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1982 J. Phys. A: Math. Gen. 15 3491

(http://iopscience.iop.org/0305-4470/15/11/026)

J. Phys. A: Math. Gen. **15** (1982) 3491–3507. Printed in Great Britain

Exact solution of non-adiabatic model Hamiltonians in solid state physics and optics

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Received 20 May 1982

Abstract. Simple non-adiabatic model Hamiltonians are treated using the realisation of the vibrational modes on Bargmann's Hilbert space of analytic functions. In this formulation the Schrödinger equation is a system of linear first-order differential equations. The energy eigenvalues are selected by the requirement that the solutions belong to the space of entire functions. The solutions are given in terms of Neumann series; the recurrence relations for the expansion coefficients have a simple structure. Under particular conditions for the interaction constant they allow for terminating Neumann series (isolated exact solutions). In the general case the conditions for the eigenvalues are transcendental equations involving a continued fraction. The continued fraction can be approximated to any desired degree of accuracy in a rapidly convergent process based on Worpitzky's theorem and its relation to conformal mapping. The eigenvalues are calculated; a physical interpretation of the solutions which makes use of intuitive arguments is also given.

1. Introduction

Until recently even the simplest non-adiabatic systems have only been treated numerically and approximately. One example is the dynamical Jahn–Teller and pseudo Jahn–Teller effect in which vibrational modes interact with electronic levels. The best understood approximate treatments by Barentzen (1979), Barentzen *et al* (1981) and Schmutz (1980) are based on work by Judd (1977). In the numerical treatment (Longuet Higgins *et al* 1958, Thorson and Moffitt 1967, Grevsmühl 1981) the eigenfunctions are expanded in the occupation number basis. Recurrence relations between the expansion coefficients are provided by the Hamiltonian matrix, which is suitably truncated and whose determinant gives the eigenvalues. For an accurate determination of the first few eigenvalues a matrix of dimension $N > 100$ is used.

A second and even simpler example, an electron hopping between two sites and interacting with one vibrational mode, has been treated numerically by Schirmer (1980). The Hamiltonian of this system makes its appearance also in optics. Here it describes a two-level atom interacting with one linearly polarised radiation mode. In contradistinction to the solid state analogue, the interaction constant is much smaller in the

0305-4470/82/113491+17$02.00

optical case. This leads to drastic simplifications: The system can be treated in RWA, i.e. by discarding half of the interaction and keeping only the nearly resonant terms. The RWA Hamiltonian can be solved exactly (Jaynes and Cummings 1963, see also Louisell 1964, 1973, Allen and Eberly 1975, Sargent *et al* 1974). The Hilbert space decomposes in a series of doublets. The solution is realistic for small detuning and not too high light intensity, as long as neighbouring doublets do not intersect (Mollow 1982). The solution has been explicitly used by Stroud (1971), Cohen-Tannoudji (1977), Series (1977), Carmichael and Walls (1976) in the theory of resonance fluorescence and the AC Stark effect. (See also Cresser *et al* 1982.)

Important progress towards an exact solution of these simple non-adiabatic model systems has been made in the Jahn–Teller field. Thorson and Moffitt (1967) had already observed that for particular rational values of the interaction constant, rational energy eigenvalues either in the ground state or in an excited state emerged from their numerical calculations. This suggests a particularly simple structure of the solutions for the set of isolated interaction constants. In an important paper, Judd (1979) derived exact rational expressions for the isolated values of the interaction constant and with those determined the coefficients of the eigenfunction in the occupation number basis. Our own contribution started from here, because we wanted in the first place an easier and more systematic way to get at Judd's isolated exact solutions. (Anybody who has tried to repeat Judd's original calculation will appreciate this point.) We hoped that a better understanding of the isolated solutions would enable us to interpolate between the different isolated solutions in one branch and thereby to find the general solution. Our approach is as follows. We convert the recurrence relations into a system of differential equations whose solutions are required to belong to the space of entire functions. This determines the eigenvalues (Reik 1980). Instead of a power series expansion of the entire functions we use a Neumann series expansion (Reik *et al* 1981a). To determine the eigenvalues with Thorson and Moffitt's (1967) accuracy only very few terms in the Neumann expansion are needed (Reik *et al* 1981b). A proof of convergence has been given (Reik and Nusser 1981); the general exact solution of the Jahn–Teller case is therefore established. Judd's isolated exact solutions correspond to terminating Neumann series (Reik *et al* 1981a). Our approach must be considered as partly experimental, as far as the derivation of the system of differential equations goes. It has however been felt from the beginning that this was a vital step and not just a trick. In this paper we want to put our approach on a firm theoretical basis and at the same time to extend its applicability to other simple non-adiabatic systems.

In § 2 we consider two non-adiabatic model Hamiltonians. By the realisation of the phonons (photons) on Bargmann's Hilbert space of analytical functions (Bargmann 1961, 1962) we obtain a system of differential equations which allows us to treat the two model Hamiltonians on the same footing and which contains the Jahn–Teller differential equations as a special case. In § 3 the solutions are expanded in Neumann series and the recurrence relations for the expansion coefficients are given. The conditions for finite Neumann series contain Judd's conditions for the isolated exact solutions as special cases. In § 4 the eigenvalues are determined by a condition involving a continued fraction. The value of the continued fraction is given by one of the two fixed points of a sequence of Moebius transformations. It can be calculated to any desired degree of accuracy depending on the length of the sequence. In § 5 we discuss special cases and give a physical interpretation of the mathematical procedure.

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

In the following we consider oversimplified model Hamiltonians which, however, contain the essential features of the non-adiabatic interaction. One of these Hamiltonians

$$H = h\omega_0(a^+_{(+)}a_{(+)} + a^+_{(-)}a_{(-)}) + \tfrac{1}{2}h\Delta\sigma_z + hk[(a_{(+)} + a^+_{(-)})\sigma_{(+)} + (a_{(-)} + a^+_{(+)})\sigma_{(-)}] \tag{2.1}$$

describes the following systems.

(a) Two circularly polarised radiation modes (+) and (−) interacting with a two-level atom.

(b) Two electronic states in a one-dimensional system with crystal momentum k_1, k_2 interacting with two degenerate phonon modes (+) and (−) of crystal momentum $\pm(k_2 - k_1)$. This is a caricature of the Fröhlich polaron (Evrard 1972).

(c) If $k_1 = -k_2$ and k_1 is equal to the Fermi momentum, we have an interaction between two degenerate electronic states and two phonons (+) and (−), which is the simplest caricature of the Peierls problem (Peierls 1956, Schuster 1975, Keller 1977).

The angular (or crystal) momentum of the system (2.1)

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

is a constant of the motion. Its eigenfunctions for positive eigenvalues are given by

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

Here j is a positive integer, ϕ and f are operator functions of the product of the creation operators for both photons, $|0\rangle$ is the vacuum state for both photons. The eigenvalues of J are positive quantities

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

We write the Hamiltonian in dimensionless form

$$H/2h\omega_0 = \tfrac{1}{2}J + h_{(+)}, \tag{2.5}$$

$$h_{(+)} = a^+_{(-)}a_{(-)} + \delta\sigma_z + \kappa[(a_{(+)} + a^+_{(-)})\sigma_{(+)} + (a_{(-)} + a^+_{(+)})\sigma_{(-)}], \tag{2.6}$$

where

$$\delta = \frac{1}{4}\frac{\Delta - \omega_0}{\omega_0}, \qquad \kappa = \frac{k}{2\omega_0}, \tag{2.7}$$

and solve the Schrödinger equation

$$h_{(+)}|\psi\rangle_{j+1/2} = \varepsilon|\psi\rangle_{j+1/2}. \tag{2.8}$$

The eigenvalue λ of the original dimensionless Hamiltonian $H/h\omega_0$ is given by

$$\lambda = 2\varepsilon + j + \tfrac{3}{2}, \tag{2.9}$$

if the zero point energies of the two photon modes are taken into account.

In order to solve (2.7), we use Bargmann's Hilbert space of analytical functions (Bargmann 1961, 1962), i.e. we map the eigenstates of the number operators $a^{+k}_{(+)}a^{+l}_{(-)}|0\rangle$ onto the powers of two complex variables ξ and η

$$a^{+k}_{(+)}a^{+l}_{(-)}|0\rangle \to \xi^k\eta^l. \tag{2.10}$$

As a consequence we have

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

and

$$|\psi\rangle_{j+1/2} \to \xi^{j}\phi(z)|\uparrow\rangle + \xi^{j+1}f(z)|\downarrow\rangle \tag{2.12}$$

where

$$z = \xi \cdot \eta. \tag{2.13}$$

The Hamiltonian $h_{(+)}$ is given by

$$h_{(+)} = \eta\,\partial/\partial\eta + \delta\sigma_z + \kappa[(\partial/\partial\xi + \eta)\sigma_{(+)} + (\partial/\partial\eta + \xi)\sigma_{(-)}]. \tag{2.14}$$

Insertion of (2.12)–(2.14) in (2.8) leads after collecting the spin up and spin down components to two coupled differential equations for $\phi(z)$ and $f(z)$

$$z\,\mathrm{d}\phi(z)/\mathrm{d}z - (\varepsilon - \delta)\phi(z) + \kappa[z\,\mathrm{d}f(z)/\mathrm{d}z + (j + 1 + z)f(z)] = 0, \tag{2.15}$$

$$\kappa(\mathrm{d}\phi(z)/\mathrm{d}z + \phi(z)) + z\,\mathrm{d}f(z)/\mathrm{d}z - (\varepsilon + \delta)f(z) = 0. \tag{2.16}$$

The eigenvalues are selected by the requirement that $\phi(z)$ and $f(z)$ belong to the space of entire functions. The fact that the differential equations are ordinary in the single variable z reflects the parabosonic nature of the Hamiltonian (2.1) (Schmutz 1980).

Eigenfunctions of the Hamiltonian (2.1) with negative eigenvalues of the angular (or crystal) momentum are found in a similar way. Note that

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

are eigenfunctions of the angular momentum operator with negative eigenvalues

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

Next write

$$H/2h\omega_0 = -\tfrac{1}{2}J + h_{(-)}, \tag{2.5a}$$

$$h_{(-)} = a^{+}_{(+)}a_{(+)} + (\delta + \tfrac{1}{2})\sigma_z + \kappa[(a_{(+)} + a^{+}_{(-)})\sigma_{(+)} + (a_{(-)} + a^{+}_{(+)})\sigma_{(-)}], \tag{2.6a}$$

and use the Bargmann Hilbert space of analytical functions

$$|\psi\rangle_{-j-1/2} = \eta^{j+1}\chi(z)|\uparrow\rangle + \eta^{j}\Omega(z)|\downarrow\rangle, \tag{2.12a}$$

$$h_{(-)} = \xi\,\partial/\partial\xi + (\delta + \tfrac{1}{2})\sigma_z + \kappa[(\partial/\partial\xi + \eta)\sigma_{(+)} + (\partial/\partial\eta + \xi)\sigma_{(-)}]. \tag{2.14a}$$

The Schrödinger equation

$$h_{(-)}|\psi\rangle_{-j-1/2} = \varepsilon|\psi\rangle_{-j-1/2} \tag{2.8a}$$

then leads to the system of differential equations for $\chi(z)$ and $\Omega(z)$

$$z\,\mathrm{d}\Omega(z)/\mathrm{d}z - (\varepsilon + \delta + \tfrac{1}{2})\Omega(z) + \kappa[z\,\mathrm{d}\chi(z)/\mathrm{d}z + (j + 1 + z)\chi(z)] = 0, \tag{2.15a}$$

$$\kappa(\mathrm{d}\Omega(z)/\mathrm{d}z + \Omega(z)) + z\,\mathrm{d}\chi(z)/\mathrm{d}z - (\varepsilon - \delta - \tfrac{1}{2})\chi(z) = 0. \tag{2.16a}$$

These are the same equations as (2.15), (2.16) with δ replaced by $-\delta - \frac{1}{2}$. One has therefore to solve equations (2.15), (2.16) for δ and $-\delta - \frac{1}{2}$ in order to get all energy

eigenfunctions. Then

$$\Omega(z,\delta)=\phi(z,-\delta-\tfrac{1}{2}), \tag{2.17}$$

$$\chi(z,\delta)=f(z,-\delta-\tfrac{1}{2}). \tag{2.18}$$

For degenerate electronic levels $\Delta=0$, $\delta=-\frac{1}{4}$ and the energy eigenstates for positive and negative angular momentum are degenerate.

We now proceed to an apparently different Hamiltonian

$$h=H/\hbar\omega_0=b^+b+(\tfrac{1}{2}+2\delta)\sigma_z+\sqrt{2}\kappa(b+b^+)(\sigma_{(+)}+\sigma_{(-)}) \tag{2.19}$$

which describes the interaction of one linearly polarised radiation mode with a spin $\frac{1}{2}$ (or equivalently a two-level atom). There is an equivalent interpretation as the Hamiltonian of a small polaron with two lattice sites under the influence of a hopping term with the transfer integral $(\frac{1}{2}+2\delta)$ (Holstein 1959, Reik 1972, Schirmer 1980). We shall show that this Hamiltonian leads to a special case of equations (2.15), (2.16) with a fictitious value $j=-\frac{1}{2}$. This is the bosonic limit, which in the Jahn–Teller case has been treated by Judd (1977), Barentzen (1979), Barentzen *et al* (1981) and Schmutz (1980).

We use again the Bargmann space, i.e.

$$b^+\to\xi, \qquad b\to \mathrm{d}/\mathrm{d}\xi, \tag{2.20}$$

$$h=\xi\,\mathrm{d}/\mathrm{d}\xi+(\tfrac{1}{2}+2\delta)\sigma_z+\sqrt{2}\kappa(\xi+\mathrm{d}/\mathrm{d}\xi)(\sigma_{(+)}+\sigma_{(-)}) \tag{2.21}$$

and the following ansatz for the wavefunction

$$|\psi_1\rangle=\phi_1(\xi)|\uparrow\rangle+(1/\sqrt{2})\xi f_1(\xi)|\downarrow\rangle. \tag{2.22}$$

The Schrödinger equation

$$h|\psi_1\rangle=\lambda|\psi_1\rangle \tag{2.23}$$

leads after collecting spin up and spin down components to the system of coupled differential equations

$$\xi\frac{\mathrm{d}\phi_1(\xi)}{\mathrm{d}\xi}+(\tfrac{1}{2}+2\delta-\lambda)\phi_1(\xi)+\kappa\left((\xi^2+1)f_1(\xi)+\xi\frac{\mathrm{d}f_1(\xi)}{\mathrm{d}\xi}\right)=0, \tag{2.24}$$

$$\kappa\left(2\phi_1(\xi)+\frac{2}{\xi}\frac{\mathrm{d}\phi_1(\xi)}{\mathrm{d}\xi}\right)+\xi\frac{\mathrm{d}f_1(\xi)}{\mathrm{d}\xi}+(-\tfrac{1}{2}-2\delta-\lambda)f_1(\xi)=0, \tag{2.25}$$

which are different from (2.15), (2.16). One recovers a special case of equations (2.15), (2.16) by substituting

$$z=\tfrac{1}{2}\xi^2, \tag{2.26}$$

$$\lambda=2\varepsilon+\tfrac{1}{2}. \tag{2.27}$$

We then obtain

$$z\,\mathrm{d}\phi_1(z)/\mathrm{d}z-(\varepsilon-\delta)\phi_1(z)+\kappa[z\,\mathrm{d}f_1(z)/\mathrm{d}z+(\tfrac{1}{2}+z)f_1(z)]=0, \tag{2.28}$$

$$\kappa\,(\mathrm{d}\phi_1(z)/\mathrm{d}z+\phi_1(z))+z\,\mathrm{d}f_1(z)/\mathrm{d}z-(\varepsilon+\delta)f_1(z)=0. \tag{2.29}$$

It is seen that (2.15), (2.16) reduce to (2.28), (2.29) for $j=-\frac{1}{2}$. The ansatz (2.22) and therefore the solutions (2.28), (2.29) do however not exhaust the eigenfunctions of the Hamiltonian (2.21). This is seen by using a second ansatz

$$|\psi_2\rangle=(1/\sqrt{2})\xi\phi_2(\xi)|\uparrow\rangle+f_2(\xi)|\downarrow\rangle.$$

By the same analysis one finds instead of (2.28), (2.29)

$$z\,\mathrm{d}f_2(z)/\mathrm{d}z-(\varepsilon+\delta+\tfrac{1}{2})f_2(z)+\kappa[z\,\mathrm{d}\phi_2(z)/\mathrm{d}z+(\tfrac{1}{2}+z)\phi_2(z)]=0, \tag{2.28a}$$

$$\kappa(\mathrm{d}f_2(z)/\mathrm{d}z+f_2(z))+z\,\mathrm{d}\phi_2(z)/\mathrm{d}z-(\varepsilon-\delta-\tfrac{1}{2})\phi_2(z)=0 \tag{2.29a}$$

and

$$f_2(z,\delta)=\phi_1(z,-\delta-\tfrac{1}{2}),\qquad \phi_2(z,\delta)=f_1(z,-\delta-\tfrac{1}{2}). \tag{2.30}$$

Schweber (1967) treated the Hamiltonian (2.19) in the Bargmann Hilbert space. His system of differential equations is slightly different from (2.24), (2.25) because a different ansatz for the wavefunctions

$$\psi=(\xi)|\uparrow\rangle+f(\xi)|\downarrow\rangle$$

was used.

We have shown that all the eigenfunctions of the Hamiltonians (2.1) and (2.19) are solutions of the differential equations (2.15), (2.16). We now proceed to the solution of these equations.

3. Expansion of the solutions in Neumann series. Elementary solutions

Equations (2.15), (2.16) for the special value $\delta=-\frac{1}{4}$ were first obtained in the context of an apparently different problem: the solution of the Longuet Higgins (Longuet Higgins *et al* 1958) and Thorson and Moffitt (1967) recurrence relation for the dynamical Jahn–Teller effect in simple systems (Reik 1980, Reik *et al* 1981b, Reik and Nusser 1981). Here we give the solution of (2.15), (2.16) for arbitrary values of δ, using a procedure (Reik *et al* 1981a) which remains applicable in the general case: the solutions $\phi(z)$ and $f(z)$ are represented by a Neumann series expansion, instead of a power series expansion,

$$\phi(z)=\frac{C}{\kappa^2}\sum_n\frac{\alpha_n}{n!\kappa^{4n}}(\kappa^2z)^{(n-j)/2}I_{n+j}(2\kappa z^{1/2}), \tag{3.1}$$

$$f(z)=\frac{C}{\kappa}\sum_n\frac{\beta_n}{n!\kappa^{4n}}(\kappa^2z)^{(n-j-1)/2}I_{n+j+1}(2\kappa z^{1/2}), \tag{3.2}$$

where C is a normalisation constant. If furthermore ε in (2.15), (2.16) is eliminated in favour of v,

$$\varepsilon=v/2-j/2-\tfrac{1}{2}-\kappa^2 \tag{3.3}$$

whose importance will become clear very shortly, then the coefficients α_n and β_n of the series expansion (3.1), (3.2) are given by the recurrence relations

$$\begin{pmatrix}\alpha_{n+1}\\ \beta_{n+1}\end{pmatrix}=\begin{pmatrix}M_{11}(n+1,n) & M_{12}(n+1,n)\\ M_{21}(n+1,n) & M_{22}(n+1,n)\end{pmatrix}\begin{pmatrix}\alpha_n\\ \beta_n\end{pmatrix} \tag{3.4}$$

where

$$M_{11}(n+1,n)=-\kappa^2(j/2+\tfrac{1}{2}-\delta+v/2), \tag{3.5}$$

$$M_{12}(n+1,n)=-\kappa^2(j/2+\tfrac{1}{2}-\delta+n-v/2), \tag{3.6}$$

$$M_{21}(n+1,n)=(\kappa^2+j/2+\tfrac{3}{2}+\delta+n-v/2)(j/2+\tfrac{1}{2}-\delta+v/2)-\kappa^2(n+1), \tag{3.7}$$

$$M_{22}(n+1,n)=(\kappa^2+j/2+\tfrac{3}{2}+\delta+n-v/2)(j/2+\tfrac{1}{2}-\delta+n-v/2)-\kappa^2(n+1). \tag{3.8}$$

From (3.5)–(3.8) one derives the expressions for the trace and the determinant of the matrix $M(n+1,n)$

$$\operatorname{Tr} M(n+1,n)=(j/2+\tfrac{3}{2}+\delta+n-v/2)(j/2+\tfrac{1}{2}-\delta+n-v/2)-\kappa^2(v+1), \tag{3.9}$$

$$\operatorname{Det} M(n+1,n)=-\kappa^4(n-v)(n+1). \tag{3.10}$$

Equation (3.4) is supplemented by the condition

$$\alpha_0=\kappa^2, \qquad \beta_0=-(\kappa^2+j/2+\tfrac{1}{2}+\delta-v/2), \tag{3.11}$$

which guarantees the regularity of $\phi(z)$, $f(z)$ at the singular point $z=0$ of the differential equations (2.15), (2.16). From (3.4)–(3.8) one finds that α_m, β_m are entire functions of κ^2 and v with j and δ as parameters; in particular $\alpha_m+\beta_m$ is a polynomial of degree m in κ^2 and of degree $2m+1$ in v. Thus for each pair of values κ^2, v one obtains a solution $\phi(z), f(z)$ of equations (2.15), (2.16). By (3.11) these solutions are regular at the origin, but in general they do not belong to the space of entire functions. (In particular, there is branching of the solutions at the singular point $z=\kappa^2$ of (2.15), (2.16).) In order to pick out the entire functions, a further implicit relation between κ^2 and v (containing j and δ as parameters)

$$\psi(\kappa^2, v; j, \delta)=0 \tag{3.12}$$

is needed, which determines v and therefore ε and λ uniquely in each state i

$$v_i=\chi_i(\kappa^2; j, \delta), \qquad i=0,1,2,\ldots,$$
$$\varepsilon_i(\kappa^2; j, \delta)=\tfrac{1}{2}\chi_i(\kappa^2; j, \delta)-j/2-\kappa^2-\tfrac{1}{2}. \tag{3.13}$$

Because there is an infinity of branches in (3.13) equation (3.12) is in general a transcendental equation. We shall derive this equation in the next section. In this section we show that (3.12) can become an algebraic equation for integer values of $v=m$ $(m=0,1,2,\ldots)$. The loci for $v=m$ in a plot of λ against κ^2 are a series of straight lines (see equations (2.9), (3.3) and the figures) which we call baselines in accordance with the notation in the theory of the dynamical Jahn–Teller effect. We therefore state that part of the eigenvalues on the baselines are determined by algebraic equations. In order to see this, note that terminating Neumann series are entire functions. For $v=m$, $\operatorname{Det} M(m+1,m)=0$. Equation (3.4) therefore allows for terminating Neumann series

$$\alpha_{m+k}=0, \qquad \beta_{m+k}=0, \qquad k=1,2,\ldots$$

provided that

$$\alpha_m+\beta_m=\psi(\kappa^2, m; j, \delta)=0. \tag{3.14}$$

But $\psi(\kappa^2, m; j, \delta)$ is a polynomial of mth degree in κ^2. Therefore (3.14) is an algebraic equation with m values of κ^2 as solutions. Those roots κ^2, which are real and positive, determine by (2.9), (3.3) eigenvalues of the Hamiltonian. The other roots are unphysical. Insertion of the l physical roots $(l\leqslant m)$ in the expressions (3.4)–(3.8) for α_n, β_n $(n\leqslant m)$ determines l eigenfunctions of the Schrödinger equation (2.15), (2.16). It should be noted that, while the Neumann series terminate, the power series for $\phi(z)$, $f(z)$ do not terminate under these conditions. This observation demonstrates the convenience of the expansion in Neumann series. The conditions for terminating

Neumann series on the baselines $v = 1$ and $v = 2$ are reproduced here:

$$\psi(\kappa^2, v=1; j, \delta) = \kappa^2(j+1+2\delta) - (j/2+1+\delta)(j/2-\delta)(j/2+\delta), \tag{3.15}$$

$$\begin{aligned}\psi(\kappa^2, v=2; j, \delta) &= -8\kappa^4(j/2+\tfrac{1}{2}+\delta) + \kappa^2\{(j/2-\tfrac{1}{2}-\delta)(j/2-\tfrac{1}{2}+\delta)(3j/2+\tfrac{5}{2}+3\delta) \\ &\quad + (j/2+\tfrac{3}{2}+\delta)(j/2+\tfrac{1}{2}-\delta)(3j/2+\tfrac{1}{2}+3\delta)\} \\ &\quad - (j/2+\tfrac{3}{2}+\delta)(j/2+\tfrac{1}{2}-\delta)(j/2+\tfrac{1}{2}+\delta) \\ &\quad \times (j/2-\tfrac{1}{2}-\delta)(j/2-\tfrac{1}{2}+\delta).\end{aligned} \tag{3.16}$$

Equations (3.15), (3.16) for $\delta = -\frac{1}{4}$ were first given by Judd (1979) using a different method.

For $j = -\frac{1}{2}$ one has

$$\psi(\kappa^2, v=m; j=-\tfrac{1}{2}, \delta) = -\psi(\kappa^2, v=m; j=-\tfrac{1}{2}, -\delta-\tfrac{1}{2}) \tag{3.17}$$

(see equations (3.15), (3.16) as example). Therefore by (2.28) the branches $\lambda_i(\kappa^2, j = -\frac{1}{2}, \delta)$ intersect the baselines, producing accidental double degeneracy at the intersections (see figures 1–3). Furthermore, for $\delta = -\frac{1}{4}$

$$\psi(\kappa^2, v=m; j=-\tfrac{1}{2}, \delta=-\tfrac{1}{4}) = 0, \tag{3.18}$$

i.e. *all* energy levels are on baselines: one has the energy level scheme of a displaced harmonic oscillator. This was first observed by Judd (1977) by inspection of the Longuet Higgins recurrence relations. Schmutz (1980) gave a very elegant explanation: he showed that the Longuet Higgins recurrence relation corresponds to a Hamiltonian of a displaced paraboson oscillator (Mukunda *et al* 1980, Sharma *et al* 1981), whose irreducible representations can be labelled by j, and where $j = -\frac{1}{2}$ is the bosonic case. Judd's observation has been used by Barentzen (1979; Barentzen *et al* 1981) in a perturbative treatment of the dynamical Jahn–Teller effect with $j + \frac{1}{2}$ as the expansion parameter.

Apart from these solutions there exist simple solutions for the ground state for $j \neq -\frac{1}{2}$. Take $v = 0$. Then the condition for terminating Neumann series

$$\alpha_0 + \beta_0 = -(j/2+\tfrac{1}{2}+\delta) = 0 \tag{3.19}$$

is independent of the coupling strength. We therefore get $\phi(z)$ and $f(z)$ as just one modified Bessel function for *all* energies on the baseline $v = 0$ provided j and δ satisfy equation (3.19). Having dealt with simple cases and algebraic equations for the eigenvalues, we proceed in the next section to the determination of the eigenvalues in the general case.

4. The eigenvalues

The recurrence relations (3.4) determine α_n, β_n for given α_{n-1}, β_{n-1}, i.e. higher expansion coefficients are calculated from below, starting with α_0, β_0 from equation (3.11). Define

$$w_n = \beta_n/\alpha_n, \tag{4.1}$$

$$W_n^{(1)} = (w_n + M_{11}(n+1,n)/M_{12}(n+1,n))M_{12}^2(n+1,n)$$
$$\times\{(M_{22}(n+1,n)/M_{12}(n+1,n)+M_{11}(n+2,n+1)/M_{12}(n+2,n+1))\}$$
$$\times(\mathrm{Det}\,M(n+1,n))^{-1}, \tag{4.2}$$

and insert the expressions for α_n, β_n. Thus $W_n^{(1)}$ calculated from below is a rational function of κ^2, v with j, δ as parameters.

On the other hand we might as well solve (3.4) for α_n, β_n in terms of $\alpha_{n+1}, \beta_{n+1}$, i.e. determine α_n, β_n from above. This gives a second relation for w_n and $W_n^{(1)}$

$$w_n = \frac{-M_{11}(n+1,n)w_{n+1}+M_{21}(n+1,n)}{M_{12}(n+1,n)w_{n+1}-M_{22}(n+1,n)} = -\frac{M_{11}(n+1,n)}{M_{12}(n+1,n)}$$
$$+\frac{\mathrm{Det}\,M(n+1,n)}{M_{12}(n+1,n)(M_{22}(n+1,n)-M_{12}(n+1,n)w_{n+1})}, \tag{4.3}$$

$$W_n^{(1)} = (1+a_n^{(1)}W_{n+1}^{(1)})^{-1}, \tag{4.4}$$

$$a_n^{(1)} = (-\mathrm{Det}\,M(n+2,n+1))[M_{12}^2(n+2,n+1)(M_{22}(n+1,n)/M_{12}(n+1,n)$$
$$+M_{11}(n+2,n+1)/M_{12}(n+2,n+1))$$
$$\times(M_{22}(n+2,n+1)/M_{12}(n+2,n+1)$$
$$+M_{11}(n+3,n+2)/M_{12}(n+3,n+2))]^{-1}. \tag{4.5}$$

The right-hand side of (4.4) can be turned into a continued fraction

$$W_n^{(1)} = \frac{1|}{|1}+\frac{a_n^{(1)}|}{|1}+\frac{a_{n+1}^{(1)}|}{|1}+\frac{a_{n+2}^{(1)}|}{|1}+\ldots \tag{4.6}$$

which is in general a transcendental function of the variables κ^2, v and the parameters j, δ and gives $W_n^{(1)}$ from above.

To determine the energy eigenvalues, fix the parameters j, δ and the interaction constant κ^2. Then equate the rational and the transcendental function of v, which determine $W_n^{(1)}$ from below and above. We interpret (4.6) as this equation with the rational function (4.2) on the LHS. The infinitely many roots of v from (4.6) give by (3.3) the energy eigenvalues ε. The value of n in (4.6) is immaterial; one could in fact start from $n = 0$ as is often done in the mathematical literature (Ince 1928, Strutt 1932, Erdelyi *et al* 1955). We determine n for computational convenience.

In order to do this, consider $a_n^{(1)}$ as a function of v for fixed values of κ^2, j, δ. Note that by (4.5), (3.5)–(3.8), (3.10)

$$\lim_{n\to\infty} a_n^{(1)} \approx n^{-2}. \tag{4.7}$$

Therefore, for v given, there is a lower bound $\bar{N}$ for the integers n defined by the following conditions

$$\bar{N} \geqslant v, \tag{4.8}$$

$$|a_n^{(1)}| \leqslant \tfrac{1}{4}, \qquad n \geqslant \bar{N}. \tag{4.9}$$

Equations (4.7)–(4.9) are illustrated in table 1; the values of $a_n^{(1)}$ are presented for three different sets of data which correspond to solutions. The integer $\bar{N}$ is also given for the three cases.

Table 1. The coefficients $a_n^{(1)}$.

	$\kappa^2 = 1$ $v = 1.569\,91$ $j = 1, \delta = 0$ $\bar{N} = 2$	$\kappa^2 = 1.55$ $v = 3.293\,04$ $j = -0.5, \delta = -1.5$ $\bar{N} = 5$	$\kappa^2 = 1.55$ $v = 0.988\,85$ $j = -0.5, \delta = -1.5$ $\bar{N} = 4$
n	$a_n^{(1)}$	$a_n^{(1)}$	$a_n^{(1)}$
0	$2.591\,146 \times 10^{-1}$	$-9.665\,076 \times 10^{-2}$	$8.381\,280 \times 10^{-3}$
1	$1.494\,599 \times 10^{-1}$	$-2.006\,342 \times 10^{-1}$	$-1.927\,225 \times 10^{0}$
2	$6.766\,662 \times 10^{-2}$	$-2.068\,532 \times 10^{-1}$	$1.130\,302 \times 10^{0}$
3	$4.113\,599 \times 10^{-2}$	$-1.096\,550 \times 10^{0}$	$2.797\,979 \times 10^{-1}$
4	$2.794\,863 \times 10^{-2}$	$6.544\,513 \times 10^{-1}$	$1.386\,903 \times 10^{-1}$
5	$2.031\,201 \times 10^{-2}$	$1.980\,296 \times 10^{-1}$	$8.528\,809 \times 10^{-2}$
6	$1.546\,167 \times 10^{-2}$	$1.057\,820 \times 10^{-1}$	$5.849\,654 \times 10^{-2}$
7	$1.217\,789 \times 10^{-2}$	$6.798\,694 \times 10^{-2}$	$4.289\,888 \times 10^{-2}$
8	$9.847\,036 \times 10^{-3}$	$4.806\,234 \times 10^{-2}$	$3.293\,061 \times 10^{-2}$
9	$8.130\,795 \times 10^{-3}$	$3.604\,610 \times 10^{-2}$	$2.613\,626 \times 10^{-2}$
10	$6.829\,487 \times 10^{-3}$	$2.815\,751 \times 10^{-2}$	$2.128\,047 \times 10^{-2}$

Conversely, choose an integer N and require

$$|a_n| \leqslant \tfrac{1}{4}, \qquad n \geqslant N. \tag{4.10}$$

Then equation (4.5) gives an upper bound for v

$$v \leqslant V(N; \kappa^2, j, \delta). \tag{4.11a}$$

We adopt this second point of view, i.e. we choose N and restrict v by (4.11a), or, if $N \leqslant V(N; \kappa^2, j, \delta)$, by

$$v \leqslant N. \tag{4.11b}$$

Then by Worpitzky's theorem (Wall 1948, Henrici 1977) the continued fraction $W_N^{(1)}$ equation (4.6) is uniformly convergent and its value and the values of all its approximants are inside the circular domain

$$|W_N^{(1)} - 4/3| \leqslant \tfrac{2}{3} \tag{4.12a}$$

in the complex $W_N^{(1)}$ plane. This is true for complex values of $a_n^{(1)}$. As in our case the $a_n^{(1)}$ are real, the continued fraction is real and its value is located on the real diameter of the Worpitzky circle

$$\tfrac{2}{3} \leqslant W_N^{(1)} \leqslant 2. \tag{4.12b}$$

The continued fraction $W_N^{(1)}$ is therefore bounded from above and below and is a smooth function of v. In order to calculate this function, i.e. the actual location of the continued fraction with a given accuracy, write equation (4.6) for $n = N$ in the following way:

$$W_N^{(1)} = (1 + a_N^{(1)} W_{N+1}^{(1)})^{-1}, \qquad W_{N+1}^{(1)} = (1 + a_{N+1}^{(1)} W_{N+2}^{(1)})^{-1}, \tag{4.13}$$

$$W_{N+m-1}^{(1)} = (1 + a_{N+m-1}^{(1)} W_{N+m}^{(1)})^{-1},$$

$$W_{N+m}^{(1)} = \frac{1|}{|1} + \frac{a_{N+m}^{(1)}|}{|1} + \frac{a_{N+m+1}^{(1)}|}{|1} + \ldots. \tag{4.14}$$

Then, as before, the continued fraction (4.14) lies in a circular domain in the complex $W^{(1)}_{N+m}$ plane with the radius $R_{N+m} = \frac{2}{3}$ whose centre is at $W^{(1)}_{0,N+m} = \frac{4}{3}$. (We disregard the additional information that $a^{(1)}_{N+m} \ldots a^{(1)}_{N+m+1} \ldots$ are real.) We interpret (4.13) as consecutive Moebius transformations which map this circle into circles in the complex $W^{(1)}_{N+m-1}$, $W^{(1)}_{N+m-2}$, $W^{(1)}_{N+1}$, $W^{(1)}_N$ planes.

The transformation formulae

$$W^{(1)}_{0,n} = (1 + a^{(1)}_n {}^* W^{(1)}_{0,n+1})/C(n), \qquad R_n = (R_{n+1}|a^{(1)}_n|)/|C(n)|,$$
$$C(n) = 1 + a^{(1)}_n W^{(1)}_{0,n+1} + a^{(1)}_n {}^* W^*_{0,n+1} + (W^{(1)}_{0,n+1} W^{(1)*}_{0,n+1} - R^2_{n+1}) a^{(1)}_n {}^* a^{(1)}_n, \tag{4.15}$$

show that on account of (4.10) all consecutive circles lie inside the first and

$$R_N < R_{N+1} < R_{N+2} < R_{N+m} = \tfrac{2}{3} \tag{4.16}$$

(of course the centres of all circles are on the real axis). How this works in practice is shown in table 2 for $N = 5$. The set of data is the same as in table 1 and the values of $a^{(1)}_n$ from table 1 have been used to calculate table 2. The number of steps for the calculation of $W^{(1)}_5$ has been determined by the requirement $R_5 \leqslant 10^{-6}$. Suppose that R_N, equation (4.16), is smaller than the required accuracy. Then each point on the real diameter of the transformed circle is equally acceptable. A particular value is obtained by a particular assignment of real values to a_{N+m+i} $(i = 0, 1, 2, \ldots)$ consistent with (4.10). This introduces a certain arbitrariness, which, under the conditions of Worpitzky's theorem, has no numerical consequences. One possible choice is the replacement of the true continued fraction by a periodic continued fraction whose first m partial numerators $a^{(1)}_N \ldots a^{(1)}_{N+m-1}$ are given by (4.5). The approximate value of the continued fraction is then equal to the fixed point of the Moebius transformation from $W^{(1)}_{N+m}$ to $W^{(1)}_N$ which lies inside the Worpitzky circle.

The elimination of $W^{(1)}_{N+m-1} \ldots W^{(1)}_{N+1}$ will now be carried out in one step. Define the iterated matrix

$$\begin{pmatrix} M_{11}(n+m,n) & M_{12}(n+m,n) \\ M_{21}(n+m,n) & M_{22}(n+m,n) \end{pmatrix}$$
$$= \begin{pmatrix} M_{11}(n+m,n+m-1) & M_{12}(n+m,n+m-1) \\ M_{21}(n+m,n+m-1) & M_{22}(n+m,n+m-1) \end{pmatrix} \times \ldots$$
$$\times \begin{pmatrix} M_{11}(n+1,n) & M_{12}(n+1,n) \\ M_{21}(n+1,n) & M_{22}(n+1,n) \end{pmatrix} \tag{4.17}$$

which describes recurrence relations with a step m

$$\begin{pmatrix} \alpha_{n+m} \\ \beta_{n+m} \end{pmatrix} = \begin{pmatrix} M_{11}(n+m,n) & M_{12}(n+m,n) \\ M_{12}(n+m) & M_{22}(n+m,n) \end{pmatrix} \begin{pmatrix} \alpha_n \\ \beta_n \end{pmatrix} \tag{4.18}$$

and

$$W^{(m)}_N = (w_N + M_{11}(N+m,N)/M_{12}(N+m,N)) M^2_{12}(N+m,N)$$
$$\times (M_{22}(N+m,N)/M_{12}(N+m,N)$$
$$+ M_{11}(N+2m,N+m)/M_{12}(N+2m,N+m))$$
$$\times (\mathrm{Det}\, M(N+m,N))^{-1}. \tag{4.19}$$

Insert the expressions for α_N, β_N from (3.4). This gives $W^{(m)}_N$ as a rational function

Table 2. Calculation of $W_5^{(1)}$ by consecutive Moebius transforms.

	$\kappa^2 = 1$ $v = 1.569\ 11$ $j = 1, \delta = 0$		$\kappa^2 = 1.55$ $v = 3.293\ 04$ $j = -0.5, \delta = -1.5$		$\kappa^2 = 1.55$ $v = 0.988\ 85$ $j = -0.5, \delta = -1.5$	
n	$W_{0,n}^{(1)}$	R_n	$W_{0,n}^{(1)}$	R_n	$W_{0,n}^{(1)}$	R_n
10			$\frac{4}{3}$	$\frac{2}{3}$	$\frac{4}{3}$	$\frac{2}{3}$
9	$\frac{4}{3}$	$\frac{2}{3}$	$9.546\ 44 \times 10^{-1}$	$2.188\ 87 \times 10^{-2}$	$9.665\ 99 \times 10^{-1}$	$1.627\ 50 \times 10^{-2}$
8	$9.870\ 82 \times 10^{-1}$	$6.395\ 91 \times 10^{-3}$	$9.561\ 31 \times 10^{-1}$	$9.617\ 44 \times 10^{-4}$	$9.691\ 51 \times 10^{-1}$	$5.033\ 89 \times 10^{-4}$
7	$9.881\ 22 \times 10^{-1}$	$7.604\ 93 \times 10^{-5}$	$9.389\ 63 \times 10^{-1}$	$5.764\ 77 \times 10^{-5}$	$9.600\ 84 \times 10^{-1}$	$1.990\ 52 \times 10^{-5}$
6	$9.849\ 51 \times 10^{-1}$	$1.140\ 72 \times 10^{-6}$	$9.096\ 48 \times 10^{-1}$	$5.045\ 93 \times 10^{-6}$	$9.468\ 24 \times 10^{-1}$	$1.043\ 84 \times 10^{-6}$
5	$9.803\ 86 \times 10^{-1}$	$2.227\ 03 \times 10^{-8}$	$8.473\ 58 \times 10^{-1}$	$7.174\ 74 \times 10^{-7}$	$9.252\ 80 \times 10^{-1}$	$7.662\ 01 \times 10^{-8}$

of the variable v with κ^2, j, δ as parameters. On the other hand we express the continued fraction $W_N^{(m)}$ by the fixed point of the Moebius formation

$$W_N^{(m)} = (1 + a_N^{(m)} W_{N+m}^{(m)})^{-1} \tag{4.20}$$

which lies inside the Worpitzky circle. This fixed point is given by

$$W_N^{(m)} = -(2a_N^{(m)})^{-1}[1 - (1 + 4a_N^{(m)})^{1/2}] \tag{4.21}$$

where

$$\begin{aligned} a_N^{(m)} = &-\mathrm{Det}\, M(N+2m, N+m) \\ &\times [M_{12}^2(N+2m, N+m)(M_{22}(N+m, N)/M_{12}(N+m, N) \\ &+ M_{11}(N+2m, N+m)/M_{12}(N+2m, N+m)) \\ &\times (M_{22}(N+2m, N+m)/M_{12}(N+2m, N+m) \\ &+ M_{11}(N+3m, N+2m)/M_{12}(N+3m, N+2m)]^{-1}. \end{aligned} \tag{4.22}$$

Equating (4.19), (4.21) leads to the following series of implicit conditions ($m = 1, 2, \ldots$)

$$\begin{aligned} \alpha_N [\![&M_{11}(N+m, N) + \{+\mathrm{Det}\, M(N+m, N)(2a_N^{(m)})^{-1}[1 - (1 + 4a_N^{(m)})^{1/2}]\}) \\ &\times [M_{12}(N+m, N)(M_{22}(N+m, N)/M_{12}(N+m, N) \\ &+ M_{11}(N+2m, N+m)/M_{12}(N+2m, N+m))]^{-1}]\!] \\ &+ \beta_N M_{12}(N+m, N) = 0 \qquad (m = 1, 2, \ldots) \end{aligned} \tag{4.23}$$

which approximate all eigenvalues v below the upper bound (4.11). The convergence with increasing m is very rapid, the more the larger N (see the next section). In this paper we choose $N = 10$. Then for $\delta = -\frac{1}{4}$ and $m = 1$ we find agreement in eight decimal places with all Thorson–Moffitt eigenvalues.

In figure 1 we plot the energy eigenvalues for $j = -\frac{1}{2}$ and resonance with respect to one photon absorption. Every second RWA doublet is indicated as a dotted line; the RWA singlet ground state coincides with $\lambda = 0$. In figures 2 and 3 the energy eigenvalues are given for $j = -\frac{1}{2}$ and resonance with respect to three and five photons. Equivalently in small polaron theory the bare bandwidth is equal to three and five times the phonon energy. The lowest small polaron band is formed by the lowest branch (as lower limit) and the lower branch of the lowest doublet (as upper limit). The figures show that if the bare bandwidth is larger than the phonon energy, then the polaron bandwidth does not go to zero as the interaction constant κ^2 is increased. This result of the exact calculation is in disagreement with Holstein's adiabatic treatment (Holstein 1959). In figures 4–6 the energy eigenvalues are plotted for $j = 1$ and $\delta = -\frac{3}{2}, -1, -\frac{1}{2}, 0, \frac{1}{2}, 1$. For $\delta = -1$ the energy of the ground state coincides with the baseline $v = 0$ in accordance with equation (3.19). In all the figures the dependence of the eigenvalues on the interaction constant and the parameter δ is very similar to that found for the $(s+p)\times\Gamma_{1u}$ pseudo Jahn–Teller system (O'Brien 1976, Grevsmühl 1981).

5. Discussion

In this section we discuss the range of applicability of equation (4.23), a few special solutions and give an intuitive interpretation of this equation.

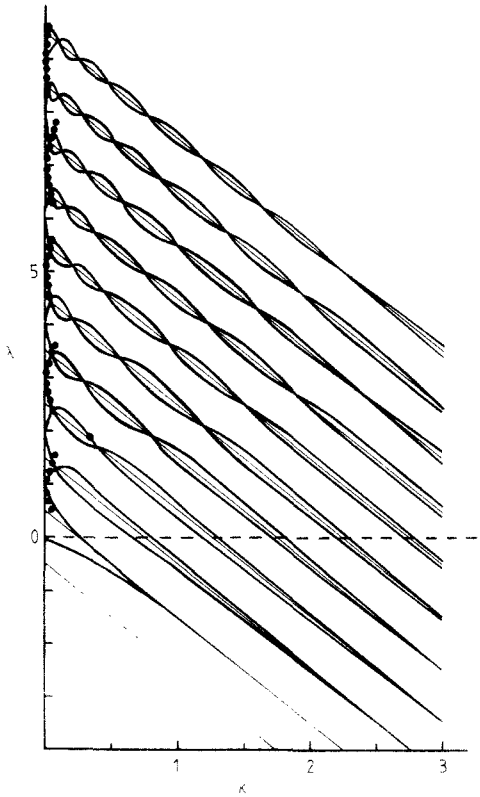

Figure 1. Energy eigenvalues λ against interaction constant κ^2 for $j=-\frac{1}{2}$, $\delta=0$ (and $\delta=-\frac{1}{2}$). Dotted lines: every second RWA doublet.

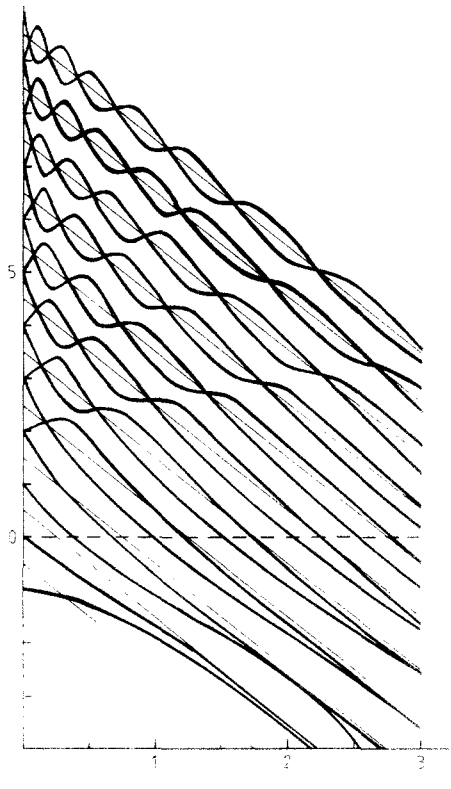

Figure 2. Energy eigenvalues λ against interaction constant κ^2 for $j=-\frac{1}{2}$, $\delta=+\frac{1}{2}$ (and $\delta=-1$).

Equation (4.23) still makes sense even for $|a_N^{(m)}|>\frac{1}{4}$ provided the radicand $1+4a_N^{(m)}$ is positive; in fact the equation remains valid under this condition as shown by the parabola theorem (Wall 1948, Jones and Thron 1980). The convergence of the roots of (4.23) towards the eigenvalues is slower than under the proper Worpitzky conditions.

We shall now discuss a few special solutions of (4.23); we refer to the less stringent condition $a_N^{(m)}\geqslant-\frac{1}{4}$.

Suppose we have chosen j and δ and the interaction constant κ^2 in such a way that there is an isolated exact solution on baseline k. A necessary condition is that vor $v=k$, $a_n^{(1)}\geqslant-\frac{1}{4}$, $n\geqslant k$. The solution is picked out by equation (4.23). Consider first the lowest possible value of $N=k$. Then Det $M(k+m,k)=0$ and $M_{11}(k+m,k)=M_{12}(k+m,k)$ (take $m=1$ in equations (3.5), (3.6) as an example). Therefore equation (4.23) reduces to $\alpha_k+\beta_k=0$, i.e. the condition for isolated exact solutions on baseline k. Consider next any value $N\geqslant k+1$; then, for the isolated exact solution $\alpha_N=\beta_N=0$, which also satisfies (4.23).

Apart from the isolated exact solutions of Judd's type other less simple solutions on the baselines exist. The last column of table 1 gives an example. Here $v\approx1$ but $a_1^{(1)}<-\frac{1}{4}$, therefore equation (4.23) is not applicable for $N=1$; $\alpha_1+\beta_1\neq0$ (see figure 3). A further example is $\kappa^2=0.55$, $j=-\frac{1}{2}$, $\delta=-\frac{3}{2}$. The non-Juddian solutions on baselines do only occur for $|\delta|>\frac{1}{4}$.

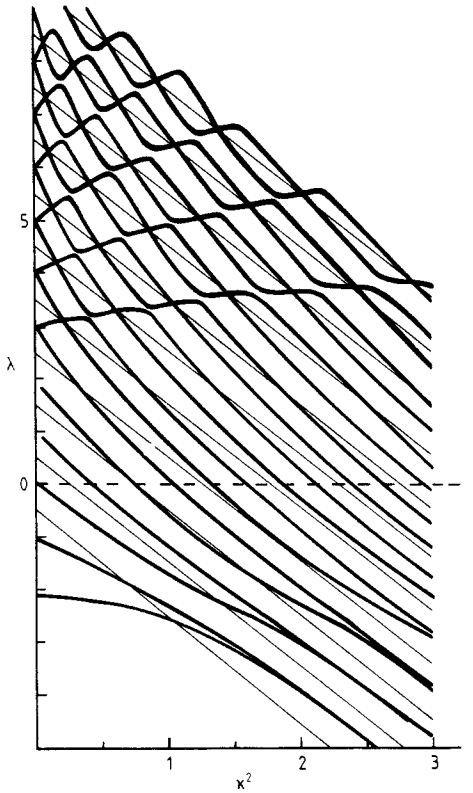

Figure 3. Energy eigenvalues λ against interaction constant κ^2 for $j=-\frac{1}{2}$, $\delta=1$ (and $\delta=-\frac{3}{2}$).

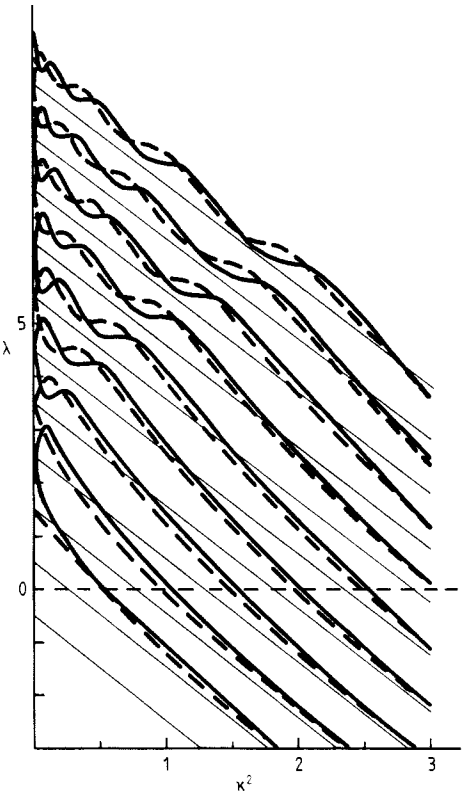

Figure 4. Energy eigenvalues λ against interaction constant κ^2. Full lines: angular momentum $J=\frac{3}{2}$, $\delta=0$ and $J=-\frac{3}{2}$, $\delta=-\frac{1}{2}$; broken lines: $J=\frac{3}{2}$, $\delta=-\frac{1}{2}$ and $J=-\frac{3}{2}$, $\delta=0$.

An intuitive interpretation of equation (4.23) can be given in the following way. Any branch in figures 1–6 intersects the baselines a number of times before it approaches one baseline asymptotically for $\kappa^2\to\infty$. Consider an example in which two consecutive intersections are Juddian on different baselines; in between the branch is in the strip $N-1<v\leq N$. The finite Neumann series for $v=N$ is embedded in the infinite Neumann series in the strip. An intuitively appealing generalisation of the isolated exact solution is obtained by studying the eigenvalue problem associated with the recurrence relation (4.18),

$$\Lambda(N+m,N)\begin{pmatrix}\alpha_N\\ \beta_N\end{pmatrix}=\begin{pmatrix}M_{11}(N+m,N) & M_{12}(N+m,N)\\ M_{21}(N+m,N) & M_{22}(N+m,N)\end{pmatrix}\begin{pmatrix}\alpha_N\\ \beta_N\end{pmatrix}. \tag{5.1}$$

The two eigenvalues

$$\Lambda=\tfrac{1}{2}\operatorname{Tr}M(N+m,N)\pm(\tfrac{1}{4}\operatorname{Tr}M(N+m,N)^2-\operatorname{Det}M(N+m,N))^{1/2} \tag{5.2}$$

are real. Denote the eigenvalue with the lower absolute value by Λ_1. Then the

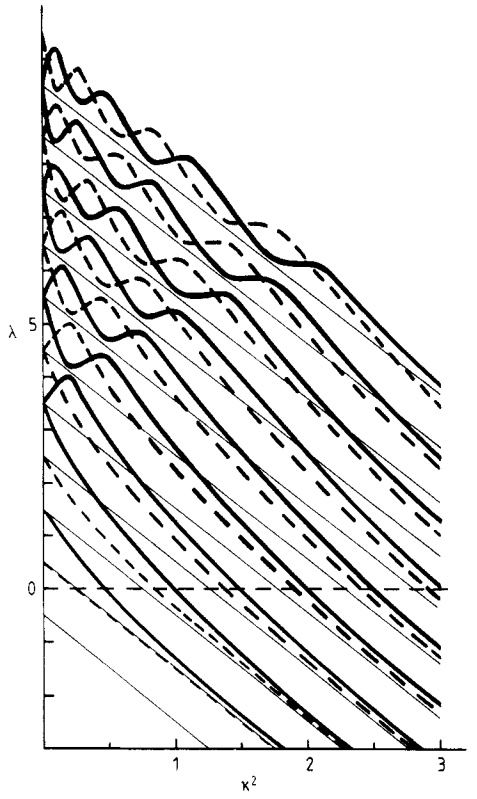

Figure 5. Energy eigenvalues λ against interaction constant κ^2. Full lines: $J=\frac{3}{2}$, $\delta=\frac{1}{2}$ and $J=-\frac{3}{2}$, $\delta=-1$; broken lines: $J=\frac{3}{2}$, $\delta=-1$ and $J=-\frac{3}{2}$, $\delta=\frac{1}{2}$.

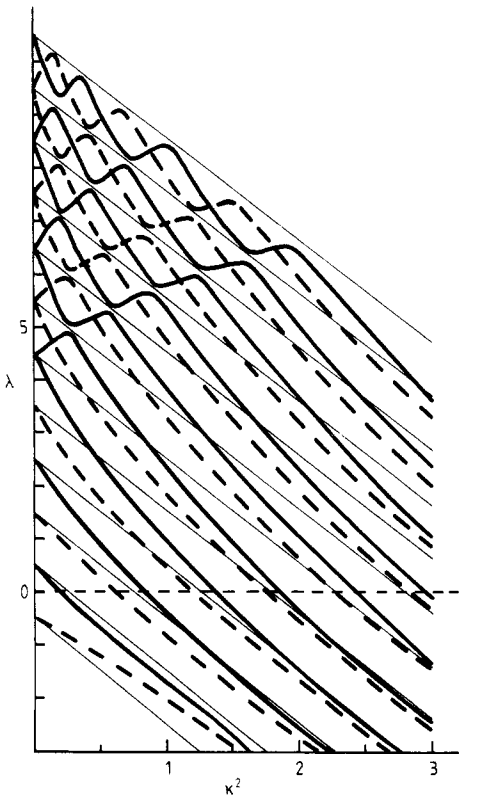

Figure 6. Energy eigenvalues λ against interaction constant κ^2. Full lines: $J=\frac{3}{2}$, $\delta=1$ and $J=-\frac{3}{2}$, $\delta=-\frac{3}{2}$; broken lines: $J=\frac{3}{2}$, $\delta=-\frac{3}{2}$ and $J=-\frac{3}{2}$, $\delta=1$.

eigenvector must satisfy the equations (3.11), (3.4) and

$$\alpha_N(M_{11}(N+m,N)-\Lambda_1(N+m,N))+\beta_N M_{12}(N+m,N)=0 \qquad (m=1,2,\ldots). \tag{5.3}$$

As for $v=N$, $\Lambda_1(N+m,N)=0$, equations (5.3) contain Judd's isolated exact solution as eigenvector of (5.1) with the eigenvalue $\Lambda_1(N+m,N)=0$. We state the following additional facts without proof. Outside the baselines equations (5.3) and (4.23) have a very similar appearance. (Insert Λ_1 in (5.3) and compare with (4.23).) Equation (5.3) holds for real values of Λ_1 i.e. under the conditions for the parabola theorem. The roots of equations (4.23) and (5.3) converge to the same limit as $m\to\infty$. In fact, the two equations reflect the element of arbitrariness in the estimate of the continued fraction. They are therefore mathematically equivalent. Equation (5.3) could have been derived along similar lines to (4.23) without referring to the eigenvalue problem (5.1).

However, because (5.3) is a consequence of (5.1) as well, we observe that the energy eigenvalues in the strip $N-1<v\leqslant N$ are selected in such a way as to make the expansion coefficients α_{N+m}, β_{N+m} $(m=1,2,\ldots)$ as small as possible under the given conditions j,δ,κ^2. This elucidates how the entire functions are picked out from the other solutions of (2.15), (2.16).

Acknowledgments

The authors thank H Risken, Ulm, for helpful and stimulating discussions. One of us (HGR) thanks Internationales Büro KFA and Conselho Nacional de Pesquisas (Brazil) for financial support during his stay at UFMG Belo Horizonte (Brazil).

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