The anharmonic oscillator problem: a new algebraic solution

1985 J. Phys. A: Math. Gen. 18 2541

(http://iopscience.iop.org/0305-4470/18/13/029)

J. Phys. A: Math. Gen. **18** (1985) 2541-2554. Printed in Great Britain

The anharmonic oscillator problem: a new algebraic solution

M Znojil, K Sandler and M Tater

Institute of Nuclear Physics, Czechoslovak Academy of Sciences, CS 250 68 Řež, Czechoslovakia

Received 25 July 1984, in final form 7 November 1984

Abstract. The second-order (one-dimensional or radial) differential Schrödinger equation with the potential $V(r)=\mu r^2+\nu r^4$ may be re-interpreted as a difference equation of the fourth order (indeed, the Hamiltonian is a pentadiagonal matrix in the standard harmonic oscillator basis $|n\rangle$, $n=0,1,\ldots$). Thus, we construct its four independent general solutions by purely algebraic means, via expansions in powers of $(n+1)^{-1/4}$. Next, preserving the analogy between difference and differential equations, the physical wavefunctions $\langle n|\psi\rangle$ and their energies are determined by the matching of the 'Jost' and 'regular' solutions. Finally, using the simplest matching condition 'at the origin', the resulting numerical algorithm is demonstrated to be both stable and quickly convergent.

1. Introduction and summary

Small vibrations in a deep potential may be described by the harmonic oscillator model. The Schrödinger equation also containing the first anharmonic correction

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}+\frac{l(l+1)}{r^2}+\mu r^2+\nu r^4-E\right)\psi(r)=0 \qquad l=0,1,\ldots \qquad \nu>0 \tag{1.1}$$

therefore finds numerous applications, e.g., in molecular physics (Lister *et al* 1978). A number of papers has been devoted to its solution; an up to date list may be found, e.g., in the papers of Arteca *et al* (1984).

One of the most interesting methodical applications of (1.1) lies in its interpretation as a zero-dimensional field model (Itzykson and Zuber 1980). Hence, a perturbative treatment of (1.1) is of particular interest—for example, Marziani (1984) recalls a number of references studying the efficiency of the resummation techniques of Borel, Padé, Aitken, continued fractions, Euler, Levin, Brezinski, Wynn and others.

Often, the inherent inconsistencies of the Rayleigh-Schrödinger perturbative approach (cf, e.g., the discussion by Flessas *et al* 1984) necessitate major modifications: Makarewicz (1984) reviews the various rearrangements of the Hamiltonians H_0 and H_1 in combination with JWKB ideas and hypervirial relations, Au *et al* (1983) recommend switching to the logarithm of ψ, Graffi and Grecchi (1975) replace the sums by matrix continued fractions, etc. The latter work also inspired the fixed-point perturbation theory (Znojil 1984a) using, in an implicit formulation, the inverse model-space dimension as a 'natural' small expansion parameter for all the anharmonic-oscillator-type Hamiltonians.

0305-4470/85/132541+14$02.25

In the present paper, we shall further develop the application of the general fixed-point perturbative idea to anharmonic oscillators (1.1). We shall start from the following three modifications of the formulation of the problem.

(i) We convert the general (non-zero) value of the anharmonic coupling ν to one (by a rescaling of the coordinate, $r \to \rho r$, with $\rho^6 \nu = 1$, and by multiplication of (1.1) by the constant ρ^2).

(ii) In the unperturbed (harmonic oscillator) basis $|n\rangle$, $n = 0, 1, \ldots$, we then rewrite the differential equation (1.1) as an algebraic linear set of equations

$$\begin{pmatrix} a_0 & b_0 & c_0 & & & \\ b_0 & a_1 & b_1 & c_1 & & \\ c_0 & b_1 & a_2 & b_2 & c_2 & \\ & c_1 & b_2 & a_3 & b_3 & c_3 \\ & & \cdot & \cdot & \cdot & \end{pmatrix} \begin{pmatrix} \langle 0|\psi\rangle \\ \langle 1|\psi\rangle \\ \langle 2|\psi\rangle \\ \langle 3|\psi\rangle \\ \ldots \end{pmatrix} = 0$$

$$a_n = 6n^2 + (11 + 6l + 2\mu)n + l^2 + (5 + \mu)l + \tfrac{1}{4}(21 + 6\mu) - E \tag{1.2}$$

$$b_n = (4n + 2l + 4 + \mu)\beta_n \qquad c_n = \beta_n \beta_{n+1}$$

$$\beta_n = (n+1)^{1/2}(n + l + \tfrac{3}{2})^{1/2}.$$

(iii) We reinterpret (1.2) as a difference equation for the projections $\langle n|\psi\rangle$ (of fourth order) (Korn and Korn 1968).

Our construction of the solution ψ and E will be based on analogies of (1.2) to the differential equations. In § 2, we explain the method on the truncated equation (1.2). In particular, we recall some relevant results of Znojil (1983, 1984b, c, to be referred to as I, II and III, respectively), notice that the truncation simplifies the asymptotic boundary conditions and introduce the (independent pairs of the) 'regular' (§ 2.1) and 'Jost' (§ 2.2) general solutions. The physical bound states are then characterised by the matching of the 'regular' and 'Jost' solutions at some four distinct points $n = K_1$, K_2, K_3 and K_4 (§ 2.3).

Our most important result is presented in § 3 where we succeed in the elimination of the infinite-dimensional limiting transition (which would be purely numerical, cf also Wilkinson 1965) and construct directly the four independent power-series general solutions to (1.2),

$$\langle n|\psi^{(j)}\rangle = \text{constant} \times (n+1)^{\text{constant}} \exp\left((n+1) \sum_{m=0}^{\infty} \frac{c_m^{(j)}}{(n+1)^{m/4}}\right)$$
$$n \geq 0 \qquad j = 1, 2, 3, 4. \tag{1.3}$$

These solutions are derived in a systematic way—the coefficients $c_m^{(i)}$ are specified here up to $m = 5$ (§ 3.4) or, implicitly, up to $m = 16$ (§ 3.5).

In § 4, we analyse the matching conditions. We prove that they are practically equivalent to the simple truncation (§ 4.1) or leading-order fixed-point prescription (§ 4.2) in the $K_i \gg 1$ asymptotic region. For $K_i = O(1)$, the matching conditions are given specific difference forms (§ 4.3 and appendix).

In § 5, we underline that Re $c_0^{(i)} = 0$ and Re $c_1^{(j)} < 0$ (for $j = 1, 2$) or Re $c_1^{(j)} > 0$ (for $j = 3, 4$). This implies that there are just two 'Jost' solutions, in full analogy with § 2. This is the most favourable situation from the purely practical point of view.

We may use (1.2) as the stable recurrences defining the components of bound states $\langle n|\psi\rangle$ from pairs of arbitrary initialisations (§ 5.1). Moreover, we may also introduce a discrete analogue of the Jost function (cf Newton 1965), the zeros of which determine the binding energies (§ 5.2). The corresponding recurrent eigenvalue/eigenvector algorithm proves to be stable and extremely efficient in the numerical tests.

We may summarise our treatment of the anharmonic oscillator (1.1) as an analytic continuation of projections $\langle n|\psi\rangle$ to the complex n-plane. It is similar to Regge theory (see Newton 1965) but its difference-equation background represents a new point of view. It enables us to represent wavefunctions by closed formulae of the type (1.3) and, presumably, to extend the non-numerical analysis to the 'Jost function' or even to its energy zeros.

Some of the present results are quite surprising.

(i) When we return to the non-rescaled problem and consider the strong anharmonic coupling $\nu \gg 1$, the present formula (1.3) contains the small expansion parameter $\nu^{-1/8}$. Its exponent differs from the usual $\nu^{-1/3}$ rule (see, e.g., Arteca *et al* 1984).

(ii) For a small coupling $\nu \ll 1$, formula (1.3) exhibits anew the non-perturbative character of the anharmonicity.

(iii) In comparison with the not very exciting zero-order result of II ($c_0^{(j)} = \mathrm{i}\pi$, $j = 1, 2, 3$ and 4), a lot of physics is clarified by the first non-trivial coefficient $c_1^{(j)}$:

(a) the double degeneracy of the 'Jost' solutions of the truncated equations (§ 2) survives the infinite-dimensional limiting transition and this is extremely favourable in the numerical context;

(b) an unexpected $n \gg 1$ asymptotic oscillation ($\mathrm{Im}\, c_1^{(j)} \neq 0$) appears, contrasting with the smooth asymptotic behaviour of the Hamiltonian itself.

(iv) The higher-order corrections ($c_m^{(j)}$, $m > 1$) keep a simple form as functions of the parameters. This clarifies the structure of ψ in a non-numerical manner—its smooth change during the transition to the double-well potential ($\mu < 0$), etc. The $m > 1$ corrections are also essential in improving the standard variational estimates.

(v) The stability and extreme efficiency of the recurrent eigenvalue/eigenvector algorithm of § 5 follows from the leading-order part of (1.3). We may expect (conjecture) that the similar properties of recurrences will remain valid for the higher anharmonicities r^{2q}, $q \geq 3$ as well.

2. The truncated Hamiltonian and the method

In the variational setting, we may truncate equation (1.2). Its cut-off $(M+1)$-dimensional subsystems for the tilded approximants of ψ

$$Q^{[M]}\tilde{\psi} = 0$$

$$Q^{[M]} = \begin{pmatrix} a_0 & b_0 & c_0 & \\ & \cdots & & \\ & c_{M-2} & b_{M-1} & a_M \end{pmatrix} \qquad \tilde{\psi} = \begin{pmatrix} \tilde{\psi}(0) \\ \cdots \\ \tilde{\psi}(M) \end{pmatrix} \tag{2.1}$$

will give the exact result in the limit $M \to \infty$ only,

$$\tilde{\psi}(n) \to \langle n|\psi\rangle \qquad \tilde{E} \to E \qquad M \to \infty.$$

For a finite $M < \infty$, the solution of (2.1) may be obtained by standard methods (Wilkinson 1965) as well as by our method (I, II, III). The latter approach may be summarised as follows.

2.1. The 'regular' $n \to n+1$ recurrences

The first row of (2.1) is a definition of $\tilde{\psi}(2)$. It is a linear function of the two unknown parameters $\tilde{\psi}(0)$ and $\tilde{\psi}(1)$. Similarly, the second row gives $\tilde{\psi}(3)$ as a function of $\tilde{\psi}(0)$ and $\tilde{\psi}(1)$ after the appropriate insertion. In this way, the general formula

$$\begin{gathered}\tilde{\psi}(k) = \alpha_k \tilde{\psi}(0) + \beta_k \tilde{\psi}(1) \\ \alpha_k = \frac{(-1)^{k+1} \det R^{(1,k)}}{c_0 c_1 \ldots c_{k-2}} \qquad \beta_k = \frac{(-1)^{k+1} \det R^{(2,k)}}{c_0 c_1 \ldots c_{k-2}} \\ R^{(j,k)}_{m1} = Q^{[k-2]}_{mj} \qquad R^{(j,k)}_{mn} = Q^{[k-1]}_{mn+1} \begin{cases} j = 1, 2 & m = 1, 2, \ldots, k-1 \\ n = 2, 3, \ldots, k-1 & k = 2, 3, \ldots \end{cases}\end{gathered} \tag{2.2}$$

is obtained (I). At an arbitrary energy, it defines the two independent 'regular' solutions (say, α_k and β_k) which satisfy even our $M = \infty$ equation (1.2) and are not normalisable in general.

In the truncated equation (2.1), the last two rows are redundant as definitions and represent rather the two independent truncation requirements

$$\tilde{\psi}(M+1) = 0 \qquad \tilde{\psi}(M+2) = 0. \tag{2.3}$$

This is a physical 'boundary condition' for our 'regular' solution (2.2). It has to fix $\tilde{\psi}(1)/\tilde{\psi}(0)$ and the energy.

A combination of (2.2) with (2.3)

$$\begin{pmatrix} \alpha_{M+1} & \beta_{M+1} \\ \alpha_{M+2} & \beta_{M+2} \end{pmatrix} \begin{pmatrix} \tilde{\psi}(0) \\ \tilde{\psi}(1) \end{pmatrix} = 0 \tag{2.4}$$

is formally equivalent to the standard secular equation

$$\det Q^{[M]} = 0 \tag{2.5}$$

of course, but it also admits systematic improvements (cf I and § 4 below).

2.2. The 'Jost' $n+1 \to n$ recurrences

In a reversed formulation of the recurrences (2.1), the 'Jost' parameters $\tilde{\psi}_J(M)$ and $\tilde{\psi}_J(M-1)$ define $\tilde{\psi}_J(M-2), \ldots$ and/or the determinantal counterpart

$$\begin{gathered}\tilde{\psi}_J(M-k) = \gamma_{M-k} \tilde{\psi}_J(M) + \delta_{M-k} \tilde{\psi}_J(M-1) \\ \gamma_k = \frac{(-1)^{k+1}}{c_{M-2} c_{M-3} \ldots c_{M-k}} \det S^{(1,k)} \qquad \delta_k = \frac{(-1)^{k+1}}{c_{M-2} c_{M-3} \ldots c_{M-k}} \det S^{(0,k)} \\ S^{(j,k)}_{mk-1} = Q^{[M]}_{M+2+m-k,M+j} \qquad S^{(j,k)}_{mn} = Q^{[M]}_{M+2+m-k,M+1+n-k} \\ n = 1, 2, \ldots, k-2 \qquad j = 0, 1 \\ m = 1, 2, \ldots, k-1 \qquad k = 2, 3, \ldots, M\end{gathered} \tag{2.6}$$

to (2.2). The remaining two rows of (1.2) or (2.1),

$$\tilde{\psi}_J(-1) = 0 \qquad \tilde{\psi}_J(-2) = 0 \tag{2.7}$$

reflect the termination of recurrences at the origin.

2.3. *The matching of solutions*

In both §§ 2.1 and 2.2, the direct generation of $\tilde{\psi}(k)$ from the respective sequence of rows (2.1) is a recurrent algorithm. It is characterised by the minimal computer storage demands (the rigorous determinantal formulae (2.3) and (2.7) necessitate a big computer) and by the possible instabilities.

We may suppress the latter shortcoming and, in analogy with the differential-equation algorithms (Korn and Korn 1968), match the 'regular' and 'Jost' solutions for an intermediate domain of indices. In the present truncated case, both these solutions contain two free parameters so that we need four conditions in general,

$$\tilde{\psi}_{\mathrm{R}}(K_i) = \tilde{\psi}_{\mathrm{J}}(K_i) \qquad i = 1, 2, 3, 4. \tag{2.8}$$

This equation also encompasses (2.3) and (2.7) as special cases.

3. The general algebraic solution for the recurrences

3.1. *Difference equation in the asymptotic region*

In the lowest-order asymptotic approximation, the recurrences (1.2) read

$$\langle M-2|\psi\rangle + 4\langle M-1|\psi\rangle + 6\langle m|\psi\rangle + 4\langle M+1|\psi\rangle + \langle M+2|\psi\rangle = 0 \qquad M \gg 1 \tag{3.1}$$

and have been analysed in I. The result $\langle M|\psi\rangle \simeq (-1)^M$ may easily be understood—it is sufficient to notice that the left-hand side of (3.1) defines just the fourth difference of the function $(-1)^M\langle M|\psi\rangle$ (Korn and Korn 1968). The general solution of (3.1), $\langle M|\psi\rangle = (-1)^M(a + bM + cM^2 + dM^3)$ remains unphysical (non-normalisable) unless $b = c = d = 0$ (II, lemma 1).

Without the inclusion of the corrections, we cannot distinguish between the $\|\psi\| < \infty$ and $\|\psi\| = \infty$ cases. Thus, we have to replace (3.1) by an improved asymptotic form of the recurrences (1.2),

$$\begin{gathered} C_1\xi(M-2) + C_2\xi(M-1) + C_3\xi(M) + C_4\xi(M+1) + C_5\xi(M+2) = 0 \\ C_i = \sum_{m=0}^{L} C_i^{(m)} \frac{1}{M}\left(1 + \frac{2-m}{M}\rho\right) + \mathrm{O}(M^{-L-1}) \\ i = 1, 2, \ldots, 5 \qquad M \geqslant 1 \qquad L > 0 \qquad \rho = \tfrac{1}{2}l + \tfrac{1}{4} \end{gathered} \tag{3.2}$$

where $\xi(M) = (-1)^M\langle M-1|\psi\rangle$ and a sample of the coefficients is given in table 1.

Table 1. The first few coefficients in equation (3.2) ($\rho = \frac{1}{2}l + \frac{1}{4}$).

m	$C_1^{(m)}$	$C_2^{(m)}$	$C_3^{(m)}$	$C_4^{(m)}$	$C_5^{(m)}$
0	1	-4	6	-4	1
1	-3	$9-\mu$	$2\mu-4$	$1-\mu$	1
2	2	$-2\rho^2+\mu-5$	$4\rho^2+1-\mu-E$	$-2\rho^2$	0
3	0	$\frac{1}{2}\rho^2(\mu-1)$	0	$\frac{1}{2}\rho^2(\mu-1)$	0
4	$-\frac{1}{2}\rho^2$	$\frac{1}{2}\rho^4-\frac{1}{2}\rho^2(1-\mu)$	0	$\frac{1}{2}\rho^4$	$-\frac{1}{2}\rho^2$

The solution of the difference equations (3.2) would be rather complicated in general. Fortunately, we may recall the estimate

$$\frac{\langle N|\psi\rangle}{\langle N-1|\psi\rangle}=-1\pm\frac{\text{const}}{N^{1/4}}+\mathrm{O}\left(\frac{1}{N^{1/2}}\right) \tag{3.3}$$

(I, theorem 3) and put $\xi(N)=\exp(f(N))$, $N\gg 1$. Then, we may expect that

$$f(N)=\mathrm{O}(N^{3/4}) \qquad f'(N)=\mathrm{O}(N^{-1/4}) \qquad f''(N)=\mathrm{O}(N^{-5/4}) \qquad \text{etc} \tag{3.4}$$

and use the approximants (truncated Taylor expansions)

$$\begin{aligned}\xi(M+n)&=\xi(M)+\frac{n}{1!}\xi'(M)+\ldots+\frac{n^K}{K!}\xi^{(K)}(M)\\&=\xi(M)\left(1+\frac{n}{1!}f'(M)+\frac{n^2}{2!}f''(M)+\ldots+\mathrm{O}\left(\frac{1}{M^{(K+1)/4}}\right)\right).\end{aligned} \tag{3.5}$$

This is our main idea—in a combination of (3.2) and (3.5), we shall postulate the compatibility of errors (3.3),

$$L+1>\tfrac{1}{4}K\geqslant L \tag{3.6}$$

and search for the coefficients in the asymptotic series (1.3).

3.2. *The first- and second-order solutions*

In the first non-trivial case with $L=1$ and $K=4$, we insert (3.5) into (3.2), omit the higher-order corrections and get the differential equation

$$\frac{\mathrm{d}^4}{\mathrm{d}M^4}\xi(M)+\frac{4}{M}\xi(M)=0. \tag{3.7}$$

When we take into account also (3.3) and the corresponding error estimate, the differential equation (3.7) becomes reducible to the algebraic equation

$$[(f'(M))^4+4/M](1+\mathrm{O}(1/M^{1/4}))=0 \tag{3.8}$$

since f'' remains negligible. In the resulting wavefunction estimate

$$\begin{aligned}&\langle M-1|\psi\rangle=(-1)^M\exp(f(M))\\&f(M)=\tfrac{4}{3}(\pm1\pm\mathrm{i})M^{3/4}+\mathrm{O}(M^{1/2})\end{aligned} \tag{3.9}$$

the first sign ambiguity distinguishes between the decreasing and increasing components while the second merely reflects their double degeneracy. The asymptotics exhibit slow oscillations—this is a rather surprising phenomenon and contrasts with the smooth behaviour of the matrix elements.

An interesting feature of (3.8) and (3.9) is a non-trivial observation that the second-order corrections drop out. Thus, we have to use the error term $\mathrm{O}(M^{1/4})$ in (3.9).

3.3. *The third-order solution*

On the $1+O(M^{-3/4})$ error level, we use (3.5) with $K=6$ and (3.2) with $L=1$. The resulting differential equation

$$\tfrac{1}{6}\xi^{(6)}(M)+\xi^{(4)}(M)+\frac{1-\mu}{M}\xi^{(2)}(M)+\frac{4}{M}\xi(M)=0 \tag{3.10}$$

and its asymptotic solution (3.9) with

$$\begin{aligned} &f(M)=\tfrac{4}{3}aM^{3/4}+bM^{1/2}+4cM^{1/4}+\ldots \\ &a=(-4)^{1/4}=\pm 1\pm \mathrm{i} \qquad b=0 \qquad c=\frac{\mu-\frac{1}{3}}{4a} \end{aligned} \tag{3.11}$$

complement (3.7) and (3.9), respectively. They have the following three interesting features.

(i) The asymptotics of $\langle N|\psi\rangle$ depend now on μ (the inverse measure of anharmonicity of the potential).

(ii) In accord with our expectations, the fundamental set of the six independent solutions of the differential equation (3.10) of the sixth order degenerates to four independent solutions in the asymptotic region.

(iii) The full degeneracy in the decreasing/increasing pair of solutions (i.e., in $\operatorname{Re} f(N)$) remains unremoved as well.

3.4. *The fourth- and fifth-order solutions*

An inclusion of the $O(M^{-3/4})$ corrections modifies (3.10) by the only additional term $4\xi^{(3)}(M)/M$ which introduces the M^{-1} correction in $f'(M)$ and adds a logarithmic correction to (3.11). Hence, the further corrections may be moved out of the exponential—the algebra (fully analogous to the preceding cases) gives

$$\langle M-1|\psi\rangle=\frac{(-1)^M Z(M)}{M^{5/8}}\exp\left(\frac{4}{3}aM^{3/4}+\frac{\mu-\frac{1}{3}}{a}M^{1/4}\right) \qquad a=(-4)^{1/4}. \tag{3.12}$$

Thus, the further corrections appear in the normalisation factor $Z=\text{constant}+O(M^{-1/4})$ and may be made arbitrarily small by our choice of the parameter $M\gg 1$.

The first non-trivial contribution to the expansion of Z necessitates $L=2$ in (3.2). Moreover, in contrast to the preceding cases, we must also incorporate the second derivative $f''(M)$ into the formulae. Then, from the related differential equation

$$\begin{aligned} &\tfrac{1}{80}\xi^{(8)}+\tfrac{1}{6}\xi^{(6)}+\left(1+\frac{2\rho-1+(1-\mu)/12}{M}\right)\xi^{(4)}+\frac{4}{M}\xi^{(3)} \\ &\qquad +\frac{1-\mu}{M}\xi^{(2)}+\left(\frac{4}{M}+\frac{4\rho-2-E}{M^2}\right)\xi=0 \qquad \rho=\tfrac{1}{2}l+\tfrac{1}{4} \end{aligned} \tag{3.13}$$

we obtain

$$\begin{aligned} &Z(M)=1+AM^{-1/4}+O(M^{-1/2}) \\ &A=a[\tfrac{1}{32}(1+\mu)^2+\rho-\tfrac{11}{20}-\tfrac{1}{4}E] \end{aligned} \tag{3.14}$$

in a straightforward way. There appears an explicit l and energy dependence here—our asymptotic formula (3.12)+(3.14) contains all the relevant parameters now.

3.5. The higher-order corrections

For $K \geqslant 9$, most of our conclusions will remain unchanged. The formulae become rather clumsy—let us close this section by the $K = 19$ example, namely, by the differential equation

$$\begin{aligned}
8 \sum_{t=1}^{8} \frac{4^t-1}{(2t+2)!} \xi^{(2t+2)} &+ \frac{8}{M} \sum_{t=1}^{7} \frac{4^t-1}{(2t+1)!}\left(1+\frac{\rho-\frac{1}{2}}{M}\right)\xi^{(2t+1)} \\
&+\frac{2}{M}\sum_{t=1}^{7}\frac{8(4^{t-1}-1)\rho-4^t+5-\mu}{(2t)!}\xi^{(2t)}+\frac{1-\mu}{M^2}\sum_{t=0}^{5}\frac{1}{(2t+1)!}\xi^{(2t+1)} \\
&+\frac{1}{M^2}\sum_{t=1}^{5}\frac{2(4^t-5)(1-\rho)+5+\mu-2\mu\rho-4\rho^2}{(2t)!}\xi^{(2t)} \\
&+\frac{(\mu-1)\rho^2}{M^3}\sum_{t=0}^{3}\frac{1}{(2t)!}\xi^{(2t)}+\frac{(1-\mu)\rho^2}{2M^4}\sum_{t=0}^{1}\frac{1}{(2t+1)!}\xi^{(2t+1)} \\
&+\frac{1}{2M^4}[\rho^4-4\rho^2-(\mu-1)(\rho-\tfrac{1}{2})\rho^2]\xi^{(2)} \\
&+\left(\frac{4}{M}+\frac{4\rho-2-E}{M^2}+\frac{2\rho^2+2(1-\mu)\rho+\mu-3}{M^4}\right)\xi=0. \qquad (3.15)
\end{aligned}$$

Its conversion into an algebraic problem would give the coefficient Z in $\langle M-1|\psi\rangle$ (3.12) valid up to the error factor $1+O(1/M^{13/4})$.

4. Properties of the 'regular' solutions

In the truncated problem of § 2, full symmetry between the 'regular' and 'Jost' solutions occurs. In the limit $M \to \infty$, only the 'regular' formula (2.2) remains valid. Fortunately, we may construct the 'Jost' solutions by the asymptotic expansion method of § 3. Thus, the formal symmetry may be restored provided only that we replace the limiting boundary condition (2.3) by the matching (2.8) at some sufficiently large but fixed values of the matching points $K_i = M_0 - i$, $M_0 \gg 1$.

In the regular solution $\tilde{\psi}(k)$, the random round-off error in $\tilde{\psi}(0)$ and $\tilde{\psi}(1)$ introduces a quickly increasing error into the higher components. For $k \gg 1$, we must compute them directly from the determinantal formula (2.2) and keep the unstable asymptotic behaviour of the $n \to n+1$ recurrences in mind. This is fully analogous to the problem encountered in solving the differential equation (e.g., Acton 1970)—we must suppress the non-physical components of ψ.

4.1. Elimination of the growing exponentials in the asymptotic region—the mechanism

For almost all energies and projections $\tilde{\psi}(1)/\tilde{\psi}(0)$, the physical normalisability requirement

$$\|\psi\| = \left(\sum_{n=0}^{\infty} |\langle n|\psi\rangle|^2\right)^{1/2} < \infty \qquad (4.1)$$

will be violated by the $k \gg 1$ part of the 'regular' solution $\psi_R(k) = \tilde{\psi}(k)$ (2.2),

$$\begin{aligned} \psi_R(k) &= (-1)^k\, e^{\gamma(k)}(A\cos\delta(k) + B\sin\delta(k))[1 + O(\exp(-2\gamma(k)))] \\ \gamma(k) &= \tfrac{4}{3}k^{3/4} + \tfrac{1}{2}(\mu - \tfrac{1}{3})k^{1/4} - \tfrac{5}{8}\ln k + \ldots \\ \delta(k) &= \tfrac{4}{3}k^{3/4} - \tfrac{1}{2}(\mu - \tfrac{1}{3})k^{1/4} + \ldots \end{aligned} \tag{4.2}$$

(cf (3.12)). Vice versa, we get the physical energy $E = E_0$ and ratio $q = \psi_R(1)/\psi_R(0) = q_0$ precisely for the physical bound states $\psi_R(k) = \langle k|\psi\rangle$, i.e., for

$$A(E_0, q_0) = 0 \qquad B(E_0, q_0) = 0 \tag{4.3}$$

(cf also equation (4.7) below). In their vicinity, we neglect the exponential corrections $O(\exp(-2\gamma))$ in (4.2), denote $v_i = (-1)^{k_i}\psi_R(k_i)\exp(-\gamma_i)$, $\gamma_i = \gamma(k_i)$, $\delta_i = \delta(k_i)$ and re-express $A = A(k)$ and $B = B(k)$ as functions of v_r and v_s for some pair of indices $r > s$,

$$\begin{aligned} \begin{pmatrix} A \\ B \end{pmatrix} &= \frac{1}{\sin\delta_{rs}}\begin{pmatrix} \sin\delta_r & -\sin\delta_s \\ -\cos\delta_r & \cos\delta_s \end{pmatrix}\begin{pmatrix} v_s \\ v_r \end{pmatrix} \\ \delta_{rs} &= \delta_r - \delta_s. \end{aligned} \tag{4.4}$$

Now, we may rewrite (4.3) as a condition $A^2 + B^2 = 0$, i.e.,

$$v_r^2 + v_s^2 - 2v_r v_s \cos\delta_{rs} = 0$$

which implies that $v_r = v_s = 0$ since $\delta_{rs} \simeq \tfrac{3}{4}(k_r - k_s)/k_s^{1/4}$ is non-zero for $k_s \gg 1$. Thus, with $k_r = k_s + 1$, we have merely rederived the truncation requirement (2.3) in a non-variational manner.

In an alternative formulation, we may consider $E \neq E_0$, $q \neq q_0$ and introduce also a discrete analogue of the derivatives which depend on the functions $\gamma(k)$ and $\delta(k)$,

$$w_{rs}^{(1)} = (v_r - v_s\cos\delta_{rs})/\sin\delta_{rs} \qquad r \neq s.$$

Then, it is easy to verify that

$$\begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} \cos\delta_s, & -\sin\delta_s \\ \sin\delta_s, & \cos\delta_s \end{pmatrix}\begin{pmatrix} v_s \\ w_{rs}^{(1)} \end{pmatrix} \tag{4.5}$$

and see that the lengths of vectors (A, B) and $(v_s, w_{rs}^{(1)})$ are equal. This simplifies (4.4) and clarifies the role of the angle $\delta(k)$ 'mixing' the non-physical 'regular' solution v with its first difference or 'derivative' $w^{(1)}$.

We may conclude that the physical asymptotics for the 'regular' solutions may be represented by a pair of requirements

$$v_s = O(\exp(-k_s^{3/2})) \qquad w_{rs}^{(1)} = O(\exp(-k_s^{3/2})). \tag{4.6}$$

In principle, they determine q_0 and energy E_0 with an arbitrary accuracy limited only by our choice of the finite matching points $k_r \gg 1$ and $k_s \gg 1$.

4.2. Physical wavefunctions—the structure

At the physical values $E = E_0$ and $q = q_0$, equation (4.2) must be replaced by the $A = B = 0$ asymptotic estimate

$$\psi_R(k) = \langle k|\psi\rangle = (-1)^k\exp(-\gamma(k))(C\cos\delta(k) + D\sin\delta(k)). \tag{4.7}$$

In essence, this may be interpreted as a matching condition (2.8) where the right-hand-side expression represents the 'Jost' asymptotic solution (1.3).

Analysing (4.7) in more detail, we may denote

$$X_i = X(k_i) = (-1)^{k_i} \exp(\gamma(k_i))\psi_R(k_i)$$

and obtain an analogue of (4.4),

$$\begin{pmatrix} C \\ D \end{pmatrix} = \frac{1}{\sin \delta_{rs}} \begin{pmatrix} \sin \delta_r & -\sin \delta_s \\ -\cos \delta_r & \cos \delta_s \end{pmatrix} \begin{pmatrix} X_s \\ X_r \end{pmatrix}. \tag{4.8}$$

With the two particular choices of $(r, s) = (2, 1)$ and $(4, 3)$, we may eliminate C and D here,

$$\sin \delta_{21} \begin{pmatrix} X_3 \\ X_4 \end{pmatrix} = \begin{pmatrix} \sin \delta_{23}, & \sin \delta_{31} \\ \sin \delta_{24}, & \sin \delta_{41} \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}. \tag{4.9}$$

This relation characterises the physical states and, in the leading-order approximation, it acquires the form

$$\begin{pmatrix} X_3 \\ X_4 \end{pmatrix} = \begin{pmatrix} -1 & 2 \\ -2 & 3 \end{pmatrix} \begin{pmatrix} X_1 \\ X_2 \end{pmatrix} \tag{4.10}$$

obtained (obtainable) also in the matrix continued-fractional formalism (III).

The numerical test of our non-truncation matching condition (4.7) is presented in table 2. We have employed the leading-order precision only, so that our results also conform with the simplified equation (4.10). We observe that our energies improve slightly the M_0-dimensional diagonalisation for the dimensions $M_0 = O(1)$ only, and reproduce it for the larger M_0.

Table 2. Coincidence of energies from the boundary condition (4.7) ($X_1 = X_2 = X_3$) with their variational counterparts (three dimensions, ground state, $\mu = 1$, $E_{\text{exact}} = 4.648\,8127$).

M_0	Present result	Variational result
9	4.650 924	4.650 939
10	4.649 433	4.649 440
11	4.648 919	4.648 920
12	4.648 824	4.648 824
13	4.648 819	4.648 819

4.3. *Matching conditions as difference relations*

When we try to understand or re-interpret the matching criteria (4.9) or (4.10), we may asume that $X_i \neq 0$ is a smooth function of the variable k_i. Then, recalling (4.5) and the definition

$$Y_{rs}^{(1)} = (X_r - X_s \cos \delta_{rs}) / \sin \delta_{rs}$$

we may derive the $A = B = 0$ formula

$$\begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} \cos \delta_s, & -\sin \delta_s \\ \sin \delta_s, & \cos \delta_s \end{pmatrix} \begin{pmatrix} X_s \\ Y_{rs}^{(1)} \end{pmatrix} \tag{4.11}$$

and eliminate the unknown parameters C and D again.

With the two pairs of subscripts (r, s) and (t, r), the two rows of the resulting relations

$$\begin{pmatrix} \cos\delta_s & -\sin\delta_s \\ \sin\delta_s & \cos\delta_s \end{pmatrix}\begin{pmatrix} X_s \\ Y_{rs}^{(1)} \end{pmatrix} = \begin{pmatrix} \cos\delta_r & -\sin\delta_r \\ \sin\delta_r & \cos\delta_r \end{pmatrix}\begin{pmatrix} X_r \\ Y_{tr}^{(1)} \end{pmatrix} \tag{4.12}$$

remain linearly dependent. Thus, we may replace δ_r by $\delta_s + \delta_{rs}$ and get the relation

$$X_r = (Y_{rs}^{(1)} - Y_{tr}^{(1)} \cos\delta_{rs})/\sin\delta_{rs}. \tag{4.13}$$

It is equivalent to a row of (4.9) and connects the physical 'regular' solution with its second derivative in the limit $\delta_{rs} \to 0$. It may again be used as a matching condition.

To conclude this section, let us summarise: for the large matching indices, $M_0 \gg 1$, the ratio between the non-physical and physical exponential factors is an extremely large number. Unless we have a computer with roughly of the order of $M_0^{3/4}$ digits, we must expect an 'underflow' $C = D = 0$ (within the round-off errors) and return to the truncation prescription (2.3). Vice versa, whenever we want to exceed the precision of the M_0-dimensional diagonalisation, we must use small M_0 and improve the asymptotic 'Jost' solution for the matching conditions. Otherwise, the physical requirement $A = B = 0$ will remain an ill-conditioned equation (see the appendix).

5. Recurrent construction of the physical bound states

5.1. *Numerical stability of the backward $n+1 \to n$ recurrences*

Numerical tests indicate that the recurrences (1.2) are stable in the decreasing $n+1 \to n$ 'Jost' direction. In the $n \gg 1$ asymptotic region, this may be proved directly. With the fundamental set of solutions

$$\begin{aligned} \psi_{(1)}(k) &= \exp(-\gamma(k)) \cos\delta(k) \qquad & \psi_{(2)}(k) &= \exp(-\gamma(k)) \sin\delta(k) \\ \psi_{(3)}(k) &= \exp(+\gamma(k)) \cos\delta(k) \qquad & \psi_{(4)}(k) &= \exp(+\gamma(k)) \sin\delta(k) \end{aligned} \tag{5.1}$$

we may rewrite any trial initialisation of (1.2) in the form of a superposition

$$\psi_J(k) = A\psi_{(3)}(k) + B\psi_{(4)}(k) + C\psi_{(1)}(k) + D\psi_{(2)}(k) \qquad k = N \gg 1. \tag{5.2}$$

Then, using the asymptotic formulae of § 3 (e.g., (3.12)), it is easy to show that the non-physical components $\psi_{(3)}(k)$ and $\psi_{(4)}(k)$ of ψ disappear for each $C \neq 0$ or $D \neq 0$ after a few iterations. Hence, the 'Jost' initialisation of (1.2) is arbitrary—it gives $A = B = 0$ (the physical 'Jost' solutions $\psi_J^{(C,D)}(k)$) for all the indices $k \leq M_0$, provided only that $M_0 \ll N$. The two-parametric family $\psi_J(k)$ which we obtain is a full analogue of the truncated example of § 2.

In the asymptotic region, the explicit form (3.12) of 'Jost' solutions enters the matching conditions (say, (4.7) or (A.1)) in the γ, δ-parametrised form. Now, we may preserve this notation and define

$$\begin{aligned} \gamma(k) &= -\tfrac{1}{2}\ln[(\psi_J^{(C_1,D_1)}(k))^2 + (\psi_J^{(C_2,D_2)}(k))^2] \\ \delta(k) &= \tan^{-1} \psi_J^{(C_1,D_1)}(k)/\psi_J^{(C_2,D_2)} \qquad k \geq 0 \end{aligned} \tag{5.3}$$

even for the recurrently computed (numerical) 'Jost' solutions (5.2) and in the non-asymptotic region. Up to the differences of the asymptotic order $O(\ln k)$, the new definition will coincide precisely with the one given in equation (4.2).

5.2. *The recurrent eigenvalue/eigenvector algorithm—'Jost function'*

Due to the monotonic n dependence of the coefficients in (1.2), we may expect the numerically stable behaviour of the backward $n+1 \to n$ recurrences even near the origin. Indeed, in contrast to our differential-equation method guide, our difference equation (1.2) does not exhibit any singularity there. Thus, the $n+1 \to n$ recurrent evaluation of the 'Jost' solutions may proceed up to $n=0$ and be complemented simply by the physical boundary condition (2.7) at the origin.

The related technicalities become extremely simple now. The two different initial values (5.2) generate the linearly independent pair of normalisable solutions $\psi_J^{(a)}(n)$ and $\psi_J^{(b)}(n)$, $n \geqslant 0$, and the remaining (first two) rows of (1.2) again represent the boundary conditions (2.7). Thus, the physical wavefunctions will have the general form

$$\langle n|\psi\rangle = C\psi_J^{(a)}(n) + D\psi_J^{(b)}(n) \qquad n \geqslant 0. \tag{5.4}$$

Its insertion into (2.7) gives the two-dimensional eigenvalue/eigenvector equation

$$\begin{gathered}\begin{pmatrix} T_{1a} & T_{1b} \\ T_{2a} & T_{2b} \end{pmatrix}\begin{pmatrix} C \\ D \end{pmatrix} = 0 \\ T_{1i} = a_0\psi_J^{(i)}(0) + b_0\psi_J^{(i)}(1) + c_0\psi_J^{(i)}(2) \qquad i = a, b \\ T_{2i} = b_0\psi_J^{(i)}(0) + a_1\psi_J^{(i)}(1) + b_1\psi_J^{(i)}(2) + c_1\psi_J^{(i)}(3). \end{gathered} \tag{5.5}$$

This specifies the non-zero coefficients C and D for a discrete set of physical binding energies only.

Obviously, the energies may be determined numerically as roots of the secular equation

$$\det\begin{pmatrix} T_{1a} & T_{1b} \\ T_{2a} & T_{2b} \end{pmatrix} = 0. \tag{5.6}$$

We may notice that this secular determinant represents a direct generalisation of the Jost function (Newton 1965) to the present difference equation case (with quotation marks).

The practical test of our algorithm and a sample of the numerical results are displayed in table 3. It illustrates both the stability of the energies and their quick rate of convergence. In principle, this convergence may be accelerated by choosing the initial values (5.2) compatible with the physical requirement (4.7). Then, a smaller dimension N or M_0 (number of iterations) will be needed in the computations. In this sense, our method should be generalised in the future—it is a significant improvement on the common truncation technique.

Table 3. Quick rate of convergence of energies E computed as roots of the 'Jost function' (5.6) ($M_0 = 0$). At $n = N$, the initialisation of $\psi_J^{(a,b)}(n)$ is random.

N	$E - E_{\text{exact}}$ ($\mu = 1$)	$E - E_{\text{exact}}$ ($\mu = 0$)
10	-0.80×10^{-6}	-0.26×10^{-6}
15	$+0.23 \times 10^{-8}$	-0.84×10^{-8}
20	$+0.48 \times 10^{-10}$	$+0.80 \times 10^{-12}$
25	$O(10^{-13})$	$O(10^{-13})$

Appendix. Matching conditions once more

When we recall the algebraic solution of § 3 or its recurrent and reparametrised form of § 5.1, we may rewrite the matching conditions (2.8) in the 4×4 matrix form

$$\begin{aligned} &\psi_{\mathrm{R}}(k_i) = AG_{i1} + BG_{i2} + CG_{i3} + DG_{i4} \qquad i = 1, 2, 3, 4 \\ &G_{i1} = \exp(\gamma_i)\cos\delta_i \qquad G_{i2} = \exp(\gamma_i)\sin\delta_i \\ &G_{i3} = \exp(-\gamma_i)\cos\delta_i \qquad G_{i4} = \exp(-\gamma_i)\sin\delta_i. \end{aligned} \tag{A1}$$

By algebraic means, the corresponding inversion G^{-1} may be performed without any loss of precision.

First, let us evaluate the determinant of the matrix G in (A1),

$$\begin{aligned} &\det G = Z_{1234} + Z_{1342} + Z_{1423} \\ &Z_{ijkl} = 2\cosh(\gamma_{ik} + \gamma_{jl})\sin\delta_{ij}\sin\delta_{kl} \\ &\gamma_{ij} = \gamma_i - \gamma_j \qquad \delta_{ij} = \delta_i - \delta_j \end{aligned} \tag{A2}$$

and notice that the cancellations take place here. Indeed, the leading-order asymptotic $O(M_0^{-1/2})$ component of (A2) becomes equal to zero as a consequence of the simple trigonometry,

$$\begin{aligned} \det G &= 2\cosh(\gamma_{13} + \gamma_{24})\sin\delta_{12}\sin\delta_{34} + \ldots \\ &= \cosh(\gamma_{13} + \gamma_{24})\cos(\delta_{12} - \delta_{34}) - \ldots \\ &= 2\sinh^2[\tfrac{1}{2}(\gamma_{13} + \gamma_{24})]2\sin^2[\tfrac{1}{2}(\delta_{12} + \delta_{34})] + \ldots . \end{aligned} \tag{A3}$$

Next, the asymptotic estimates

$$\begin{aligned} &\gamma_{ij} = (i-j)(\rho + b\rho^3) \qquad \delta_{ij} = (i-j)(\rho - b\rho^3) \\ &\rho = \text{constant}/M_0^{1/4} \qquad b = \text{constant} \times (1 + O(\rho)) \end{aligned} \tag{A4}$$

based on (3.12) imply that the coefficient in (A3) is also equal to zero in the asymptotic region,

$$\begin{aligned} \det G &= 4\sinh^2[\tfrac{1}{2}(4\rho + 4b\rho^3)]\sin^2(\rho - b\rho^3) + \ldots \\ &= 16[\sinh(2\rho + 2b\rho^3)\sin(\rho - b\rho^3) \\ &\quad + \sinh(\rho + b\rho^3)\sin(2\rho + 2b\rho^3)]\sinh(\rho + b\rho^3)\sin(\rho - b\rho^3) \\ &\quad \times\{\sinh^2[\tfrac{1}{2}(\rho + b\rho^3)] + \sin^2[\tfrac{1}{2}(\rho - b\rho^3)]\} = 32\rho^6(1 + O(\rho^3)). \end{aligned} \tag{A5}$$

Thus, the resulting determinant is of the order of magnitude $O(M_0^{-3/2})$. This would deteriorate the quality of a numerical solution of equation (A1).

Of course, the algebraic inversion will be equivalent to equations (4.9) or (4.13). For completeness, let us give the resulting formulation of the physical requirement $A = B = 0$,

$$\begin{aligned} &\sum_{j=1}^{4} \tilde{G}_{ij}\tilde{\psi}_{\mathrm{R}}(k_j) = 0 \qquad i = 1, 2 \\ &\tilde{G}_{11} = \sin\delta_2\sin\delta_{34}\exp(\gamma_2 - \gamma_3 - \gamma_4) + \sin\delta_3\sin\delta_{42}\exp(\gamma_3 - \gamma_4 - \gamma_2) \\ &\qquad + \sin\delta_4\sin\delta_{23}\exp(\gamma_4 - \gamma_2 - \gamma_3) \end{aligned} \tag{A6}$$

and notice that the omitted coefficients may be generated by a sequence of replacements

$$\tilde{G}_{1j+1} = \tilde{G}_{1j}\ (\text{subscript}\ j+1 \rightarrow \text{subscript}\ j) \qquad j = 1, 2, 3$$

$$\tilde{G}_{2j} = \tilde{G}_{1j}\ (\sin \delta_m \rightarrow \cos \delta_m,\ m \neq j) \qquad j = 1, 2, 3, 4.$$

References

Acton F S 1970 *Numerical Methods that Work* (New York: Harper and Row)
Arteca G A, Fernández F M and Castro E A 1984 *J. Math. Phys.* **25** 932, 2377
Au C K, Rogers G W and Aharonov Y 1983 *Phys. Lett.* **95A** 287
Graffi S and Grecchi V 1975 *Lett. Nuovo Cimento* **12** 425
Itzykson C and Zuber J B 1980 *Quantum Field Theory* (New York: McGraw-Hill)
Korn G A and Korn T M 1968 *Mathematical Handbook* (New York: McGraw-Hill)
Lister D G, MacDonald J N and Owen N L 1978 *Internal Rotation and Inversion* (London: Academic)
Makarewicz J 1984 *J. Phys. A: Math. Gen.* **17** 1449
Marziani M F 1984 *J. Phys. A: Math. Gen.* **17** 547
Newton R G 1965 *Scattering Theory of Waves and Particles* (New York: McGraw-Hill)
Flessas G P, Whitehead R R and Rigas A 1984 *J. Math. Phys.* **25** 910
Wilkinson J H 1965 *The Algebraic Eigenvalue Problem* (Oxford: Clarendon)
Znojil M 1983 *J. Phys. A: Math. Gen.* **16** 293
—— 1984a *J. Math. Phys.* **25** 2979
—— 1984b *J. Phys. A: Math. Gen.* **17** 1603
—— 1984c *J. Phys. A: Math. Gen.* **17** 1611