the calculation of eigenstates and eigenvalues of the QES potentials is the use of orthogonal polynomials. Bender and Dunne showed [9] that there is a correspondence between the QES models in quantum mechanics and the set of orthogonal polynomials $P_m(E)$, which are polynomials in energy $E$. This paper is devoted to describing the eigenstates and eigenvalues of the Rabi Hamiltonian by using the Bender and Dunne method, in the framework of quasi exact solvability.

The paper is organized as follows. In section 2 we transform the Rabi Hamiltonian into the quasi exactly solvable differential equation form and discuss the determination of the condition for quasi exact solvability. In section 3 we present a solution for the eigenstates and eigenvalues of the Rabi Hamiltonian. The relation between Rabi system and quasi exactly solvable Pöschl–Teller system is also discussed in this section. In section 4 we compare our results with those obtained by other methods. In section 5 finally we comment on the validity of our method and suggest the possible extensions of the problem.

## 2. Quasi exact form of the Rabi Hamiltonian

In the cyclooctatetraene molecular ion, which is a particular case of molecules having a fourfold axis symmetry, in the resonant excitation of double molecules or dimers, a doubly degenerate state becomes coupled by a single mode. This system is known as the $E \otimes \beta$ Jahn–Teller system which helps us to understand the more complex cases of the Jahn–Teller effect. The $E \times \beta$ Jahn–Teller system coupled to a system executing harmonic oscillations whose energy eigenvalues differ by $2\mu$ is characterized by the Rabi Hamiltonian [6]:

$$H = a^+a + \kappa\sigma_3(a^+ + a) + \mu(\sigma^+ + \sigma^-) \tag{1}$$

where $\sigma^\pm = \frac{1}{2}(\sigma_1 \pm \mathrm{i}\sigma_2)$ and $\sigma_1, \sigma_2, \sigma_3$ are Pauli matrices and the parameter $\kappa$ is a linear coupling constant. Hamiltonian (1) can be expressed as a differential equation in the Bargmann–Fock space by using the realizations of the bosonic operators,

$$a^+ = z \qquad a = \frac{\mathrm{d}}{\mathrm{d}z}. \tag{2}$$

In this formulation, the Schrödinger equation consists of two independent sets of linear first-order differential equations. Substituting (2) into (1) we obtain a system of two linear differential equations for the functions $\psi_1(z)$ and $\psi_2(z)$:

$$(z+\kappa)\frac{\mathrm{d}\psi_1(z)}{\mathrm{d}z} + (\kappa z - E)\psi_1(z) + \mu\psi_2(z) = 0 \tag{3$a$}$$

$$(z-\kappa)\frac{\mathrm{d}\psi_2(z)}{\mathrm{d}z} - (\kappa z + E)\psi_2(z) + \mu\psi_1(z) = 0 \tag{3$b$}$$

where $E$ is the eigenvalue of the Rabi Hamiltonian. We eliminate $\psi_2(x)$ between the two equations, and substituting

$$z = \kappa(2x-1) \qquad \psi_1(x) = \mathrm{e}^{-2\kappa^2 x}\Re(x) \tag{4}$$

we obtain a second-order differential equation

$$x(1-x)\frac{\mathrm{d}^2\Re(x)}{\mathrm{d}x^2} + [\kappa^2(4x^2 - 2x - 1) + E(2x-1) - x + 1]\frac{\mathrm{d}\Re(x)}{\mathrm{d}x} + [\kappa^4(-4x+3) - E^2 + 2E\kappa^2(-2x+1) + \mu^2]\,\Re(x) = 0. \tag{5}$$

In order to understand quasi exact solvability of (5) the standard way is to demonstrate that the Hamiltonian can be expressed in terms of generators of the Lie algebra. Let us consider the algebra $su(1,1)$ expressed in the following form:

$$J_- = \frac{\mathrm{d}}{\mathrm{d}x} \qquad J_0 = x\frac{\mathrm{d}}{\mathrm{d}x} - j \qquad J_+ = x^2\frac{\mathrm{d}}{\mathrm{d}x} - 2jx. \tag{6}$$

The generators obey the commutation relation

$$[J_+, J_-] = -2J_0 \qquad [J_0, J_\pm] = \pm J_\pm. \tag{7}$$

If $2j$ is a positive integer, the algebra possesses $(2j+1)$-dimensional subspace

$$\Re(x) = \{1, x, x^2, \ldots, x^{2j}\}. \tag{8}$$

We first introduce the following linear and bilinear combination of the algebraic operators:

$$T = -J_+J_- + J_-J_0 - jJ_- + 4\kappa^2 J_+ - (4\kappa^2 - 2j + 1)J_0 + \mu^2 \tag{9}$$

for which one can define the spectral problem

$$T\Re(x) = \lambda\Re(x) \tag{10}$$

where $\lambda$ is a spectral parameter. The algebraic structure (9) is quasi exactly solvable [11]. The insertion of (6) into (9) leads to the following differential equation:

$$x(1-x)\frac{\mathrm{d}^2\Re(x)}{\mathrm{d}x^2} + [2j(2x-1) + (x-1)(4\kappa^2 x - 1)]\frac{\mathrm{d}\Re(x)}{\mathrm{d}x} \\ + [\mu^2 + j(1-2j) + 4\kappa^2(1-2x) - \lambda]\,\Re(x) = 0. \tag{11}$$

Equations (5) and (11) are identical under the conditions

$$E = 2j - \kappa^2 \qquad \lambda = j(1 + 2j - 4\kappa^2). \tag{12}$$

Thus we have shown that the Rabi Hamiltonian is QES. There are various techniques to solve (11). Here we obtain its solution with the theory of orthogonal polynomials.

## 3. Determination of eigenvalues and eigenfunction of the Rabi Hamiltonian

In this section we seek a solution for (11) to obtain eigenfunction and eigenvalues of the QES. Since the function $\Re(x) = \{1, x, x^2, \ldots, x^{2j}\}$ forms a basis function for $su(1,1)$ algebra, we search for a solution of (11) by substituting the polynomial of degree $2j$,

$$\Re(x) = \sum_{m=0}^{2j} a_m x^m. \tag{13}$$

The wavefunction is itself the generating function of the energy polynomials. The eigenvalues are then produced just by the roots of such polynomials. Therefore (13) can be written in the form

$$\Re(x) = \sum_{m=0}^{2j} a_m P_m(\kappa) x^m. \tag{14}$$

Substituting (14) in (11) and carrying out a straightforward calculation, we obtain the expression

$$\Re(x) = 1 + \frac{4P_{2j-1}(\kappa)(\kappa x)^{2j}}{\mu^2} + \sum_{m=1}^{2j-1} P_m(\kappa)(x)^m. \tag{15}$$

Here $P_m(\kappa)$ satisfies the recurrence relation

$$(m+1)(m+1-2j)P_{m+1}(\kappa) + [(m-2j)(2j - 4\kappa^2 - m) + \mu^2]P_m(\kappa) \\ + 4\kappa^2(m-1-2j)P_{m-1}(\kappa) = 0 \tag{16}$$

with the initial conditions $P_{-1}(\kappa) = 0$ and $P_0(\kappa) = 1$. Certain properties of the polynomial $P_m(\kappa)$ have been discussed in some recent works [12]. If $\kappa_j$ is a root of the polynomial

$P_{m+1}(\kappa)$, the series (15) truncates at $m \geqslant 2j+1$ and $\kappa_j$ belongs to the spectrum of the Rabi Hamiltonian. Therefore the solution given in (15) terminates at $m = 2j$ and it becomes a polynomial of degree $2j$. The first four of them are given by

$$P_1(\kappa) = \mu^2 \tag{17a}$$

$$P_2(\kappa) = \mu^2(4\kappa^2 + \mu^2 - 1) \tag{17b}$$

$$P_3(\kappa) = \mu^2(32\kappa^4 + 4(3\mu^2 - 8)\kappa^2 + \mu^2(\mu^2 - 5) + 4) \tag{17c}$$

$$P_4(\kappa) = \mu^2(384\kappa^6 + 16(11\mu^2 - 54)\kappa^4 + 8(3\mu^4 - 29\mu^2 + 54)\kappa^2 + \mu^2(\mu^2 - 7)^2 - 36) \tag{17d}$$

for $j = 0, 1/2, 1, 3/2$, respectively. The components of the eigenfunctions are expressed as

$$\psi_1(x) = N_1\,\mathrm{e}^{-\kappa^2 x}\Re(x) \tag{18a}$$

$$\psi_2(x) = N_2\,\mathrm{e}^{-\kappa^2 x}(2(j - \kappa^2 x)\Re(x) - x\Re'(x)) \tag{18b}$$

where $N_1$ and $N_2$ are normalization constants. It is obvious that the degrees of polynomials in the expressions for $\psi_1(x)$ and $\psi_2(x)$ are $2j$ and $2j+1$, respectively. The polynomials given in (17*a*)–(17*c*) are exactly the same results obtained by the method of Juddian isolated exact solution [3, 10]. In the following section we discuss the results.

## 4. Results

The eigenfunctions can be obtained for a given $j$. As an example consider the $j = 1/2$ case. The polynomial $P_m(\kappa)$ appears as the coefficient in the wavefunction. The series terminate when $P_2(\kappa) = 0$. The zeros of the $P_2(\kappa)$ are given by

$$\mu = 0 \qquad \mu = \pm\sqrt{1 - 4\kappa^2}. \tag{19}$$

Under the assumption $\mu \neq 0$ we obtain the exact solution of the Rabi Hamiltonian, and its normalized eigenfunctions can be written as

$$\psi_1(x) = \frac{(8 + 4\mu^2 + \mu^4)\,\mathrm{e}^{-\kappa^2 x}}{2\kappa^2\mu^4}\left(1 + \frac{4\kappa^2}{\mu^2}x\right) \tag{20a}$$

$$\psi_2(x) = \frac{(728 - 288\mu^2 - 19\mu^4 + 6\mu^6 + \mu^8)\,\mathrm{e}^{-\kappa^2 x}}{32\kappa^6}((1 + 2\kappa^2)x - 1)(\mu^2 + 4\kappa^2 x) \tag{20b}$$

with the eigenvalues

$$E = 1 - \kappa^2. \tag{21}$$

The condition for the normalizabilty of the functions is given by

$$\mathrm{Re}(\kappa^2) > 0 \qquad \text{and} \qquad -\frac{\pi}{4} < \arg(\kappa) < \frac{\pi}{4}. \tag{22}$$

When $j = 1$ the roots of the polynomial $P_3(\kappa)$ can be obtained from (17*c*) and they read

$$\mu = 0 \qquad \mu = \sqrt{\tfrac{5}{2} - 6\kappa^2 \pm \sqrt{16\kappa^4 + 8\kappa^2 + 9}}. \tag{23}$$

The corresponding eigenfunctions are obtained by evaluating (20*a*) and (20*b*). The unnormalized eigenfunctions for $j = 1$ are given by

$$\begin{aligned}\psi_1(x) &= \mathrm{e}^{-\kappa^2 x}\left(1 + (8\kappa^2 + \mu^2 - 4)\left(x + \frac{4\kappa^2}{\mu^2}x^2\right)\right)\\ \psi_2(x) &= 2 + (14\kappa^2 + 2\mu^2 - 9)x - [8\kappa^2 + \mu^2 - 4]\\ &\quad\times\left[\left(1 + 2\kappa^2 - \frac{8\kappa^2}{\mu^2}\right)x^2 - \frac{4\kappa^2(1 + 2\kappa^2)x^3}{\mu^2}\right].\end{aligned} \tag{24}$$

We have checked that the eigenfunctions are normalizable under the condition given in (22).

Another interesting property of the Rabi Hamiltonian is its relation with the Pöschl–Teller potential. When we transform the resulting differential equation (5) in the form of the Schrödinger equation, the Pöschl–Teller potential naturally appears. In order to transform (5) in the form of the Schrödinger equation we introduce the variable

$$x = -\sinh \alpha y \tag{25}$$

and define the wavefunction

$$\psi(x) = \mathrm{e}^{-\kappa^2 \cosh 2\alpha y} (\cosh \alpha y)^{2j+\frac{1}{2}} (\sinh \alpha y)^{2j-\frac{1}{2}} \Re(-\sinh \alpha y) \tag{26}$$

to obtain the Schrödinger equation

$$-\frac{1}{2}\frac{\mathrm{d}^2\psi(x)}{\mathrm{d}x^2} + V(x)\psi(x) = E_{\mathrm{PT}}\psi(x) \tag{27}$$

where the potential and eigenvalues are respectively

$$\begin{aligned} V(x) = \frac{\alpha^2}{8}(16j^2 - 1)\mathrm{cosech}^2\,\alpha y - \frac{\alpha^2}{8}(4j+1)(4j+3)\mathrm{sech}^2\,\alpha y \\ + 4\alpha^2\kappa^2 \sinh^2 \alpha y (1 + 2\kappa^2 + 2\kappa^2 \sinh^2 \alpha y). \end{aligned} \tag{28}$$

$$E_{\mathrm{PT}} = 2\alpha^2(\kappa^2(4j+2) + \mu^2). \tag{29}$$

The potential $V(x)$ is the quasi exactly solvable Pöschle–Teller potential. When $\kappa \to 0$ the potential reduces to the exactly solvable Pöschle–Teller potential.

## 5. Conclusion

We have presented the quasi exact solution of the Rabi Hamiltonian which implies that $E \otimes \epsilon$ JT system also has a quasi exact solution. The existence of a quasi exact solution does not of course allow for the general solution of the Rabi Hamiltonian. These solutions have a direct practical importance for checking the precision of analytical and numerical approximations. Another important result of this paper is that the eigenfunctions possess explicit expressions. The method given here can be extended to other JT or multi-dimensional atomic system problems. A further interesting implication of the method is the existence of the relations between the QES Pöschl–Teller family potentials and the Rabi systems.

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