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Treatment of the generalised $E \times \varepsilon$ Jahn–Teller Hamiltonian in polar coordinates

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Abstract. The generalised $E \times \varepsilon$ Jahn-Teller Hamiltonian is treated in configuration space using polar coodinates. The expansion in radial oscillator states leads to simple recurrence relations. These are equivalent to a system of two ordinary linear first-order differential equations. The isolated exact solutions are polynomials multiplied with a exponential function in this formulation. They are also calculated in configuration space. The connection of the present treatment with Reik's treatment is established. This leads to a new understanding of Reik's Neumann series expansion.

1. Introduction

Recently, a new method of treating the generalised $E \times \varepsilon$ Jahn-Teller Hamiltonian was suggested by Reik *et al* (1982) and Reik (1984). The Hamiltonian

$$H' = \frac{1}{2m}(p_A^2 + p_B^2) + \tfrac{1}{2}m\omega_0^2(q_A^2 + q_B^2) + \hbar k(m\omega_0/\hbar)^{1/2}(q_A\sigma_x - q_B\sigma_y) + \tfrac{1}{2}\hbar\Delta\sigma_z \qquad (1.1)$$

which reduces for $\Delta = 0$ to the $E \times \varepsilon$ Jahn-Teller Hamiltonian, was formulated in Bargman's Hilbert space of analytical functions. The Schrödinger equation is a system of linear first-order differential equations in this formulation. The energy eigenvalues are determined by the requirement that the solutions of the above system of differential equations are entire functions. The solution of this problem was given in terms of a Neumann series expansion. It was shown that for particular values of the interaction constant κ the Neumann series expansion terminates. These terminating Neumann series correspond to the isolated exact solutions (Judd 1979). The general case was solved using a rapidly converging continued fraction procedure.

In this paper, we will give a different treatment of the generalised $E \times \varepsilon$ Jahn-Teller Hamiltonian (1.1). In § 2, we will introduce polar coordinates and expand the vibronic part of the wavefunction in a radial oscillator basis. This leads to simple recurrence relations, which are equivalent to a system of linear ordinary differential equations of *first* order. These equations are manipulated in § 3 to find the isolated exact solutions in our treatment. The essential point is the extraction of an exponential function from the wavefunctions. This new system of differential equations is connected to the system of differential equations in Reik's treatment by a series of manipulations containing a Laplace transform (Reik *et al* 1981). In this formulation, the isolated exact solutions correspond to a terminating power series expansion. For this reason, we are interested in the wavefunctions in configuration space which correspond to the powers r^n. These functions, which we call $S_n^j(\phi, \rho, \kappa)$, form a complete (but not orthogonal) set and are given explicitly in § 3. The isolated exact solutions in configuration space are given by a finite sum of the functions $S_n^j(\phi, \rho, \kappa)$. In § 4, the correspondence between the present treatment and Reik's treatment is established. It turns out that the Neumann series expansion can be immediately transformed to the configuration space.

2. The treatment of the Hamiltonian in polar coordinates and expansion of the eigenstates in the radial oscillator basis

We now introduce polar coordinates

$$\begin{aligned} q_A &= r\cos\phi \\ q_B &= r\sin\phi \end{aligned} \tag{2.1}$$

to treat the Hamiltonian (1.1). In the new coordinates, the Hamiltonian is

$$\begin{aligned} H' = &-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial r^2}+\frac{1}{r}\frac{\partial}{\partial r}+\frac{1}{r^2}\frac{\partial^2}{\partial^2\phi}\right)+\tfrac{1}{2}m\omega_0 r^2 \\ &+\hbar k(m\omega_0/\hbar)^{1/2} r(e^{i\phi}\sigma_{(-)}+e^{-i\phi}\sigma_{(+)})+\tfrac{1}{2}\hbar\Delta\sigma_z. \end{aligned} \tag{2.2}$$

Further we introduce the new Hamiltonian $H = H'/\hbar\omega$, the new constants $\kappa = k/2\omega_0$ and $\delta = \frac{1}{4}(\Delta-\omega_0)/\omega_0$ and the new coordinate $\rho = m\omega_0 r/\hbar$. The Hamiltonian H is now given by

$$H = -\frac{1}{2}\left(\frac{\partial^2}{\partial\rho^2}+\frac{1}{\rho}\frac{\partial}{\partial\rho}+\frac{1}{\rho^2}\frac{\partial^2}{\partial^2\phi}\right)+\tfrac{1}{2}\rho^2+2\kappa\rho(e^{i\phi}\sigma_{(-)}+e^{-i\phi}\sigma_{(+)})+\bar{\delta}\sigma_z \tag{2.3}$$

in dimensionless units, where $\bar{\delta} = (2\delta+\frac{1}{2})$. The constants are chosen to achieve agreement with Reik's treatment. The total angular momentum

$$I = -i(\partial/\partial\phi)+\tfrac{1}{2}\sigma_z \tag{2.4}$$

is a constant of the motion. Thus the operator I commutes with the Hamiltonian

$$\{I, H\} = 0 \tag{2.5}$$

as can be easily seen. Therefore, the eigenstates of H can be labelled with the eigenvalues of I.

Consider now the eigenvalue problem

$$I|\psi\rangle_{j+1/2} = (j+\tfrac{1}{2})|\psi\rangle_{j+1/2}. \tag{2.6}$$

It is solved by the states

$$|\psi\rangle_{j+1/2} = F(\rho)\, e^{ij\phi}|\uparrow\rangle + G(\rho)\exp[i(j+1)\phi]|\downarrow\rangle \tag{2.7}$$

where $F(\rho)$ and $G(\rho)$ are not determined. The spectrum of I is obtained by the requirement that the states $|\psi\rangle_{j+1/2}$ should not change when replacing ϕ by $\phi+2\pi$. For this to be true, j must be a positive or negative integer. The Schrödinger equation

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

gives, after collecting the spin-up and spin-down components, the following system of coupled ordinary differential equations of second order:

$$\begin{aligned} -\frac{1}{2}\left[\frac{d^2}{d\rho^2}+\frac{1}{\rho}\frac{d}{d\rho}-\left(\frac{j}{\rho}\right)^2-\rho^2-2\bar{\delta}+2\lambda\right]F(\rho)+2\kappa\rho G(\rho)=0 \\ -\frac{1}{2}\left[\frac{d^2}{d\rho^2}+\frac{1}{\rho}\frac{d}{d\rho}-\left(\frac{j+1}{\rho}\right)^2-\rho^2+2\bar{\delta}+2\lambda\right]G(\rho)+2\kappa\rho F(\rho)=0. \end{aligned} \tag{2.9}$$

Putting

$$\begin{aligned} F(\rho) &= \rho^{|j|}\exp(-\rho^2/2)f(\rho) \\ G(\rho) &= \rho^{|j+1|}\exp(-\rho^2/2)g(\rho) \end{aligned} \tag{2.10}$$

and $t=\rho^2$, we find

$$\begin{aligned} &\left(t\frac{d^2}{dt^2}+[(|j|+1)-t]\frac{d}{dt}-\frac{|j|+1}{2}+\tfrac{1}{2}(\lambda-\bar{\delta})\right)f(t)-\kappa t^{(1+|j+1|-|j|)/2}g(t)=0 \\ &\left(t\frac{d^2}{dt^2}+[(|j+1|+1)-t]\frac{d}{dt}-\frac{|j+1|+1}{2}+\tfrac{1}{2}(\lambda+\bar{\delta})\right)g(t)-\kappa t^{(1-|j+1|+|j|)/2}f(t)=0. \end{aligned} \tag{2.11}$$

Note that equations (2.11) are reproduced by the simultaneous transformations

$$\begin{aligned} &j\to -j-1 \\ &\bar{\delta}\to-\bar{\delta} \\ &f(t)\to g(t) \\ &g(t)\to f(t). \end{aligned} \tag{2.12}$$

For this reason, it is sufficient to solve the problem for $j\geqslant 0$. For $j\geqslant 0$, equations (2.11) become

$$\left(t\frac{d^2}{dt^2}+(j+1-t)\frac{d}{dt}-\frac{j+1}{2}+\tfrac{1}{2}(\lambda-\bar{\delta})\right)f(t)-\kappa t g(t)=0 \tag{2.13}$$

$$\left(t\frac{d^2}{dt^2}+(j+2-t)\frac{d}{dt}-\frac{j+2}{2}+\tfrac{1}{2}(\lambda-\bar{\delta})\right)g(t)-\kappa f(t)=0.$$

To solve the equations, let us remark that for $\kappa=0$ and $\bar{\delta}=0$ the Hamiltonian H simply describes a two-dimensional harmonic oscillator. For the eigenstate with angular momentum j and energy $2n+j+1$ we have

$$f_{nj}(t)=c_{nj}\,{}_1F_1(-n,j+1,t). \tag{2.14}$$

Here c_{nj} is a normalisation constant and ${}_1F_1(-n,j+1,t)$ is a confluent hypergeometric function. We now expand the eigenfunctions in the general case with respect to the described oscillator states, which surely form a complete set of functions:

$$f(t)=\sum_{n=0}^{\infty}a_n\,{}_1F_1(-n,j+1,t) \tag{2.15}$$

$$g(t)=\sum_{n=0}^{\infty}b_n\,{}_1F_1(-n,j+2,t).$$

The insertion of (2.15) in (2.13) leads to the recurrence relations

$$
\begin{aligned}
&[-\tfrac{1}{2}(j+1)+\tfrac{1}{2}(\lambda-\bar{\delta})-(n+1)]a_{n+1}-\kappa(j+1)b_{n+1}=-\kappa(j+1)b_n \\
&\kappa\frac{(n+1)}{(j+1)}a_{n+1}=\kappa\frac{(j+1+n)}{(j+1)}a_n+[\tfrac{1}{2}(j+2)-\tfrac{1}{2}(\lambda+\bar{\delta})+n]b_n.
\end{aligned}
\tag{2.16}
$$

We have made use of the formulae

$$
\left[t\frac{d^2}{dt^2}+(j+1-t)\frac{d}{dt}-\left(\frac{j+1}{2}+\tfrac{1}{2}(\lambda-\bar{\delta})\right)\right]{}_1F_1(-n,j+1,t)
$$

$$
=\left(-\frac{j+1}{2}+\tfrac{1}{2}(\lambda-\bar{\delta})-n\right){}_1F_1(-n,j+1,t) \tag{2.17}
$$

$$(j+1){}_1F_1(-n,j+1,t)=-n{}_1F_1(-n-1,j+2,t)+(j+1+n){}_1F_1(-n,j+2,t)$$

$$t{}_1F_1(-n,j+2,t)=(j+1)[{}_1F_1(-n,j+1,t)-{}_1F_1(-n-1,j+1,t)]$$

to arrive at (2.16). Note that the recurrence relations (2.16) terminate for negative values of n ($a_{-i}=b_{-i}=0$, $i=1,2\ldots$) when the initial condition

$$[-\tfrac{1}{2}(j+1)+\tfrac{1}{2}(\lambda-\bar{\delta})]a_0-\kappa(j+1)b_0=0 \tag{2.18}$$

is valid. They can be formed to

$$
\begin{pmatrix} a_{n+1} \\ b_{n+1} \end{pmatrix}=\hat{M}(n)\begin{pmatrix} a_n \\ b_n \end{pmatrix}=\begin{pmatrix} M_{11}(n) M_{12}(n) \\ M_{21}(n) M_{22}(n) \end{pmatrix}\begin{pmatrix} a_n \\ b_n \end{pmatrix} \tag{2.19}
$$

where

$$
\begin{aligned}
&M_{11}(n)=(n+1+j)/(n+1) \\
&M_{12}(n)=\frac{(j+1)}{\kappa(n+1)}\left(\frac{j+2}{2}-\frac{\lambda+\bar{\delta}}{2}+n\right) \\
&M_{21}(n)=\frac{(j+1+n)}{\kappa(j+1)(n+1)}\left(-\frac{j+1}{2}+\frac{\lambda-\bar{\delta}}{2}-n-1\right) \\
&M_{22}(n)=1+\frac{1}{\kappa^2(n+1)}\left(-\frac{j+1}{2}+\frac{\lambda-\bar{\delta}}{2}-(n+1)\right)\left(\frac{j+2}{2}-\frac{\lambda+\bar{\delta}}{2}+n\right) \\
&\det\hat{M}(n)=\frac{(n+j+1)}{(n+1)}.
\end{aligned}
\tag{2.20}
$$

Since $j\geqslant 0$, $\det\hat{M}(n)\neq 0$ for $n=0,1,2,\ldots$. Therefore the recurrence relations (2.16) do not terminate for positive values of n. There are two solutions of (2.19) with different behaviour for large n:

$$
\begin{aligned}
&\lim_{n\to\infty}\left(\frac{a_{n+1}}{a_n}\right)_1=\lim_{n\to\infty}\left(\frac{b_{n+1}}{b_n}\right)_1\sim\operatorname{Tr}\hat{M}(n)\sim-\frac{n}{\kappa^2} \\
&\lim_{n\to\infty}\left(\frac{a_{n+1}}{a_n}\right)_2=\lim_{n\to\infty}\left(\frac{b_{n+1}}{b_n}\right)_2\sim\frac{\det\hat{M}(n)}{\operatorname{Tr}\hat{M}(n)}\sim-\frac{\kappa^2}{n}.
\end{aligned}
\tag{2.21}
$$

Only the second solution is the physical solution, since the expansion (2.15) must be convergent. This solution can be obtained using a continued fraction procedure which is described in detail by Reik *et al* (1982).

3. Isolated exact solutions in configuration space and expansion of the eigenstates in a new basis

The recurrence relations (2.16) are equivalent to the following system of ordinary differential equations of first order:

$$
\begin{aligned}
&w\frac{\mathrm{d}f}{\mathrm{d}w}+\left(\frac{j+1}{2}-\frac{\lambda+\bar{\delta}}{2}\right)f(w)+\kappa(j+1)(1-w)g(w)=0\\
&\kappa(w-1)\frac{\mathrm{d}f}{\mathrm{d}w}+\kappa(j+1)f(w)+(j+1)w\frac{\mathrm{d}g}{\mathrm{d}w}+(j+1)\left(\frac{j+2}{2}-\frac{\lambda+\bar{\delta}}{2}\right)g(w)=0.
\end{aligned}
\tag{3.1}
$$

This can be seen when $f(w)$ and $g(w)$ are written as a power series of the complex variable w:

$$
\begin{aligned}
f(w)&=\sum_{n=0}^{\infty}a_n w^n\\
g(w)&=\sum_{n=0}^{\infty}b_n w^n.
\end{aligned}
\tag{3.2}
$$

In other words, the power series expansion (3.2) corresponds to the expansion of the vibronic components of the wavefunction in a radial oscillator basis. Note that equation (3.1) is now a system of differential equations of *first* order in contrast to the Schrödinger equation (2.9) in configuration space.

The behaviour at large n of the physical solution in (2.21) suggests the ansatz

$$
\begin{aligned}
f(w)&=\exp(-\kappa^2 w)\tilde{f}(w)\\
g(w)&=\exp(-\kappa^2 w)\tilde{g}(w)
\end{aligned}
\tag{3.3}
$$

for the solution of (3.1). This leads to

$$
\begin{aligned}
&\kappa(j+1)(1-w)\tilde{g}(w)+w\frac{\mathrm{d}\tilde{f}}{\mathrm{d}w}+\left(\frac{j+1}{2}-\frac{\lambda-\bar{\delta}}{2}-\kappa^2 w\right)\tilde{f}(w)=0\\
&(j+1)w\frac{\mathrm{d}\tilde{g}}{\mathrm{d}w}+(j+1)\left(\frac{j+2}{2}-\frac{\lambda+\bar{\delta}}{2}-\kappa^2 w\right)\tilde{g}(w)\\
&\qquad+\kappa(w-1)\frac{\mathrm{d}\tilde{f}}{\mathrm{d}w}+\kappa(j+1+\kappa^2-\kappa^2 w)\tilde{f}(w)=0.
\end{aligned}
\tag{3.4}
$$

We now put $-\kappa^2 w=r$, $(j+1)\tilde{g}(w)=x_2(r)$, $\tilde{f}(w)=x_1(r)$ and $\lambda=v+1/2-2\kappa^2$. The complex variable r just introduced should not be confused with the radius r introduced by equation (2.1). Furthermore, we multiply the first equation in (3.4) with κ and subtract it from the second equation in (3.4). The result is

$$
\begin{aligned}
&(\kappa+r/\kappa)x_2(r)+r(\mathrm{d}/\mathrm{d}r)x_1(r)-(-\kappa-\tfrac{1}{2}j-\tfrac{1}{2}\bar{\delta}-\tfrac{1}{4}+\tfrac{1}{2}v-r)x_1(r)=0\\
&r(\mathrm{d}/\mathrm{d}r)x_2(r)-(-\tfrac{1}{2}j+\bar{\delta}-\tfrac{3}{4}+\tfrac{1}{2}v)x_2(r)+\kappa^3(\mathrm{d}x_1/\mathrm{d}r)+\kappa(\tfrac{1}{2}j-\tfrac{1}{2}\bar{\delta}+\tfrac{3}{4}+\tfrac{1}{2}v)x_1(r)=0.
\end{aligned}
\tag{3.5}
$$

These are exactly the equations obtained by Reik *et al* (1981) for $\bar{\delta}=0$ using a very different method. It was shown that a power series expansion for $x_1(r)$ and $x_2(r)$ terminates for particular values of the coupling constant κ. These terminating power series exhaust all classes of isolated exact solutions. We are now going to calculate the state in configuration space which corresponds to the power r^n. Remember the correspondence

$$r^n \leftrightarrow (-\kappa^2 w)^n \exp(-\kappa^2 w) \tag{3.6}$$

$$w^n \leftrightarrow e^{ij\phi}\rho^j \exp(-\rho^2/2)\,{}_1F_1(-n, j+1, \rho^2) \tag{3.7}$$

for the spin-up component and

$$w^n \leftrightarrow \exp[i(j+1)\phi]\rho^{j+1} \exp(-\rho^2/2)\,{}_1F_1(-n, j+2, \rho^2) \tag{3.8}$$

for the spin-down component. We restrict ourselves now to the case of the spin-up component. (The spin-down component case is obtained by replacing j by $j+1$.)

Since

$$(-\kappa^2 w)^n \exp(-\kappa^2 w) = \sum_{\nu=0}^{\infty} (-\kappa^2)^{\nu+n} w^{n+\nu}/\nu! \tag{3.9}$$

we have to calculate the series

$$\sum_{\nu=0}^{\infty} [(-\kappa^2)^{\nu+n}/\nu!]\, e^{ij\phi}\rho^j \exp(-\rho^2/2)\,{}_1F_1(-(n+\nu), j+1, \rho^2). \tag{3.10}$$

For $n=0$ this is simple and we find the correspondence

$$r^0 \leftrightarrow \exp(-\kappa^2 w) \leftrightarrow e^{ij\phi}[j!\exp(-\kappa^2)/\kappa^j] \exp(-\rho^2/2) I_j(2\kappa\rho). \tag{3.11}$$

Here $I_j(2\kappa\rho)$ is the jth modified Bessel function.

To proceed in the case $n \neq 0$, we make use of

$$(-\kappa^2 w)^n = \frac{(-\kappa^2)^n}{(-i)^n} \int_{-\infty}^{\infty} \delta^{(n)}(p)\, e^{ipw}\, dp \tag{3.12}$$

to write

$$(-\kappa^2 w)^n \exp(-\kappa^2 w) = \frac{(-\kappa^2)^n}{(-i)^n} \int_{-\infty}^{\infty} \delta^{(n)}(p) \exp[iw(p+i\kappa^2)]\, dp. \tag{3.13}$$

Using the correspondence (3.11) for $i(p+i\kappa^2)$ instead of $-\kappa^2$ we find, after some algebra,

$$r^n \leftrightarrow (-\kappa^2 w)^n \exp(-\kappa^2 w) \leftrightarrow n!j!(-1)^n \kappa^{2n-j} \times \exp(ij\phi - \kappa^2 - \rho^2/2) \sum_{k=0}^{n} \frac{1}{(n-k)!}\frac{1}{k!}(-\rho)^k I_{j+k}(2\kappa\rho). \tag{3.14}$$

We now introduce the notation

$$S_n^j(\phi, \rho, \kappa) = n!j!(-1)^n \kappa^{2n-j} \exp(ij\phi - \rho^2/2 - \kappa^2) \sum_{k=0}^{n} \frac{1}{(n-k)!}\frac{1}{k!}(-\rho)^k I_{j+k}(2\kappa\rho). \tag{3.15}$$

Since $\lim_{\rho\to 0} S_n^j \sim \rho^j$ and

$$I_{j+k}(2\kappa\rho) = \frac{e^{2\kappa\rho}}{(2\pi 2\kappa\rho)^{1/2}}\left(1 + O\left(\frac{1}{2\kappa\rho}\right)\right)$$

the functions $S_n^j(\phi, \rho, \kappa)$ do belong to the Hilbert space. Further, they form a complete but not orthogonal set because of their construction from the radial oscillator states.

The power series expansion of $x_1(r)$ and $x_2(r)$ corresponds to the expansion of the vibronic component of the wavefunction in configuration space with respect to the complete set of functions $S^j_n(\phi, \rho, \kappa)$. Let us conclude this section with the remark that the isolated exact solutions are given in configuration space by a finite superposition of the functions $S^j_n(\phi, \rho, \kappa)$.

4. Connection of the present treatment with Reik's treatment of the generalised $E \times \varepsilon$ Jahn–Teller Hamiltonian

In Reik's treatment (Reik *et al* 1982), the Schrödinger equation is formulated in Bargmann's Hilbert space of analytical functions. It was shown that the eigenvalue problem can be formed to the problem of finding entire functions $\phi(z)$ and $f(z)$, which are a solution of the coupled differential equations

$$z\frac{\mathrm{d}\phi}{\mathrm{d}z} - (\varepsilon - \delta)\phi(z) + \kappa\left(z\frac{\mathrm{d}f}{\mathrm{d}z} + (j+1+z)f(z)\right) = 0 \qquad (4.1)$$

$$\kappa\left(\frac{\mathrm{d}\phi}{\mathrm{d}z} + \phi(z)\right) + z\frac{\mathrm{d}f}{\mathrm{d}z} - (\varepsilon + \delta)f(z) = 0$$

where $\varepsilon = \frac{1}{2}(\lambda - j - \frac{3}{2})$. Equations (4.1) are connected with equations (3.5) by a series of manipulations, which include a Laplace transform. This series of manipulations is given by Reik *et al* (1981) for $\delta = -\frac{1}{4}$. For general values of δ it is not changed. When a power series expansion of $x_1(r)$ and $x_2(r)$ is transformed back, a Neumann series expansion of $\phi(z)$ and $f(z)$ is obtained. It was found that the following correspondence exists:

$$r^n \leftrightarrow z^{(n-j)/2} I_{n+j}(2\kappa\sqrt{z}) \qquad (4.2)$$

for the spin-up component and

$$r^n \leftrightarrow z^{[n-(j+1)]/2} I_{n+j+1}(2\kappa\sqrt{z}) \qquad (4.3)$$

for the spin-down component. Due to the results of § 3 (equation (3.14)) we have now established the correspondence

$$z^{(n-j)/2} I_{n+j}(2\kappa\sqrt{z}) \leftrightarrow (\sqrt{\pi} j!)^{-1} S^j_n(\phi, \rho, \kappa). \qquad (4.4)$$

The constant $(\sqrt{\pi} j!)^{-1}$ was included to achieve coincidence in normalisation of both functions. Therefore the solution given by Reik *et al* (1982) in terms of a Neumann series expansion can be immediately transformed to configuration space with the help of (4.4).

5. Discussion

We have presented the treatment of the generalised $E \times \varepsilon$ Jahn–Teller Hamiltonian in polar coordinates. The crucial point is that the expansion of the vibronic part of the wavefunction in radial oscillator states leads to the *simple* recurrence relations (2.16). These are equivalent to the system of *first*-order differential equations (3.1). After the extraction of an exponential function from the wavefunction, the isolated exact solutions are found and the relation to Reik's treatment is given. Because of relation (4.4), the Neumann series expansion for the solution of the system of differential equations (4.1) leads to the same 'algebra' as the expansion of the vibronic part of the wavefunction in terms of the complete set of functions $(\sqrt{\pi} j!)^{-1} S_n^j(\phi, \rho, \kappa)$ in configuration space. This 'algebra' can be used for a solution of the general problem in terms of a continued fraction procedure. Since this procedure has been worked out in great detail (Reik *et al* 1982, Reik 1984) and the corresponding results presented, we do not repeat it here.

The main purpose of this paper is to illuminate the rather formal Neumann series expansion in the light of the presented treatment in configuration space. We have seen that the nth term in the Neumann series expansion corresponds to a series of radial oscillator states, starting with the state of energy $2n+j+1$ (see (3.14), (3.15) and (4.4)). Since this series can be calculated analytically (see (3.14)), the present treatment gives some information about the behaviour of the vibronic part of the wavefunction in configuration space.

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