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

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Dedicated to the memory of H Risken

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Abstract. The eigenvalue problem for the Rabi and $E \otimes \varepsilon$ Jahn–Teller Hamiltonians in Bargmann's Hilbert space is a system of two first-order differential equations for the two-component wavefunctions for which entire solutions are sought. The concept of the generalized potential has been introduced in a previous paper together with a particular example. Here we treat a simpler potential $N(z)$ which satisfies a second-order ordinary differential equation closely related to the differential equation of the confluent Heun functions. The component wavefunctions are linear in the potential and its first derivative. The coefficients of $N(z)$ and $\mathrm{d}N(z)/\mathrm{d}z$ are functions of z and the physical parameters which are identical in all eigenstates. The relation to the previous example is fully discussed.

1. Introduction

The analytical theory of the Rabi and the $E \otimes \varepsilon$ Jahn–Teller system was prompted by two algebraic discoveries: the Longuet Higgins *et al* (1958) recurrence relations can be solved exactly for the fictitious value $j = -1/2$ of the orbital angular momentum and the detuning $\delta = -1/4$ (Judd 1977) and for arbitrary angular momenta and detunings for isolated values of the interaction constant κ between bosons and fermions (Judd 1979). The latter solutions are known as Juddian isolated exact solutions.

In Bargmann (1961, 1962), his theory on a Hilbert space of analytical functions leads to a system of two ordinary differential equations for the component wavefunctions in the complex domain. The differential equations have two regular singular points. The first is at $z = 0$ with the exponents $0, -j - 1$. The second singular point is at $z = \kappa^2$ with the exponents $0, v$ (where v is Judds (1977, 1979) baseline parameter). Finally, there is an irregular singularity at infinity.

The Juddian isolated exact solutions are now easily classified: an isolated exact solution is obtained for integer v *and* for those values of the interaction constant κ for which the second singularity becomes *apparent*. It is no surprise that the component wavefunctions are terminating series of functions whose differential equations have singularities at infinity and $z = 0$, only with singular properties which are compatible with those of the component wavefunctions (Reik *et al* 1982, 1987).

In this paper, we consider the general case where the second singularity is *real* and we adopt the following strategy: we construct a differential equation for a function $N(z)$ whose main ingredient is a confluent Heun operator which has the same real singularities as the differential equations for the component wavefunctions, i.e. $z = 0$ (exponents $0, -j - 1$),

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$z = \kappa^2$ (exponents $0, v+1$) and an irregular singularity at infinity. Furthermore, there is a term providing an additional singularity which is *apparent* for *all* values of the physical parameters. (The position of the apparent singularity depends on v.) By a suitable choice of the additional term, $N(z)$ becomes a generalized potential in the following sense: both component wavefunctions which solve the original equations in Bargmann's Hilbert space are linear forms in $N(z)$ and its first derivative $\mathrm{d}N(z)/\mathrm{d}z$.

The paper is organized as follows. In section 2, we collect some material from our previous publications: we give the differential equations for the component wavefunctions in Bargmann's Hilbert space (z-domain) and in the r-domain (which is related to the Laplace transform) and introduce the concept of the generalized potential. The equations in the r-domain are particularly easy to work with and we solve them in section 3. In section 4 and 5, we give the theory in the z-domain. Section 6 deals with a different choice of the generalized potential and the relation between the potentials. In section 7, we summarize the results and discuss their relation to work by O'Brien (1964) and Ham (1987) and some practical and mathematical aspects of the theory.

2. The equations for the component wavefunctions. The generalized potential

In this section, we study first a canonically transformed version of the standard $E \otimes \varepsilon$ Jahn–Teller Hamiltonian in terms of the configuration coordinates and momenta (O'Brien 1964, Englman 1972 and, more recently, Eiermann and Wagner 1992). This version clearly shows the close relation with the Rabi system. The transformed Hamiltonian

$$H = a^+_{(+)}a_{(+)} + a^+_{(-)}a_{(-)} + 1 + (1/2 + 2\delta)\sigma_z + 2\kappa[(a_{(+)} + a^+_{(-)})\sigma_{(+)} + (a_{(-)} + a^+_{(+)})\sigma_{(-)}] \tag{2.1}$$

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

$$J = a^+_{(+)}a_{(+)} - a^+_{(-)}a_{(-)} + \tfrac{1}{2}\sigma_z \tag{2.2}$$

is a constant of motion with the eigenfunction

$$|\psi\rangle_{j+1/2} = [a^+_{(+)}]^j \phi(a^+_{(+)}a^+_{(-)})|0\rangle|\uparrow\rangle + [a^+_{(+)}]^{j+1} f(a^+_{(+)}a^+_{(-)})|0\rangle|\downarrow\rangle \tag{2.3}$$

for $j = 0, 1, 2, \ldots$. Here, $\sigma_z|\uparrow\rangle = |\uparrow\rangle$, $\sigma_z|\downarrow\rangle = -|\downarrow\rangle$, $|0\rangle$ is the vacuum state for both bosons $a_{(+)}|0\rangle = a_{(-)}|0\rangle = 0$ and $\phi(a^+_{(+)}a^+_{(-)})$, $f(a^+_{(+)}a^+_{(-)})$ are power series in the product of the creation operators starting with power zero. Furthermore

$$J|\psi\rangle_{j+1/2} = (j + 1/2)|\psi\rangle_{j+1/2}. \tag{2.4}$$

Equations (2.3) and (2.4) still make sense for negative integer j provided that the power series for ϕ and f begin with the powers $-j$ and $-j-1$, respectively.

In the eigenvalue problem

$$H|\psi\rangle_{j+1/2} = \lambda|\psi\rangle_{j+1/2} = (v + 1/2 - 2\kappa^2)|\psi\rangle_{j+1/2} \tag{2.5}$$

we introduce Judd's baseline parameter v (Judd 1979) instead of λ as the new eigenvalue. Furthermore, we apply Bargmann's method (Bargmann 1961, 1962, Schweber 1967), i.e.

we map the creation operators onto two complex variables ξ and η by $a^+_{(+)} \to \xi$, $a^+_{(-)} \to \eta$ which entails $a_{(+)} \to \partial/\partial\xi$, $a_{(-)} \to \partial/\partial\eta$. The Hamiltonian, the angular momentum and the eigenfunctions are given by

$$H = \xi\partial/\partial\xi + \eta\partial/\partial\eta + 1 + (1/2 + 2\delta)\sigma_z + 2\kappa[(\partial/\partial\xi + \eta)\sigma_{(+)} + (\partial/\partial\eta + \xi)\sigma_{(-)}] \tag{2.6}$$

$$J = \xi\partial/\partial\xi - \eta\partial/\partial\eta + (1/2)\sigma_z \tag{2.7}$$

$$|\psi\rangle_{j+1/2} = \xi^j\phi(z)|\uparrow\rangle + \xi^{j+1}f(z)|\downarrow\rangle \tag{2.8}$$

where $z = \xi\cdot\eta$. In order to calculate the component wavefunctions $\phi(z)$ and $f(z)$ we insert (2.6) and (2.8) into (2.5) and collect the spin-up and spin-down components. We obtain the following system of ordinary first-order differential equations for $\phi(z)$ and $f(z)$

$$z\,\mathrm{d}\phi(z)/\mathrm{d}z - (v/2 - j/2 - 1/2 - \delta - \kappa^2)\phi(z) + \kappa[z\,\mathrm{d}f(z)/\mathrm{d}z + (j + 1 + z)f(z)] = 0 \tag{2.9}$$

and

$$\kappa[\mathrm{d}\phi(z)/\mathrm{d}z + \phi(z)] + z\,\mathrm{d}f(z)/\mathrm{d}z - (v/2 - j/2 - 1/2 + \delta - \kappa^2)f(z) = 0. \tag{2.10}$$

The system (2.9) and (2.10) has two regular singular points at $z = 0$ and $z = \kappa^2$ and an irregular singular point at infinity. The exponents at the singular point $z = 0$ are 0 and $-j-1$ and the difference between the exponents is integer. For $j \geqslant 0$, we have $0 > -j-1$. Therefore, the solution with the exponent $-j-1$ contains logarithmic terms. On the other hand, the solution $\phi(z)$, $f(z)$, as a power series of positive powers (including zero), is regular at the origin. Conversely, for negative integers j, we have $-j-1 \geqslant 0$ and the solution with the exponent 0 is irregular. Equations (2.9) and (2.10) allow for the regular expansions in the vicinity of the origin which we had already anticipated. 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 expansions of the regular solutions $\phi(z)$, $f(z)$ at the origin have an infinite radius of convergence, i.e. that $\phi(z)$ and $f(z)$ are entire functions, selects the eigenvalues v and, hence, the eigenvalues λ of the Hamiltonian. (In this case, $\xi^j\phi(\xi\cdot\eta)$, $\xi^{j+1}f(\xi\cdot\eta)$ are entire in ξ and η which is the original form of Bargmann's quantization.)

We turn now to the Rabi Hamiltonian

$$H = a^+a + 1/2 + (1/2 + 2\delta)\sigma_z + \sqrt{2}\kappa(a^+ + a)(\sigma_{(+)} + \sigma_{(-)}). \tag{2.11}$$

With the Bargmann mapping $a^+ \to \xi$, $a \to \mathrm{d}/\mathrm{d}\xi$, the Hamiltonian takes the form

$$H = \xi\mathrm{d}/\mathrm{d}\xi + 1/2 + (1/2 + 2\delta)\sigma_z + \sqrt{2}\kappa(\xi + \mathrm{d}/\mathrm{d}\xi)(\sigma_{(+)} + \sigma_{(-)}). \tag{2.12}$$

The eigenfunctions of (2.12) for a definite parity are given by

$$|\psi\rangle = \phi(z,\delta)|\uparrow\rangle + (1/\sqrt{2})\xi f(z,\delta)|\downarrow\rangle. \tag{2.13}$$

Here, $z = \xi^2/2$ and the component wavefunctions $\phi(z,\delta)$ and $f(z,\delta)$ satisfy (2.9) and (2.10) for $j = -1/2$.

The eigenfunctions with the opposite parity have the form

$$|\psi\rangle = (1/\sqrt{2})\xi f(z, -\delta - 1/2)|\uparrow\rangle + \phi(z, -\delta - 1/2)|\downarrow\rangle \qquad (2.14)$$

and the component wavefunctions $\phi(z, -\delta - 1/2)$ and $f(z, -\delta - 1/2)$ satisfy (2.9) and (2.10) for $j = -1/2$ and δ replaced by $-\delta - 1/2$.

The eigenvalues λ or v in (2.5) are selected by the requirement that the component wavefunctions $\phi(z, \delta)$, $f(z, \delta)$ and $\phi(z, -\delta - 1/2)$, $f(z, -\delta - 1/2)$ are entire functions of ξ. Therefore the eigenvalue problems of the $E \otimes \varepsilon$ Jahn–Teller and Rabi Hamiltonians are mathematically identical (save for different values of the angular-momentum quantum number j).

The importance of the fictitious case $j = -1/2$ as the limiting case in the $E \otimes \varepsilon$ Jahn–Teller system was first observed by Judd (1977) when analysing the structure of the Longuet–Higgins *et al* (1958) recurrence relation. An ingenious perturbation scheme based on this observation, in which the deviation of the angular momentum from the fictitious value is used as the expansion parameter, has been devised by Barentzen (1979) and Barentzen *et al* (1981). Neither Judd nor Barentzen noticed the intimate relationship between the Jahn–Teller and Rabi systems since they restricted themselves to the detuning $\delta = -1/4$. In this case, the Rabi system reduces to the displaced harmonic oscillator where the states with positive and negative parity are degenerate.

Having dealt with the physics of (2.9) and (2.10), we proceed to the solution of the equations. We Laplace transform (2.9) and (2.10) and denote the Laplace transforms of the component wavefunctions by $\phi(p)$, $f(p)$. Since the Laplace transforms of $\mathrm{d}\phi(z)/\mathrm{d}z$, $\mathrm{d}f(z)/\mathrm{d}z$ depend on $\phi(z = 0)$ and $f(z = 0)$, we have to distinguish between the cases $j \geqslant 0$ and $j < 0$; we restrict ourselves to the latter case. We obtain

$$-p\,\mathrm{d}\phi(p)/\mathrm{d}p - (v/2 - j/2 + 1/2 - \delta - \kappa^2)\phi(p) + \kappa(-[p+1]\,\mathrm{d}f(p)/\mathrm{d}p + jf(p)) = 0 \qquad (2.15)$$

and

$$\kappa(p+1)\phi(p) - p\,\mathrm{d}f(p)/\mathrm{d}p - (v/2 - j/2 + 1/2 + \delta - \kappa^2)f(p) = 0. \qquad (2.16)$$

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

$$\phi(p) = p^{j-1}\exp(\kappa^2/p)X_1(\kappa^2/p) \qquad (2.17)$$

$$f(p) = p^{j}\exp(\kappa^2/p)X_2(\kappa^2/p) \qquad (2.18)$$

and eliminate the independent variable p in favour of $r = \kappa^2/p$. We get the following system of first-order differential equations in the r-domain:

$$r\,\mathrm{d}X_1(r)/\mathrm{d}r - (v/2 + j/2 - 1/2 - \delta - \kappa^2 - r)X_1(r) + \kappa(\kappa^2 + r)\,\mathrm{d}X_2(r)/\mathrm{d}r + \kappa(\kappa^2 - j + r)X_2(r) = 0 \qquad (2.19)$$

and

$$\kappa(1 + r/\kappa^2)X_1(r) + r\,\mathrm{d}X_2(r)/\mathrm{d}r - (v/2 + j/2 + 1/2 + \delta - \kappa^2 - r)X_2(r) = 0. \qquad (2.20)$$

We also use the linear combination $(2.19) - \kappa(2.20) = 0$

$$r\,\mathrm{d}X_1(r)/\mathrm{d}r - (v/2 + j/2 - 1/2 - \delta)X_1(r) + \kappa^3\,\mathrm{d}X_2(r)/\mathrm{d}r + (v/2 - j/2 + 1/2 + \delta)\kappa X_2(r) = 0 \qquad (2.21)$$

instead of (2.19). The system of equation in the r-domain has two irregular singular points at $r = 0$ and at infinity; however, solutions in power series are admitted (Ince 1956, p 417)

$$X_i(r) = \sum_{n=0} X_i^{(n)} r^n \qquad i = 1, 2 \tag{2.22}$$

which, for the eigenvalues v, are entire functions. The inversion of the Laplace transform gives the eigensolutions of (2.9) and (2.10).

There are two methods of solution for (2.20) and (2.21). The first method treats (2.20) and (2.21) on the same footing. The power series (2.22) are inserted and the recurrence relations for the coefficients $X^{(n)}$ are solved simultaneously. The eigensolutions together with the eigenvalues v are picked out either by matrix truncation (O'Brien 1971, O'Brien and Pooler 1979, O'Brien and Evangelou 1980, review by Pooler 1984) or by a continued fraction procedure (Swain 1972, 1973, Reik *et al* 1982, Risken 1984).

The second strategy was invented by Reik (1993) and, henceforth, this paper is referred to as [I]. The method is modelled on the potential theory and treats (2.20) and (2.21) on a different footing: an ansatz is made for the components $X_1(r), X_2(r)$ of a complex two-dimensional vector field in terms of a scalar field $X(r)$, the generalized potential.

$$X_1(r) = [\alpha + (\beta + \zeta r)\,\mathrm{d}/\mathrm{d}r + (-\nu\kappa^3 - \overline{\nu}\kappa^3 r)\,\mathrm{d}^2/\mathrm{d}r^2]X(r) \tag{2.23}$$

and

$$X_2(r) = [\gamma + (\chi + \mu r)\,\mathrm{d}/\mathrm{d}r + (\nu r + \overline{\nu} r^2)\,\mathrm{d}^2/\mathrm{d}r^2]X(r). \tag{2.24}$$

Since $X_1(r), X_2(r)$ are entire functions in the eigenstates, $X(r)$ is also entire. The coefficients $\alpha, \beta, \zeta, \gamma, \chi, \mu, \nu, \overline{\nu}$ are adjustable. We insert (2.23) and (2.24) into (2.21). The resulting second-order differential equation is satisfied by *any* entire function $X(r)$, provided we dispose of the coefficients (see Reik (1993) (hereafter referred to as [I]), equations (4.11)–(4.16)). Insertion of (2.23) and (2.24) [I; (4.11)–(4.16)] into (2.20) gives a third-order differential equation by which $X(r)$ is actually determined. The ansatz (2.23) and (2.24) has the advantage that, once $X(r)$ is entire, each term on the right-hand side is manifestly entire.

We do, however, feel that (2.23) and (2.24) is not the most basic ansatz (in particular, when we look into the consequences in the z-domain [I; sections 5–7]). A theory which is modelled on the potential theory should allow for vector components $X_1(r), X_2(r)$ which are of *first* order in the generalized potential and, as a consequence, for a second-order differential equation for the potential. We have found a new ansatz which satisfies these requirements. In the next three sections we shall use this ansatz for the solution of (2.20) and (2.21) in the r-domain and (2.9) and (2.10) in the z-domain.

3. Solution in the r-domain

In this section, we solve the differential equations (2.20) and (2.21) with the new ansatz for the components $X_1(r), X_2(r)$ of a two-dimensional complex vector field in terms of a potential field $M(r)$

$$X_1(r) = -\kappa^3 (r - r_0)^{-1} [\mathrm{d}M(r)/\mathrm{d}r - (\rho/r_0)M(r)] \tag{3.1}$$

and

$$X_2(r) = (r - r_0)^{-1} [r\,\mathrm{d}M(r)/\mathrm{d}r - \rho M(r)]. \tag{3.2}$$

The parameters r_0, ρ will presently be determined as functions of κ, j, δ and the eigenvalue v. Since the entire solutions $X_1(r)$, $X_2(r)$ of (2.20) and (2.21) are sought, $M(r)$ must be entire and, in addition, the function $r_0\,\mathrm{d}M(r)/\mathrm{d}r - \rho M(r)$ must have a simple zero at $r = r_0$. Equation (3.1) can be rewritten as

$$rX_1(r) + \kappa^3 X_2(r) = \kappa^3(\rho/r_0)M(r) \tag{3.3}$$

and

$$r_0 X_1(r) + \kappa^3 X_2(r) = \kappa^3\,\mathrm{d}M(r)/\mathrm{d}r. \tag{3.4}$$

In (2.21), we express $r\,\mathrm{d}X_1(r)/\mathrm{d}r + \kappa^3\,\mathrm{d}X_2(r)/\mathrm{d}r$ by (3.3) and the component wavefunctions $X_1(r)$, $X_2(r)$ by (3.1) and (3.2). We obtain a differential equation of first order for $M(r)$

$$\begin{aligned}[\kappa^2(v/2 + j/2 + 1/2 - \delta - \rho) + r(\kappa^2\rho/r_0 + v/2 - j/2 + 1/2 + \delta)]\,\mathrm{d}M(r)/\mathrm{d}r \\ - \rho[(\kappa^2/r_0)(v/2 + j/2 + 1/2 - \delta) + v/2 - j/2 + 1/2 + \delta]M(r) = 0.\end{aligned} \tag{3.5}$$

This equation is satisfied by all entire functions $M(r)$, provided we put

$$\rho = v/2 + j/2 + 1/2 - \delta \tag{3.6}$$

and

$$r_0 = -\kappa^2(v/2 + j/2 + 1/2 - \delta)/(v/2 - j/2 + 1/2 + \delta) \tag{3.7}$$

in *all* eigenstates. We shall, however, continue to use ρ and r_0 in subsequent equations as abbreviations for the right-hand side of (3.6) and (3.7).

Next we derive the equation by which $M(r)$ and the eigenvalue v are actually determined. We insert (3.1) and (3.2) into (2.20) and obtain a second-order differential equation for the potential $M(r)$. Define a special double-confluent Heun operator $[\mathrm{DCH}]_{j+1,v+1}$ (Schmidt and Wolf 1994)

$$\begin{aligned}[\mathrm{DCH}]_{j+1,v+1} = r^2\,\mathrm{d}^2/\mathrm{d}r^2 + (-\kappa^4 - [j + v + 1]r + r^2)(\mathrm{d}/\mathrm{d}r) \\ + (v/2 + j/2 + 1/2 - \delta)(v/2 + j/2 + 3/2 + \delta) - \kappa^2(v + 1) - r(v + 1).\end{aligned} \tag{3.8}$$

Then we have

$$SM(r) = (r - r_0)[\mathrm{DCH}]_{j+1,v+1}M(r) - r_0[r\,\mathrm{d}M(r)/\mathrm{d}r - \rho M(r)] = 0 \tag{3.9a}$$

$$= (r - r_0)\{[\mathrm{DCH}]_{j+1,v+1}M(r) - r_0\,\mathrm{d}M(r)/\mathrm{d}r\} - r_0[r_0\mathrm{d}M(r)/\mathrm{d}r - \rho M(r)] = 0. \tag{3.9b}$$

The differential equation (3.9*a,b*) has irregular singularities at $r = 0$ and at infinity which are due to the double-confluent Heun operator in the first term of (3.9*a,b*) and an apparent singularity at $r = r_0$ with the exponents 0 and 2 from the second term (Ince 1956, p 406). The solution with the exponent 0 does not contain logarithmic terms. Therefore, both partners of the fundamental system in the vicinity of r_0 are analytical functions. As a consequence, it is seen that the function $r_0\,\mathrm{d}M(r)/\mathrm{d}r + \rho M$ has a simple zero at $r = r_0$ as required. In the vicinity of the origin, the physical solution is a power series which, for the eigenvalues v, defines an entire function. The comparison of (3.9*a,b*) and (3.1) and (3.2) shows that the component wavefunctions $X_1(r)$, $X_2(r)$ can also be written as

$$X_2(r) = (1/r_0)[\mathrm{DCH}]_{j+1,v+1}M(r) \tag{3.10}$$

$$r_0 X_1(r) = -\kappa^3((1/r_0)[\mathrm{DCH}]_{j+1,v+1}M(r) - \mathrm{d}M(r)/\mathrm{d}r) \tag{3.11a}$$

and

$$rX_1(r) = -(\kappa^3/r_0)([\mathrm{DCH}]_{j+1,v+1}M(r) - \rho M(r)). \tag{3.11b}$$

To check the consistency of (3.10), (3.11) and (3.1), (3.2), insert (3.10), (3.11), (3.6) and (3.7) into (2.21). Then, equations (3.9*a,b*) are reobtained. If (3.10), (3.11), (3.6) and (3.7) are inserted into (2.20), we get a differential equation of third order

$$TM(r) = (r_0 r(\mathrm{d}/\mathrm{d}r) + r_0 r - r_0[v/2 + j/2 + 3/2 + \delta] - \kappa^4)SM(r) = 0 \tag{3.12}$$

which is satisfied by all solutions of the second-order differential equations (3.9*a,b*) $SM(r) = 0$ (Ince 1956, p 127).

We can, of course, also start by considering (3.10) and (3.11) as an ansatz for the component wavefunctions in terms of an entire potential where ρ and r_0 are *adjustable parameters*. Insertion of (3.10) and (3.11) into (2.20) and (2.21) gives a differential equation of second order *and* a differential equation of third order for $M(r)$. These differential equations do *not* contradict each other *if* we dispose of ρ and r_0 by (3.6) and (3.7). Under these conditions, equations (3.9*a,b*) and (3.12) are reobtained.

Having dealt with the component wavefunctions $X_1(r)$, $X_2(r)$ and the potential $M(r)$ in the r-domain, we now turn to the solutions $\phi(z)$ and $\kappa f(z)$ of equations (2.9) and (2.10) in the z-domain.

4. The component wavefunctions in the z-domain. First point of view

Once we have found the entire solutions $M(r)$ of (3.9*a,b*) and the eigenvalues v in the eigenstates of the Hamiltonian, we also know the component wavefunctions $\kappa f(z)$ and $\phi(z)$ in the z-domain. We calculate the potential $N(z)$ whose Laplace transform $N(p)$ is related to $M(r)$ by

$$N(p) = \kappa^4 p^j \exp(\kappa^2/p)M(\kappa^2/p). \tag{4.1}$$

Furthermore, define a special confluent Heun operator [CH] (Slavyanov 1994)

$$\begin{aligned}[\mathrm{CH}] = {} & z(z-\kappa^2)(\mathrm{d}^2/\mathrm{d}z^2) + [(j+2)(z-\kappa^2) - (v+1)z](\mathrm{d}/\mathrm{d}z) \\ & - \kappa^2(z-\kappa^2) + (v/2 - j/2)^2 - (1/2+\delta)^2 - \kappa^2(v+1).\end{aligned} \tag{4.2}$$

Then the component wavefunctions $\kappa f(z)$ and $\phi(z)$ are given by

$$\kappa f(z) = (1/\kappa^3 r_0)[\mathrm{CH}]N(z) \tag{4.3}$$

$$\phi(z) = -(1/\kappa^3 r_0)\{[\mathrm{CH}]N(z) - (v/2 + j/2 + 1/2 - \delta)N(z)\} \tag{4.4}$$

and

$$\kappa f(z) + \phi(z) = (1/\kappa^3 r_0)(v/2 + j/2 + 1/2 - \delta)N(z). \tag{4.5}$$

To prove (4.3), we Laplace transform the equation

$$\kappa f(p) = (1/\kappa^3 r_0)\{p^2(\mathrm{d}^2/\mathrm{d}p^2) + [\kappa^2 p^2 + p(-j+v+3) + \kappa^2](\mathrm{d}/\mathrm{d}p) \\ - j + v + 1 + \kappa^4 + \Lambda - jp\kappa^2\}N(p) \tag{4.6}$$

where

$$\Lambda = (v/2 - j/2)^2 - (1/2+\delta)^2 - \kappa^2(v+1) \tag{4.7}$$

and insert (4.1) and (2.18). Finally, we replace p by κ^2/r and obtain (3.10) which proves (4.3). Equation (4.4) is proved using the same technique.

In this section, we have obtained the solution of (2.9) and (2.10) in the z-domain using results from the r-domain. In the next section, we derive the same results without reference to the r-domain.

5. Solution in the z-domain. Second point of view

In this section, we give a direct calculation for the two components $\phi(z)$ and $\kappa f(z)$ of the complex vector field in terms of the potential $N(z)$. We find, by the same method as in section 3,

$$\phi(z) = (\rho/\kappa^3 r_0)(z - z_0)^{-1}[z\,\mathrm{d}N(z)/\mathrm{d}z + (z+j+1)N(z)] \tag{5.1}$$

and

$$\kappa f(z) = (\rho/\kappa^3 r_0)(z - z_0)^{-1}[-z\,\mathrm{d}N(z)/\mathrm{d}z + (v/2 - j/2 - 1/2 - \delta - \kappa^2)N(z)]. \tag{5.2}$$

The functions in the square brackets of (5.1) and (5.2) must have simple zeros at $z = z_0$. This requirement entails

$$z_0 = -v/2 - j/2 - 1/2 + \delta + \kappa^2 = \kappa^2 - \rho \tag{5.3}$$

and, hence,

$$\kappa f(z) + \phi(z) = (\rho/\kappa^3 r_0)N(z) \tag{5.4}$$

in accordance with (4.5). All functions $\phi(z)$ and $\kappa f(z)$, defined by (5.1) and (5.2), solve (2.9). We insert (5.1) and (5.2) into (2.10), multiply the equation by $(z - z_0)^2$ and get a second-order differential equation for $N(z)$

$$UN(z) = (z - z_0)[\mathrm{CH}]N(z) + \rho[z\,\mathrm{d}N(z)/\mathrm{d}z - (v/2 - j/2 - 1/2 - \delta - \kappa^2)N(z)] \tag{5.5a}$$

$$= (z - z_0)\{[\mathrm{CH}]N(z) - \rho N(z)\} + \rho[z\mathrm{d}N(z)/\mathrm{d}z + (z+j+1)N(z)] = 0 \tag{5.5b}$$

with the [CH] defined as in (4.2). The differential equation (5.5*a,b*) has regular singularities at $z = 0$ (exponents $0, -j-1$) and $z = \kappa^2$ (exponents $0, v+1$) and an irregular singularity at infinity. The exponents of the potential $N(z)$ close to the regular singular points are in agreement with the exponents of the component wavefunctions $\kappa f(z)$ and $\phi(z)$. On account of the second term in (5.5*a,b*), there is an apparent singularity at $z = z_0$ with the exponents 0, 2. The solution with the exponent 0 does not contain logarithmic terms (Ince 1956, p 406). Therefore, all solutions of (5.5*a,b*) are holomorphic in the vicinity of z_0. Furthermore, (5.5*a,b*), (5.1) and (5.2) show that the component wavefunctions can also be written as

$$\kappa f(z) = (1/\kappa^3 r_0)[\mathrm{CH}]N(z) \tag{5.6}$$

and

$$\phi(z) = -(1/\kappa^3 r_0)([\mathrm{CH}]N(z) - \rho N(z)) \tag{5.7}$$

in accordance with (4.3) and (4.4).

6. Comparison with the previous treatment

We come back to the theory given in [I] and to equations (2.23) and (2.24) for the component wavefunctions $X_1(r), X_2(r)$ in terms of the potential $X(r)$. If care is taken of [I; (4.11)–(4.16)], these equations can be written as

$$X_1(r) = -\kappa^3[(\nu+\overline{\nu}r_0)\rho^2/r_0^2 - \{2\nu\rho/r_0 + \overline{\nu}(\rho-2) + \overline{\nu}\rho r/r_0\}\,\mathrm{d}/\mathrm{d}r + (\nu+\overline{\nu}r)\,\mathrm{d}^2/\mathrm{d}r^2]X(r) = L_1X(r) \tag{6.1}$$

and

$$X_2(r) = [(\nu+\overline{\nu}r_0)\rho(\rho-1)/r_0 + \{-\nu\rho + [\nu\rho/r_0 + 2\overline{\nu}(\rho-1)]r\}\,\mathrm{d}/\mathrm{d}r + (\nu r+\overline{\nu}r^2)\,\mathrm{d}^2/\mathrm{d}r^2]X(r) = L_2X(r) \tag{6.2}$$

with ρ and r_0 given by (3.6) and (3.7).

Now we can factorize the operators L_1 and L_2

$$\begin{aligned} L_1 &= -\kappa^3(r-r_0)^{-1}[\mathrm{d}/\mathrm{d}r - \rho/r_0]L_s \\ L_2 &= (r-r_0)^{-1}[r\,\mathrm{d}/\mathrm{d}r - \rho]L_s \end{aligned} \tag{6.3}$$

with

$$L_s = (r-r_0)[(\nu+\overline{\nu}r)\,\mathrm{d}/\mathrm{d}r - \nu\rho/r_0 - (\nu+\overline{\nu}r)/(r-r_0) - \overline{\nu}(\rho-1)]. \tag{6.4}$$

The proof is by inspection. L_s depends linearly on $(\nu,\overline{\nu})$. The component wavefunctions in (3.1), (3.2) and (6.1), (6.2) are the same. The comparison yields the relation between $M(r)$ and $X(r)$

$$M(r) = L_sX(r) \tag{6.5}$$

where only X depends on $(\nu,\overline{\nu})$.

Next we rederive the results of [I] in the z-domain. In order to shorten the calculations, we restrict ourselves to the case $\nu=0$ for the rest of this section. The Laplace transform of the potential $D(z)$ corresponding to $X(r)$ is given by [I; (5.7*b*)]

$$D(p) = \kappa^4p^{j-2}\exp(\kappa^2/p)X(\kappa^2/p). \tag{6.6}$$

We insert (6.6) into (6.5) and use (6.4) for $\nu=0$. The resulting equation for $M(\kappa^2/p)$ is put into (4.1). We get

$$N(p) = \overline{\nu}\{[r_0p^3 - \kappa^2p^2]\,\mathrm{d}/\mathrm{d}p + [-\kappa^4 + p\kappa^2(r_0-\rho+j-2) + p^2r_0(\rho-j+1)]\}D(p) \tag{6.7}$$

and, after inversion,

$$\begin{aligned} N(z) &= HD(z) \\ &= \overline{\nu}\{-\kappa^4 + \kappa^2[r_0-\rho+j]\,\mathrm{d}/\mathrm{d}z \\ &\quad + [r_0(\rho-j-2)+\kappa^2z]\,\mathrm{d}^2/\mathrm{d}z^2 - r_0z\,\mathrm{d}^3/\mathrm{d}^3z\}D(z). \end{aligned} \tag{6.8}$$

Insertion of (6.8) into (4.5) gives

$$\begin{aligned}\kappa f(z)+\phi(z) &= (1/\kappa^3 r_0)(v/2+j/2+1/2-\delta)N(z)\\ &= (1/\kappa^3 r_0)\rho N(z)\\ &= (\overline{v}\rho/\kappa^3 r_0)\{-\kappa^4+\kappa^2[r_0-\rho+j]\,\mathrm{d}/\mathrm{d}z\\ &\quad +[r_0(\rho-j-2)+\kappa^2 z]\,\mathrm{d}^2/\mathrm{d}z^2 - r_0 z\,\mathrm{d}^3/\mathrm{d}z^3\}D(z)\end{aligned} \tag{6.9}$$

in agreement with [I; (5.10)($\nu = 0$)]. Equations (5.1), (5.2) and (6.8) show that

$$\phi(z) = K_1 D(z) \tag{6.10a}$$

$$K_1 = \overline{v}(\rho/\kappa^3 r_0)(z-z_0)^{-1}(z\,\mathrm{d}/\mathrm{d}z + z + j + 1)H \tag{6.10b}$$

and

$$\kappa f(z) = K_2 D(z) \tag{6.11a}$$

$$K_2 = \overline{v}(\rho/\kappa^3 r_0)(z-z_0)^{-1}(-z\,\mathrm{d}/\mathrm{d}z + v/2 - j/2 - 1/2 - \delta - \kappa^2)H \tag{6.11b}$$

where the operators K_1, K_2 are already factorized. Multiplying out the right-hand sides of (6.10*b*) and (6.11*b*), we obtain

$$\begin{aligned}K_1 = \overline{v}\kappa\{&-(\rho/r_0+1)+[-\rho(\rho-j+1)+2(j+1)]\kappa^{-2}\,\mathrm{d}/\mathrm{d}z\\ &+[(j+1)(\rho-j-2)+(\rho/r_0+2)\kappa^2 z]\kappa^{-4}\,\mathrm{d}^2/\mathrm{d}z^2\\ &+[\rho-2j-4]\kappa^2 z\kappa^{-6}\,\mathrm{d}^3/\mathrm{d}z^3 - \kappa^4 z^2\kappa^{-8}\,\mathrm{d}^4/\mathrm{d}z^4 + \kappa^{-3}(z-z_0)^{-1}Q\end{aligned} \tag{6.10c}$$

$$\begin{aligned}K_2 = \overline{v}\kappa\{&1+2[\rho-j-1]\kappa^{-2}\,\mathrm{d}/\mathrm{d}z+[\rho(\rho-1)+(j+1)(j+2-2\rho)-2\kappa^2 z]\kappa^{-4}\,\mathrm{d}^2/\mathrm{d}z^2\\ &-2[\rho-j-2]\kappa^2 z\kappa^{-6}\,\mathrm{d}^3/\mathrm{d}z^3+\kappa^4 z^2\kappa^{-8}\,\mathrm{d}^4/\mathrm{d}z^4\} - \kappa^{-3}(z-z_0)^{-1}Q\end{aligned} \tag{6.11c}$$

where Q is defined by [I; (6.1*a*), (6.2), (6.3)] and $QD(z) = 0$ since $\phi(z)$ and $\kappa f(z)$ are holomorphic in the vicinity of $z = z_0$. By insertion of (6.10*c*) and (6.11*c*) into (6.10*a*) and (6.11*a*), equations [I; (5.8), (5.9)] are reproduced.

7. Summary and discussion

The results of this paper can be summarized as follows. The eigenvalue problem of the Rabi and the $E \otimes \varepsilon$ Jahn–Teller Hamiltonian amounts to finding the entire solutions $X_1(r), X_2(r)$ of (2.20) and (2.21) together with the eigenvalues λ. The solutions to the problem are accomplished in two steps.

(i) Consider the subspace of entire functions $M(r)$ for which the expression $r_0(\mathrm{d}M(r)/\mathrm{d}r) - \rho M(r)$ with ρ and r_0 defined by (3.6) and (3.7) has a simple zero at $r = r_0$. All functions in this subspace are called potentials. By (3.1) and (3.2), *each* potential generates a vector field with the components $X_1(r), X_2(r)$ which satisfy (2.21).

(ii) Equation (3.9a,b) selects those potentials whose associated vector fields $X_1(r)$, $X_2(r)$ *also* satisfy (2.20). The eigenvalues v are also determined. The procedure in the r-domain and in the z-domain exactly parallel each other. The theory given in [I] is also incorporated.

We are now going to discuss the results but, for conciseness, we restrict ourselves to the r-domain. Equations (3.1) and (3.2) give the *complete* interdependence of the components $X_1(r)$, $X_2(r)$ if the wavefunctions are in all eigenstates. A relation between the component wavefunctions in the domain of the configuration coordinates has been found by O'Brien (1964) on plausible and intuitive grounds. Ham (1987) showed that this relation is a consequence of Berry's geometrical phase. (See also Chancey and O'Brien (1988) for an application to a different Jahn–Teller system.) We would like to look into this problem using the complete information which is now at our disposal and transforming our equations to the configuration coordinate domain. This program will be carried out in a forthcoming paper and might give a more detailed understanding of the work by O'Brien and Ham.

In this paper, we have argued that the potential $M(r)$ is more fundamental than $X(r)$. However, the recurrence relations for $X(r)$ with $\nu = 0$ are easier to solve than for $M(r)$: the physical solutions of [I; (4.18), (4.19)] and of (3.9a,b) are power series

$$X(r) = (\kappa^2)^{-j-1} \sum_{n=0} D_n r^n \tag{7.1}$$

and

$$M(r) = \sum_{n=0} M_n r^n \tag{7.2}$$

and from (6.5) ($\nu = 0$), we have

$$M_n = (\kappa^2)^{-j-1} \overline{\nu}[(n-1-\rho)D_{n-1} - r_0(n+1-\rho)D_n]. \tag{7.3}$$

Insertion of (7.1) in [I; (4.18), (4.19)] gives a three-term recurrence relation

$$\begin{aligned} D_{n+1}\kappa^4(n+1)(\overline{\nu}[n+3]+\overline{\mu}) - D_n[n(n-j-v) + (v/2+j/2-1/2-\delta)(v/2+j/2+1/2+\delta) - \kappa^2 v] \\ \times (\overline{\nu}[n+1] + \overline{\mu}) - D_{n-1}(n-v-1)(\overline{\nu}n + \overline{\mu}) = 0 \end{aligned} \tag{7.4}$$

and

$$\overline{\mu} = -\overline{\nu}(\rho - 1) \tag{7.5}$$

while the recurrence relation for M_n is four term

$$\begin{aligned} M_{n+1}\kappa^4 r_0(n+1) - M_n[r_0 n(n-j-v-2) + r_0(n-\rho) + r_0(v/2+j/2+1/2-\delta) \\ \times (v/2+j/2+3/2+\delta) - r_0\kappa^2(v+1) + \kappa^4 n] \\ + M_{n-1}[-r_0(n-v-2) + (n-1)(n-j-v-3) + (v/2+j/2+1/2-\delta) \\ \times (v/2+j/2+3/2+\delta) - \kappa^2(v+1)] - M_{n-2}(n-v-3) = 0. \end{aligned} \tag{7.6}$$

It is therefore expedient to solve (7.4) for the eigenvalue and for D_n and calculate M_n by (7.3). For integer v, the recurrence relations allow for polynomial solutions of $M(r)$ and $X(r)$ which upon insertion into (3.1), (3.2) and (2.23), (2.24) give the Juddian isolated exact solutions for the component wavefunction (Judd 1979). In the general case, we have for the coefficients of the physical solutions the limit behaviour $\lim M_{n+1}/M_n = \lim D_{n+1}/D_n \approx -n^{-1}$.

The double-confluent Heun equation

$$[\mathrm{DCH}]_{j,v}\mathcal{M}(r) = 0 \qquad \mathcal{M}(r) = \sum_{n=0} \mathcal{M}_n r^n \tag{7.7}$$

with the recurrence relation

$$\mathcal{M}_{n+1}\kappa^4(n+1) - \mathcal{M}_n[n(n-j-v) + (v/2 + j/2 - 1/2 - \delta)(v/2 + j/2 + 1/2 + \delta) - \kappa^2 v] \\ - \mathcal{M}_{n-1}(n - v - 1) = 0 \tag{7.8}$$

also allows for polynomial solutions for integer v (see also Schmidt and Wolf 1994, section 3). Furthermore, for the entire solutions of (7.7), in the general case, we have $\lim \mathcal{M}_{n+1}/\mathcal{M}_n \approx -n^{-1}$. We, therefore, believe that virtually the whole body of results for the double-confluent Heun equation, as given by Schmidt and Wolf (1994), can be taken over to the more general equations (3.9*a*) and (3.9*b*) with only minor quantitative changes.

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