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1984 J. Phys. A: Math. Gen. 17 3441

(http://iopscience.iop.org/0305-4470/17/18/014)

J. Phys. A: Math. Gen. 17 (1984) 3441-3448. Printed in Great Britain

Fixed-point perturbation theory and the potential $r^2+\lambda r^2/(1+gr^2)$: I. Analysis of convergence

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Received 3 April 1984

Abstract. The simplest illustration of the recently suggested asymptotic-perturbative approach to the band-matrix Hamiltonians is found in the harmonic oscillator complemented by the non-polynomial anharmonicity $\lambda r^2/(1+gr^2)$. In the paper, the detailed construction of the effective Hamiltonian is given and the convergence of its fixed-point expansion is shown.

1. Introduction

The reasons for study of the various anharmonic oscillators range from the purely phenomenological needs of quantum mechanics up to the perturbative and field-theoretical methodology (Itzykson and Zuber 1980). In particular, a number of papers (the updated list of references may be found, e.g. in Choudhury and Mukherjee 1983) have been devoted to the one-body problem

$$[H_0+\lambda r^2/(1+gr^2)]|\psi\rangle = E|\psi\rangle$$
$$H_0=-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+r^2=\sum_{n=0}^{\infty}|n\rangle\varepsilon_n\langle n| \qquad (1.1)$$
$$\varepsilon_n=4n+2l+3, \qquad l=-1,0 \text{ or } 0,1,\ldots .$$

After the discovery by Flessas (1979) of the exceptional elementary solutions of (1.1), Whitehead *et al* (1982) converted the differential equation (1.1) into the simple algebraic set

$$Q_{(N)}\begin{pmatrix} z_0 \\ z_1 \\ \cdots \\ z_{N-1} \end{pmatrix}=0 \qquad (1.2)$$

$$Q_{(N)}=\begin{pmatrix} a_0 & b_0 & & & & \\ b_0 & a_1 & b_1 & & & \\ & b_1 & a_2 & b_2 & & \\ & & & \cdots & & \\ & & & & b_{N-2} & a_{N-1} \end{pmatrix}$$

where $N \geqslant 1$ and the harmonic-oscillator basis is used:

$$\begin{aligned} z_k &= (\varepsilon_k - E + \lambda/g)\langle k|\psi\rangle, \\ a_k &= \tfrac{1}{2}g\varepsilon_k + 1 - \lambda(\lambda + g\varepsilon_k - gE)^{-1}, \\ b_{k-1} &= g[k(k+l+\tfrac{1}{2})]^{1/2}, \qquad k = 0, 1, \ldots, N-1. \end{aligned} \tag{1.3}$$

In this formulation, we may classify all the elementary solutions easily by the choice of $N \geqslant 1$, $N < \infty$.

With $N = \infty$, the algebraic equation (1.2) becomes equivalent precisely to the original differential Schrödinger eigenvalue problem (1.1) (Znojil 1983, hereafter referred to as P). This makes the anharmonicity $r^2/(1+gr^2)$ one of the simplest interactions from the formal point of view.

Equation (1.1) appears to be suitable for testing the various computational and perturbative algorithms (Lai and Lin 1982, Bessis *et al* 1983). In the present paper, we intend to use it as the simplest non-trivial test and illustration of efficiency of our general 'fixed-point' perturbation theory (FPPT, Znojil 1984a).

In § 2, we recall the main result of P, namely, the continued-fractional form of solution to (1.1). In § 3, this enables us to obtain a simple implicit equation for energies which is suitable for application of the general fixed-point expansion technique. In § 4 we shall analyse its convergence. The results will be summarised in § 5.

2. Recurrences for wavefunctions

Equation (1.2) alone (without (1.3)) is simply a general set of the homogeneous three-term recurrences. In the light of their mathematical theory (see e.g. Korn and Korn 1968, § 20.4-4) they resemble the ordinary second-order linear differential equation. In particular, we may use the explicit determinantal solution

$$z_n = z_0 \frac{(-1)^n}{b_0 b_1 \ldots b_{n-1}} \det Q_{(n)}, \qquad n = 1, 2, \ldots \tag{2.1}$$

which is 'regular in the origin' (Znojil 1984b). We may also find some analogue of the oscillation theorem so that the 'physical' solutions may be specified by the asymptotic boundary-type conditions $z_N = 0$ or

$$\det Q_{(N)} = 0 \tag{2.2}$$

in the limit $N \to \infty$ (cf P and the so-called Hill-determinant method and its modifications (Ginsburg 1982)).

2.1. *The truncation of recurrences*

In the present case, we may interpret (2.2) simply on the variational grounds, i.e., as a secular equation pertaining to the truncation of (1.2) (cf P for details). With the matrix elements defined by the analytic formula (1.3), we may eliminate at least part of its numerical character by the factorisation

$$Q_{(N)} = \begin{pmatrix} 1 & w_0 & & \\ & 1 & w_1 & \\ & & \cdots & \\ & & & 1 \end{pmatrix} \times \begin{pmatrix} f_0^{-1} & & & \\ & f_1^{-1} & & \\ & & \ddots & \\ & & & f_{N-1}^{-1} \end{pmatrix} \times \begin{pmatrix} 1 & & & \\ d_1 & 1 & & \\ & d_2 & 1 & \\ & & \cdots & \\ & & d_{N-1} & 1 \end{pmatrix} \tag{2.3}$$

$$w_k = b_k f_{k+1} = d_{k+1}, \qquad k = 0, 1, \ldots, N-2.$$

It is defined by the recurrences

$$f_k^{-1} = a_k - b_k^2 f_{k+1}, \qquad k = 0, 1, \ldots, N-1, \qquad f_N = 0, \tag{2.4}$$

i.e., in terms of the analytic continued fractions

$$f_k = \cfrac{1}{a_k - b_k^2 \cfrac{1}{a_{k+1} - b_{k+1}^2 \cfrac{1}{a_{k+2} - \ldots}}} \tag{2.5}$$

$$b_{N-1} = 0, \; N \to \infty$$

(Wall 1948).

The determinant in (2.2) may be identified with the product of the diagonal matrix elements in (2.3). We may ignore the singularities here ($f_{m+1} = \infty$ implies that $f_m = 0$ and $f_{m+1} f_m = b_m^{-2}$, $m \geqslant 0$) so that the secular eigenvalue condition (2.2) may be given the (precisely equivalent) continued-fractional form

$$f_0^{-1} = 0. \tag{2.6}$$

Having solved (2.6), we may use its byproducts (2.5) and also rewrite (2.1):

$$\langle n|\psi\rangle = (-1)^n \frac{\text{constant}}{n+\delta} b_0 f_1 \ldots b_{n-1} f_n$$

$$\text{constant} = \langle 0|\psi\rangle \cdot \delta, \tag{2.7}$$

$$\delta = \tfrac{1}{4}(2l + 3 - E + \lambda/g), \qquad n = 0, 1, 2, \ldots .$$

This form of eigenvectors proves to be useful especially for an investigation of their convergence in the norm (cf P again).

2.2. Leading-order asymptotic estimate and the acceleration of convergence of the auxiliary continued fractions

For the matrix elements (1.3), the asymptotic behaviour of f_k, $k \gg 1$ has already been investigated in P. This study was based on an observation that the auxiliary mapping

$$\mu_{(k)}: x = (k+1) f_{k+1} \to y = k f_k$$

becomes almost independent of k for $k \gg 1$. Hence the sequence of ratios

$$\langle k|\psi\rangle / \langle k-1|\psi\rangle = -b_{k-1} f_k (1 + \mathrm{O}(k^{-1}))$$

may only oscillate or accumulate near one of the fixed points of $\mu_{(k)}$. Moreover we may easily verify that our mapping $\mu_{(k)}$ has a simple form

$$y = \frac{1 + \mathrm{O}(k^{-1})}{2g - x(g^2 + \mathrm{O}(k^{-1}))}, \qquad k \gg 1 \tag{2.8}$$

compatible with the accumulation. In this case, we obtain an estimate:

$$b_{k-1} f_k = 1 + \mathrm{O}(k^{-1/2}). \tag{2.9}$$

A more detailed analysis as performed in P shows that any prescription compatible with the second-order formula

$$b_{k-1}f_k = 1-(gk)^{-1/2}+c(k)$$
$$c(k)\neq 2(gk)^{-1/2}+O(k^{-1}) \tag{2.10}$$

guarantees the normalisability of ψ in (1.1). *Vice versa* equation (2.10), $k=N$, is equivalent to the continued-fractional initialisation $f_N=0$ in the limit $N\to\infty$, accelerating only its convergence for $c(N)=O(N^{-1})$.

In the light of the standard theory (Wall 1948), we may accelerate the convergence in a systematic way by the redefinitions

$$f_k = f_k^{(0)} = f_k^{(1)} + h_k^{(0)}, \qquad k=1,2,\ldots \tag{2.11}$$

of the continued fractions. The subtracted quantity $h_k^{(0)}$ should be a good approximation to f_k. In essence, just an iterative application of this idea is the essence of the FPPT in application to the present anharmonic oscillator with the tridiagonal Q or Hamiltonian $H\approx Q+EI$.

3. Fixed-point perturbation series

3.1. *Secular equation*

In the continued-fractional formula (2.7) we may use the identity

$$\frac{1}{f_1f_2\ldots f_n} = \det\begin{pmatrix} a_1 & b_1 & & \\ b_1 & a_2 & b_2 & \\ & \ldots & & \\ & & b_{n-1} & a_n \end{pmatrix} - b_n^2 f_{n+1}\det\begin{pmatrix} a_1 & b_1 & & \\ b_1 & a_2 & b_2 & \\ & \ldots & & \\ & & b_{n-2} & a_{n-1} \end{pmatrix} \tag{3.1}$$
$$n=2,3,\ldots$$

and express the products of f_k as functions of the single continued fraction f_{n+1}. This will simplify also the projections $\langle m|\psi\rangle$, $m=0,1,\ldots,n$.

In a similar way, we may also replace the secular equation (2.6) by the requirement

$$\det Q_{(n+1)} = b_n^2 f_{n+1}\det Q_{(n)}, \qquad n\geqslant 1 \tag{3.2}$$

containing the same continued-fractional 'input' f_{n+1}. It is solvable numerically with an arbitrary precision, provided only that the input function f_{n+1} is known. Here, it is to be represented by the FPPT series. Its construction (present §) and proof of convergence (§ 4) are easy. Moreover, after a modification (Znojil 1984c), also its form becomes simple even when compared with the continued-fractional expansion. Nevertheless, the main merit of the FPPT form of f_{n+1} will lie in its extremely rapid rate of convergence.

3.2. *Leading-order fixed-point approximant*

Formulae (3.1) and (3.2) enable us to choose $n\gg 1$ and vary the input f_{n+1} without causing any significant errors. This is the essence of the numerical algorithm of Lanczos (Wilkinson 1965)—the higher matrix elements of $Q_{(\infty)}$ do not carry any important information about the low-lying spectrum of energies in most of the applications.

Alternatively, we may preserve the precision of energies by an improved evaluation of f_{n+1} at $n=O(1)$, still keeping in mind the low information content of the higher matrix elements. This is the essence of the present FPPT approach.

From the formal point of view, we have to take into account the smooth part of the matrix Q by a sort of interpolation procedure. Indeed, as a consequence of (1.3) or (2.10), we may expect that $f_k \approx f_{k+1} \approx$ fixed point (cf also P or § 2.2). In this way, the definition

$$h_k^{-1} = a_k - b_k^2 h_k \tag{3.3}$$

inspired by (2.4) is to be used in (2.11). Of course, it is ambiguous,

$$h_k = (2b_k^2)^{-1}[a_k \pm (a_k^2 - 4b_k^2)^{1/2}] \tag{3.4}$$

but, fortunately, the physical requirement (2.10) enables us to eliminate the wrong sign without any difficulty (see below).

3.3. Iterated subtractions

We may insert $f_m = h_m^{(0)} + f_m^{(1)}$, $m=k,\ k+1$ and re-write (2.4) as a mapping $f_{k+1}^{(1)} \rightarrow f_k^{(1)}$ generating the corrections to the fixed-point approximation. Of course, such a procedure may be repeated giving

$$f_k = h_k^{(0)} + h_k^{(1)} + \ldots + h_k^{(M-1)} + f_k^{(M)}, \qquad M \geq 1 \tag{3.5}$$

in the Mth step.

We may notice that all the higher-order mappings acquire the same fractional form

$$f_k^{(M)} = \frac{A_k^{(M)} + B_k^{(M)} f_{k+1}^{(M)}}{C_k^{(M)} + D_k^{(M)} f_{k+1}^{(M)}}, \qquad k = 1, 2, \ldots. \tag{3.6}$$

Hence, the parameters may be generated by the recurrent prescriptions

$$\begin{aligned} &D_k^{(M)} = D_k^{(M-1)}, \qquad C_k^{(M)} = C_k^{(M-1)} + D_k^{(M-1)} h_{k+1}^{(M-1)}, \\ &B_k^{(M)} = B_k^{(M-1)} - D_k^{(M-1)} h_k^{(M-1)}, \\ &A_k^{(M)} = B_k^{(M)}(h_{k+1}^{(M-1)} - h_k^{(M-1)}), \qquad k = 1, 2, \ldots,\ M = 1, 2, \ldots. \end{aligned} \tag{3.7}$$

With the initial choice

$$A_k^{(0)} = 1, \qquad B_k^{(0)} = 0, \qquad C_k^{(0)} = a_k, \qquad D_k^{(0)} = -b_k^2 \qquad k = 1, 2, \ldots \tag{3.8}$$

they correspond to the original definition (3.4).

It is important to notice here that the higher-order fixed points

$$\begin{aligned} h_k^{(M)} &= \frac{A_k^{(M)} + B_k^{(M)} h_k^{(M)}}{C_k^{(M)} + D_k^{(M)} h_k^{(M)}} \\ &= (1/2D_k^{(0)})[B_k^{(M)} - C_k^{(M)} \pm [(B_k^{(M)} - C_k^{(M)})^2 + 4A_k^{(M)} D_k^{(0)}]^{1/2}], \\ &M > M_0 \end{aligned} \tag{3.9}$$

are unique. Their sign must be chosen in such a way that they remain small, $|h_k^{(M)}| \ll |h_k^{(M-1)}|$. Otherwise, we would reintroduce the root eliminated in the preceding step.

3.4. *Modifications*

In place of f_k we may consider any product $\tilde{f}_k = f_k \times$some function of k. In the fixed-point formalism of § 3.3, this corresponds merely to a change of the initialisation (3.8). At the same time, it could improve the properties of the FPPT expansion (3.5).

In the present example, a non-trivial modification $f_k \to \tilde{f}_k$ is in fact desirable. Indeed, (3.3) implies that

$$
\begin{aligned}
& b_{k-1}h_k = 1-(gk)^{-1/2}+c(k) \\
& c(k) = [(g/k)^{1/2}+\mathrm{O}(k)^{-1}]/[1+(1-g)^{1/2}]
\end{aligned}
\tag{3.10}
$$

which ceases to be real (for $g > 1$) in the very first iteration. Fortunately it is sufficient to replace f_k by the 'tilded' $\tilde{f}_k = b_{k-1}f_k$ and similarly (3.3) by the 'more natural' definition $\tilde{f}_k \approx \tilde{f}_{k+1} \approx G_k$, i.e.,

$$
\begin{aligned}
& h_k^{(0)} = G_k b_{k-1}^{-1} \\
& G_k = [a_k b_{k-1}^{-1} - b_k b_{k-1}^{-1} G_k]^{-1}.
\end{aligned}
\tag{3.11}
$$

Then *mutatis mutandis* we obtain

$$
h_k^{(0)} = (2b_k b_{k-1})^{-1}[a_k - (a_k^2 - 4b_k b_{k-1})^{1/2}]
\tag{3.12}
$$

which gives the optimal error $c(k) = \mathrm{O}(1/k)$ in (2.10).

Resulting formulae are only slightly more complicated—as an example, the first mapping of corrections

$$
f_k^{(1)} = \frac{h_k^{(0)} b_k (b_k h_{k+1}^{(0)} - b_{k-1} h_k^{(0)}) + h_k^{(0)} b_k^2 f_{k+1}^{(1)}}{1/h_k^{(0)} - b_k (b_k h_{k+1}^{(0)} - b_{k-1} h_k^{(0)}) - b_k^2 f_{k+1}^{(1)}}
\tag{3.13}
$$

gives the 'maximal' acceleration of the continued-fractional convergence in the first-order algorithm.

4. Convergence of the fixed-point expansion

4.1. *Algebraic proof*

The asymptotic behaviour of continued fractions (2.5) is closely related to their convergence, as well as to the asymptotic smoothness of matrix $Q_{(\infty)}$ (P). Here we intend to relate them also to the convergence of our FPPT.

From the purely formal point of view, any finite form of (3.5) remains merely an algebraic equivalence transformation $f_k^{(0)} \to f_k^{(M)}$. Hence, it is necessary to analyse the remainder $f_k^{(M)}$ for $M \gg 1$. It may be simplified by the relations

$$
\begin{aligned}
& B_k^{(M+1)} - C_k^{(M+1)} = B_k^{(M)} - C_k^{(M)} - 2D_k^{(0)} h_k^{(M)} - D_k^{(0)} \Delta_k^{(M)} \\
& \Delta_k^{(M)} = h_{k+1}^{(M)} - h_k^{(M)}
\end{aligned}
\tag{4.1}
$$

and

$$
\begin{aligned}
(B_k^{(M+1)} - C_k^{(M+1)})^2 + 4A_k^{(M+1)} D_k^{(0)} \\
&= (B_k^{(M)} - C_k^{(M)})^2 + 4A_k^{(M)} D_k^{(0)} + 2D_k^{(0)} (B_k^{(M)} + C_k^{(M)}) \Delta_k^{(M)} \\
&\quad + (D_k^{(0)} \Delta_k^{(M)})^2
\end{aligned}
\tag{4.2}
$$

which follow from (3.7) and imply that

$$h_k^{(M)} = \Delta_k^{(M-1)} \frac{2B_k^{(M)}}{C_k^{(M)} - B_k^{(M)}} \left[1 + \left(1 + \frac{4B_k^{(M)} D_k^{(0)}}{(C_k^{(M)} - B_k^{(M)})^2} \Delta_k^{(M-1)} \right)^{1/2} \right]^{-1}. \tag{4.3}$$

Hence, we may conclude that

$$h_k^{(M)} / h_k^{(M-1)} = \mathrm{O}(k^{-1}), \qquad M > M_0 \tag{4.4}$$

so that, provided that the higher-order roots do not become complex, the asymptotic series (3.5) will converge very quickly. At the same time, the rate of convergence will be controlled by the parameter k^{-1}, the magnitude of which is fully at our disposal and may be chosen smaller for the less smooth matrices $Q_{(\infty)}$. In the present example (1.1), the 'smoothness' of Q is such that we may use $M_0 = 0$ in (4.4).

4.2. Geometric picture

In an alternative formulation of the convergence question, we may recall the particular initial values (say, (3.8)) and obtain

$$\begin{aligned} &B_k^{(M+1)} = b_k^2 (f_k^{(0)} - f_k^{(M+1)}), \qquad C_k^{(M+1)} = 1/f_k^{(0)} + b_k^2 f_{k+1}^{(M+1)}, \\ &D_k^{(M+1)} = -b_k^2. \end{aligned} \tag{4.5}$$

This enables us to rewrite (3.6) in a simple $f_k^{(0)}$-dependent and very transparent form

$$f_k^{(M)} = \frac{b_k^2 f_k^{(0)2} (\Delta_k^{(M-1)} + f_{k+1}^{(M)})}{1 + b_k^2 f_k^{(0)} (\Delta_k^{(M-1)} + f_{k+1}^{(M)})}. \tag{4.6}$$

The Raabe criterion of convergence (Korn and Korn 1968) necessitates that

$$|b_{k-1} f_k| < 1 - k^{-1} = |b_{k-1} / b_n|$$

for large k. As a consequence we may put $b_k f_k = \cos\varphi$ where the real angle φ lies somewhere within the interval $(0, \pi)$. In this notation, the fixed points of the mapping (4.6) acquire a simple form

$$\begin{aligned} &h_k^{(M+1)} = \Delta_k^{(M)} (2\cos^2\varphi) / z_{(+)} \\ &z_{(\pm)} = \sin^2\varphi + b_k \Delta_k^{(M)} \cos\varphi \pm [(\sin^2\varphi + b_k \Delta_k^{(M)} \cos\varphi)^2 + 4 b_k \Delta_k^{(M)} \cos^3\varphi]^{1/2}. \end{aligned} \tag{4.7}$$

Obviously, for the presumably small $\Delta_k^{(M)}$, we must avoid the singularity and use the plus-sign here. Then, we have

$$h_k^{(M+1)} = \Delta_k^{(M)} \frac{\cos^2\varphi}{\sin^2\varphi} \left(1 - b_k \Delta_k^{(M)} \frac{\cos\varphi}{\sin^4\varphi} + \mathrm{O}(b_k \Delta_k^{(M)})^2 \right) \tag{4.8}$$

which confirms the estimate (4.4) in an explicit way.

On the boundary of the above-mentioned interval, we would put $b_k f_k = \pm 1 = \pm B_k f_k$ and get the formula

$$h_k^{(M+1)} = \pm (\Delta_k^{(M)} B_k^{-1})^{1/2} - \tfrac{1}{2} \Delta_k^{(M)} (1 + \mathrm{O}(\Delta_k^{(M)} B_k)^{1/2}) \tag{4.9}$$

differing from (4.8) in an essential way. Such a case gives a slower convergence. In the present example, it is not encountered since (2.10) implies that $\varphi \neq 0, \pi$, at least for $k > k_0$.

5. Summary

The Schrödinger eigenvalue problem (1.1) has been interpreted as the three-term recurrences (1.2) plus the physical 'boundary conditions' in the preceding paper P. The general 'regular-type' solutions (2.2) have been made physical by their asymptotic restriction (2.10).

In the present continuation, the 'Jost-type' solutions (2.7) and (3.5) become physical after their restriction (3.2) 'near the origin'. In this way, a complete algebraic symmetry between $n=0$ and $n=\infty$ is established, complementing the numerical tests as given in P.

The present tridiagonal matrix representation of the Hamiltonian ($H \approx Q+EI$, which depends on energy in this form) is well suited for application of the FPPT idea. Indeed, the matrix Q is asymptotically 'smooth' (this supports (implies) a quick convergence of the FPPT) and its matrix elements are simple functions of the indices (this simplifies the algebraic construction of the FPPT formulae). Moreover, the one-dimensional character of the tridiagonal partitions of Q (i.e., its tridiagonality) simplifies the rigorous analysis of convergence—its demonstration is our main result. When compared with the standard perturbation theories, an easy analysis of convergence in FPPT is its important merit.

In the practical applications of our FPPT formulae, we may encounter essentially the two types of problems:

(1) An algebraic construction of the explicit higher-order corrections is a comparatively tedious task—we must solve the quadratic algebraic equations.

(2) The formulae contain the square roots—a non-trivial analysis of existence of the real solutions is sometimes needed.

Both these problems are only technical in nature. They may be completely avoided via a modification of the FPPT formalism. This will be described, for the present example (1.1), in the forthcoming paper (Znojil 1984c).

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