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Exact solution of the $E \otimes \varepsilon$ Jahn–Teller and Rabi Hamiltonian by generalised spheroidal wavefunctions?

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Abstract. The Schrödinger equation for the $E \otimes \varepsilon$ Jahn-Teller and Rabi systems in Bargmann's Hilbert space is a system of two ordinary differential equations of first order for the spin up and down components of the wavefunctions. This system has two regular and one irregular singular points. The energy eigenvalues are selected by the requirement that the solutions belong to the space of entire functions. The differential equations of the generalised spheroidal wavefunctions have the same singular points and the same exponents at each singular point. It is therefore conjectured that the component wavefunctions in the excited state i can be expanded in $i+4$ generalised spheroidal wavefunctions. The energy eigenvalues $v^{(i)}$ $(i=0,1,\ldots,5)$ calculated with the conjectured component wavefunctions agree with numerical values within the computational error. The same is true for the coefficients of the Neumann expansion of the component wavefunctions. A proof is still missing.

1. Introduction

Non-adiabatic model systems like the $E \otimes \varepsilon$ Jahn-Teller system and the Rabi Hamiltonian outside the rotating wave approximation (RWA) are interesting in their own right. The latter system is also practically important for the treatment of the one-atom maser (Meschede *et al* 1985, Rempe *et al* 1987). In the experimental set-up, atoms prepared in a high Rydberg state (Gallas *et al* 1985, Haroche and Raimond 1985) cross a microwave cavity tuned to a particular transition. In the theoretical treatment (Jaynes and Cummings 1963, Yoo and Eberly 1985, Filipowicz *et al* 1986a,b, Knight 1986) the authors use RWA for simplicity although the interaction between atomic levels and radiation scales with a high power of the principal quantum number.

The first step towards the exact solution of these model systems was taken by Judd (1979) in an important paper. He solved the Longuet Higgins (Longuet Higgins *et al* 1958) recurrence relations for the $E \otimes \varepsilon$ and $\Gamma_8 \otimes \tau_2$ Jahn-Teller systems in closed rational form for isolated values of the interaction constant (Juddian isolated exact solutions). The next step was taken by us. We formulated the $E \otimes \varepsilon$ Jahn-Teller and the Rabi Hamiltonian in Bargmann's Hilbert space of analytical functions (Bargmann 1961, 1962, Schweber 1967). We obtained a system of two linear first-order differential equations for the component wavefunctions, and expanded the wavefunctions in Neumann series. These series terminate for the isolated exact solutions (Reik *et al* 1982, 1985, Kus 1985, Kus and Lewenstein 1986).

In general the Neumann series are infinite but they converge much faster than the power series expansion which correspond to the occupation number representation. A thorough numerical study of the convergence properties has been made by Nusser (1983).

In this paper we ask ourselves the question whether we can find new expansion functions which allow for a finite expansion of the wavefunction in the general case. For the Juddian isolated exact solutions this expansion must reduce to the finite Neumann series.

Our answer to this question is only partial. By comparing the pole structure of the system of differential equations for the wavefunctions with the pole structure of the differential equation for the expansion functions of the Neumann series we pinpoint the analytical reason for the infinite Neumann expansions: one regular singular point in the system is an ordinary point in the differential equation for the expansion functions. We generalise the differential equation for the expansion functions so that the point in question becomes a regular singular point. The expansion functions defined in this way should therefore allow for finite expansions of the component wavefunctions unless we have missed a very subtle point.

The paper is organised as follows. In § 2 we formulate the Hamiltonians in Bargmann's Hilbert space of analytical functions. The Neumann expansions are given in § 3. In § 4 we prove that the Neumann expansions are infinite except for the Juddian isolated exact solutions by looking at the unphysical solutions for the component wavefunctions. The new expansion functions and their eigenvalues are studied in § 5. These functions turn out to be the generalised spheroidal wavefunctions of Leitner and Meixner (1960). In § 6 an ansatz for the component wavefunctions is made in terms of a finite series of generalised spheroidal wavefunctions. In § 7 we use this ansatz to calculate the eigenvalues of the $E\otimes\varepsilon$ Jahn–Teller system and the Rabi system up to the fifth excited state. The results of this calculation are in agreement with the results of a numerical calculation within the limits of accuracy.

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

In the following we consider two model Hamiltonians which contain the essential features of the non-adiabatic interactions. The first is a canonically transformed form of the generalised $E\otimes\varepsilon$ Jahn–Teller Hamiltonian (Reik *et al* 1982)

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

which describes two boson modes $(+)$ and $(-)$ interacting with a two-level system. The level separation is $1+4\delta$ ($\sigma_z^2=1$). The operator

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

is a constant of motion,

$$[J, H] = 0 \qquad (2.3)$$

with the eigenfunctions

$$|\Psi\rangle_{j+1/2} = [a^+_{(+)}]^j\Phi(a^+_{(+)}a^+_{(-)})|0\rangle|\uparrow\rangle + [a^+_{(+)}]^{j+1}f(a^+_{(+)}a^+_{(-)})|0\rangle|\downarrow\rangle \qquad (2.4)$$

$$J|\Psi\rangle_{j+1/2} = (j+\tfrac{1}{2})|\Psi\rangle_{j+1/2} \qquad j=0,1,2,\ldots. \qquad (2.5)$$

Here $|0\rangle$ is the vacuum state for both phonons and Φ, f are arbitrary functions of the products of the two creation operators.

We write the Hamiltonian in the form

$$\tfrac{1}{2}H = \tfrac{1}{2}J + \tfrac{1}{2} + h_{(+)} \qquad (2.6)$$

where

$$h_{(+)} = a^{+}_{(-)}a_{(-)} + \delta\sigma_z + \kappa[(a_{(+)} + a^{+}_{(-)})\sigma_{(+)} + (a_{(-)} + a^{+}_{(+)})\sigma_{(-)}]. \tag{2.7}$$

On account of (2.3) the eigenfunctions of the Hamiltonian (2.1) are of the form (2.4)

$$H|\Psi\rangle_{j+1/2} = \lambda|\Psi\rangle_{j+1/2} \tag{2.8}$$

and satisfy the equivalent Schrödinger equation

$$h_{(+)}|\Psi\rangle_{j+1/2} = \varepsilon|\Psi\rangle_{j+1/2} \tag{2.9}$$

where the eigenvalue ε is related to λ by (2.7),

$$\lambda = 2\varepsilon + j + \tfrac{3}{2}. \tag{2.10}$$

We now use Bargmann's method (Bargmann 1961, 1962, Schweber 1967, Perelomov 1986, Klauder and Skagerstam 1985) for the solution of the eigenvalue problem (2.9), i.e. we map the creation operators onto two complex variables ξ and η

$$a^{+}_{(+)} \to \xi \qquad a^{+}_{(-)} \to \eta \tag{2.11}$$

which entails

$$a_{(+)} \to \partial/\partial\xi \qquad a_{(-)} \to \partial/\partial\eta. \tag{2.12}$$

The Hamiltonian $h_{(+)}$, the operator J and the eigenfunctions are given by

$$h_{(+)} = \eta\,\partial/\partial\eta + \delta\sigma_z + \kappa[(\partial/\partial\xi + \eta)\sigma_{(+)} + (\partial/\partial\eta + \xi)\sigma_{(-)}] \tag{2.13}$$

$$J = \xi\,\partial/\partial\xi - \eta\,\partial/\partial\eta + \tfrac{1}{2}\sigma_z \tag{2.14}$$

$$|\Psi\rangle_{j+1/2} = \xi^{j}\Phi(z)|\uparrow\rangle + \xi^{j+1}f(z)|\downarrow\rangle \tag{2.15}$$

where $z = \xi\cdot\eta$. We insert (2.13) and (2.15) into (2.9) and collect the spin up and down components. This gives the following system of ordinary linear first-order differential equations for the functions $\Phi(z), f(z)$:

$$z\,\mathrm{d}\Phi(z)/\mathrm{d}z - (\varepsilon - \delta)\Phi(z) + \kappa[z\,\mathrm{d}f(z)/\mathrm{d}z + (j + 1 + z)f(z)] = 0 \tag{2.16}$$

$$\kappa(\mathrm{d}\Phi(z)/\mathrm{d}z + \Phi(z)) + z\,\mathrm{d}f(z)/\mathrm{d}z - (\varepsilon + \delta)f(z) = 0. \tag{2.17}$$

This system of differential equations is the Schrödinger equation in Bargmann's Hilbert space. Till now j has been restricted to positive integers including zero. Equations (2.16) and (2.17) still make sense for negative values of j provided one requires that the component wavefunctions $\xi^{j}\Phi(z)$ and $\xi^{j+1}f(z)$ belong to the space of entire functions of ξ and η.

In the following we introduce Judd's baseline parameter (Judd 1979) v instead of λ and ε by

$$\varepsilon = \tfrac{1}{2}v - \tfrac{1}{2}j - \tfrac{1}{2} - \kappa^2 \qquad \lambda = v + \tfrac{1}{2} - 2\kappa^2. \tag{2.18}$$

Next we cast (2.16) and (2.17) in a form which exhibits the pole structure

$$\frac{\mathrm{d}\Phi(z)}{\mathrm{d}z} = \left(\frac{\frac{1}{2}v - \frac{1}{2}j - \frac{1}{2} - \delta}{z - \kappa^2}\right)\Phi(z) - \left(\frac{\kappa(\frac{1}{2}v + \frac{1}{2}j + \frac{1}{2} + \delta)}{z - \kappa^2} + \kappa\right)f(z) \tag{2.19}$$

$$\frac{\mathrm{d}f(z)}{\mathrm{d}z} = \left(\frac{\frac{1}{2}v - \frac{1}{2}j - \frac{1}{2} - \delta - \kappa^2}{\kappa z} - \frac{\frac{1}{2}v - \frac{1}{2}j - \frac{1}{2} - \delta}{\kappa(z - \kappa^2)}\right)\Phi(z) + \left(-\frac{j+1}{z} + \frac{\frac{1}{2}v + \frac{1}{2}j + \frac{1}{2} + \delta}{z - \kappa^2}\right)f(z). \tag{2.20}$$

The system (2.19) and (2.20) has two regular singular points at $z'=0$ and $z'=\kappa^2$ and an irregular singular point at infinity. In the neighbourhood of each regular singular point there are in general two linearly independent multiplicative solutions (Ince 1956, Whittaker and Watson 1958)

$$\Phi(z)=(z-z')^{\gamma_{1/2}}L(z-z') \qquad L=\sum l_n(z-z')^n \tag{2.21}$$

$$f(z)=(z-z')^{\gamma_{1/2}}M(z-z') \qquad M=\sum m_n(z-z')^n \tag{2.22}$$

with functions $L(z-z')$, $M(z-z')$ which are regular in the vicinity of z'. In the exceptional case where the exponents γ_1 and γ_2 differ by an integer, there exists at least the multiplicative solution for the higher exponent. The second solution contains logarithmic terms.

The two exponents γ_1, γ_2 at the regular singular points of the system (2.19) and (2.20) are given in the first two lines of table 1.

Table 1. Regular singular points and exponents for various differential equations from the text.

Differential equation	Function	Singular point z'	γ_1	γ_2
(2.19) and (2.20)	$\Phi(z), f(z)$	0	0	$-j-1$
		κ^2	0	v
(2.27) and (2.28)	$\Phi^{(m)}(z), f^{(m)}(z)$	0	0	$-\frac{1}{2}$
	$m=\pm\frac{1}{2}$	κ^2	0	v
(4.1)	$w(\bar{j}-n;z)$	0	0	$-\bar{j}+n$
(5.1)	$u(\bar{j},\bar{v};\Lambda;z)$	0	0	$-\bar{j}$
		κ^2	0	$\bar{v}$

For the eigenvalues $v^{(i)}$ in the excited state i the regular solution with the exponent $\gamma_1=0$ centred at $z'=\kappa^2$ has an infinite radius of convergence. The same is true for the regular solution centred at $z'=0$ with the higher exponent (γ_1 (for $j>0$) or γ_2 (for $j<0$)). Both solutions are identical everywhere in the complex z plane and the component wavefunctions $\xi^j\Phi(z)$, $\xi^{j+1}f(z)$ are entire in ξ and η.

We now turn to the second non-adiabatic model, the Rabi system (Schweber 1967, Reik *et al* 1982, 1985, Kus 1985, Kus and Lewenstein 1986, Schmutz 1986) with the Hamiltonian

$$H=a^+a+\tfrac{1}{2}+(\tfrac{1}{2}+2\delta)\sigma_z+\sqrt{2}\kappa(a^++a)(\sigma_{(+)}+\sigma_{(-)}). \tag{2.23}$$

After the Bargmann mapping the Hamiltonian takes the form

$$H=\xi\,\mathrm{d}/\mathrm{d}\xi+\tfrac{1}{2}+(\tfrac{1}{2}+2\delta)\sigma_z+\sqrt{2}\kappa(\xi+\mathrm{d}/\mathrm{d}\xi)(\sigma_{(+)}+\sigma_{(-)}). \tag{2.24}$$

The eigenvalues λ are determined by the requirement that the up and down components of the wavefunctions

$$\Psi^{(m)}=(\xi/\sqrt{2})^{m+1/2}\Phi^{(m)}(\xi)|\uparrow\rangle+(\xi/\sqrt{2})^{-m+1/2}f^{(m)}(\xi)|\downarrow\rangle \tag{2.25}$$

($m=\pm\frac{1}{2}$) belong to the space of entire functions. We introduce a new independent variable $z=\frac{1}{2}\xi^2$, insert (2.24) and (2.25) in the Schrödinger equation and collect the spin up and down components. We then obtain the following system of differential equations:

$$z\,\mathrm{d}\Phi^{(m)}(z)/\mathrm{d}z-[\varepsilon-\delta-\tfrac{1}{2}(m+\tfrac{1}{2})]\Phi^{(m)}(z)$$
$$+\kappa\{[z^{-m+1/2}-\tfrac{1}{2}(m-\tfrac{1}{2})z^{-m-1/2}]f^{(m)}(z)$$
$$+z^{-m+1/2}\,\mathrm{d}f^{(m)}(z)/\mathrm{d}z\}=0 \qquad (2.26)$$

$$\kappa\{[z^{m+1/2}+\tfrac{1}{2}(m+\tfrac{1}{2})z^{m-1/2}]\Phi^{(m)}(z)+z^{m+1/2}\,\mathrm{d}\Phi^{(m)}(z)/\mathrm{d}z\}$$
$$+z\,\mathrm{d}f^{(m)}(z)/\mathrm{d}z-[\varepsilon+\delta+\tfrac{1}{2}(m+\tfrac{1}{2})]f^{(m)}(z)=0 \qquad (2.27)$$

$$\lambda=2\varepsilon+1=v+\tfrac{1}{2}-2\kappa^2. \qquad (2.28)$$

For $m=-\frac{1}{2}$ (2.26) and (2.27) are identical to (2.16) and (2.17) with $j=-\frac{1}{2}$, and for $m=\frac{1}{2}$ to equations (2.28*a*) and (2.29*a*) of Reik *et al* (1982). The properties of the solutions close to the regular singular points can be read off from table 1, lines 3 and 4.

The generalised $E\otimes\varepsilon$ Jahn–Teller system and the Rabi Hamiltonian can therefore be treated on the same footing provided one allows for positive and negative integer values of j as well as the value $j=-\frac{1}{2}$ in the system (2.16) and (2.17).

3. Neumann expansion of the component wavefunctions

In the following we restrict ourselves to $\bar{j}, j<0$ and define the functions

$$w(\bar{j}-n;\,z)=(\kappa^2 z)^{-(\bar{j}-n)/2}I_{-\bar{j}+n}(2\kappa z^{1/2})$$
$$=(\kappa^2 z)^{-(\bar{j}-n)}\sum_{k=0}^{\infty}\frac{(\kappa^2 z)^k}{\Gamma(k+1)\Gamma(-\bar{j}+n+k+1)} \qquad (3.1)$$

where $I_\nu(2\kappa z^{1/2})$ is a modified Bessel function.

We expand $\Phi(z), f(z)$ in Neumann series:

$$\Phi(z)=\kappa^{-2}\sum_{n=0}^{\infty}\frac{A_n}{n!\kappa^{4n}}\,w(j-n;\,z) \qquad (3.2)$$

$$f(z)=\kappa^{-1}\sum\frac{B_n}{n!\kappa^{4n}}\,w(j+1-n;\,z). \qquad (3.3)$$

Insertion of (3.2) and (3.3) in (2.16) and (2.17) gives the following recurrence relations for the expansion coefficients:

$$\begin{pmatrix}B_{n+1}\\A_{n+1}\end{pmatrix}=\begin{pmatrix}\bar{M}_{11}(n+1,n) & \bar{M}_{12}(n+1,n)\\ \bar{M}_{21}(n+1,n) & \bar{M}_{22}(n+1,n)\end{pmatrix}\begin{pmatrix}B_n\\A_n\end{pmatrix} \qquad (3.4)$$

where

$$\bar{M}_{11}(n+1,n)=-\kappa^2(-\tfrac{1}{2}j+\tfrac{1}{2}+\delta+\tfrac{1}{2}v) \qquad (3.5)$$

$$\bar{M}_{12}(n+1,n)=-\kappa^2(-\tfrac{1}{2}j+\tfrac{1}{2}+\delta+n-\tfrac{1}{2}v) \qquad (3.6)$$

$$\bar{M}_{21}(n+1,n)=(\kappa^2-\tfrac{1}{2}j+\tfrac{1}{2}+n-\tfrac{1}{2}v)(-\tfrac{1}{2}j+\tfrac{1}{2}+\delta+\tfrac{1}{2}v)-\kappa^2(n+1) \qquad (3.7)$$

$$\bar{M}_{22}(n+1,n)=(\kappa^2-\tfrac{1}{2}j+\tfrac{1}{2}+n-\tfrac{1}{2}v)(-\tfrac{1}{2}j+\tfrac{1}{2}+\delta+n-\tfrac{1}{2}v)-\kappa^2(n+1) \qquad (3.8)$$

and

$$\det\bar{M}(n+1,n)=-\kappa^4(n-v)(n+1). \qquad (3.9)$$

Equation (3.4) is supplemented by the initial condition

$$B_0=\kappa^2 \qquad A_0=-(\kappa^2-\tfrac{1}{2}j-\tfrac{1}{2}-\delta-\tfrac{1}{2}v). \tag{3.10}$$

The recurrence relation (3.4) can be solved using a continued fraction technique which determines the eigenvalues $v^{(i)}$ in the excited states i. The Neumann expansion (3.2) and (3.3) converges much more rapidly than the power series expansion for $\Phi(z), f(z)$ (Nusser 1983).

We now turn to the Juddian isolated exact solutions. Note that all matrix elements $\bar{M}_{ik}(n+1, n)$ as well as A_0 and B_0 are linear in κ^2. Therefore A_n and B_n are polynomials of degree $n+1$ in κ^2. However the sums A_n+B_n are polynomials of degree n in κ^2. Equations (3.4)-(3.9) show that for integer values $v=N$ the series terminate, i.e.

$$A_{N+1}=A_{N+2}=\ldots=B_{N+1}=B_{N+2}=\ldots=0 \tag{3.11}$$

provided

$$A_N+B_N=0. \tag{3.12}$$

Since A_N+B_N is a polynomial of Nth degree in κ^2, equation (3.12) has N roots $\kappa_1^2, \ldots, \kappa_N^2$. The positive roots are the physical values for the interaction constant for Juddian isolated exact solutions on baseline N.

4. The unphysical solution of (2.16) and (2.17)

The straightforward calculation shows that the Neumann series (3.2) and (3.3) are infinite except for the Juddian isolated exact solutions. The reason is that $z=\kappa^2$ is an ordinary point in the differential equation

$$\frac{\mathrm{d}^2 w(\bar{j}-n; z)}{\mathrm{d}z^2}+\frac{\bar{j}-n+1}{z}\frac{\mathrm{d}w(\bar{j}-n; z)}{\mathrm{d}z}-\frac{\kappa^2}{z}w(\bar{j}-n; z)=0 \qquad \bar{j}<0 \tag{4.1}$$

satisfied by the expansion functions (3.1), while $z=\kappa^2$ is a regular singular point in the system (2.19) and (2.20). This distinction is not important for integer values of v, hence the finite Neumann series for Juddian isolated exact solutions. These statements will now be proved.

Note that for non-integer $\bar{j}$ a second solution of (4.1) is given by

$$\begin{aligned}\tilde{w}(\bar{j}-n; z)&=(\kappa^2 z)^{-(\bar{j}-n)/2} I_{\bar{j}-n}(2\kappa z^{1/2})\\ &=\sum\frac{(\kappa^2 z)^k}{\Gamma(k+1)\Gamma(+\bar{j}-n+k+1)}.\end{aligned} \tag{4.2}$$

For negative integers $\bar{j}$ the right-hand sides of (3.1) and (4.2) become identical. In this case the second solution is defined by the limit

$$\tilde{w}(\bar{j}-n; z)=\lim_{\Delta\to 0}(\tilde{w}(\bar{j}+\Delta-n; z)-w(\bar{j}-\Delta-n; z))/2\Delta \tag{4.3}$$

where $\tilde{w}(\bar{j}+\Delta-n; z)$, $w(\bar{j}-\Delta-n; z)$ are given by (4.2) and (3.1) respectively. The solution (4.3) contains logarithmic terms.

The analytical structure (4.2) and (4.3) is due to the fact that $z=0$ is a regular singular point of (4.1) (see table 1). The point at infinity is an irregular singular point in (4.1).

For a given eigenvalue v we obtain a second solution of (2.16) and (2.17) by the expansion

$$\tilde{\Phi}(z) = \kappa^{-2} \sum_{n=0}^{\infty} \frac{A_n}{n!\,\kappa^{4n}} \tilde{w}(j-n;\, z) \tag{4.4}$$

$$\tilde{f}(z) = \kappa^{-1} \sum_{n=0}^{\infty} \frac{B_n}{n!\,\kappa^{4n}} \tilde{w}(j+1-n;\, z) \tag{4.5}$$

with $\tilde{w}(j-n;\, z)$ given by (4.2) or (4.3).

The coefficients A_n, B_n are the same as in (3.2) and (3.3). In order to see this, note that for the derivation of (3.4)-(3.10) the differential recurrence relations for $w(\bar{j}-n;\, z)$ have been used, e.g.

$$\mathrm{d}w(j-n;\, z)/\mathrm{d}z = \kappa^2 w(j+1-n;\, z) \tag{4.6}$$

which we obtained from those for the modified Bessel functions. The differential recurrence relations for $w(\bar{j}-n;\, z)$ are true for any solution of (4.1), including (4.2) and (4.3). Therefore (4.4) and (4.5) is a second solution of (2.16) and (2.17). We call $\Phi(z), f(z)$ ((3.2) and (3.3)) the physical solution and $\tilde{\Phi}(z), \tilde{f}(z)$ ((4.4) and (4.5)) the unphysical solution of (2.16) and (2.17).

Let us now look at the point $z = 0$ which is a regular singular point in (2.19) and (2.20) and in (4.1).

The exponents γ_1 for these equations are the same and the exponents γ_2 differ by integers n (see table 1). Therefore the physical solution and the unphysical solution and their expansion functions (3.1) and (4.2) and (4.3) have the same analytical structure in the vicinity of $z = 0$. It should therefore in principle be possible to represent the physical solution and the unphysical solution of (2.16) and (2.17) by finite expansions (3.2) and (3.3) and (4.4) and (4.5), as far as this singularity is concerned. Let us now turn to the second regular singular point $z = \kappa^2$ of (2.16) and (2.17) and assume first that the eigenvalue v is non-integer. Since the physical solution (3.2) and (3.3) and the unphysical solution (4.4) and (4.5) are linearly independent and since the physical solution is by construction regular at $z = \kappa^2$, the unphysical solution must be multivalued.

On the other hand, each of the expansion functions (4.2) and (4.3) is regular at $z = \kappa^2$ since this point is an ordinary point of the differential equation (4.1). In order to expand a multivalued function by a series of functions which are regular at the branch point, infinitely many terms are required. Therefore the expansions (4.4) and (4.5) of the unphysical solution *and hence* the expansions (3.2) and (3.3) of the physical solution are infinite.

Assume next an integer eigenvalue v. Then the unphysical solution is regular at $z = \kappa^2$ as are the expansion functions. Therefore the Neumann series representing the Juddian isolated exact solutions are finite.

5. Natural expansion functions

The analysis in the preceding section shows that the differential equations (2.19) and (2.20) and the differential equation (4.1) have two singular points in common: the regular singular point $z = 0$ and the irregular singular point at infinity. Furthermore, the analytical structure of both solution and expansion functions is the same in the vicinity of these singular points. Therefore the expansions (3.2) and (3.3) are rapidly converging.

The foregoing analysis also shows that natural expansion functions can be constructed which allow in principle for finite expansions of $\Phi(z), f(z)$. A necessary condition is that in the differential equation of the natural expansion functions $z=\kappa^2$ is a regular singular point with the exponents $\gamma_1=0$, $\gamma_2=v+m$ $(m=1,2,3,\ldots)$, while nothing is changed at the singular point $z=0$ and at the point at infinity. In this case the analytical structure of both solution and natural expansion functions is the same in the vicinity of *all* singular points of (2.19) and (2.20). There is only one second-order differential equation which satisfies this requirement:

$$\frac{d^2u(\bar{j},\bar{v};\Lambda;z)}{dz^2}+\left(\frac{\bar{j}+1}{z}+\frac{1-\bar{v}}{z-\kappa^2}\right)\frac{du(\bar{j},\bar{v};\Lambda;z)}{dz}+\left(-\frac{\kappa^2}{z}+\frac{\Lambda}{z(z-\kappa^2)}\right)u(\bar{j},\bar{v};\Lambda;z)=0 \tag{5.1}$$

(see table 1 for the exponents). In particular we have

$$u(\bar{j},1;0;z)=w(\bar{j}-n;z). \tag{5.2}$$

Equation (5.1) is one of the confluent forms of Heun's wave equation (Heun 1889, Erdelyi *et al* 1953). It has been treated by Lambe and Ward (1934). The transformed function $\Psi(\xi)=\xi^{\bar{j}+1/2}(1-\xi^2)^{-v/2}u(\kappa^2\xi^2)$, $\kappa^2\xi^2=z$ is a generalised spheroidal wavefunction (Leitner and Meixner 1960, Meixner *et al* 1980), which for $\bar{j}=-\frac{1}{2}$ (Rabi system) reduces to an ordinary spheroidal wavefunction. The reference to Heun's equation and to the generalised spheroidal wavefunctions indicates that the natural expansion functions are more involved than the familiar functions of mathematical physics. In Ince's (1956) classification (5.1) is derived from a differential equation with seven elementary singularities (exponent difference $\frac{1}{2}$) while (4.1) is obtained by the confluence of five elementary singularities.

Therefore the solution of (5.1) which is regular in the vicinity of $z=0$ (exponent $\gamma_2=-\bar{j}$) has a finite radius of convergence except for particular values of Λ, the eigenvalues of (5.1) which are transcendental functions of j, v, κ^2. We shall now find solutions $u(\bar{j},v;\Lambda_l;z)$ of (5.1) which are regular at $z=\kappa^2$ together with their eigenvalues Λ_l $(l=0,1,2,\ldots)$.

In order to do this we expand

$$u(\bar{j},\bar{v};\Lambda;z)=\sum\frac{C_n(\bar{j},\bar{v};\Lambda)}{n!\kappa^{4n}}w(\bar{j}-n;z) \tag{5.3}$$

and standardise the functions $u(\bar{j},\bar{v};\Lambda;z)$ by

$$C_0(\bar{j},\bar{v};\Lambda)=1. \tag{5.3a}$$

Insertion of (5.3) in (5.1) gives the recurrence relations

$$\begin{gathered}-C_{n+1}(\bar{j},\bar{v};\Lambda)+C_n(\bar{j},\bar{v};\Lambda)[(n-\bar{j})(n+1-\bar{v})+\Lambda]\\ +C_{n-1}(\bar{j},\bar{v};\Lambda)\kappa^4 n(n-\bar{v})=0 \qquad n=0,1,2,\ldots\end{gathered} \tag{5.4}$$

$$C_{-1}(\bar{j},\bar{v};\Lambda)=0.$$

We get a feeling for the eigenvalue spectrum by looking at the coefficients $C_n(\bar{j},\bar{v};\Lambda)$ in the limit $n\to\infty$. There are two types of limits. In the first type the second and third terms in (5.4) are of the same order of magnitude while the first is small. Therefore we have

$$\lim_{n\to\infty} C_n(\bar{j}, \bar{v}; \Lambda)/C_{n-1}(\bar{j}, \bar{v}; \Lambda) = -\kappa^4 \tag{5.5}$$

and the expansion (5.3) is regular at $z=\kappa^2$.

In the second type the first and second terms in (5.3) are of the same order of magnitude, while the last term is small. We obtain

$$\lim_{n\to\infty} C_{n+1}(\bar{j}, \bar{v}; \Lambda)/C_n(\bar{j}, \bar{v}; \Lambda) = n^2. \tag{5.6}$$

The limit (5.6) would lead to a non-analytic behaviour of the expansion (5.3) at $z=\kappa^2$, which must be suppressed by the choice of the eigenvalues. For $\kappa^2 \to 0$ one obtains the approximate eigenvalues

$$\Lambda_l^{(0)}(\bar{j}, \bar{v}) = -(l-\bar{j})(l+1-\bar{v}) \qquad (l=0,1,2,\ldots) \tag{5.7}$$

by which the onset of the unwanted limit behaviour is stopped in the lth recurrence relation (5.4).

Figure 1 shows the $\bar{v}$ dependence of the exact eigenvalue $\Lambda_l(\bar{j}, \bar{v})$ for $\bar{j} = -\frac{1}{2}, -5$ and $\kappa^2 = 1, 2, 3$. The curves are labelled from up to down with $\Lambda_0(\bar{j}, \bar{v})$ for the uppermost curve.

The exact eigenvalues $\Lambda_l(\bar{j}, \bar{v})$ and the expansion coefficients $C_n(\bar{j}, \bar{v}; \Lambda_l)$ are calculated by a standard continued fraction technique (Perron 1955, Wall 1973, Henrici 1977, Jones and Thron 1980, Risken 1984).

The recurrence relation is turned into the form

$$C_n(\bar{j}, \bar{v}; \Lambda)/C_{n-1}(\bar{j}, \bar{v}; \Lambda) = -\kappa^4 n(n-\bar{v})\bar{W}_n(\bar{j}, \bar{v}; \Lambda)/[(n-\bar{j})(n+1-\bar{v})+\Lambda] \tag{5.8}$$

where $\bar{W}_n(\bar{j}, \bar{v}; \Lambda)$ is a continued fraction given by

$$\bar{W}_n(\bar{j}, \bar{v}; \Lambda) = 1/(1+\bar{s}_n \bar{W}_{n+1}(\bar{j}, \bar{v}; \Lambda)) \tag{5.9}$$

$$\bar{s}_n = \kappa^4(n+1)(n+1-\bar{v})/[(n-\bar{j})(n+1-\bar{v})+\Lambda][(n+1-\bar{j})(n+2-\bar{v})+\Lambda] \tag{5.10}$$

$$\lim_{n\to\infty} \bar{W}_n(\bar{j}, \bar{v}; \Lambda) = 1. \tag{5.11}$$

From (5.11) and (5.8) $C_n(\bar{j}, \bar{v}; \Lambda)/C_{n-1}(\bar{j}, \bar{v}; \Lambda)$ tends to the limit (5.5). Therefore $u(j, v; \Lambda_l; z)$ is regular in the vicinity of $z=\kappa^2$.

We now show that the series (5.3) terminate for $v=N$. From (5.4) we have

$$C_1(\bar{j}, \bar{v}; \Lambda) = C_0(\bar{j}, \bar{v}; \Lambda)[-\bar{j}(1-\bar{v})+\Lambda] \tag{5.12}$$

$$C_2(\bar{j}, \bar{v}; \Lambda) = C_0(\bar{j}, \bar{v}; \Lambda)\{[-\bar{j}(1-\bar{v})+\Lambda][(1-\bar{j})(2-\bar{v})+\Lambda]+\kappa^4(1-\bar{v})\}. \tag{5.13}$$

From (5.9) and (5.10), $\bar{W}_2(\bar{j}, 1; \Lambda)$ is finite and $\bar{W}_1(\bar{j}, 1; \Lambda) = 1$. From (5.8) $C_n(j, 1; \Lambda) = 0$ $(n=1,2,\ldots)$. From (5.12) we have $\Lambda_0(\bar{j}, 1) = 0$. Furthermore, by (5.9) and (5.10) $\bar{W}_3(\bar{j}, 2; \Lambda)$ is finite and $\bar{W}_2(\bar{j}, 2; \Lambda) = 1$. By (5.8), $C_n(j, 2; \Lambda) = 0$, $(n=2,3,\ldots)$. From (5.13) we have $(\bar{j}+\Lambda)\Lambda - \kappa^4 = 0$. The roots of this equation are the two highest eigenvalues $\Lambda_0(\bar{j}, 2)$, $\Lambda_1(\bar{j}, 2)$. For $v=N$ we obtain $C_n(j, N; \Lambda) = 0$ $(n=N, N+1, \ldots)$ and equations of Nth degree in Λ, whose roots are the highest eigenvalues $\Lambda_0(\bar{j}, N)\ldots\Lambda_{N-1}(\bar{j}, N)$ (see figure 1 and the plots in Reik and Doucha (1986a, b)).

These results show that the isolated exact solutions can be expanded in a finite series of natural expansion functions.

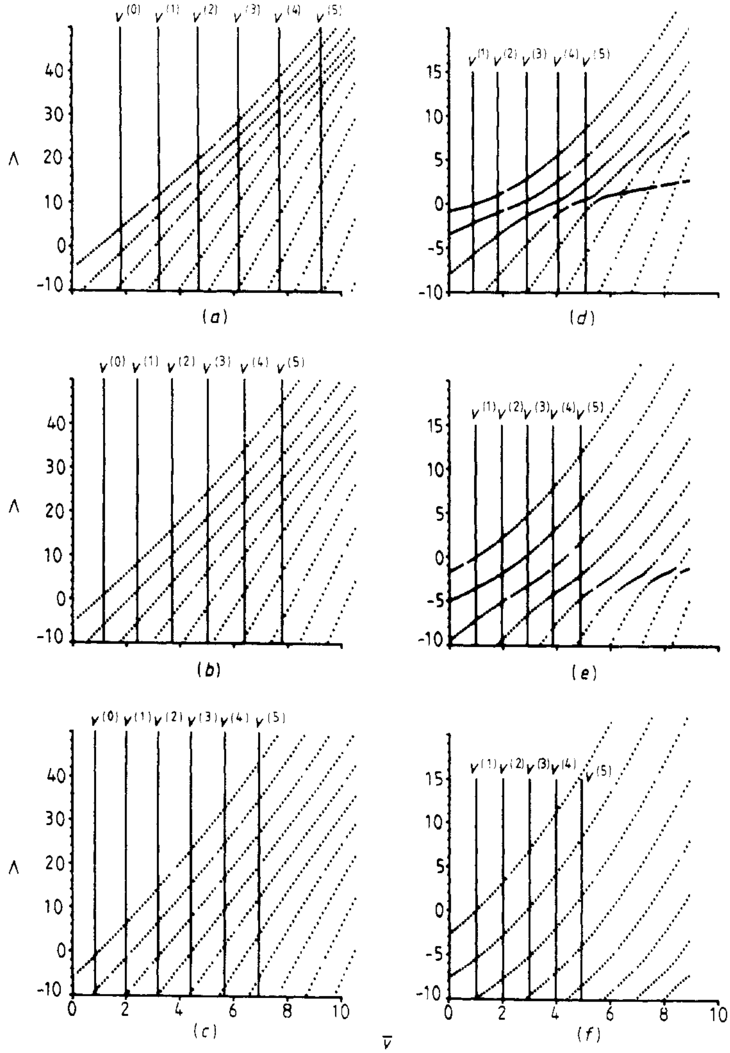

Figure 1. Eigenvalues $\Lambda(\bar{j}, \bar{v})$ of (5.1) against $\bar{v}$ and eigenvalues $v^{(i)}$ of the Hamiltonian. (a), (b), (c): $\bar{j} = -5$; (d), (e), (f): $\bar{j} = -\frac{1}{2}$; (a), (d): $\kappa^2 = 1$; (b), (e): $\kappa^2 = 2$; (c), (f): $\kappa^2 = 3$.

6. The conjecture

In the following we concentrate on $\Phi(z)$. We conjecture that in each eigenstate i $(i = 0, 1, 2, \ldots)$ of the Hamiltonian the function $\Phi(z)$ is a finite linear combination of eigenfunctions of (5.1):

$$\Phi(z)\kappa^2/A_0 = \bar{\Phi}(z) = \sum_{\{l\}} x_l^{(i)} u(j, v^{(i)}; \Lambda_l; z) + \sum_{\{l'\}} x_{l'}^{(i)} u(j, v^{(i)} + 1; \Lambda_{l'}; z)$$
$$+ \sum_{\{l''\}} x_{l''}^{(i)} u(j-1, v^{(i)}; \Lambda_{l''}; z). \tag{6.1}$$

The finite sets of integers $\{l\}\{l'\}\{l''\}$ in the eigenstate i label the eigenfunctions of (5.1) by labelling the eigenvalues $\Lambda_l(j, v^{(i)})$, $\Lambda_{l'}(j, v^{(i)} + 1)$, $\Lambda_{l''}(j-1, v^{(i)})$.

Equation (6.1) is obviously correct for all Juddian isolated exact solutions; we believe that it is also true in the general case.

We now look at the consequences of (6.1). We rewrite (3.2) as

$$\bar{\Phi}(z)=\sum_{n=0}^{\infty}\frac{\bar{A}_n^{(i)}}{n!\,\kappa^{4n}}\,w(j-n;z)\qquad \bar{A}_n=A_n/A_0. \tag{6.2}$$

In (6.1) we expand $u(j, v^{(i)}; \Lambda_l; z)$ by using (5.3). Comparison with (6.2) gives

$$\bar{A}_n^{(i)}=\sum_{\{l\}}x_l^{(i)}C_n(j,v^{(i)};\Lambda_l)+\sum_{\{l'\}}x_{l'}^{(i)}C_n(j,v^{(i)}+1;\Lambda_{l'})$$
$$+n\kappa^4\sum_{\{l''\}}x_{l''}^{(i)}C_{n-1}(j-1,v^{(i)};\Lambda_{l''}). \tag{6.3}$$

Equation (6.3) shows that the expansion coefficients $\bar{A}_n^{(i)}$ of the infinite expansions (6.2) are given in terms of $x_l^{(i)}$, $x_{l'}^{(i)}$, $x_{l''}^{(i)}$, i.e. by a finite number of coefficients.

We use (6.3) to calculate the coefficients $x_l^{(i)}$, $x_{l'}^{(i)}$, $x_{l''}^{(i)}$ and the eigenvalues $v^{(i)}$. In order to do this we need the recurrence relations for $\bar{A}_n^{(i)}$:

$$-\bar{A}_{n+1}^{(i)}+\bar{A}_n^{(i)}[(n-j)(n+1-v^{(i)})+R(j,v^{(i)};n)]$$
$$+\bar{A}_{n-1}^{(i)}\kappa^4 n(n-1-v^{(i)})(1+O(n))=0\qquad n=0,1,2,\ldots \tag{6.4}$$

$$R(j,v^{(i)};n)=j(1-v^{(i)})-\kappa^2(v^{(i)}+1)+(\tfrac{1}{2}v^{(i)}+\tfrac{1}{2}j-\tfrac{1}{2})^2-\delta^2$$
$$-\kappa^2(\tfrac{1}{2}v^{(i)}-\tfrac{1}{2}j+\tfrac{1}{2}+\delta)O(n) \tag{6.5}$$

$$O(n)=\frac{(\frac{1}{2}v^{(i)}+\frac{1}{2}j-\frac{1}{2}+\delta-\kappa^2-n)(\frac{1}{2}v^{(i)}-\frac{1}{2}j+\frac{1}{2}+\delta)+\kappa^2(n+1)}{(\frac{1}{2}v^{(i)}+\frac{1}{2}j-\frac{1}{2}+\delta-\kappa^2-n)(\frac{1}{2}v^{(i)}-\frac{1}{2}j+\frac{1}{2}+\delta)+\kappa^2 n}-1. \tag{6.6}$$

Equation (6.9) shows that $O(n)$ is only slightly n dependent and that

$$\lim_{n\to\infty}O(n)=0. \tag{6.7}$$

Therefore the n dependence of $R(j, v^{(i)}; n)$ is also slight. Equations (6.4)-(6.6) are obtained from (3.4) by eliminating B_n in favour of A_n and inserting the matrix elements $\bar{M}_{lk}(n+1, n)$ given by (3.5)-(3.8). The similarity of the recurrence relations (6.4) and (5.4) is obvious.

We insert (6.3) in (6.4) and take care of (5.4). On account of the similarity of (6.4) and (5.4) a lot of terms cancel and we obtain the following infinite system of equations for $x_l^{(i)}$, $x_{l'}^{(i)}$, $x_{l''}^{(i)}$:

$$\sum_{\{l\}}x_l^{(i)}\Gamma^{(l)}(j,v^{(i)};n)+\sum_{\{l'\}}x_{l'}^{(i)}\Gamma^{(l')}(j,v^{(i)};n)$$
$$+\sum_{\{l''\}}x_{l''}^{(i)}\Gamma^{(l'')}(j,v^{(i)};n)=0\qquad n=0,1,2,\ldots. \tag{6.8}$$

The coefficients $\Gamma^{(l)}(j, v^{(i)}; n)\ldots$ are given by

$$\Gamma^{(l)}(j,v^{(i)};n)=C_n(j,v^{(i)};\Lambda_l)[R(j,v^{(i)};n)-\Lambda_l(j,v^{(i)})]$$
$$+C_{n-1}(j,v^{(i)};\Lambda_l)\kappa^4 n[-1+(n-1-v^{(i)})O(n)] \tag{6.9}$$

$$\Gamma^{(l')}(j,v^{(i)};n)=C_n(j,v^{(i)}+1;\Lambda_{l'})[n-j+R(j,v^{(i)};n)-\Lambda_{l'}(j,v^{(i)}+1)]$$
$$+C_{n-1}(j,v^{(i)}+1;\Lambda_{l'})\kappa^4 n[(n-1-v^{(i)})O(n)]. \tag{6.10}$$

Equations (6.8)-(6.10) hold for $n = 0, 1, 2, \ldots$. For $\Gamma^{(l'')}(j, v^{(i)}; n)$ we have

$$\Gamma^{(l'')}(j, v^{(i)}; O) = -\kappa^4 \tag{6.11}$$

$$\begin{aligned} \Gamma^{(l'')}(j, v^{(i)}; n) = {} & C_{n-1}(j-1, v^{(i)}; \Lambda_{l''})\kappa^4 n[v^{(i)}(1 - j/n) + R(j, v^{(i)}; n) \\ & - \Lambda_{l''}(j-1, v^{(i)})(1 + 1/n)] \\ & + C_{n-2}(j-1, v^{(i)}; \Lambda_{l''})\kappa^8 n(n-1)[(n-1-v^{(i)})O(n) - (n-1-v^{(i)})/n] \\ & \qquad n = 1, 2, 3, \ldots . \end{aligned} \tag{6.12}$$

Equations (6.8)-(6.12) are exact, provided (6.1) is true.

In this section we have studied the consequences of the conjecture (6.1). In the next section we test the conjecture by looking at the numerical results.

7. Numerical tests and conclusion

We are unable to produce a proof of the existence of the finite expansion (6.1). In order to test the conjecture we therefore resort to an experimental method. We again concentrate on $\bar{\Phi}^{(i)}(z)$.

Firstly we compute the eigenvalues $v^{(i)}$ $(i = 0, 1, \ldots, 5)$ and the function $\bar{\Phi}^{(i)}(z)$ *numerically*, for the $E \otimes \varepsilon$ Jahn-Teller system, $j = -5$, and for the Rabi system in resonance ($\delta = 0, j = -\frac{1}{2}$). In both cases the calculations are done for $\kappa^2 = 1, 2, 3$, i.e. for intermediate coupling strengths. The accuracy is 14 digits for $v^{(i)}$ and 12 digits for the expansion coefficients. Tables 2 and 3 reproduce part of the numerical results, namely the eigenvalues $v^{(i)}$ and the expansion coefficients $\bar{A}_{30}^{(i)}$.

On the other hand we retrieve the numerical results analytically. We get an (almost?) perfect agreement by the following ansatz (6.1). The function $\bar{\Phi}^{(i)}(z)$ is a linear

Table 2. Eigenvalues $v^{(i)}$ and expansion coefficients for the $E \otimes \varepsilon$ Jahn-Teller system: $j = -5$; $\delta = -\frac{1}{4}$. Comparison of theory and numerical results.

κ^2	i	$v^{(i)}$	$\bar{A}_{30}/\kappa^{120}30!$
1	0	1.807 908 143 174 33	$0.661\,104\,470\,110 \times 10^{-41}$
	1	3.230 447 186 234 13	$-0.188\,019\,234\,776 \times 10^{-39}$
	2	4.691 814 839 406 83	$-0.753\,174\,918\,665 \times 10^{-38}$
	3	6.185 475 515 737 38	$0.520\,727\,692\,133 \times 10^{-36}$
	4	$7.705\,524\,947\,42\vert 2\,29$	$-0.334\,281\,394\vert\,113 \times 10^{-35}$
	5	$9.245\,284\,153\,134\vert\,07$	$0.174\,079\,154\,96\vert\,4 \times 10^{-34}$
2	0	1.155 700 586 767 41	$0.320\,258\,560\,758 \times 10^{-41}$
	1	2.410 473 848 595 95	$0.692\,297\,327\,712 \times 10^{-40}$
	2	3.703 255 956 915 27	$0.620\,229\,925\,625 \times 10^{-39}$
	3	5.031 377 988 860 47	$-0.919\,069\,547\,083 \times 10^{-39}$
	4	6.391 634 367 557 46	$-0.130\,148\,452\,183 \times 10^{-36}$
	5	7.780 716 338 148 78	$-0.236\,158\,659\,81\vert 5 \times 10^{-35}$
3	0	0.830 619 167 673 44	$-0.103\,567\,331\,204 \times 10^{-41}$
	1	1.992 351 939 048 10	$-0.497\,830\,387\,849 \times 10^{-42}$
	2	3.183 761 950 583 83	$0.928\,098\,320\,98\vert 0 \times 10^{-40}$
	3	4.405 489 647 509 39	$0.127\,884\,593\,549 \times 10^{-38}$
	4	5.657 087 439 413 53	$0.953\,445\,244\,318 \times 10^{-38}$
	5	$6.937\,322\,111\,700\,9\vert 6$	$0.186\,531\,019\,850 \times 10^{-37}$

Table 3. Eigenvalues $v^{(i)}$ and expansion coefficients for the Rabi Hamiltonian, resonance $\delta = 0$. Comparison of theory and numerical results.

κ^2	i	$v^{(i)}$	$\bar{A}_{30}/\kappa^{120}30!$
1	0	−0.046 542 813 266 11	$-0.919\,613\,114\,436 \times 10^{-36}$
	1	0.881 871 010 221 75	$0.623\,348\,836\,145 \times 10^{-35}$
	2	1.817 318 472 374 84	$-0.101\,693\,548\,038 \times 10^{-33}$
	3	2.895 658 140 333 02	$-0.622\,348\,803\,8357 \times 10^{-34}$
	4	4.065 153 260 607 55	$0.762\,337\,886\,782 \times 10^{-34}$
	5	5.088 533 004 140 9|7	$0.143\,057\,107\,756 \times 10^{-34}$
2	0	−0.016 933 609 795 5|2	$-0.558\,734\,025\,936 \times 10^{-36}$
	1	0.977 386 552 475 84	$-0.170\,842\,031\,858 \times 10^{-35}$
	2	1.956 870 464 881 66	$-0.291\,483\,569\,428 \times 10^{-35}$
	3	2.906 150 208 827 90	$0.199\,506\,216\,080 \times 10^{-34}$
	4	3.858 908 985 755 25	$-0.212\,694\,223\,405 \times 10^{-33}$
	5	4.887 788 230 923 86	$-0.142\,239\,940\,070 \times 10^{-33}$
3	0	−0.010 895 822 541 24	$-0.146\,529\,586\,5 \vert 24 \times 10^{-36}$
	1	0.987 870 665 601 40	$-0.507\,845\,919\,\vert 316 \times 10^{-36}$
	2	1.985 515 250 463 30	$-0.156\,442\,331\,56 \vert 8 \times 10^{-35}$
	3	2.978 772 227 312 16	$-0.395\,257\,464\,710 \times 10^{-35}$
	4	3.958 872 745 098 19	$-0.543\,222\,142\,165 \times 10^{-35}$
	5	4.918 117 909 470 29	$0.404\,136\,205\,817 \times 10^{-34}$

combination of $i+4$ natural expansion functions. The choice of the functions does not depend on j, δ and κ^2 and $\{l\} = 0, 1, \ldots, i+1, \{l'\} = i, \{l''\} = i$.

In order to calculate the $i+4$ coefficients $x_l^{(i)}, x_{l'}^{(i)}, x_{l''}^{(i)}$ of the natural expansion (6.1) we take the first $i+4$ equations of the system (6.8). We fix κ^2, δ and j and compute the eigenvalues $v^{(i)}$ by putting the determinant equal to zero. In tables 2 and 3 a vertical line is inserted after the last decimal place for which the results of this method agree with the results of the numerical method. We then solve the equations for the coefficients $x_l^{(i)}, x_{l'}^{(i)}, x_{l''}^{(i)}$ of the natural expansions. Finally we calculate the coefficients $\bar{A}_n^{(i)}$ of the Neumann expansion for $\bar{\Phi}^{(i)}(z)$. The values obtained by this method agree very well with the results of the numerical computation. For $n = 30$ this is shown in the last column of tables 2 and 3. The end of the agreement is indicated by a vertical line as before.

We did not trim our procedure of retrieving the eigenvalues and the expansion coefficients to the same degree of computational sophistication that is available for the numerical method. We attribute the remaining incomplete agreement in tables 2 and 3 to this fact.

In any case, the numerical correspondences which have been established for the ansatz (6.1) are far from being accidental. Of course, the expansion can still be infinite but then the convergence is fabulously fast. We therefore *believe* that the answer to the question raised in the title of this paper is in the affirmative. But this question can only be *settled* by a proof.

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