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Analytical treatment of a two-level system with transitive and displacive vibronic coupling

H G Reik†, N Klenner† and H Nusser‡

† Fakultät für Physik, Universität Freiburg, D-7800 Freiburg, West Germany
‡ Institut für Theoretische Physik III, Universität Stuttgart, D-7000 Stuttgart, West Germany

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Abstract. The eigenvalue problem of a Hamiltonian which has been used as a model in exciton dynamics and in the theory of non-radiative transitions is formulated in Bargmann's Hilbert space of analytical functions. For particular combinations of the parameters of the Hamiltonian one finds exact solutions which are elementary transcendental functions. In the general case the eigenvalues and the eigenfunctions are determined by matrix continued fractions. The eigenfunctions can be represented accurately by Neumann expansions with very few terms.

1. Introduction

Recently Friesner and Silbey (1981) and Wagner (1983) and his collaborators (Denner and Wagner 1984, Benk and Sigmund 1985) have studied a very interesting model. The model consists of an electronic two-level system with a level separation ε, a phonon with creation and annihilation operators b^+, b and a linear vibronic coupling. The Hamiltonian is given by

$$H = b^+b + \tfrac{1}{2} + \tfrac{1}{2}\varepsilon\sigma_z' + \tfrac{1}{4}\sqrt{2}D(b+b^+)\sigma_z' + \tfrac{1}{4}\sqrt{2}\Delta_w(b+b^+)\sigma_x' \tag{1.1}$$

in Wagner's notation. Here σ_i are the spin operators ($\sigma_i^2 = 1$) and D and Δ_w are, respectively, the displacive and transitive vibronic interaction constants. In introducing this notation it is tacitly assumed that σ_z' is diagonal. The model is a caricature of real systems in the exciton dynamics of dimers and in the theory of non-radiative transitions. The caricature is studied because it can be diagonalised numerically. One can therefore test different approximation schemes and hope to learn something about the applicability of these schemes in less simple and more realistic vibronic systems. The questions Friesner and Silbey and Wagner and collaborators are asking themselves are therefore primarily of a physical nature. However, one can also investigate the exact structure of the spectrum and the eigenstates of the Hamiltonian (1.1) and this mathematical aspect of the problem will be treated in this paper. The paper is organised as follows. In § 2 we transform the Hamiltonian (1.1) into a more convenient form and formulate the eigenvalue problem in Bargmann's Hilbert space of analytical functions (Bargmann 1961, 1962). In this formalism the Schrödinger equation is a system of two coupled linear first-order differential equations for the two-component wavefunctions of a complex variable ξ. The solutions are required to belong to the space of entire functions; this determines the eigenvalues. In § 3 we show that an enumerable sequence of

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isolated parameter values exists for which the eigenvalues are determined by algebraic equations. In this case the eigenfunctions are elementary entire functions. The low-lying isolated eigenvalues and eigenfunctions can be written down easily. The higher states become increasingly more complicated in practice (although by no means less elementary in principle). The states have the same properties as the isolated exact solutions in Jahn-Teller systems which were first discussed in a important paper by Judd (1979); for this reason we call them Juddian isolated exact solutions.

In § 4 we start from the isolated exact solutions and adapt a continued fraction procedure by Reik *et al* (1982, hereafter referred to as I) to determine the eigenvalues in the general case. The convergence of the continued fraction is rather poor because the isolated exact solutions are pathologically simple. On the other hand, a Neumann expansion with very few terms reproduces the eigenfunctions extremely well in the general case as well as for the isolated exact solutions (§ 5). We are then led to a matrix continued fraction procedure for the determination of the eigenvalues which converges extremely rapidly.

2. Transformation of the Hamiltonian and analytical formulation of the eigenvalue problem

We now transform the Hamiltonian by a rotation in spin space

$$\begin{aligned} \sigma_x' &= \sigma_x \cos\alpha - \sigma_z \sin\alpha \\ \sigma_z' &= \sigma_x \sin\alpha + \sigma_z \cos\alpha \end{aligned} \tag{2.1}$$

and obtain instead of (1.1)

$$\begin{aligned} H = b^+b + \tfrac{1}{2} + \tfrac{1}{2}\varepsilon(\sigma_z \cos\alpha + \sigma_x \sin\alpha) + \sqrt{2}\,(b+b^+)[\tfrac{1}{4}\sigma_x(D\sin\alpha + \Delta_w \cos\alpha) \\ + \tfrac{1}{4}\sigma_z(D\cos\alpha - \Delta_w \sin\alpha)]. \end{aligned} \tag{2.2}$$

We require in particular that the phonons interact only with σ_x, i.e. that the Hamiltonian is of the form

$$H = b^+b + \tfrac{1}{2} + (\tfrac{1}{2} + 2\delta)\sigma_z + 2\rho\sigma_x + \sqrt{2}\kappa(b+b^+)\sigma_x, \tag{2.3}$$

which is a generalisation of equation (2.19) of I. Equation (2.3) is a complete Rabi Hamiltonian where a photon field, which is linearly polarised in the x direction, interacts with a spin-$\frac{1}{2}$ system in a static field. For $\rho \neq 0$ the static field is not perpendicular to the polarisation direction (see figure 1).

A comparison of equations (2.2) and (2.3) gives relations between the parameters of the Hamiltonians (1.1) and (2.3) which we collect in table 1. The relations with the parameters of Friesner and Silbey are also included.

Friesner and Silbey (1981) also use the spin rotation (2.1) in going from their equation (11) to equation (15), but they require a phonon interaction with the σ_z component only.

In order to solve the Schrödinger equation

$$H|\psi\rangle = \lambda|\psi\rangle \tag{2.4}$$

$$|\psi\rangle = \zeta(b^+)|0\rangle|\uparrow\rangle_x + X(b^+)|0\rangle|\downarrow\rangle_x \tag{2.5}$$

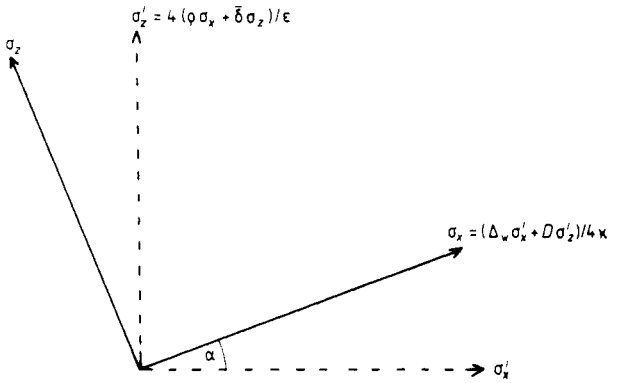

Figure 1. Rotation in spin space.

Table 1. Relations between the parameters of the model used by different authors.

Friesner and Silbey (1981, equation (11))	Wagner's group	This paper
Δ_{FS}	$\frac{1}{2}\epsilon$	$2(\bar{\delta}^2+\rho^2)^{1/2}$
γ	$\frac{1}{2}D$	$2\kappa\rho/(\bar{\delta}^2+\rho^2)^{1/2}$
v	$\frac{1}{2}\Delta_w$	$2\kappa\bar{\delta}/(\bar{\delta}^2+\rho^2)^{1/2}$
$\Delta_{FS}v/2(\gamma^2+v^2)^{1/2}$	$\epsilon\Delta_w/4(D^2+\Delta_w^2)^{1/2}$	$\bar{\delta}=\frac{1}{4}+\delta$
$\Delta_{FS}\gamma/2(\gamma^2+v^2)^{1/2}$	$\epsilon D/4(D^2+\Delta_w^2)^{1/2}$	ρ
$\frac{1}{2}(\gamma^2+v^2)^{1/2}$	$\frac{1}{4}(D^2+\Delta_w^2)^{1/2}$	κ

where

$$b|0\rangle = 0 \tag{2.6}$$

$$\begin{aligned} &\sigma_z|\uparrow\rangle_z = |\uparrow\rangle_z \qquad |\uparrow\rangle_x = \tfrac{1}{2}\sqrt{2}(|\uparrow\rangle_z + |\downarrow\rangle_z) \qquad \sigma_x|\uparrow\rangle_x = |\uparrow\rangle_x \\ &\sigma_z|\downarrow\rangle_z = -|\downarrow\rangle_z \qquad |\downarrow\rangle_x = \tfrac{1}{2}\sqrt{2}(|\uparrow\rangle_z - |\downarrow\rangle_z) \qquad \sigma_x|\downarrow\rangle_x = -|\downarrow\rangle_x, \end{aligned} \tag{2.7}$$

i.e. in order to determine the functions $\zeta(b^+)$ and $X(b^+)$ of the creation operator together with the eigenvalues, we introduce Bargmann's Hilbert space of analytical functions (Bargmann 1961, 1962). In Bargmann's method the eigenstates of the number operator are mapped onto the powers of a complex variable ξ:

$$b^{+n}|0\rangle \to \xi^n. \tag{2.8}$$

As a consequence we have

$$b^+ \to \xi \qquad b \to \mathrm{d}/\mathrm{d}\xi \tag{2.9}$$

so that the Hamiltonian and the eigenfunctions are written as

$$H = \xi(\mathrm{d}/\mathrm{d}\xi) + \tfrac{1}{2} + 2\bar{\delta}\sigma_z + 2\rho\sigma_x + \sqrt{2}\kappa[(\mathrm{d}/\mathrm{d}\xi) + \xi]\sigma_x \tag{2.10}$$

$$\bar{\delta} = (\tfrac{1}{4} + \delta) \tag{2.11}$$

$$|\psi\rangle = \zeta(\xi)|\uparrow\rangle_x + X(\xi)|\downarrow\rangle_x. \tag{2.12}$$

Inserting (2.10) and (2.12) into the Schrödinger equation (2.4) and collecting the

components of $|\uparrow\rangle_x$ and $|\downarrow\rangle_x$ gives the following system of linear first-order differential equations for $\zeta(\xi)$ and $X(\xi)$:

$$(\xi+\sqrt{2}\kappa)(\mathrm{d}\zeta(\xi)/\mathrm{d}\xi)-(\lambda-\tfrac{1}{2}+2\kappa^2-2\rho)\zeta(\xi)+\sqrt{2}\kappa(\xi+\sqrt{2}\kappa)\zeta(\xi)+2\bar{\delta}X(\xi)=0 \quad (2.13)$$

$$(\xi-\sqrt{2}\kappa)(\mathrm{d}X(\xi)/\mathrm{d}\xi)-(\lambda-\tfrac{1}{2}+2\kappa^2+2\rho)X(\xi)-\sqrt{2}\kappa(\xi-\sqrt{2}\kappa)X(\xi)$$
$$+2\bar{\delta}\zeta(\xi)=0. \quad (2.14)$$

The component function must belong to the space of entire functions. This determines the eigenvalues.

The solution of (2.13) and (2.14) for $\bar{\delta}=0$ is trivial:

$$\zeta^{(+)}(\xi)=(\xi+\sqrt{2}\kappa)^{\lambda-\frac{1}{2}+2\kappa^2-2\rho}\exp(-\sqrt{2}\kappa\xi)$$
$$X^{(+)}(\xi)=0 \quad (2.15)$$

$$\zeta^{(-)}(\xi)=0$$
$$X^{(-)}(\xi)=(\xi-\sqrt{2}\kappa)^{\lambda-\frac{1}{2}+2\kappa^2+2\rho}\exp(+\sqrt{2}\kappa\xi). \quad (2.16)$$

The requirement that the solutions (2.15) and (2.16) belong to the space of entire functions selects the eigenvalues

$$\lambda_N^{(+)}=N+\tfrac{1}{2}-2\kappa^2+2\rho \quad (2.15a)$$

$$\lambda_N^{(-)}=N+\tfrac{1}{2}-2\kappa^2-2\rho. \quad (2.16a)$$

All eigenfunctions are now entire and the eigenvalues lie on a series of equidistant straight lines in a λ against κ^2 plot. We call these lines the (+) and (−) baselines in accordance with the notation introduced in the theory of the Jahn-Teller effect (Longuet Higgins *et al* 1958, Thorson and Moffitt 1967, Judd 1977). For $\bar{\delta}\neq 0$ ($\delta\neq-\frac{1}{4}$) the λ against κ^2 plot is much more involved, but it has a beautiful structure (see figures 1-3 of I and figures 2-7 of this paper). As a result of this, the (+) and (−) baselines are the loci of simple solutions and there are exactly N of them on the (+) baseline N and the (−) baseline N. (Solutions with negative κ^2 are, of course, unphysical.)

We shall investigate these simple isolated exact solutions, the so-called Juddian isolated exact solutions (Judd 1979), in the next section. There are more solutions with energies on the (+) baseline N and (−) baseline N which are more complicated and which we shall discuss only briefly at the end of the next section.

3. Juddian isolated exact solutions

In the general case $\bar{\delta}\neq 0$ and for energies on the (+) baseline N and (−) baseline N one still has particularly simple solutions which, in a way, remember the structure (2.15) and (2.16) of the solutions in the special case $\bar{\delta}=0$: they correspond to one particular displacement of the phonons. These solutions are, however, only possible for particular values of the interaction constant κ^2, hence the name isolated exact solutions. We shall treat only the solutions on the (+) baselines as the method can be taken over literally for the treatment of isolated exact solutions on the (−) baselines.

In order to obtain the isolated exact solutions on the (+) baselines put

$$\zeta^{(+)}(\xi)=\mu(\xi)\exp(-\sqrt{2}\kappa\xi) \qquad X^{(+)}(\xi)=\gamma(\xi)\exp(-\sqrt{2}\kappa\xi), \quad (3.1)$$

i.e. extract a factor $\exp(-\sqrt{2}\kappa\xi)$ from the solution. Insertion of (3.1) into (2.13) and

(2.14) then gives the following system of differential equations for $\mu(\xi)$ and $\gamma(\xi)$:

$$(\xi+\sqrt{2}\kappa)(\mathrm{d}\mu(\xi)/\mathrm{d}\xi)-(\lambda-\tfrac{1}{2}+2\kappa^2-2\rho)\mu(\xi)+2\bar{\delta}\gamma(\xi)=0 \tag{3.2}$$

$$(\xi-\sqrt{2}\kappa)(\mathrm{d}\gamma(\xi)/\mathrm{d}\xi)-(\lambda-\tfrac{1}{2}+2\kappa^2+2\rho)\gamma(\xi)-2\sqrt{2}\kappa(\xi-\sqrt{2}\kappa)\gamma(\xi)+2\bar{\delta}\mu(\xi)=0. \tag{3.3}$$

This system of differential equations has two regular singular points, $\xi_1=-\sqrt{2}\kappa$ and $\xi_2=+\sqrt{2}\kappa$, and one irregular singular point at infinity. We expand $\mu(\xi)$ and $\gamma(\xi)$ around ξ_1,

$$\mu(\xi)=\sum_{n=0}\mu_n^{(1)}(\xi+\sqrt{2}\kappa)^n \tag{3.4}$$

$$\gamma(\xi)=\sum_{n=0}\gamma_n^{(1)}(\xi+\sqrt{2}\kappa)^n, \tag{3.5}$$

and obtain the following recurrence relations:

$$(n-\lambda+\tfrac{1}{2}-2\kappa^2+2\rho)\mu_n^{(1)}+2\bar{\delta}\gamma_n^{(1)}=0 \tag{3.6}$$

$$2\bar{\delta}\mu_n^{(1)}-2\sqrt{2}\kappa(n+1)\gamma_{n+1}^{(1)}+(n-\lambda+\tfrac{1}{2}+6\kappa^2-2\rho)\gamma_n^{(1)}-2\sqrt{2}\kappa\gamma_{n-1}^{(1)}=0. \tag{3.7}$$

Using (3.6) and (3.7) one can calculate $\mu_n^{(1)}$ and $\gamma_n^{(1)}$ as functions of the parameters λ, κ^2, ρ and $\bar{\delta}$. In general the radius of convergence of (3.4) and (3.5) is $2\sqrt{2}\kappa$. One possibility for an infinite radius of convergence, which makes $\mu(\xi)$ and $\gamma(\xi)$ entire functions, is that the series (3.4) and (3.5) terminate. This happens for particular energy values on the (+) baselines,

$$\lambda=N+\tfrac{1}{2}-2\kappa^2+2\rho, \tag{3.8}$$

and we shall carry out the procedure for $N=1$ and $N=2$. For $N=1$ and $n=0$, 1 equation (3.6) gives

$$\gamma_0^{(1)}=1 \qquad \mu_0^{(1)}=2\bar{\delta} \tag{3.9}$$

$$\gamma_1^{(1)}=0 \qquad \mu_1^{(1)} \text{ arbitrary.} \tag{3.10}$$

On the other hand, from (3.7) and (3.8) with $N=1$, $n=0$ we have

$$2\sqrt{2}\kappa\gamma_1^{(1)}=2\bar{\delta}\mu_0^{(1)}+(-1+8\kappa^2-4\rho)\gamma_0^{(0)}. \tag{3.11}$$

By (3.10) the left-hand side of (3.11) is zero. Insertion of (3.9) on the right-hand side gives

$$\kappa^2=\tfrac{1}{8}+\tfrac{1}{2}\rho-\tfrac{1}{2}\bar{\delta}^2 \tag{3.12}$$

as the condition for the interaction constant κ^2 of the isolated exact solution on the first (+) baseline. We will now show that the expansions (3.4) and (3.5) can be made to terminate.

By (3.10) the coefficient $\mu_1^{(1)}$ is still arbitrary. We dispose of it by putting

$$\mu_1^{(1)}=\sqrt{2}\kappa/\bar{\delta}. \tag{3.13}$$

Then (3.7) $\{n=1\}$ shows that $\gamma_2^{(1)}=0$, which implies $\mu_2^{(1)}=0$, (3.6) $\{n=2\}$, etc.

For Juddian isolated exact solutions on the (+) baseline $N=2$ one proceeds as follows. From (3.6) $\{N=2, n=0, 1, 2\}$ we obtain

$$\gamma_0^{(1)}=1 \qquad \mu_0^{(1)}=\bar{\delta} \tag{3.14}$$

$$\mu_1^{(1)}=2\bar{\delta}\gamma_1^{(1)} \tag{3.15}$$

$$\gamma_2^{(1)}=0 \qquad \mu_2^{(1)} \text{ arbitrary.} \tag{3.16}$$

On the other hand, (3.7) gives for $n = 0, 1$

$$\gamma_1^{(1)} = \frac{1}{\sqrt{2}\kappa}(\bar{\delta}^2 - 1 + 4\kappa^2 - 2\rho) \tag{3.17}$$

$$\gamma_2^{(1)} = \frac{1}{2\sqrt{2}\kappa}[\bar{\delta}\mu^{(1)} + (-\tfrac{1}{2} + 4\kappa^2 - 2\rho)\gamma_1^{(1)}] - \tfrac{1}{2}\gamma_0^{(1)} \tag{3.18}$$

and by (3.15)

$$\gamma_2^{(1)} = \frac{1}{2\sqrt{2}\kappa}(2\bar{\delta}^2 - \tfrac{1}{2} + 4\kappa^2 - 2\rho)\gamma_1^{(1)} - \tfrac{1}{2}\gamma_0^{(1)}. \tag{3.19}$$

The left-hand side of (3.19) is zero on account of (3.16). Insertion of (3.17) on the right-hand side gives a quadratic equation for the values of κ^2 which correspond to Juddian isolated exact solutions on the second (+) baseline:

$$\kappa^4 + \kappa^2(\tfrac{3}{4}\bar{\delta}^2 - \tfrac{1}{2} - \rho) + \tfrac{1}{4}(\bar{\delta}^2 - \tfrac{1}{4} - \rho)(\tfrac{1}{2}\bar{\delta}^2 - \tfrac{1}{2} - \rho) = 0. \tag{3.20}$$

The series (3.4) and (3.5) can also be made to terminate in this case if we dispose of $\mu_2^{(1)}$ in the following way:

$$\mu_2^{(1)} = \sqrt{2}\kappa\gamma_1^{(1)}/\bar{\delta}. \tag{3.21}$$

For arbitrary values of $\mu_1^{(1)}$ $\{N = 1\}$ and $\mu_2^{(1)}$ $\{N = 2\}$ the series (3.4) and (3.5) do not terminate and their radius of convergence is $2\sqrt{2}\kappa$. We are therefore forced to select the terminating series as the eigenfunctions of the isolated exact solutions. The generalisation of the procedure for arbitrary N is now obvious and we obtain N isolated values of κ^2 on the (+) baseline N. Negative roots are unphysical and have to be discarded. The positive roots of (3.12), (3.20), etc, correspond to Juddian isolated exact solutions of (3.2) and (3.3). The functions $\mu(\xi)$ and $\gamma(\xi)$ are polynomials in $(\xi + \sqrt{2}\kappa)$ of degree N and $N-1$, respectively. In physical terms the component functions $\zeta^+(\xi)$ and $X^+(\xi)$ are linear combinations of the ground and excited states of displaced harmonic oscillators with the displacement $\xi_1 = -\sqrt{2}\kappa$ up to the excited state N and $N-1$, respectively.

It is easy to investigate the isolated exact solutions on the (−) baselines by extracting a factor $\exp(+\sqrt{2}\kappa\xi)$ from the functions $\zeta(\xi)$ and $X(\xi)$ and expanding about the singular point ξ_2. In particular, one obtains the conditions for κ^2 on the (−) baseline N if ρ is replaced by $-\rho$ in the corresponding conditions for the (+) baselines.

In figures 2-7 the energy levels are given as a function of κ^2 (λ against κ^2 plots) for particular values of the parameters $\bar{\delta}$ and ρ. For $N = 1$ and $N = 2$ the values of κ^2 which correspond to isolated exact solutions on the (+) and (−) baselines are indicated by circles. One gets an accidental double degeneracy of the isolated exact solutions for $\rho = 0$, i.e. if the (+) and (−) baselines N coalesce (see figures 1-3 of I) and for $\rho = \frac{1}{4}m$ $(m = 1, 2, \ldots)$ (see figures 4 and 7). In the last case with $m = 1$ the (+) baseline N and the (−) baseline $N+1$ coalesce. Equations (3.12) and (3.20) in this case become

$$\kappa^2 = \tfrac{1}{4} - \tfrac{1}{2}\bar{\delta}^2 \tag{3.12a}$$

$$(\kappa^2 - \tfrac{1}{4} + \tfrac{1}{2}\bar{\delta}^2)(\kappa^2 + \tfrac{1}{4}\bar{\delta}^2) = 0 \tag{3.20a}$$

and the physical root of (3.20a) coincides with (3.12a). In the case of accidental double degeneracy the general solution of (3.2) and (3.3), and hence of (2.13) and (2.14), is an entire function (Ince 1956).

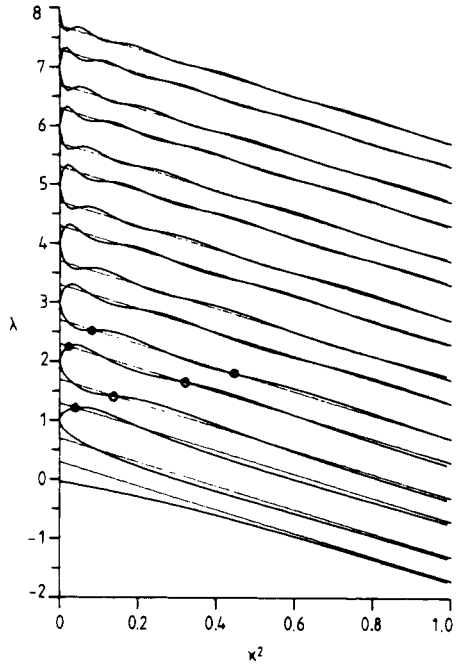

Figure 2. Energy levels as a function of the interaction constant κ^2 for $\bar{\delta} = 0.25$ ($\delta = 0$), $\rho = 0.1$. The circles are the Juddian isolated exact solutions on the first and second (+) and (−) baselines.

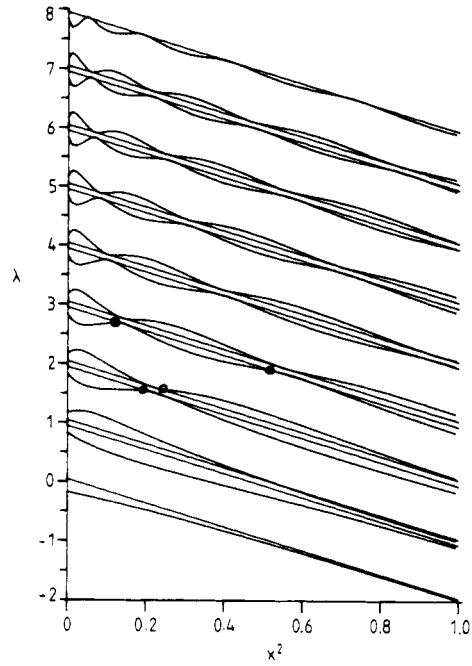

Figure 3. As figure 2, but for $\bar{\delta} = 0.25$ ($\delta = 0$), $\rho = 0.225$.

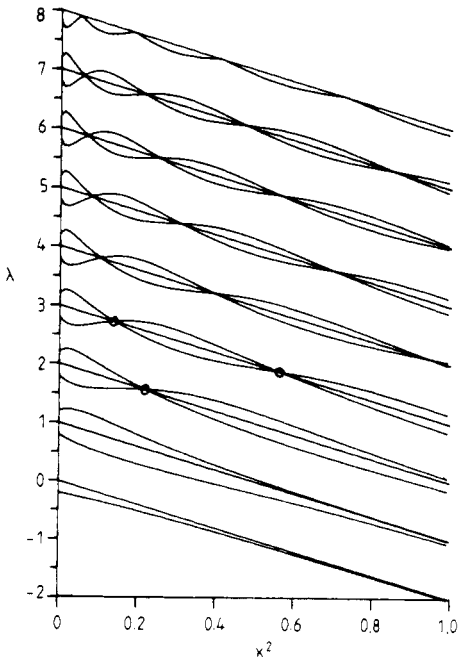

Figure 4. As figure 2, but for $\bar{\delta} = 0.25$ ($\delta = 0$), $\rho = 0.25$.

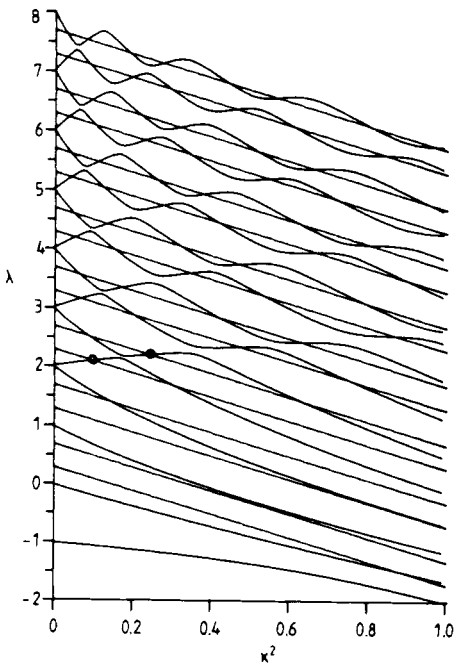

Figure 5. As figure 2, but for $\bar{\delta} = 0.75$ ($\delta = 0.5$), $\rho = 0.1$.

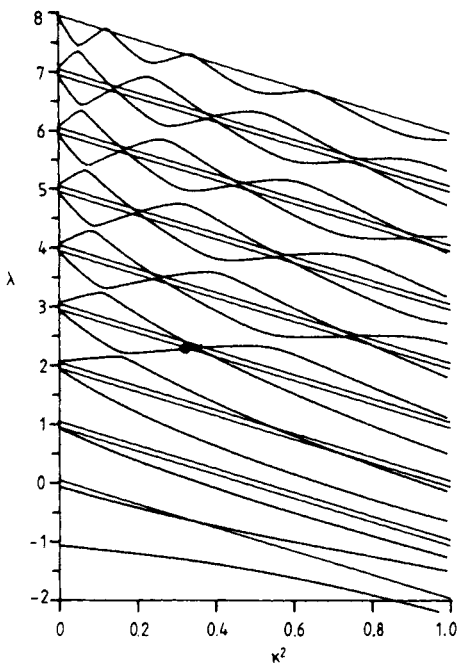

Figure 6. As figure 2, but for $\bar{\delta}=0.75$ ($\delta=0.5$), $\rho=0.225$.

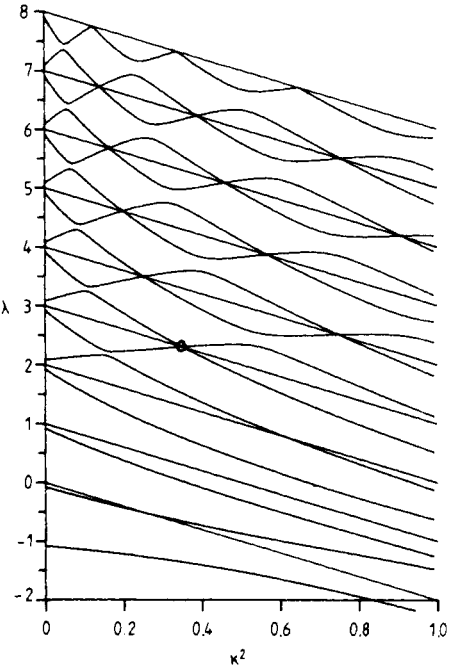

Figure 7. As figure 2, but for $\bar{\delta}=0.75$ ($\delta=0.5$), $\rho=0.25$.

Isolated exact solutions have been discovered in simple Jahn-Teller systems by Judd (1979). They have been further discussed by Reik *et al* (1981, 1982), Reik and Kaspar (1983) and Loorits (1983). The Juddian isolated exact solutions of (3.3) and (3.4) for $\rho=0$ were first given in I.

Figures 2-7, and in particular figure 2, show that apart from the Juddian isolated exact solutions there are other solutions with the eigenvalue on the same baseline whose interaction constant κ^2 does not satisfy (3.12), (3.20), etc. The recurrence relations (3.6) and (3.7) in this case show that

$$\begin{aligned} &\mu_n^{(1)}=0 \qquad n=0,1\ldots,N-1 \\ &\gamma_n^{(1)}=0 \qquad n=0,1\ldots,N \\ &\mu_N^{(1)}=\text{arbitrary}. \end{aligned} \tag{3.22}$$

The higher coefficients are given by the recurrence relations (3.6) and (3.7). The functions $\mu^{(1)}(\xi)$ and $\gamma^{(1)}(\xi)$ are therefore power series in $(\xi+\sqrt{2}\kappa)$ with the first term of power N and $N+1$, respectively. Apart from the particular property (3.22) the non-Juddian solutions on the baselines share all further properties with the solutions in the general case which we treat in the next two sections.

4. The eigenfunctions and eigenvalues outside the baselines; a continued fraction procedure for the eigenvalues

The Juddian isolated exact solutions on the (+) and (−) baselines preserve the displacement of the phonons in the solutions (2.15) and (2.16) (for $\bar{\delta}=0$) for finite $\bar{\delta}$,

i.e. in the presence of terms which would like to, and in general do, scramble the (+) and (−) displacements. One could also say that the isolated exact solutions somehow manage to unscramble the different displacements of the phonons which are present for arbitrary values of the parameters in the Hamiltonian. Therefore the method of the last section is ideally suited for the treatment of the isolated exact solutions.

However, outside the (+) baselines (3.1) puts an undue emphasis on one particular displacement and the expansions (3.4) and (3.5) have to correct this by producing (among others) a term $\exp(2\sqrt{2}\kappa\xi)$ which, in (3.1), gives the admixture of the second displacement $\exp(\sqrt{2}\kappa\xi)$. Such a term is produced by an infinite power series and therefore the convergence of (3.4) and (3.5) will be rather slow (from a physicist's point of view). Nevertheless, we use the expansions (3.4) and (3.5) for an important mathematical and computational reason: the recurrence relations for $\gamma_n^{(1)}$ and $\mu_n^{(1)}$ are tridiagonal. They share this property only with the expansion around the second singular point $\xi_2 = +\sqrt{2}\kappa$ and with the equivalent expansions around $\xi_1 = -\sqrt{2}\kappa$ and $\xi_2 = +\sqrt{2}\kappa$ for which the factor $\exp(+\sqrt{2}\kappa\xi)$ is extracted from the solution.

For $\rho \neq 0$ all other expansions have more complicated recurrence relations and most of them do not compensate for this by an improvement in convergence.

We shall now show how (3.4) and (3.5) manage to produce a term $\exp(2\sqrt{2}\kappa\xi)$ by looking at the properties of the recurrence relations at infinity. Eliminate $\mu_n^{(1)}$ in (3.7) in favour of $\gamma_n^{(1)}$:

$$2\sqrt{2}\kappa(n+1)\gamma_{n+1}^{(1)} + \left(-n - \tfrac{1}{2} + \lambda - 6\kappa^2 + 2\rho + \frac{4\bar{\delta}^2}{n + \frac{1}{2} - \lambda - 2\kappa^2 + 2\rho}\right)\gamma_n^{(1)} + 2\sqrt{2}\kappa\gamma_{n-1}^{(1)} = 0. \tag{4.1}$$

For $n \to \infty$ (see Erdelyi *et al* 1955)

$$\gamma_n^{(1)} = t\gamma_{n-1}^{(1)} \qquad \gamma_{n+1}^{(1)} = t^2\gamma_{n-1}^{(1)} \tag{4.2}$$

and (4.1) becomes a quadratic equation for t. If only the leading terms in n are kept the quadratic equation

$$2\sqrt{2}\kappa n t^2 - nt + 2\sqrt{2}\kappa = 0 \tag{4.1a}$$

has the solutions

$$t_1 \approx 1/2\sqrt{2}\kappa \tag{4.3}$$

$$t_2 \approx 2\sqrt{2}\kappa/n. \tag{4.4}$$

The root (4.3) describes a geometrical series whose radius of convergence is $2\sqrt{2}\kappa$. This series must be discarded and this is only possible for the energy eigenvalues. The second root t_2 corresponds to the expansion of the exponential function $\exp(2\sqrt{2}\kappa\xi)$ and furnishes us with the required admixture of the second displacement of the phonon in the eigenfunctions. One could now calculate the eigenvalues directly by a continued fraction procedure based on the tridiagonal recurrence relation (4.1). However, we want to use a method from I which will be generalised further in the next section. Therefore we expand the functions $\mu(\xi)$ and $\gamma(\xi)$ around the second singular point $\xi_2 = +\sqrt{2}\kappa$. Instead of (3.4) and (3.5) we then have

$$\mu(\xi) = \sum_{n=0} \mu_n^{(2)}(\xi - \sqrt{2}\kappa)^n \tag{4.5}$$

$$\gamma(\xi) = \sum_{n=0} \gamma_n^{(2)}(\xi - \sqrt{2}\kappa)^n. \tag{4.6}$$

We furthermore put

$$\mu_n^{(2)} = (2\sqrt{2}\kappa)^n \bar{\mu}_n^{(2)}/n! \tag{4.7}$$

$$\gamma_n^{(2)} = (2\sqrt{2}\kappa)^n \bar{\gamma}_n^{(2)}/n! \tag{4.8}$$

because we expect that $\lim_{n\to\infty} \bar{\mu}_n^{(2)} = \lim_{n\to\infty} \bar{\gamma}_n^{(2)} \to 1$. Finally, the energy λ is eliminated in favour of v,

$$\lambda = v + \tfrac{1}{2} - 2\kappa^2, \tag{4.9}$$

so that v = constant defines a parallel to the baselines.

Insertion of (4.5)-(4.9) in (3.2) and (3.3) leads to the following recurrence relations:

$$\begin{pmatrix} \bar{\mu}_{n+1}^{(2)} \\ \bar{\gamma}_{n+1}^{(2)} \end{pmatrix} = \begin{pmatrix} \bar{M}_{11}(n+1, n)\bar{M}_{12}(n+1, n) \\ \bar{M}_{21}(n+1, n)\bar{M}_{22}(n+1, n) \end{pmatrix} \begin{pmatrix} \bar{\mu}_n^{(2)} \\ \bar{\gamma}_n^{(2)} \end{pmatrix} \tag{4.10}$$

where the matrix elements and the determinant are given by

$$\bar{M}_{11}(n+1, n) = \frac{(-1)}{8\kappa^2}(n - v + 2\rho) \tag{4.11}$$

$$\bar{M}_{12}(n+1, n) = \frac{(-1)}{8\kappa^2}(2\bar{\delta}) \tag{4.12}$$

$$\bar{M}_{21}(n+1, n) = \frac{2\bar{\delta}(n - v + 2\rho)}{8\kappa^2(n + 1 - v - 2\rho)} \tag{4.13}$$

$$\bar{M}_{22}(n+1, n) = \frac{(2\bar{\delta})^2 + 8\kappa^2(n+1)}{8\kappa^2(n + 1 - v - 2\rho)} \tag{4.14}$$

$$\det \bar{M}(n+1, n) = -\frac{(n+1)(n - v + 2\rho)}{8\kappa^2(n + 1 - v - 2\rho)}. \tag{4.15}$$

The recurrence relations are supplemented by the initial conditions

$$\bar{\mu}_0^{(2)} = v + 2\rho \qquad \bar{\gamma}_0^{(2)} = 2\bar{\delta} \tag{4.16}$$

for the regular expansion (4.5) and (4.6) around the regular singular point ξ_2. Equation (4.15) shows that the expansions (4.5) and (4.6) can be made to terminate for $v = n + 2\rho$, i.e. on the (+) baselines. The theory of the isolated exact solutions can be set up starting from here. However, we want to embark directly on the calculation of the eigenvalues in the general case.

The recurrence relations (4.10) determine $\bar{\mu}_n^{(2)}$ and $\bar{\gamma}_n^{(2)}$ for given $\bar{\mu}_{n-1}^{(2)}$ and $\bar{\gamma}_{n-1}^{(2)}$, i.e. higher expansion coefficients are calculated from below starting with $\bar{\mu}_0^{(2)}$ and $\bar{\gamma}_0^{(2)}$ (equations (4.16)). Therefore by (4.11)-(4.14) $\bar{\mu}_n^{(2)}$ and $\bar{\gamma}_n^{(2)}$ are rational functions of v, κ^2, $\bar{\delta}$, ρ, and so are the right-hand sides and of the following two equations which define the quantities w_n and $W_n^{(1)}$ as rational functions of $\bar{\mu}_n^{(2)}$, $\bar{\gamma}_n^{(2)}$ and the matrix elements (4.11)-(4.14):

$$w_n = \bar{\gamma}_n^{(2)}/\bar{\mu}_n^{(2)} \tag{4.17}$$

$$W_n^{(1)} = \frac{\left(w_n + \dfrac{\bar{M}_{11}(n+1, n)}{\bar{M}_{12}(n+1, n)}\right)\bar{M}_{12}^2(n+1, n)\left(\dfrac{\bar{M}_{22}(n+1, n)}{\bar{M}_{12}(n+1, n)} + \dfrac{\bar{M}_{11}(n+2, n+1)}{\bar{M}_{12}(n+2, n+1)}\right)}{\det \bar{M}(n+1, n)}. \tag{4.18}$$

On the other hand, we might as well invert (4.10), i.e. solve for $\bar{\mu}_n^{(2)}$ and $\bar{\gamma}_n^{(2)}$ in terms of $\bar{\mu}_{n+1}^{(2)}$ and $\bar{\gamma}_{n+1}^{(2)}$. This determines $\bar{\mu}_n^{(2)}$ and $\bar{\gamma}_n^{(2)}$ from above and corresponds to the following equations for w_n and $W_n^{(1)}$:

$$w_n = \frac{-\bar{M}_{11}(n+1,n)w_{n+1} + \bar{M}_{21}(n+1,n)}{\bar{M}_{12}(n+1,n)w_{n+1} - \bar{M}_{22}(n+1,n)} \tag{4.19}$$

$$= -\frac{\bar{M}_{11}(n+1,n)}{\bar{M}_{12}(n+1,n)} + \frac{\det \bar{M}(n+1,n)}{\bar{M}_{12}(n+1,n)(\bar{M}_{22}(n+1,n) - \bar{M}_{12}(n+1,n)w_{n+1})}$$

$$W_n^{(1)} = \frac{1}{1 + a_n^{(1)} W_{n+1}^{(1)}} \tag{4.20}$$

$$a_n^{(1)} = \frac{-\det \bar{M}(n+2,n+1)}{\bar{M}_{12}^2(n+2,n+1)\left(\dfrac{\bar{M}_{22}(n+1,n)}{\bar{M}_{12}(n+1,n)} + \dfrac{\bar{M}_{11}(n+2,n+1)}{\bar{M}_{12}(n+2,n+1)}\right)\left(\dfrac{\bar{M}_{22}(n+2,n+1)}{\bar{M}_{12}(n+2,n+1)} + \dfrac{\bar{M}_{11}(n+3,n+2)}{\bar{M}_{12}(n+3,n+2)}\right)}. \tag{4.21}$$

The right-hand side of equation (4.20) can be turned into a continued fraction,

$$W_n^{(1)} = \frac{1|}{|1} + \frac{a_n^{(1)}|}{1} + \frac{a_{n+1}^{(1)}|}{|1} + \frac{a_{n+2}^{(1)}|}{|1} + \ldots, \tag{4.22}$$

which is a transcendental function of the variable v for given values of the parameters κ^2, $\bar{\delta}$ and ρ of the Hamiltonian. If we equate (4.18) and (4.22) we obtain

$$\bar{\mu}_n^{(2)}\left(\bar{M}_{11}(n+1,n) - \frac{\det \bar{M}(n+1,n)\, W_n^{(1)}}{\bar{M}_{12}(n+1,n)\left(\dfrac{\bar{M}_{22}(n+1,n)}{\bar{M}_{12}(n+1,n)} + \dfrac{\bar{M}_{11}(n+2,n+1)}{\bar{M}_{12}(n+2,n+1)}\right)}\right)$$
$$+ \bar{\gamma}_n^{(2)} \bar{M}_{12}(n+1,n) = 0 \tag{4.18a}$$

with the transcendental function $W_n^{(1)}$ given by (4.22). The infinitely many roots v_i ($i = 0, 1, 2, \ldots$) of (4.18a) are independent of n and give by (4.9) the eigenvalues λ_i of the Hamiltonian. If we are interested only in the low-lying energy levels $v < \bar{V}$ the calculation of the eigenvalues can be considerably simplified by a particular choice of an integer $N > \bar{N}$ so that the continued fraction (4.22) has no poles for $v < \bar{V}$. Note that

$$\lim_{n\to\infty} a_n^{(1)} \to 8\kappa^2 n^{-1}. \tag{4.23}$$

Therefore for $v < \bar{V}$ there is an integer $\bar{N}$ such that

$$|a_N^{(1)}| < \tfrac{1}{4} \qquad N > \bar{N}. \tag{4.24}$$

Hence by Worpitzky's theorem (Perron 1977, Henrici 1977, Jones and Thron 1980, Wall 1948)

$$\tfrac{2}{3} \leqslant W_N^{(1)} \leqslant 2 \tag{4.25}$$

so that $W_N^{(1)}$ is a smooth function of v which approaches unity for increasing N. This function can be approximated to any desired degree of accuracy by a periodic continued fraction with period m where $W_N^{(1)} = 1$ for $m = 0$. We therefore have the following recipe for the determination of the low-lying energy levels. Choose an integer N so that Worpitzky's theorem holds and approximate $W_N^{(1)}$ with the desired accuracy using

a periodic continued fraction with period m. Then calculate $\bar{\mu}_N^{(2)}$ and $\bar{\gamma}_N^{(2)}$ by (4.10)-(4.16). Finally insert $W_N^{(1)}$, $\bar{\mu}_N^{(2)}$ and $\bar{\gamma}_N^{(2)}$ in (4.18a) and determine the roots of the equation. Columns 1 and 2 of table 2 show that $N = 33$, $m = 2$ is sufficient to compute the ground-state energy with an accuracy of eight decimal places; column 1 of table 3 gives the first 10 energy levels calculated with $N = 50$, $m = 1$. The λ against κ^2 plots (figures 2-7) are also calculated with this method as well as with the method of the next section.

Table 2. Convergence of the ground-state energy.

This paper $\bar{\delta} = -\frac{1}{4}$ ($\delta = -0.5$) $\rho = 0.2$ $\kappa^2 = 1$			This paper $\bar{\delta} = -\frac{1}{4}$ ($\delta = -0.5$) $\rho = 0$ $\kappa^2 = 1$			Paper I $\bar{\delta} = -\frac{1}{4}$ ($\delta = -0.5$) $\rho = 0$ $\kappa^2 = 1$		
N	m	$\lambda_0^{(N,m)}$	N	m	$\lambda_0^{(N,m)}$	N	m	$\lambda_0^{(N,m)}$
30	2	−1.932 199 89	30	2	−1.546 542 66	2	1	−1.546 566 67
33	2	−1.932 199 89	33	2	−1.546 542 81	3	1	−1.546 542 03
			35	2	−1.546 542 81	4	1	−1.546 542 83
						5	1	−1.546 542 81

Table 3. The low-lying eigenvalues of the Hamiltonian.

	Equation (4.18a) $N = 50$ $m = 1$ $\kappa^2 = 1$ $\bar{\delta} = 0.75$ ($\delta = 0.5$) $\rho = 0.10$	Equation (5.37a) $N = 6$ $m = 0$ $\kappa^2 = 1$ $\bar{\delta} = 0.75$ ($\delta = 0.5$) $\rho = 0.10$	Equation (5.37a) $N = 10$ $m = 0$ $\kappa^2 = 1$ $\bar{\delta} = 0.75$ ($\delta = 0.5$) $\rho = 0.10$
i	$\lambda_i^{(N,m)}$	$\lambda_i^{(N,m)}$	$\lambda_i^{(N,m)}$
0	−2.012 638 90	−2.012 638 90	−2.012 638 90
1	−1.658 467 96	−1.658 467 96	−1.658 467 96
2	−1.158 465 75	−1.158 465 51	−1.158 465 75
3	−0.695 688 18	−0.695 687 68	−0.695 688 18
4	−0.115 337 37	−0.115 342 86	−0.115 337 37
5	0.477 953 88	0.477 941 09	0.477 953 88
6	1.121 189 36	1.121 298 57	1.121 189 36
7	1.766 486 93	1.766 625 08	1.766 486 93
8	2.414 675 51	2.413 717 57	2.414 675 51
9	2.634 392 29	2.634 156 76	2.634 392 29

The present method requires an expansion of the component wavefunctions whose expansion coefficients satisfy the recurrence relations (4.10). This is also true for a different expansion in I (for $\rho = 0$) where correct emphasis was placed on the two different displacements of the phonons from the start. In that case the quantity $a_n^{(1)}$ ((4.20) and (4.21)) which regulates the convergence of the continued fraction varies infinitely as n^{-2}. The convergence is therefore much better, as is clearly seen by a comparison of columns 2 and 3 of table 2. For $\rho \neq 0$ this expansion has more

complicated recurrence relations and therefore no longer allows for the determination of the eigenvalues by the scalar continued fraction method (equation (4.18*a*)). In the next section we shall calculate the eigenvalues and eigenfunctions for $\rho \neq 0$ by a matrix continued fraction method. A preliminary look at columns 2 and 3 of table 3 shows that a very rapid convergence of the eigenvalues is achieved using this method. (For a good exposition of the use of matrix continued fractions in physics see Risken (1984).)

5. Reformulation of the problem: matrix continued fraction procedure for the energy levels

It was shown in I that for $\rho = 0$ the Hilbert space and the spectrum of the Hamiltonian (2.10) decompose into two subspaces in which the component functions of the spin-up and spin-down components in the z direction have definite parities:

$$|\psi\rangle_1 = \varphi_1(z)|\uparrow\rangle_z + \tfrac{1}{2}\sqrt{2}\xi f_1(z)|\downarrow\rangle_z \tag{5.1}$$

$$|\psi\rangle_2 = \tfrac{1}{2}\sqrt{2}\xi\varphi_2(z)|\uparrow\rangle_z + f_2(z)|\downarrow\rangle_z. \tag{5.2}$$

Here

$$z = \tfrac{1}{2}\xi^2. \tag{5.3}$$

The functions $\varphi_i(z)$ and $f_i(z)$ have been expanded in Neumann series in the following way:

$$\begin{aligned}
\varphi_1(z) &= \frac{1}{\kappa^2}\sum_{n=0}\frac{\alpha_n^{(1)}}{n!\kappa^{4n}}(\kappa^2 z)^{\frac{1}{4}+\frac{1}{2}n} I_{n-\frac{1}{2}}(2\kappa z^{1/2}) \\
f_1(z) &= \frac{1}{\kappa}\sum_{n=0}\frac{\beta_n^{(1)}}{n!\kappa^{4n}}(\kappa^2 z)^{-\frac{1}{4}+\frac{1}{2}n} I_{n+\frac{1}{2}}(2\kappa z^{1/2}) \\
f_2(z) &= \frac{1}{\kappa^2}\sum_{n=0}\frac{\alpha_n^{(2)}}{n!\kappa^{4n}}(\kappa^2 z)^{\frac{1}{4}+\frac{1}{2}n} I_{n-\frac{1}{2}}(2\kappa z^{1/2}) \\
\varphi_2(z) &= \frac{1}{\kappa}\sum_{n=0}\frac{\beta_n^{(2)}}{n!\kappa^{4n}}(\kappa^2 z)^{-\frac{1}{4}+\frac{1}{2}n} I_{n+\frac{1}{2}}(2\kappa z^{1/2}).
\end{aligned} \tag{5.4}$$

The modified Bessel functions of half-integer order are elementary functions which contain the positive and negative exponentials $\exp(\sqrt{2}\kappa\xi)$ and $\exp(-\sqrt{2}\kappa\xi)$ on the same footing. If (5.1) and (5.2) are written in terms of the spin components $|\uparrow\rangle_x$ and $|\downarrow\rangle_x$ the parity argument shows that it is impossible to single out one exponential only in (5.1) and (5.2). However, by linear combination of (5.1) and (5.2) one can prepare either the (+) or the (−) deformation of the phonons separately. These linear combinations of (5.1) and (5.2) are eigenstates of the Hamiltonian if there is an accidental degeneracy of the two parts of the spectrum (see figures 1-3 of I). In short, for $\rho = 0$ Juddian isolated exact solutions always occur in pairs.

The results of § 3 show that for $\rho \neq 0$ and $\rho \neq \frac{1}{4}m$ the Juddian isolated exact solutions are non-degenerate, as are all eigenstates. The Hilbert space no longer decomposes and the eigenfunctions must be of the general structure

$$|\psi\rangle = (\varphi_1(z) + \tfrac{1}{2}\sqrt{2}\xi\varphi_2(z))|\uparrow\rangle_z + (\tfrac{1}{2}\sqrt{2}\xi f_1(z) + f_2(z))|\downarrow\rangle_z. \tag{5.5}$$

This can also be seen by noting that the $\rho\sigma_x$ term in (2.10) flips $|\uparrow\rangle_z$ and $|\downarrow\rangle_z$ without doing anything to the phonons. Inserting (5.5) into (2.4) and (2.10) and collecting the

spin-up and spin-down components according to the parity gives the following system of first-order differential equations:

$$\begin{pmatrix} z & \kappa z & 0 & 0 \\ \kappa & z & 0 & 0 \\ 0 & 0 & z & \kappa z \\ 0 & 0 & \kappa & z \end{pmatrix} \begin{pmatrix} \mathrm{d}\varphi_1(z)/\mathrm{d}z \\ \mathrm{d}f_1(z)/\mathrm{d}z \\ \mathrm{d}f_2(z)/\mathrm{d}z \\ \mathrm{d}\varphi_2(z)/\mathrm{d}z \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{2}v-\kappa^2-\bar{\delta} & -\kappa(z+\frac{1}{2}) & -\rho & 0 \\ -\kappa & \frac{1}{2}v-\kappa^2-\frac{1}{2}+\bar{\delta} & 0 & -\rho \\ -\rho & 0 & \frac{1}{2}v-\kappa^2+\bar{\delta} & -\kappa(z+\frac{1}{2}) \\ 0 & -\rho & -\kappa & \frac{1}{2}v-\kappa^2-\frac{1}{2}-\bar{\delta} \end{pmatrix} \begin{pmatrix} \varphi_1(z) \\ f_1(x) \\ f_2(z) \\ \varphi_2(z) \end{pmatrix} \tag{5.6}$$

where the eigenvalue λ has been eliminated in favour of v (equation (4.9)). This system of four differential equations decomposes into two systems of two differential equations for $\rho = 0$.

Insertion of (5.4) into (5.6) leads after a lengthy but straightforward calculation to the following recurrence relations:

$$\begin{pmatrix} \boldsymbol{a}_{n+1} \\ \boldsymbol{b}_{n+1} \end{pmatrix} = \begin{pmatrix} \boldsymbol{M}_{11}(n+1, n; \bar{\delta}) & \boldsymbol{M}_{12}(n+1, n; \bar{\delta}) \\ \boldsymbol{M}_{21}(n+1, n; \bar{\delta}) & \boldsymbol{M}_{22}(n+1, n; \bar{\delta}) \end{pmatrix} \begin{pmatrix} \boldsymbol{a}_n \\ \boldsymbol{b}_n \end{pmatrix} \tag{5.7}$$

where the vectors $\boldsymbol{a}_n$ and $\boldsymbol{b}_n$ are defined by

$$\boldsymbol{a}_n = \begin{pmatrix} \alpha_n^{(1)} \\ \beta_n^{(1)} \end{pmatrix} \qquad \boldsymbol{b}_n = \begin{pmatrix} \alpha_n^{(2)} \\ \beta_n^{(2)} \end{pmatrix} \tag{5.8}$$

and $\boldsymbol{M}(n+1, n; \bar{\delta})$ is a supermatrix (Gantmacher 1958) whose elements $\boldsymbol{M}_{ik}$ are matrices:

$$\boldsymbol{M}_{11}(n+1, n; \bar{\delta}) = \begin{pmatrix} M_{11}(n+1, n; \bar{\delta}) & M_{12}(n+1, n; \bar{\delta}) \\ M_{21}(n+1, n; \bar{\delta}) & M_{22}(n+1, n; \bar{\delta}) \end{pmatrix} \tag{5.9}$$

$$\boldsymbol{M}_{12}(n+1, n; \bar{\delta}) = \begin{pmatrix} M_{13}(n+1, n; \bar{\delta}) & M_{14}(n+1, n; \bar{\delta}) \\ M_{23}(n+1, n; \bar{\delta}) & M_{24}(n+1, n; \bar{\delta}) \end{pmatrix}. \tag{5.10}$$

Their elements are given by

$$M_{11}(n+1, n; \bar{\delta}) = -\kappa^2(\tfrac{1}{2}+\tfrac{1}{2}v-\bar{\delta}) \tag{5.11}$$

$$M_{12}(n+1, n; \bar{\delta}) = -\kappa^2(n+\tfrac{1}{2}-\tfrac{1}{2}v-\bar{\delta}) \tag{5.12}$$

$$M_{21}(n+1; n; \bar{\delta}) = -\kappa^2(n+1)-\rho^2+(n+1-\tfrac{1}{2}v+\kappa^2+\bar{\delta})(\tfrac{1}{2}+\tfrac{1}{2}v-\bar{\delta}) \tag{5.13}$$

$$M_{22}(n+1; n; \bar{\delta}) = -\kappa^2(n+1)+\rho^2+(n+1-\tfrac{1}{2}v+\kappa^2+\bar{\delta})(n+\tfrac{1}{2}-\tfrac{1}{2}v-\bar{\delta}) \tag{5.14}$$

$$M_{13}(n+1, n; \bar{\delta}) = \kappa^2\rho \tag{5.15}$$

$$M_{14}(n+1, n; \bar{\delta}) = -\kappa^2\rho \tag{5.16}$$

$$M_{23}(n+1, n; \bar{\delta}) = \rho(-n-\tfrac{1}{2}+v-\kappa^2) \tag{5.17}$$

$$M_{24}(n+1, n; \bar{\delta}) = \rho(2n+\tfrac{3}{2}-v+\kappa^2+2\bar{\delta}). \tag{5.18}$$

As a consequence of the structure of (5.6) we have the reciprocal relations

$$\boldsymbol{M}_{21}(n+1, n; \bar{\delta}) = \boldsymbol{M}_{12}(n+1, n; -\bar{\delta}) \tag{5.19}$$

$$\boldsymbol{M}_{22}(n+1, n; \bar{\delta}) = \boldsymbol{M}_{11}(n+1, n; -\bar{\delta}). \tag{5.20}$$

Furthermore there are two independent supplementary initial conditions

$$\boldsymbol{a}_0^{(1)} = \begin{pmatrix} \kappa^2 \\ \frac{1}{2}v - \kappa^2 - \bar{\delta} \end{pmatrix} \qquad \boldsymbol{b}_0^{(1)} = \begin{pmatrix} 0 \\ -\rho \end{pmatrix} \tag{5.21}$$

$$\boldsymbol{a}_0^{(2)} = \begin{pmatrix} 0 \\ -\rho \end{pmatrix} \qquad \boldsymbol{b}_0^{(2)} = \begin{pmatrix} \kappa^2 \\ \frac{1}{2}v - \kappa^2 + \bar{\delta} \end{pmatrix} \tag{5.22}$$

which are obtained by a Fuchsian analysis of the regular expansion (5.4) of the solution around the singular point $z = 0$ of the system (5.6). The general initial condition compatible with the requirement of local regularity is therefore

$$\boldsymbol{a}_0 = \eta_1 \boldsymbol{a}_0^{(1)} + \eta_2 \boldsymbol{a}_0^{(2)} \qquad \boldsymbol{b}_0 = \eta_1 \boldsymbol{b}_0^{(1)} + \eta_2 \boldsymbol{b}_0^{(2)} \tag{5.23}$$

with coefficients η_1 and η_2 which will be determined along with the eigenfunctions, i.e. by the requirement of global regularity. The general solution of the recurrence relations is then given by

$$\boldsymbol{a}_n = \eta_1 \boldsymbol{a}_n^{(1)} + \eta_2 \boldsymbol{a}_n^{(2)} \qquad \boldsymbol{b}_n = \eta_1 \boldsymbol{b}_n^{(1)} + \eta_2 \boldsymbol{b}_n^{(2)} \tag{5.23a}$$

and $\boldsymbol{a}_n^{(1)}$ and $\boldsymbol{b}_n^{(1)}$ are the solutions of the recurrence relations for the initial conditions $\boldsymbol{a}_0^{(1)}$, $\boldsymbol{b}_0^{(1)}$, etc. It is seen that $\boldsymbol{a}_n^{(1)}$, $\boldsymbol{b}_n^{(1)}$, etc are entire functions of v, κ^2, $\bar{\delta}$ and ρ and that on account of the reciprocal relations (5.19) and (5.20) the symmetry of the initial conditions is propagated:

$$\boldsymbol{b}_n^{(2)}(\bar{\delta}) = \boldsymbol{a}_n^{(1)}(-\bar{\delta}) \qquad \boldsymbol{a}_n^{(2)}(\bar{\delta}) = \boldsymbol{b}_n^{(1)}(-\bar{\delta}). \tag{5.24}$$

The determinant of the 4×4 matrix $\boldsymbol{M}(n+1, n; \bar{\delta})$ is given by

$$\det \boldsymbol{M}(n+1, n; \bar{\delta}) = \kappa^8 (n+1)^2 (v - n - 2\rho)(v - n + 2\rho) \tag{5.25}$$

and shows that (5.7) allows for Juddian isolated exact solutions on the (+) and (−) baselines.

The formal structure of (4.10) and (5.7) is the same except that in (5.7) we have supermatrices instead of matrices. One can therefore set up a procedure for the determination of the eigenvalues in analogy to § 4 only if correct care is taken of the non-commutativity of the supermatrix elements. We expect a rapid convergence of the eigenvalues as correct emphasis is placed on the (+) and (−) displacements of the phonons in the ansatz (5.4) for the component wavefunction. In analogy with (4.17) and (4.18) we define two matrices $\boldsymbol{w}_n$ and $\boldsymbol{W}_n^{(1)}$ by the vectors $\boldsymbol{b}_n$ and $\boldsymbol{a}_n$ (equations (5.23*a*)) which are calculated from below and therefore are entire rational functions of v (and the parameters κ^2, $\bar{\delta}$, ρ):

$$\boldsymbol{b}_n = \boldsymbol{w}_n \boldsymbol{a}_n \tag{5.26}$$

$$\boldsymbol{W}_n^{(1)} = \boldsymbol{M}_{12}(\boldsymbol{w}_n + \boldsymbol{M}_{12}^{-1}\boldsymbol{M}_{11})(\boldsymbol{M}_{22}\boldsymbol{M}_{12}^{-1}\boldsymbol{M}_{11} - \boldsymbol{M}_{21})^{-1}(\bar{\boldsymbol{M}}_{12}^{-1}\bar{\boldsymbol{M}}_{11} + \boldsymbol{M}_{22}\boldsymbol{M}_{22}^{-1}). \tag{5.27}$$

Here

$$\begin{aligned} \boldsymbol{M}_{ik} &= \boldsymbol{M}_{ik}(n+1, n; \bar{\delta}) \\ \bar{\boldsymbol{M}}_{ik} &= \boldsymbol{M}_{ik}(n+2, n+1; \bar{\delta}) \\ \bar{\bar{\boldsymbol{M}}}_{ik} &= \boldsymbol{M}_{ik}(n+3, n+2; \bar{\delta}). \end{aligned} \tag{5.27a}$$

The right-hand side of (5.27) is therefore a matrix whose elements are rational functions of v (and the parameters κ^2, $\bar{\delta}$, ρ).

Next we invert the recurrence relations. We then get, in analogy with (4.20),

$$\boldsymbol{W}_n^{(1)} = (\mathbf{1} + \boldsymbol{A}_n^{(1)} \boldsymbol{W}_{n+1}^{(1)} \boldsymbol{C}_n^{(1)})^{-1} \tag{5.28}$$

which defines the matrix $\boldsymbol{W}_n^{(1)}$ from above. Here

$$\boldsymbol{A}_n^{(1)} = -(\bar{\boldsymbol{M}}_{12}^{-1}\bar{\boldsymbol{M}}_{11} + \boldsymbol{M}_{22}\boldsymbol{M}_{12}^{-1})^{-1}\bar{\boldsymbol{M}}_{12}^{-1} \tag{5.29}$$

$$\boldsymbol{C}_n^{(1)} = (\bar{\bar{\boldsymbol{M}}}_{12}^{-1}\bar{\bar{\boldsymbol{M}}}_{11} + \bar{\boldsymbol{M}}_{22}\bar{\boldsymbol{M}}_{12}^{-1})^{-1}(\bar{\boldsymbol{M}}_{22}\bar{\boldsymbol{M}}_{12}^{-1}\bar{\boldsymbol{M}}_{11} - \bar{\boldsymbol{M}}_{21}). \tag{5.30}$$

The right-hand side of (5.28) can be turned in a matrix continued fraction (Risken 1984),

$$\boldsymbol{W}_n^{(1)} = (\mathbf{1} + \boldsymbol{A}_n^{(1)}(\mathbf{1} + \boldsymbol{A}_{n+1}^{(1)}(\mathbf{1} + \boldsymbol{A}_{n+2}^{(1)}(\mathbf{1} + \ldots)\boldsymbol{C}_{n+2}^{(1)})^{-1}\boldsymbol{C}_{n+1}^{(1)})^{-1}\boldsymbol{C}_n^{(1)})^{-1}, \tag{5.31}$$

by which $\boldsymbol{W}_n^{(1)}$ is determined unambiguously as a transcendental function of v (and the parameters κ^2, $\bar{\delta}$, ρ).

A closer inspection of $\boldsymbol{A}_n^{(1)}$ and $\boldsymbol{C}_n^{(1)}$ using (5.9)-(5.20) shows that for $v < \bar{V}$ there is an integer $\bar{N}$ so that for all integers $N > \bar{N}$ the convergence criteria of Denk and Riederle (1982) (see also Denk 1984) are satisfied. These criteria are the matrix analogues of the Worpitzky-Pringsheim conditions. The matrix $\boldsymbol{W}_N^{(1)}$ is then a smooth function of $v < \bar{V}$ for fixed values of the parameters κ^2, $\bar{\delta}$ and ρ. We defer the actual calculation of this function. Instead we assume, for the time being, that the function is known and insert it on the left-hand side of (5.27) for $n = N$. Equation (5.27) is then written in the form

$$\boldsymbol{W}_N^{(1)}(\bar{\boldsymbol{M}}_{12}^{-1}\bar{\boldsymbol{M}}_{11} + \boldsymbol{M}_{22}\boldsymbol{M}_{12})^{-1}(\boldsymbol{M}_{22}\boldsymbol{M}_{12}^{-1}\boldsymbol{M}_{11} - \boldsymbol{M}_{21}) = \boldsymbol{M}_{12}\boldsymbol{w}_N + \boldsymbol{M}_{11}. \tag{5.27b}$$

Now, while $\boldsymbol{W}_N^{(1)}$ is unambiguously defined by (5.31), $\boldsymbol{w}_N$ (equation (5.26)) is not. We can, however, remove the ambiguity in (5.27*b*) by multiplying this equation from the right by the vector $\boldsymbol{a}_N$. This gives

$$(\boldsymbol{M}_{11} - \boldsymbol{L})\boldsymbol{a}_N + \boldsymbol{M}_{12}\boldsymbol{b}_N = 0 \tag{5.32}$$

where

$$\boldsymbol{L} = \boldsymbol{W}_N^{(1)}(\bar{\boldsymbol{M}}_{12}^{-1}\bar{\boldsymbol{M}}_{11} + \boldsymbol{M}_{22}\boldsymbol{M}_{12}^{-1})^{-1}(\boldsymbol{M}_{22}\boldsymbol{M}_{12}^{-1}\boldsymbol{M}_{11} - \boldsymbol{M}_{21}). \tag{5.33}$$

Equation (5.32) contains, apart from the supermatrix elements, the matrix $\boldsymbol{W}_N^{(1)}$ and the vectors $\boldsymbol{a}_N$ and $\boldsymbol{b}_N$ and is a condition which determines the coefficients η_1 and η_2 (equation (5.23*a*)). Insertion of (5.23*a*) in (5.32) gives

$$\eta_1 \boldsymbol{v}_N + \eta_2 \boldsymbol{u}_N = 0 \tag{5.34}$$

where the vectors $\boldsymbol{v}_N$ and $\boldsymbol{u}_N$,

$$\boldsymbol{v}_N = \begin{pmatrix} v_{N1} \\ v_{N2} \end{pmatrix} \qquad \boldsymbol{u}_N = \begin{pmatrix} u_{N1} \\ u_{N2} \end{pmatrix}, \tag{5.35}$$

are defined by

$$\begin{aligned} \boldsymbol{v}_N &= (\boldsymbol{M}_{11} - \boldsymbol{L})\boldsymbol{a}_N^{(1)} + \boldsymbol{M}_{12}\boldsymbol{b}_N^{(1)} \\ \boldsymbol{u}_N &= (\boldsymbol{M}_{11} - \boldsymbol{L})\boldsymbol{a}_N^{(2)} + \boldsymbol{M}_{12}\boldsymbol{b}_N^{(1)}. \end{aligned} \tag{5.36}$$

Equation (5.34) can only be satisfied if the vectors $\boldsymbol{v}_N$ and $\boldsymbol{u}_N$ are parallel. This entails the condition

$$\det\begin{pmatrix} v_{N1} & u_{N1} \\ v_{N2} & u_{N2} \end{pmatrix} = 0. \tag{5.37}$$

As the vector components are given as functions of v (and the parameters κ^2, $\bar{\delta}$, ρ) the roots of this equation for $v < \bar{V}$ determine by (4.9) the low-lying energy levels λ_i of the Hamiltonian. For each root v_i there is a solution $\eta_1^{(i)}$, $\eta_2^{(i)}$ of (5.34) and hence of the vectors $\boldsymbol{a}_n^{(i)}$, $\boldsymbol{b}_n^{(i)}$ which determine the eigenfunctions of the eigenstate i.

We are still left with the actual calculation of the matrix $\boldsymbol{W}_N^{(1)}$, which we had postponed. We assume, subject to later verification, that it is possible to find a reasonably small value of N for which $\boldsymbol{W}_N^{(1)}$ in (5.33) can be approximated by the unit matrix. Next we multiply equation (5.34) by the matrix $\bar{\boldsymbol{M}}_{12}(\boldsymbol{M}_{22}\boldsymbol{M}_{12}^{-1} + \bar{\boldsymbol{M}}_{12}^{-1}\bar{\boldsymbol{M}}_{11})$ and obtain

$$\eta_1 \boldsymbol{v}'_N + \eta_2 \boldsymbol{u}'_N = 0 \tag{5.34a}$$

$$\begin{aligned} \boldsymbol{v}'_N &= (\bar{\boldsymbol{M}}_{11}\boldsymbol{M}_{11} + \bar{\boldsymbol{M}}_{12}\boldsymbol{M}_{21})\boldsymbol{a}_N^{(1)} + (\bar{\boldsymbol{M}}_{12}\boldsymbol{M}_{22} + \bar{\boldsymbol{M}}_{11}\boldsymbol{M}_{12})\boldsymbol{b}_N^{(1)} \\ \boldsymbol{u}'_N &= (\bar{\boldsymbol{M}}_{11}\boldsymbol{M}_{11} + \bar{\boldsymbol{M}}_{12}\boldsymbol{M}_{21})\boldsymbol{a}_N^{(2)} + (\bar{\boldsymbol{M}}_{12}\boldsymbol{M}_{22} + \bar{\boldsymbol{M}}_{11}\boldsymbol{M}_{12})\boldsymbol{b}_N^{(2)}. \end{aligned} \tag{5.36a}$$

The vectors $\boldsymbol{v}'_N$ and $\boldsymbol{u}'_N$ are now entire rational functions of v (and the parameters κ^2, $\bar{\delta}$, ρ). Therefore the equation

$$\det \begin{pmatrix} v'_{N1} & u'_{N1} \\ v'_{N2} & u'_{N2} \end{pmatrix} = 0 \tag{5.37a}$$

contains all roots v_i of the equation (5.37) but all poles of (5.37) have been eliminated. Columns 2 and 3 of table 3 show the 10 lowest eigenvalues of the Hamiltonian which have been calculated by (5.37a) for $N = 6$ and $N = 10$. The convergence is very rapid indeed and the assumption made for $\boldsymbol{W}_N^{(1)}$ is fully satisfied for $N = 10$.

In this formalism the isolated exact solutions are obtained in the following way. On the (+) and (−) baselines N the determinant of the 4×4 matrix $\boldsymbol{M}(n+1, n; \bar{\delta})$ is zero by (5.25). As a consequence (Gantmacher 1958) the determinant of the 2×2 matrix $\boldsymbol{M}_{22}\boldsymbol{M}_{12}^{-1}\boldsymbol{M}_{11} - \boldsymbol{M}_{21}$ is also zero and so is det L. Therefore the isolated exact solutions have to satisfy the conditions

$$\begin{aligned} &\eta_1(\boldsymbol{M}_{11}\boldsymbol{a}_N^{(1)} + \boldsymbol{M}_{12}\boldsymbol{b}_N^{(1)}) + \eta_2(\boldsymbol{M}_{11}\boldsymbol{a}_N^{(2)} + \boldsymbol{M}_{12}\boldsymbol{b}_N^{(2)}) = 0 \\ &\eta_1 \boldsymbol{L}\boldsymbol{a}_N^{(1)} + \eta_2 \boldsymbol{L}\boldsymbol{a}_N^{(2)} = 0. \end{aligned}$$

The calculation is more complicated than in § 3 because we start from a expansion of the wavefunctions in which the displacements are scrambled.

6. Discussion

The methods and results of the preceding section can be summarised as follows. The component wavefunctions are linear combinations of the ground and excited states of two displaced harmonic oscillators with displacements ξ_1 and ξ_2. Therefore we start from the expansion (5.4) and (5.5) of the wavefunction in which correct emphasis is placed on the two different displacements ξ_1 and ξ_2 of the phonons. This leads to a two-term recurrence relation between four component vectors and the condition for the eigenvalues of the Hamiltonian involves a matrix continued fraction with excellent convergence properties. For this reason the actual calculation of the matrix continued fraction can be avoided. Furthermore by (5.34a) and (5.36a) the conditions for the eigenvalues do not involve any inverted matrices. The determinantal equation (5.37a) is therefore free of poles. Furthermore the slope of the determinant at the zeros can

be made very large for reasonable values of N, so that the roots of the determinantal equation can be determined very accurately.

During the preparation of this paper we learnt that the Hamiltonian (1.1) and its eigenvalue problem are also being studied by the groups of Sigmund (Stuttgart) and Reineker (Ulm) (Durst *et al* 1985). They work in the occupation number representation of the Hamiltonian (1.1), which in Bargmann's method corresponds to a power series expansion of $\zeta(\xi)$ and $X(\xi)$ in (2.12). The recurrence relations are not tridiagonal. As the power series expansions have to produce the exponential functions $\exp(\sqrt{2}\kappa\xi)$ and $\exp(-\sqrt{2}\kappa\xi)$, the convergence of the expansion must be the same as in § 4. Durst (1984) compared the low-lying eigenvalues calculated by the two methods for some parameters and found complete agreement in all cases.

Finally it should be mentioned that a zero determinant (5.25) is necessary but by no means sufficient to give terminating series for the eigenfunction. The symmetry of the supermatrix in (5.2) and the existence of two independent initial conditions (5.21) and (5.22) is absolutely vital. We know of counterexamples for rather similar Hamiltonians where one cannot satisfy the recurrence relations by terminating series in spite of a zero determinant.

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