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A generalized potential in the theory of the Rabi and $E \otimes \varepsilon$ Jahn–Teller system

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Abstract. The eigenvalue problem for the Rabi and the $E \otimes \varepsilon$ Jahn–Teller Hamiltonian in Bargmann's Hilbert space of analytical functions is a system of two first-order differential equations for the two-component wavefunctions, whose entire solutions (the eigenstates) are sought. We show that each eigenstate is a terminating series in the derivatives of a scalar entire function $D(z)$, called the generalized potential, which satisfies a higher-order differential equation. The coefficients of the terminating series depend on the physical parameters and are polynomials in the independent variable z . The coefficients are identical in all eigenstates.

1. Introduction

The eigenvalue problem for the $E \otimes \varepsilon$ Jahn–Teller system was first solved numerically by Longuet Higgins *et al* (1958). The calculation was refined by O'Brien (1971) and O'Brien and Pooler (1979) and extended to other Jahn–Teller and pseudo-Jahn–Teller systems (e.g. O'Brien and Evangelou (1980), Grevsmühl (1981), Pooler (1984)).

The eigenvalue problem for the full Rabi Hamiltonian (outside the rotating-wave approximation) was solved by Swain (1972, 1973). Swain worked with the recurrence relations in the occupation number representation and calculated the eigenvalues and eigenstates by a continued-fraction technique.

In 1977 Judd (1977) observed that, for a fictitious value of the angular momentum, the Longuet-Higgins recurrence relations become the recurrence relations of the displaced harmonic oscillator. Since the recurrence relations for the Rabi system also become the recurrence relations for the displaced harmonic oscillator for the level-splitting zero, Judd's observation indicated that the $E \otimes \varepsilon$ Jahn–Teller system and the Rabi system might be mathematically identical (except for different values of the physical parameters). Furthermore, Judd's observation was the starting point for an ingenious perturbation scheme by Barentzen (1979) and Barentzen *et al* (1981).

The next step for the $E \otimes \varepsilon$ Jahn–Teller system was also taken by Judd (1979). In retrospect, the results of his important paper can be summarized as follows. For energy eigenvalues on baseline N the Longuet-Higgins recurrence relations can be solved exactly for N isolated values of the vibronic coupling constant κ^2 , which are the zeros of a polynomial of degree N . In 1979 the situation was different: the result was only exemplified for the baselines 1 and 2. The calculation was something like an escape from a labyrinth and any attempt to tackle $N > 2$ led into 'a morass of algebra', to use Judd's own words.

It was at this point that analytical methods entered the stage. Reik *et al* (1982) (referred to as I) formulated the $E \otimes \varepsilon$ Jahn–Teller problem and the full Rabi problem in Bargmann's

(1961, 1962) Hilbert space of analytical functions. They obtained a system of two first-order differential equations for the component wavefunctions which are identical for the two systems. We have now the whole body of methods from the theory of differential equations in the complex domain at our disposal. It is easy to systematically rederive the Juddian isolated exact solutions in the general form stated above. Furthermore, expansions of the component wavefunctions in series of special functions can be given which converge much more rapidly than the power series expansion which correspond to the occupation-number representation (Nusser 1984). The fastest convergence is obtained by an expansion in generalized spheroidal wavefunctions (Reik *et al* 1987), henceforth referred to as II).

In this paper we introduce a new concept in the analytical theory of nonadiabatic model systems. For each eigenstate we construct a scalar entire function $D(z)$ with the following property. Both component wavefunctions are terminating series in the derivatives of $D(z)$ with coefficients which are polynomials in the independent variable z . For this reason we call $D(z)$ the generalized potential. The paper is organized as follows. In section 2 we collect some material from our earlier publications; in particular, we derive a system of first-order differential equations for the component wavefunctions. In section 3 we Laplace-transform the equations and formulate the theory with the reciprocal $r = \kappa^2/p$ as an independent variable. The equations in the r domain are particularly easy to work with. The expressions for the component wavefunctions $X_1(r)$, $X_2(r)$ in terms of the generalized potential $X(r)$ are given in section 4, together with the differential equations for $X(r)$. In the following three sections we invert the equations in the r domain and get the corresponding results in Bargmann's Hilbert space for the independent variable z . In section 8 we discuss the relation between the results of this paper and the earlier analytical work in I and II.

2. Model Hamiltonians and the Schrödinger equation in Bargmann's Hilbert space of analytical functions

We consider first a canonically transformed version of the $E \otimes \varepsilon$ Jahn-Teller Hamiltonian

$$H = a_{(+)}^+ a_{(+)}^+ + a_{(-)}^+ a_{(-)}^+ + 1 + (1/2 + 2\delta)\sigma_z + 2\kappa \left[(a_{(+)}^+ + a_{(-)}^+) \sigma_{(+)}^+ + (a_{(-)}^+ + a_{(+)}^+) \sigma_{(-)}^+ \right] \quad (2.1)$$

which describes two-boson modes (+) and (-) interacting with a two-level system. The level separation is $1 + 4\delta$. The angular momentum

$$J = a_{(+)}^+ a_{(+)}^+ - a_{(-)}^+ a_{(-)}^+ + (1/2)\sigma_z \quad (2.2)$$

is a constant of motion with the eigenfunctions

$$|\psi\rangle_{j+1/2} = \left[a_{(+)}^+ \right]^j \phi(a_{(+)}^+, a_{(-)}^+) |0\rangle |\uparrow\rangle + \left[a_{(+)}^+ \right]^{j+1} f(a_{(+)}^+, a_{(-)}^+) |0\rangle |\downarrow\rangle \quad (2.3)$$

$$J|\psi\rangle_{j+1/2} = (j + 1/2) |\psi\rangle_{j+1/2} \quad (j = 0, 1, 2, \dots). \quad (2.4)$$

Here $|0\rangle$ is the vacuum state for both phonons, and ϕ and f are power series in the product $a_{(+)}^+ a_{(-)}^+$ of the creation operators starting with the power zero. Equations (2.3) and (2.4) still make sense for negative integers j provided the power series for ϕ and f begin with the powers $-j$ and $-j - 1$, respectively. We write the Hamiltonian as $H = J + 1 + 2h_{(+)}$ with

$$h_{(+)} = a_{(-)}^+ a_{(-)} + \delta\sigma_z + \kappa \left[(a_{(+)} + a_{(-)}^+) \sigma_{(+)} + (a_{(-)} + a_{(+)}^+) \sigma_{(-)} \right]. \quad (2.5)$$

The eigenfunctions of the Hamiltonian are of the form (2.3)

$$H|\psi\rangle_{j+1/2} = \lambda|\psi\rangle_{j+1/2} \tag{2.6}$$

and satisfy the equivalent Schrödinger equation

$$h_{(+)}|\psi\rangle_{j+1/2} = \varepsilon|\psi\rangle_{j+1/2} \tag{2.7}$$

where λ and ε are related by $\lambda = j + 3/2 + 2\varepsilon$. We introduce Judd’s baseline parameter v (Judd 1979) instead of ε by $\varepsilon = v/2 - j/2 - 1/2 - \kappa^2$. The eigenvalue λ of the Hamiltonian is therefore expressed in terms of the eigenvalue v :

$$\lambda = v + 1/2 - 2\kappa^2. \tag{2.8}$$

We now apply Bargmann’s method (Bargmann 1961, 1962, Schweber 1967, Klauder and Skagerstam 1985, Perelomov 1986) for the solution of the eigenvalue problem (2.7), i.e. we map the creation operators onto two complex variables ξ and η by $a_{(+)}^+ \rightarrow \xi$, $a_{(-)}^+ \rightarrow \eta$, which entails $a_{(+)} \rightarrow \partial/\partial\xi$, $a_{(-)} \rightarrow \partial/\partial\eta$. The Hamiltonian $h_{(+)}$, the angular momentum and the eigenfunctions are given as

$$\%ofl h_{(+)} = \eta\partial/\partial\eta + \delta\sigma_z + \kappa \left[\left(\partial/\partial\xi + \eta \right) \sigma_{(+)} + \left(\partial/\partial\eta + \xi \right) \sigma_{(-)} \right] \tag{2.9}$$

$$J = \xi\partial/\partial\xi - \eta\partial/\partial\eta + (1/2)\sigma_z \tag{2.10}$$

$$|\psi\rangle_{j+1/2} = \xi^j \phi(z) | \uparrow \rangle + \xi^{j+1} f(z) | \downarrow \rangle \tag{2.11}$$

where $z = \xi \cdot \eta$. The eigenvalues v are selected by the requirement that $\xi^j \phi(z)$ and $\xi^{j+1} f(z)$ belong to the space of entire functions in ξ and η . Therefore, (2.11) makes sense for positive and negative integers j provided that the power series for $\phi(z)$ and $f(z)$ begin with the power zero for positive j and the powers z^{-j} , z^{-j-1} respectively for negative j . The Schrödinger equation (2.7) (2.9) in Bargmann’s Hilbert space allows for these expansions for positive and negative j and for no others as we shall presently see.

Insert (2.9) (2.11) in (2.7) and collect the spin up and spin down components. Then the following system of ordinary linear first-order differential equations is obtained:

$$z \, d\phi(z)/dz - (v/2 - j/2 - 1/2 - \delta - \kappa^2)\phi(z) + \kappa [z \, df(z)/dz + (j + 1 + z)f(z)] = 0 \tag{2.12}$$

$$\kappa [d\phi(z)/dz + \phi(z)] + z \, df(z)/dz - (v/2 - j/2 - 1/2 + \delta - \kappa^2)f(z) = 0. \tag{2.13}$$

These two equations constitute the Schrödinger equation in Bargmann’s Hilbert space. The system of (2.12) and (2.13) has two regular singular points $z = 0$ and $z = \kappa^2$ and an irregular singularity at infinity. The exponents at the singular point $z = 0$ are 0 and $-j - 1$ and the difference of the exponents is integer. For $j > 0$ we have $0 > -j - 1$. Therefore, the solution with the exponent $-j - 1$ is logarithmically divergent at $z = 0$. On the other hand, the solution $\phi(z)$, $f(z)$ as series of positive powers including zero is regular at the origin. Conversely, for negative integers j we have $-j - 1 > 0$, and the solution with the smaller exponent 0 is irregular. The power series for f and ϕ , which begin with the powers $-j - 1$ and $-j$, respectively, are regular at the origin. The regular singular point $z = \kappa^2$ has the exponents 0 and v , and since v is in general non-integer, the solution with the exponent 0 is regular at $z = \kappa^2$.

The requirement that the regular solution at the origin has an infinite radius of convergence, i.e. that f and ϕ are entire functions, selects the eigenvalues v and hence the eigenvalues λ of the Hamiltonian.

Apart from (2.12) and (2.13), we also use the linear combination (2.12) $-\kappa(2.13) = 0$:

$$(z - \kappa^2) \, d\phi(z)/dz - (v/2 - j/2 - 1/2 - \delta)\phi(z) + \kappa(z + v/2 + j/2 + 1/2 + \delta - \kappa^2)f(z) = 0. \tag{2.14}$$

Any two of the three equations (2.12)–(2.14) can be picked out to solve the eigenvalue problem.

We turn now to the Rabi Hamiltonian

$$H = a^+ a + 1/2 + (1/2 + 2\delta)\sigma_z + \sqrt{2}\kappa(a^+ + a)(\sigma_{(+)} + \sigma_{(-)}) \quad (2.15)$$

which can be treated on the same footing. With the Bargmann mapping $a^+ \rightarrow \xi$, $a \rightarrow d/d\xi$ the Hamiltonian takes the form

$$H = \xi d/d\xi + 1/2 + (1/2 + 2\delta)\sigma_z + \sqrt{2}\kappa(\xi + d/d\xi)(\sigma_{(+)} + \sigma_{(-)}). \quad (2.16)$$

The eigenvalue λ are selected by the requirement that the spin up and spin down components of the wavefunctions

$$|\psi^{(m)}\rangle = (\xi/\sqrt{2})^{m+1/2} \phi^{(m)}(\xi, \delta) |\uparrow\rangle + (\xi/\sqrt{2})^{-m+1/2} f^{(m)}(\xi, \delta) |\downarrow\rangle \quad (2.17)$$

($m = \pm 1/2$) belong to the space of entire functions. We introduce a new independent variable $z = (1/2)\xi^2$, insert (2.16) and (2.17) in the Schrödinger equation and collect the spin-up and down components. We then obtain the following system of differential equations

$$\begin{aligned} z d\phi^{(m)}(z, \delta)/dz - [v/2 - 1/4 - \delta - \kappa^2 - (1/2)(m + 1/2)] \phi^{(m)}(z, \delta) \\ + \kappa z^{-m+1/2} df^{(m)}(z, \delta)/dz \\ + \kappa [z^{-m+1/2} - (1/2)(m - 1/2)z^{-1/2-m}] f^{(m)}(z, \delta) = 0 \end{aligned} \quad (2.18)$$

$$\begin{aligned} \kappa [z^{m+1/2} d\phi^{(m)}(z, \delta)/dz + (z^{m+1/2} + (1/2)(m + 1/2)z^{m-1/2}) \phi^{(m)}(z, \delta)] \\ + z df^{(m)}(z, \delta)/dz \\ - [v/2 - 1/4 + \delta - \kappa^2 + (1/2)(m + 1/2)] f^{(m)}(z, \delta) = 0 \end{aligned} \quad (2.19)$$

and λ is given by (2.8). For $m = -1/2$ (2.18) (2.19) reduce to (2.12) (2.13) for $j = -1/2$ and for $m = 1/2$ we have

$$\phi^{(1/2)}(z, \delta) = f^{(-1/2)}(z, -\delta - 1/2) \quad (2.20)$$

$$f^{(1/2)}(z, \delta) = \phi^{(-1/2)}(z, -\delta - 1/2) \quad (2.21)$$

so that the eigenvalue problem associated with (2.12) (2.13) exhausts the spectrum of the $E \otimes \varepsilon$ Jahn–Teller system and the Rabi Hamiltonian and gives all the eigenfunctions.

3. Laplace transform of (2.12), (2.13). The equations in the r domain

So far we were able to treat (2.12) and (2.13) for negative and positive values of j on the same footing by properly selecting the expansion of $\phi(z)$ and $f(z)$ at the origin. We now Laplace-transform (2.12), (2.13) and denote the Laplace transforms of the component wavefunctions by $\phi(p)$, $f(p)$. Since the Laplace transform of the first derivative $d\phi(z)/dz$ depends upon the initial value $\phi(0)$, the two cases $j \geq 0$ and $j < 0$ must now be considered separately. Since for the Rabi Hamiltonian $j = -1/2$, we give the theory for $j < 0$. We obtain

$$\begin{aligned} -p d\phi(p)/dp - (v/2 - j/2 + 1/2 - \delta - \kappa^2)\phi(p) \\ + \kappa(-[p + 1]df(p)/dp + jf(p)) = 0 \end{aligned} \quad (3.1)$$

$$\kappa\phi(p)[p + 1] - p df(p)/dp - (v/2 - j/2 + 1/2 + \delta - \kappa^2)f(p) = 0. \quad (3.2)$$

Next we introduce two new dependent variables instead of $\phi(p)$ and $f(p)$

$$\phi(p) = p^{j-1} \exp(\kappa^2/p) X_1(\kappa^2/p) \quad (3.3)$$

$$f(p) = p^j \exp(\kappa^2/p) X_2(\kappa^2/p) \quad (3.4)$$

and eliminate the independent variable p in favor of the variable $r = \kappa^2/p$. By this procedure we get a system of differential equations for $X_1(r)$ and $X_2(r)$:

$$r \frac{dX_1(r)}{dr} - (v/2 + j/2 - 1/2 - \delta - \kappa^2 - r)X_1(r) + \kappa(\kappa^2 + r)\frac{dX_2(r)}{dr} + \kappa[\kappa^2 - j + r]X_2(r) = 0 \quad (3.5)$$

$$\kappa X_1(r)(1 + r/\kappa^2) + r \frac{dX_2(r)}{dr} - X_2(r)(A_0 - r) = 0 \quad (3.6)$$

with

$$A_0 = v/2 + j/2 + 1/2 + \delta - \kappa^2. \quad (3.7)$$

In order to study the singularities of (3.5), (3.6) we solve for $dX_1(r)/dr$ and $dX_2(r)/dr$:

$$\begin{aligned} dX_1(r)/dr = & X_1(r) \left\{ (v/2 + j/2 - 1/2 - \delta + \kappa^2)/r + \kappa^4/r^2 \right\} \\ & - X_2(r) \left\{ (v/2 - j/2 + 1/2 + \delta - \kappa^2)/r + \kappa^2 A_0/r^2 \right\} \end{aligned} \quad (3.5a)$$

$$dX_2(r)/dr = -X_1(r)\kappa^{-1}(1 + \kappa^2/r) + X_2(r)(A_0/r - 1). \quad (3.6a)$$

The system (3.5), (3.6) has two irregular singular points at $r = 0$ and at infinity; however, solutions in power series are admitted

$$X_i(r) = \sum_{\ell=0} X_i^{(\ell)} r^\ell \quad i = 1, 2 \quad (3.8)$$

which, for the eigenvalues v , turn out to be entire functions. Apart from (3.5) and (3.6), we also study the linear combination $\kappa^{-1}(3.5) - (3.6) = 0$:

$$\begin{aligned} \kappa^{-1}r \frac{dX_1(r)}{dr} + \kappa^2 \frac{dX_2(r)}{dr} - X_1(r)\kappa^{-1}(v/2 + j/2 - 1/2 - \delta) \\ + X_2(r)(A_0 + \kappa^2 - j) = 0 \end{aligned} \quad (3.9)$$

and any two of the three equations (3.5), (3.6) and (3.9) can be picked out to solve the eigenvalue problem in the r domain.

4. Solution in the r domain. The concept of the generalized potential

We turn to the solution of the differential equations (3.6), (3.9). We make an ansatz for the components $X_1(r)$, $X_2(r)$ of a complex two-dimensional vector field in terms of a scalar field $X(r)$ which we call the generalized potential

$$X_1(r) = [\alpha + (\beta + \zeta r)d/dr + (-v\kappa^3 - \bar{v}\kappa^3 r)d^2/dr^2] X(r) \quad (4.1)$$

$$X_2(r) = [\gamma + (\chi + \mu r)d/dr + (vr + \bar{v}r^2)d^2/dr^2] X(r). \quad (4.2)$$

The ansatz contains two free parameters \bar{v} , v whose values determine the gauge. The rest of the coefficients α , β , ζ , γ , χ , μ will presently be determined as functions of the parameters κ , j , δ and the eigenvalue v . To this end, insert the ansatz (4.1), (4.2) in (3.9). Since $\kappa^{-1}r X_1(r) + \kappa^2 X_2(r)$ is of first order in $X(r)$ we obtain a second-order differential equation

$$\left[(a_0^{(2)} + a_1^{(2)}r + a_2^{(2)}r^2)d^2/dr^2 + (a_0^{(1)} + a_1^{(1)}r)d/dr + a_0^{(0)} \right] X(r) = 0 \quad (4.3)$$

where

$$a_0^{(2)} = \kappa^2 [(v/2 + j/2 + 1/2 - \delta)v + \chi] \quad (4.4)$$

$$a_1^{(2)} = \beta/\kappa + \mu\kappa^2 + v(A_0 + \kappa^2 - j) + \bar{v}\kappa^2(v/2 + j/2 + 1/2 - \delta) \quad (4.5)$$

$$a_2^{(2)} = \zeta/\kappa + \bar{v}(A_0 + \kappa^2 - j) \quad (4.6)$$

$$a_0^{(1)} = -\beta(v/2 + j/2 - 1/2 - \delta)/\kappa + (\gamma + \mu)\kappa^2 + \chi(A_0 + \kappa^2 - j) \quad (4.7)$$

$$a_1^{(1)} = \alpha/\kappa + \mu(A_0 + \kappa^2 - j) - \zeta(v/2 + j/2 - 3/2 - \delta)/\kappa \quad (4.8)$$

$$a_0^{(0)} = -\alpha(v/2 + j/2 - 1/2 - \delta)/\kappa + \gamma(A_0 + \kappa^2 - j). \quad (4.9)$$

The differential equation is satisfied by *any* entire $X(r)$ provided we put

$$a_i^{(\ell)} = 0 \quad i = 0, \dots, \ell \quad \ell = 0, 1, 2. \quad (4.10)$$

Equations (4.3)–(4.10) are an analogue of the electrostatic equation $\nabla \times \nabla\phi = 0$, which is satisfied by *all* harmonic functions. Equations (4.10) are six linear inhomogeneous equations for the six ansatz coefficients α , β , ζ , γ , χ and μ with the solution

$$\chi = -(v/2 + j/2 + 1/2 - \delta)v \quad (4.11)$$

$$\zeta = -\kappa(v/2 - j/2 + 1/2 + \delta)\bar{v} \quad (4.12)$$

$$\mu = (v/2 - j/2 + 1/2 + \delta)v/\kappa^2 - 2(v/2 + j/2 - 1/2 - \delta)\bar{v} \quad (4.13)$$

$$\beta = -2\kappa(v/2 - j/2 + 1/2 + \delta)v + \kappa^3(v/2 + j/2 - 3/2 - \delta)\bar{v} \quad (4.14)$$

$$\alpha = -\kappa(v/2 - j/2 + 1/2 + \delta)(\bar{\mu} + \bar{v}) \quad (4.15)$$

$$\gamma = -(v/2 + j/2 - 1/2 - \delta)(\bar{\mu} + \bar{v}) \quad (4.16)$$

where $\bar{\mu}$ is a shorthand:

$$\bar{\mu} = (v/2 - j/2 + 1/2 + \delta)v/\kappa^2 - (v/2 + j/2 + 3/2 - \delta)\bar{v}. \quad (4.17)$$

The coefficients in (4.1), (4.2) have the same dependence on κ , j , δ and v and the gauge parameters v , \bar{v} in the ground state and the excited states, i.e. for different potential functions $X(r)$. Of course they are numerically different since they depend on the eigenvalue v .

We proceed now to the equation by which the potential function $X(r)$ is actually determined. We insert (4.1), (4.2), (4.11)–(4.17) into (3.6) and obtain (the calculation is lengthy)

$$O \left[(v + \bar{v}r)dX(r)/dr + (\bar{v} + \bar{\mu})X(r) \right] - vr d^2X/dr^2 + [A_0v - \kappa^4\bar{v} - r(v + \bar{v}\kappa^2)](dX(r)/dr) = 0 \quad (4.18)$$

where O is the operator of a special double confluent Heun equation (Schmidt and Wolf 1993) with two irregular singular points at $r = 0$ and $r \rightarrow \infty$:

$$O = r^2 d^2/dr^2 + (-\kappa^4 - r[j + v - 1] + r^2)d/dr - \kappa^2v + [j/2 + v/2 - 1/2 - \delta][j/2 + v/2 + 1/2 + \delta] - rv. \quad (4.19)$$

Equation (4.18) is therefore of third order. The entire solutions $X(r)$ for the eigenvalues v give, via (4.1), (4.2), the component wavefunctions $X_1(r)$, $X_2(r)$ in the ground state and the excited states which are solutions of the system (3.6), (3.7).

In order to find the entire solutions of (4.18) and (4.19), we expand the potential field $X(r)$ in a power series

$$X(r) = (\kappa^2)^{-j-1} \sum_{n=0} D_n r^n. \quad (4.20)$$

Insertion in (4.18), (4.19) gives the recurrence relation

$$\begin{aligned} & D_{n+2}(-v\kappa^4)(n+2)(n+1) + D_{n+1}(n+1) \\ & \times [vn(n-1-v-j) - v\{\kappa^2v - (v/2 + j/2 - 1/2 - \delta) \\ & \times (v/2 + j/2 + 1/2 + \delta) - A_0\} - \kappa^4\{\bar{v}(n+3) + \bar{\mu}\}] \\ & + D_n [vn(n-v-2) - \kappa^2\bar{v}n + \{\bar{v}(n+1) + \bar{\mu}\}] \end{aligned}$$

$$\begin{aligned} & \times \{n(n - j - v) - \kappa^2 v + (v/2 + j/2 - 1/2 - \delta)(v/2 + j/2 + 1/2 + \delta)\} \\ & + D_{n-1}(\bar{v}n + \bar{\mu})(n - 1 - v) = 0 \end{aligned} \tag{4.21}$$

which, as shown by the last term, allows for terminating power series (4.20) for integer eigenvalues v . One has therefore Juddian isolated exact solutions for the *potential*. From these solutions we obtain the Juddian isolated exact solutions for the *component wavefunctions* (Judd 1979, Reik *et al* 1981, 1982, 1983, 1985, Kus 1985) by (4.1), (4.2), (4.11)–(4.17). The recurrence relation (4.21) is in general four-term but becomes a three-term recurrence relation in the special gauge $v = 0$. The eigenvalue v and the expansion coefficients D_n of the entire functions $X(r)$ in the eigenstates are found by the continued-fraction technique for the solution of recurrence relations (Erdelyi *et al* 1953 (p 60), Risken 1984).

The power-series expansions for the component wavefunctions are given by

$$\begin{aligned} X_1(r) = (\kappa^2)^{-j-1} \sum_{n=0} r^n [D_n(\alpha + \zeta n) + D_{n+1}(n + 1)(\beta - \bar{v}\kappa^3 n) \\ - D_{n+2}\bar{v}\kappa^3(n + 2)(n + 1)] \end{aligned} \tag{4.22}$$

$$X_2(r) = (\kappa^2)^{-j-1} \sum_{n=0} r^n [D_n(\gamma + \mu n + \bar{v}n(n - 1)) + D_{n+1}(n + 1)(\chi + \nu n)] \tag{4.23}$$

as shown by (4.1), (4.2) and (4.20).

5. The component wavefunctions and the potential in Bargmann's Hilbert space

In the last section we solved the eigenvalue problem in the r domain and obtained the component wavefunctions $X_1(r), X_2(r)$, the potential $X(r)$ and the eigenvalues v in the eigenstates. In this section we go back to Bargmann's Hilbert space and see how the component wavefunctions $\phi(z), f(z)$ and the potential $D(z)$ look like in the z domain. We do this by first going from the r domain to the Laplace transforms $\phi(p), f(p)$ of the component wavefunctions and the Laplace transform of the potential $D(p)$. Finally we invert the Laplace transforms.

We insert (4.23) in (3.4) and obtain $f(p)$:

$$\begin{aligned} f(p) = (\kappa^2)^{-j-1} p^j \exp(\kappa^2/p) \\ \times \sum_{n=0} (\kappa^2/p)^n [D_n(\gamma + \mu n + \bar{v}n(n - 1) + D_{n+1}(n + 1)(\chi + \nu n)]. \end{aligned} \tag{5.1}$$

We invert this equation (Erdelyi *et al* 1954 (p 197, equation (18))) and get the component wavefunction $f(z)$ in the z domain

$$f(z) = \sum_{n=0} [D_n(\gamma + \mu n + \bar{v}n(n - 1) + D_{n+1}(n + 1)(\chi + \nu n)] w(j + 1 - n; z) \tag{5.2}$$

where

$$w(\bar{j} - n; z) = (\kappa^2 z)^{-(\bar{j}+n)/2} I_{-\bar{j}+n}(2\kappa z^{1/2}). \tag{5.3}$$

Equation (5.2) is the Neumann expansion of $f(z)$. We have the following relation between the three consecutive functions $w(j - n; z)$, $w(j + 1 - n; z)$ and $w(j + 2 - n; z)$:

$$nw(j + 1 - n; z) = (j + 1)w(j + 1 - n; z) - w(j - n; z) + \kappa^2 z w(j + 2 - n; z) \tag{5.4a}$$

and hence

$$\begin{aligned} n^2 w(j + 1 - n; z) = w(j - 1 - n; z) - (2j + 1)w(j - n; z) \\ + [(j + 1)^2 - 2\kappa^2 z] w(j + 1 - n; z) + (2j + 3)\kappa^2 z w(j + 2 - n; z) \\ + \kappa^4 z^2 w(j + 3 - n; z). \end{aligned} \tag{5.4b}$$

Equation (5.4a) is derived, using the differential recurrence relations for the modified Bessel functions (Magnus *et al* 1966 p 67). We rewrite (5.2) by inserting (5.4a), (5.4b). This gives

$$\begin{aligned}
 f(z) = \sum_{n=0} D_n \{ & \bar{v}w(j-1-n; z) + [-\mu + v - 2j\bar{v}]w(j-n; z) \\
 & + [\mu(j+1) + \gamma - \chi - 2(j+1)v + \bar{v}(j+1)j - 2\kappa^2 z \bar{v}] \\
 & \times w(j+1-n; z) + [\chi(j+2) + v(j+2)(j+1) \\
 & + \{\mu - 2v + 2(j+1)\bar{v}\}\kappa^2 z]w(j+2-n; z) \\
 & + [\{\chi + 2(j+2)v\}\kappa^2 z + \bar{v}\kappa^4 z^2]w(j+3-n; z) \\
 & + v\kappa^4 z^2 w(j+4-n; z) \}. \quad (5.5)
 \end{aligned}$$

Since

$$\kappa^{-2} dw(\bar{j}-n; z)/dz = w(\bar{j}+1-n; z) \quad (5.6)$$

the curly bracket in (5.5) is linear in the derivatives $d^\ell w(j-1-n; z)/dz^\ell$ ($\ell = 0, 1, 2, 3, 4, 5$) labelled by n with coefficients, which do *not* depend on n . Therefore, we infer that

$$D(z) = \sum_{n=0} D_n w(j-1-n; z) \quad (5.7a)$$

is the Neumann expansion of the potential in the z domain. For the Laplace transform $D(p)$ equation (5.7a), (4.20) implies

$$D(p) = \kappa^4 p^{j-2} \exp(\kappa^2/p) X(\kappa^2/p) \quad (5.7b)$$

$$= (\kappa^2)^{-j+1} p^{j-2} \exp(\kappa^2/p) \sum_{n=0} D_n (\kappa^2/p)^n \quad (5.7c)$$

since inversion of (5.7c) leads back to (5.7a). Equation (5.5) is now rewritten as

$$\begin{aligned}
 f(z) = \{ & \bar{v} + [-\mu + v - 2j\bar{v}] \kappa^{-2} d/dz \\
 & + [\mu(j+1) + \gamma - \chi - 2(j+1)v + \bar{v}(j+1)j - 2\kappa^2 z \bar{v}] \kappa^{-4} d^2/dz^2 \\
 & + [\chi(j+2) + v(j+2)(j+1) + \{\mu - 2v + 2(j+1)\bar{v}\}\kappa^2 z] \kappa^{-6} d^3/dz^3 \\
 & + [\{\chi + 2(j+2)v\}\kappa^2 z + \bar{v}\kappa^4 z^2] \kappa^{-8} d^4/dz^4 \\
 & + v\kappa^4 z^2 \kappa^{-10} d^5/dz^5 \} D(z). \quad (5.8)
 \end{aligned}$$

By the same method we get the component wavefunction $\phi(z)$:

$$\begin{aligned}
 \phi(z) = \kappa^{-2} \{ & -[\zeta + \bar{v}\kappa^3] + [\alpha - \beta + \zeta j - v\kappa^3 + 2\bar{v}\kappa^3 j] \kappa^{-2} d/dz \\
 & + [\beta(j+1) + 2(j+1)v\kappa^3 - \bar{v}\kappa^3(j+1)j \\
 & + (\zeta + 2\bar{v}\kappa^3)\kappa^2 z] \kappa^{-4} d^2/dz^2 \\
 & + [-v\kappa^3(j+2)(j+1) + \{\beta - \bar{v}\kappa^3 2(j+1) + 2v\kappa^3\}\kappa^2 z] \kappa^{-6} d^3/dz^3 \\
 & + [-2v\kappa^3(j+2) - \bar{v}\kappa^3 \kappa^2 z] \kappa^2 z \kappa^{-8} d^4/dz^4 \\
 & - v\kappa^3 \kappa^4 z^2 \kappa^{-10} d^5/dz^5 \} D(z). \quad (5.9)
 \end{aligned}$$

The component wavefunctions are of fifth order in $D(z)$ in the general case and of fourth order in the special gauge $v = 0$. Note that $\phi(z)$ and $-\kappa f(z)$ have common terms. For $\phi(z) + \kappa f(z)$ we get the following expression

$$\begin{aligned}
 \phi(z) + \kappa f(z) = \kappa^{-2} \{ & \zeta + [\alpha - \beta + \zeta j - \mu\kappa^3] \kappa^{-2} d/dz \\
 & + [\beta(j+1) + \gamma\kappa^3 + \mu(j+1)\kappa^3 - \chi\kappa^3 + \zeta\kappa^2 z] \kappa^{-4} d^2/dz^2
 \end{aligned}$$

$$\begin{aligned}
 &+ [\chi\kappa^3(j+2) + (\beta + \mu\kappa^3)\kappa^2z] \kappa^{-6} d^3/dz^3 \\
 &+ \chi\kappa^3\kappa^2z\kappa^{-8} d^4/dz^4 \} D(z)
 \end{aligned}
 \tag{5.10}$$

which is of fourth order in the general gauge and of third order in the special gauge $\nu = 0$. Recall that $\alpha, \beta, \gamma, \mu, \chi$ and ζ are shorthand for the RHS of (4.11)–(4.16). Close to the regular singular point $z = 0$ of the system (2.12), (2.13), the entire solutions $f(z), \phi(z)$ are power series. The series for $\phi(z)$ begins with z^{-j} . On the other hand, the expansion of $D(z)$ (5.7a) in view of (5.3) begins with the power z^{-j+1} . Therefore, (5.9) contains dangerous terms with the powers z^{-j-2}, z^{-j-1} which in fact cancel out. Similarly there are no dangerous terms left over in (5.8).

6. The differential equation for $D(z)$. First point of view

The procedure for the solution of the eigenvalue problem (2.12), (2.13) in Bargmann’s Hilbert space can be summarized as follows:

- (i) Determine the eigenvalues v and the expansion coefficients D_n by solving the recurrence relation (4.21).
- (ii) Calculate $D(z)$ (5.7a) and the component wavefunctions $f(z), \phi(z)$ (5.8), (5.9).

We are therefore able to calculate everything in the z domain and in particular get the results already obtained in I and II. It is however interesting from the theoretical point of view to study the differential equation satisfied by $D(z)$ as well.

If the component wavefunctions are inserted into (2.12), (2.13) we obtain two differential equations of different order for $D(z)$. Since $f(z), \phi(z)$ (5.8), (5.9) solve the eigenvalue problem (2.12), (2.13), it is obvious that the two differential equations for the potential have the solution $D(z)$ (5.7a) in common. This entails a relation between the two differential equations for $D(z)$ which we also derive. From now on we use the special gauge $\nu = 0$ which simplifies the equations without loss of mathematical insight. We begin by inserting (5.8), (5.9) in (2.12). Since this equation contains the differential quotients only in the linear combination $d\phi(z)/dz + \kappa df(z)/dz$ and since $\phi(z) + \kappa f(z)$, (5.10) is of third order in $D(z)$ in the special gauge $\nu = 0$, we get a differential equation of fourth order:

$$\begin{aligned}
 Q \cdot D(z) = & \bar{\nu}z^2(z - \kappa^2)d^4D(z)/dz^4 \\
 & + \{-\bar{\nu}\kappa^2z[(3/2)j - v/2 + 7/2 + \delta] \\
 & + \bar{\nu}z^2[(3/2)j - (3/2)v + 5/2 + \delta]\} d^3D(z)/dz^3 \\
 & + \{\bar{\nu}\kappa^2[-j^2/2 + vj/2 - 2j + v/2 - 3/2 - \delta - j\delta] \\
 & + \bar{\nu}z[2\kappa^4 - \kappa^2(v+1) + (3/4)v^2 - v - \delta + (3/4)j^2 + 1/4 - j - (3/2)jv \\
 & + j\delta - \delta v] - 2\bar{\nu}\kappa^2z^2\} d^2D(z)/dz^2 + \\
 & + \{\bar{\nu}[j/2 - v/2 - 1/2 - \delta][j/2 - v/2 + 1/2 + \delta][j/2 - v/2 - 1/2 + \delta] \\
 & + \bar{\nu}\kappa^2[v(v/2 - j/2 + 1/2 - \delta) - j] + \bar{\nu}\kappa^4[(3/2)j - v/2 + 3/2 + \delta] \\
 & + \bar{\nu}\kappa^2z[-(3/2)j + (3/2)v - 1/2 - \delta]\} dD(z)/dz \\
 & + \bar{\nu}\kappa^2\{\kappa^2(z - \kappa^2) + \kappa^2(v+1) \\
 & - [j/2 - v/2 - 1/2 - \delta][j/2 - v/2 + 1/2 + \delta]\} D(z) = 0.
 \end{aligned}
 \tag{6.1a}$$

After regrouping the terms, (6.1a) can be cast in a concise form

$$QD(z) = P \{ \bar{v} d^2(zD(z))/dz^2 + [\bar{v}(j-1) + \bar{\mu}] dD(z)/dz - \bar{v}\kappa^2 D(z) + \kappa^2(\bar{v} + \bar{\mu})(d^2D(z)/dz^2 + dD(z)/dz) = 0 \quad (6.2)$$

where P is the operator of a special confluent Heun equation with two regular singular points $z = 0$, $z = \kappa^2$ and an irregular singularity at infinity (Slavyanov 1993):

$$P = z(z - \kappa^2)d^2/dz^2 + [(j+2)(z - \kappa^2) - (v+1)z] d/dz - \kappa^2(z - \kappa^2) - \kappa^2(v+1) + [j/2 - v/2 - 1/2 - \delta][j/2 - v/2 + 1/2 + \delta]. \quad (6.3)$$

The identity of the differential equations (6.1a) and (6.1b), (6.1c) is proved by inspection. The identity of the terms in the fourth and zeroth order can be read off immediately.

Next we turn to the differential equation (2.14) which is also solved by the component wavefunctions $f(z)$, $\phi(z)$ (5.8), (5.9). Insertion gives a differential equation of the fifth order in $D(z)$, which can be written as (the calculation is lengthy)

$$RD(z) = (d/dz - 1)QD(z) = 0. \quad (6.2)$$

Therefore (6.2) is automatically satisfied by any solution of (6.1) and in particular by the entire solution (5.7a) which completes the proof. Relation (6.2) between the differential equations $RD(z) = 0$ and $QD(z) = 0$ is a special case of a general relation between two differential equations of different order which have one (or more) solutions in common (Ince 1956 (p 126)).

7. The differential equation for $D(z)$. Second point of view

There is also a systematic way of deriving differential equation (6.1b), (6.1c) for $D(z)$. We start from (4.18), (4.19) in the r domain and work in the special gauge $v = 0$. In (4.18), (4.19) we change the independent variable from r to p and eliminate the dependent variable $X(\kappa^2/p)$ in favour of $D(p)$ by (5.7b). We obtain

$$\{d/dp(p^2 d/dp) + (\kappa^2 + [j+v-1]p + \kappa^2 p^2)d/dp - \kappa^2 v + [j/2 + v/2 - 1/2 - \delta][j/2 + v/2 + 1/2 + \delta] + \kappa^4 + (j-1)\kappa^2/p\} \Theta(p) + \Lambda(p) = 0 \quad (7.1)$$

where

$$\Theta(p) = p^{-j+1} \{-\bar{v} p^2 dD(p)/dp + D(p) \{[\bar{v}(j-1) + \bar{\mu}]p - \bar{v}\kappa^2\}\} \quad (7.2a)$$

$$= p^{-j+1} \vartheta(p) \quad (7.2b)$$

and

$$\Lambda(p) = p^{-j+1} \bar{v}\kappa^2(p+1) \{p^2 dD(p)/dp + D(p) (\kappa^2 - [j-2]p)\} \quad (7.3a)$$

$$= p^{-j+1} \lambda(p). \quad (7.3b)$$

A comparison of (7.2a) and (7.3a) shows that

$$\lambda(p) = -\kappa^2(p+1) \{\vartheta(p) - (\bar{v} + \bar{\mu})pD(p)\}. \quad (7.4)$$

We insert (7.2b), (7.3b) into (7.1) and factor out p^{-j+1} . We get the equation

$$\{p^2 d^2/dp^2 + (\kappa^2 + [-j+v+3]p + \kappa^2 p^2)d/dp - (j-1)(v+1) - \kappa^2 v + [j/2 + v/2 - 1/2 - \delta][j/2 + v/2 + 1/2 + \delta] + \kappa^4 - (j-1)\kappa^2 p\} \vartheta(p) + \lambda(p) = 0 \quad (7.5)$$

which we now invert

$$\begin{aligned} & \{z(z - \kappa^2)(d^2/dz^2 + [(j + 1)(z - \kappa^2) - vz] d/dz \\ & \quad - \kappa^2(z - \kappa^2) - \kappa^2v + [j/2 - v/2 - 1/2 - \delta] \\ & \quad \times [j/2 - v/2 + 1/2 + \delta])\} \vartheta(z) + \lambda(z) = 0. \end{aligned} \tag{7.6}$$

The inversion of (7.2), (7.3) gives $\vartheta(z)$ and $\lambda(z)$ in terms of $D(z)$ and its derivatives

$$\vartheta(z) = \bar{v} d^2(zD(z))/dz^2 + (\bar{v}[j - 1] + \bar{\mu})dD(z)/dz - \bar{v}\kappa^2 D(z) \tag{7.7}$$

$$\begin{aligned} \lambda(z) = & -\kappa^2 [\bar{v}d^3(zD(z))/dz^3 + \bar{v}d^2(zD(z))/dz^2 + \bar{v}(j - 2)d^2D(z)/dz^2 \\ & - \bar{v}(\kappa^2 - j + 2)dD(z)/dz + \kappa^2\bar{v}D(z)]. \end{aligned} \tag{7.8a}$$

A second useful expression for $\lambda(z)$ is obtained by inverting (7.4)

$$\lambda(z) = -\kappa^2 [d\vartheta(z)/dz + \vartheta(z) - (\bar{v} + \bar{\mu})(d^2D(z)/dz^2 + dD(z)/dz)]. \tag{7.8b}$$

Finally, inserting of (7.7), (7.8b) into (7.6) we obtain the differential equation (6.1b), (6.1c) for $D(z)$. The same method can also be used in the general gauge.

8. Discussion

In this section we analyse the calculations which led to the solution of the eigenvalue problem for the Rabi and $E \otimes \varepsilon$ Jahn–Teller system in the r - and the z -domain from the logical point of view and try to get the gist of the matter as clearly as possible. We begin with the r domain. The solution is achieved in three steps:

(1). We chose the ansatz (4.1), (4.2) in such a way that upon insertion of (4.1), (4.2) into (3.5), (3.6), two differential equations of the same (third) order are obtained,

$$\frac{d^3X}{dr^3}(vr^2 + \bar{v}r^3) + \frac{d^2X}{dr^2} \sum_0^3 b_i^{(2)}r^i + \frac{dX}{dr} \sum_0^2 b_i^{(1)}r^i + X \sum_0^1 b_i^{(0)}r^i = 0 \tag{8.1}$$

$$\frac{d^3X}{dr^3}(vr^2 + \bar{v}r^3) + \frac{d^2X}{dr^2} \sum_0^3 c_i^{(2)}r^i + \frac{dX}{dr} \sum_0^2 c_i^{(1)}r^i + X \sum_0^1 c_i^{(0)}r^i = 0 \tag{8.2}$$

and that the coefficients of the same derivatives in the two equations are polynomials of the same degree. (It is clear that $b_{\ell+1}^{(\ell)} = c_{\ell+1}^{(\ell)}$, $\ell = 0, 1, 2$.) Subtraction of (8.2) from (8.1) gives

$$\frac{d^2X}{dr^2} \sum_0^2 (b_i^{(2)} - c_i^{(2)})r^i + \frac{dX}{dr} \sum_0^1 (b_i^{(1)} - c_i^{(1)})r^i + X(b_0^{(0)} - c_0^{(0)}) = 0. \tag{8.3}$$

(2). Equations (8.1) and (8.2) are free of contradictions if the polynomials with the same superscript are identical or, equivalently, if all polynomials in (8.3) are equal to zero. The condition of solvability (4.10),

$$b_i^{(\ell)} - c_i^{(\ell)} = a_i^{(\ell)} = 0 \quad i = 0, \dots, \ell \quad \ell = 0, 1, 2 \tag{8.4}$$

is satisfied by (4.11)–(4.17).

(3). The entire solution of the identical equations (8.1), (8.2) are sought.

We turn now to the discussion of the calculations in the z domain. Likewise, there are three steps which are equivalent to the three steps in the r domain although the procedure is not identical.

(1). We chose the ansatz (5.8), (5.9). Upon insertion in (2.12), (2.13) we obtain two differential equations of the sixth order (note that $\nu \neq 0$)

$$\bar{R}_1 D(z) = 0 \quad (8.5)$$

$$\bar{R}_2 D(z) = 0 \quad (8.6)$$

whose coefficients of $d^6 D/dz^6$ are identical. Subtraction of (8.5), (8.6) gives a differential equation of fifth order:

$$\bar{Q} D(z) = 0. \quad (8.7)$$

It is impossible to put the coefficients of all derivatives in (8.7) equal to zero by analogy with (8.3), (8.4). Equivalently, (8.5) and (8.6) cannot be made *identical*.

(2). In order to make (8.5), (8.6) *compatible*, we determine the ansatz coefficients χ , ζ , μ , β , α and γ by (4.11)–(4.17). This assignment entails that

$$\bar{R}_1 = (p(z)d/dz + q(z))\bar{Q} \quad (8.8)$$

i.e. that the system of fundamental solutions of (8.5) contains the fundamental solutions of (8.7). In this case (8.6) is also satisfied by all solutions of (8.7). (In the special gauge $\nu = 0$ the operator \bar{Q} is of fourth order and $p(z) = q(z) = 1$; see (6.2)).

(3) The entire solution of (8.7) is sought.

While it is fairly easy to guess the ansatz (4.1), (4.2) in the r domain by looking at (3.6) and (3.7), equations (5.8) and (5.9) are very hard to guess. For this reason we obtained the equations in the z domain systematically by inverting (4.1) and (4.2).

Equations (4.1), (4.2) and (5.8), (5.9) show that the component wavefunctions $X_1(r)$, $X_2(r)$ in the r domain as well as the component wavefunctions $\phi(z)$, $f(z)$ in the z domain are firmly entangled. Ham (1987) showed that a relation between the component wavefunctions in the domain of the configuration coordinates found by O'Brien (1964) is a consequence of Berry's geometrical phase (see also Chancey and O'Brien (1988) for a generalisation). We should like to transform our equations into this domain and make contact with the work of O'Brien and Ham.

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