A simplified fixed-point perturbation theory. II. An application to the first few Pade potentials



1987 J. Phys. A: Math. Gen. 20 1751

(http://iopscience.iop.org/0305-4470/20/7/021)

J. Phys. A: Math. Gen. **20** (1987) 1751-1760. Printed in the UK

# A simplified fixed-point perturbation theory: II. An application to the first few Padé potentials

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Received 13 June 1986, in final form 28 August 1986

**Abstract.** In the radial Schrödinger equation for bound states, central potentials $V(r) = V_{\text{Coulomb}} + V_{\text{short-range}}$ are considered, with $V_{\text{short-range}}$ replaced by its $[p-j, p]$ Padé approximants, $p > j \geq 1$. The earlier method is completed and a few coefficients of the fixed-point perturbation theory asymptotic expansions of the effective Hamiltonians are evaluated in REDUCE for $p \leq 3$.

## 1. Introduction

An algebraic construction of the exact effective Hamiltonians as described in I (Znojil 1987) is an extremely suitable task for computer symbolic manipulation. Indeed, the underlying fixed-point perturbation theory (FPPT) is a simple idea which leads to complicated equations, but their final solution remains comparatively simple again. In the present paper, we intend to illustrate this statement by a number of examples.

Bearing in mind the phenomenological needs, we shall consider the three-dimensional (radial) Schrödinger equation

$$\left(-\frac{d^2}{dr^2}+\frac{l(l+1)}{r^2}+V(r)\right)\psi(r)=E_V\psi(r) \qquad l=0,1,\ldots \tag{1.1a}$$

where the potential $V(r)$ behaves like a Coulomb force at both $r \approx 0$ and $r \to \infty$. In the 'realistic' situations of this type, we may write $V(r)$ as a superposition of the Coulombic term with a force regular at the origin and decreasing to infinity. Thus, in the light of the methodical considerations of I, we shall assume that

$$V(r)=\frac{a}{r}+\frac{B(r)}{C(r)} \tag{1.1b}$$

$$B(r)=\sum_{i=0}^{p-1} b_i r^i$$

$$C(r)=1+\sum_{j=1}^{p} c_j r^j > 0 \qquad r \geq 0,\ p \geq 1,\ c_p > 0.$$

The Coulomb + Padé force (1.1$b$) contains $2p+1$ free parameters in general. In atoms and molecules, they may be employed in a phenomenological description of the screening and polarisation effects, whereas in nuclear physics, the Padé component of $V(r)$ may simulate strong interactions, etc. The flexibility and complexity of $V(r)$ (1.1$b$) is only limited by our choice of the integer $p$.

0305-4470/87/071751+10$02.50  

Methodically, the Schrödinger eigenvalue problem (1.1) leads to a number of open questions: how to compute the matrix elements in the purely variational context (cf, e.g., the special $p=1$ example of Mitra (1978)), how to take the corrections into account, etc. In the light of I, all these problems may be reduced to mere technical questions. Their systematic analysis is done for $p \leqslant 3$ here. For the higher values of $p$, the search for answers may become rather difficult again, but the algebraic method itself remains the same.

In § 2, we shall start from the change of variables proposed in I. In analogy with the $p=2$ example of I (where $a=0$, $b_1=0$ and $c_1=0$ have been chosen in addition), we shall show how the band matrix equivalent of (1.1) may be obtained for an arbitrary $p \geqslant 1$. In § 3, we start from a recurrent and difference-equation re-interpretation of this linear algebraic set of equations $A\varphi=0$ (§ 3.1). Then, in the standard perturbative spirit (cf, e.g., Kumar 1962), we describe FPPT as an algebraic power-series expansion of the Feshbach effective Hamiltonian (§ 3.2).

In a systematic way, the $p=2$ and $p=3$ examples are considered in §§ 4 and 5, respectively. We employ REDUCE and define the first few FPPT contributions as functions of the corresponding $2p+1$ coupling constants. These results are summarised in § 6.

## 2. The difference Schrödinger equation

In accord with I, we intend to represent the class of eigenvalue problems (1.1) in a Sturmian basis. In the first step, we have to change the variables

$$\begin{aligned} &E_V=-k^2<0 \qquad && r=x^2/2k>0 \qquad && \psi(r)=x^{1/2}\chi(x) \\ &l=\tfrac{1}{2}(L-\tfrac{1}{2}) && a=-\tfrac{1}{2}k\varepsilon. \end{aligned} \tag{2.1}$$

As a consequence, our new 'canonical' Schrödinger equation

$$\left(H_0+\frac{x^2}{k^2}\,\frac{B(x^2/2k)}{C(x^2/2k)}\right)\chi(x)=\varepsilon\chi(x) \tag{2.2}$$

is equivalent to (1.1). It contains the perturbed harmonic-oscillator Hamiltonian

$$H_0=-\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{L(L+1)}{x^2}+x^2$$

rather than the screened Coulombic one.

In the second step, we shall factorise the anharmonicity in (2.2). In a non-unique way, we shall write

$$\begin{aligned} &\frac{x^2}{k^2}\,\frac{B(x^2/2k)}{C(x^2/2k)}=\frac{\tilde{G}(x)}{\tilde{U}(x)\tilde{V}(x)} \\ &\tilde{G}(x)=\sum_{m=1}^{p}\tilde{G}_m x^{2m} \\ &\tilde{U}(x)=\prod_{i=1}^{p_1}(x^2+\tilde{U}_i) \qquad \tilde{V}(x)=\prod_{j=1}^{p_2}(x^2+\tilde{V}_j) \end{aligned} \tag{2.3}$$

where $p_1+p_2=p$ and the non-negative numbers $\tilde{U}_i \notin (-\infty, 0\rangle$ and $\tilde{V}_j \notin (-\infty, 0\rangle$ will be complex in general. This enables us to rewrite our Schrödinger differential equation (2.2) in its final form $A\varphi = 0$,

$$[\tilde{U}(x)(H_0-\varepsilon)\tilde{V}(x)+\tilde{G}(x)]\psi(x)=0. \tag{2.4}$$

The new wavefunctions $\varphi(x)=\tilde{V}^{-1}(x)\chi(x)$ are square integrable if and only if their original form $\psi(r)$ describes a bound state (I)—we may expand them in the standard and complete harmonic oscillator basis $|n\rangle$,

$$\begin{aligned} &\varphi(x)=\sum_{m=0}^{\infty}\langle x|m\rangle\varphi_m \\ &H_0|n\rangle=(4n+2L+3)|n\rangle \qquad n=0,1. \end{aligned} \tag{2.5}$$

In this representation, (2.4) acquires a new infinite-dimensional algebraic form

$$\sum_{n=0}^{\infty} A_{mn}\varphi_n = 0 \qquad m=0,1,\ldots \tag{2.6}$$

where $A_{mn}=0$ whenever $|m-n|>p$ (cf also Znojil 1986).

In analogy with I, it is easy to evaluate the matrix elements in (2.6). In particular, we may derive the asymptotic form of the matrix $A$,

$$\begin{aligned} &A_{mn}=4N^{p+1}\binom{2p}{p+m-n}(1+O(N^{-1})) \\ &N=\max(m,n)\gg 1 \end{aligned} \tag{2.7}$$

and see immediately that the product $(-1)^n\varphi_n$ is almost constant for $n\gg 1$. Moreover, we may expect that

$$\varphi_n=(-1)^n\exp(\tilde{d}_1 n^{(2p-1)/2p}+\tilde{d}_2 n^{(2p-2)/2p}+\ldots) \qquad n\geqslant n_0\gg 1 \tag{2.8}$$

or

$$\frac{\mathrm{d}}{\mathrm{d}n}\ln[(-1)^n\varphi_n]=\frac{2p-1}{2p}\tilde{d}_1+\ldots=\sum_{m=0}^{K} d_m\rho^m+O(\rho^{K+1}) \qquad K\geqslant 0,\ \rho=n^{-1/2p}\ll 1 \tag{2.9}$$

where the FPPT expansion coefficients $d_m$ or $\tilde{d}_m$ are to be determined from a compatibility of (2.9) with our difference Schrödinger equation (2.6) at the sufficiently large indices $n\geqslant n_0\gg 1$.

## 3. Jost solutions and effective Hamiltonians

### *3.1. Boundary conditions*

Whenever $m\geqslant p$, our infinite-dimensional equation (2.6) may be treated as a difference equation. In general, it possesses precisely $2p$ independent solutions

$$\varphi_n=\varphi_n^{(\sigma)} \qquad \sigma=\pm 1,\pm 2,\ldots,\pm p,\ n=0,1,\ldots \tag{3.1}$$

(Nörlund 1923). The remaining 'redundant' $p$ rows of (2.6) are equivalent to the boundary condition

$$\varphi_{-1}=\varphi_{-2}=\ldots=\varphi_{-p}=0 \tag{3.2}$$

'in the origin'. On the contrary, the 'regular' solutions satisfying (3.2) are just some arbitrary values $\varphi_0, \varphi_1, \ldots, \varphi_{p-1}$ complemented by their continuation $\varphi_p, \varphi_{p+1}, \ldots$ obtainable directly from the $m = 0, 1, \ldots$, respective rows of (2.6). These regular solutions form a subclass of (3.1)—we shall denote them by the negative superscripts here

$$\varphi_n^{(\mathrm{reg})} = \sum_{\sigma=1}^{p} \varphi_n^{(-\sigma)} g^{(-\sigma)}. \tag{3.3}$$

The regular solutions (3.3) of (2.6) will not be normalisable in general. On the other hand, the bound-state condition

$$\sum_{n=0}^{\infty} \varphi_n^* \varphi_n < \infty \tag{3.4}$$

will specify the physical and unique superposition (3.3).

Obviously, the convergence of the norm (3.4) is necessary for the very existence of our fundamental expansion (2.5). It controls a large-$n$ behaviour of $\varphi_n$ (3.1). In analogy with I, it may also specify some $p$ independent 'Jost' solutions given, e.g., by their asymptotic expansion (2.8) for $n \geqslant n_0 \gg 1$. We may denote them by a positive upper index and write

$$\varphi_n^{(\mathrm{Jost})} = \sum_{\sigma=1}^{p} \varphi_n^{(\sigma)} g^{(\sigma)}. \tag{3.5}$$

Again, the respective $m = n_0 + p - 1, n_0 + p - 2, \ldots$ rows of (2.6) specify the components $\varphi_{n_0-1}^{(\mathrm{Jost})}, \varphi_{n_0-2}^{(\mathrm{Jost})}, \ldots$ in a recurrent manner. Obviously, this solution remains incompatible with the first $p$ redundant rows of (2.6), i.e. with the boundary conditions (3.2).

In a fully summetric way, we may start from both the regular and Jost initial values and treat (2.6) simply as recurrences with the $2p$ matching conditions

$$\varphi_{n_i}^{(\mathrm{phys})} = \varphi_{n_i}^{(\mathrm{Jost})} = \varphi_{n_i}^{(\mathrm{reg})} \qquad p \leqslant n_i < n_0, \; i = 1, 2, \ldots, 2p. \tag{3.6}$$

Of course, such a choice is redundant. Whenever we choose a matching point $n_i$ such that $0 \leqslant n_i < p$, the corresponding item (3.6) becomes trivial and fixes merely one of the 'regular' coefficients $g^{(\sigma)}$, $\sigma < 0$. On the contrary, a choice of $n_i \geqslant n_0$ lowers the freedom in (3.5). Thus, with all $n_i \notin \langle p, n_0)$, we are left with $p$ matching conditions (3.6) only. In particular, we may use $p$ free Jost parameters $g^{(\sigma)}$, $\sigma > 0$ and all $n_i < 0$ (Znojil *et al* 1985) or, alternatively, regular $\sigma < 0$ and all $n_i \geqslant n_0$ (Znojil 1984a, Fernandez *et al* 1986).

### *3.2. Re-interpretation of the Feshbach method*

Linear equations of the type (2.6) are often treated as $N \to \infty$ limits of their finite $N$-dimensional subsystems. In the spirit of Feshbach (1958), we may analyse the $N \to \infty$ limit also by means of the projection operator

$$P = \sum_{m=0}^{M-1} |m\rangle\langle m| \tag{3.7}$$

on the so-called model space with the fixed and finite dimension $M < \infty$. Indeed, with $M < N < \infty$, a separation of (2.6) into its $P$-projected and complementary parts

$$PA(P+Q)\varphi = 0 \qquad Q = 1 - P \qquad QA(Q+P)\varphi = 0$$

enables us to eliminate formally, with $\det QAQ \neq 0$,

$$Q\varphi = -\frac{1}{QAQ} QAP\tilde{\varphi} \qquad \tilde{\varphi} = P\varphi \tag{3.8}$$

and get the finite-dimensional equivalent

$$A^{\text{eff}}\tilde{\varphi} = 0 \tag{3.9}$$

of (2.6) with the so-called effective Hamiltonian (Feshbach 1958)

$$A^{\text{eff}} = PAP - PAQ\frac{1}{QAQ}QAP. \tag{3.10}$$

In the latter operator, the $N \to \infty$ limiting transition may be replaced by the perturbation expansions (Kumar 1962), matrix continued-fractional analysis (Graffi and Grecchi 1975), etc.

In general, the $(2p+1)$-diagonal matrix structure of $A$ implies that $A^{\text{eff}}_{mn} = A_{mn}$ for $m$ or $n$ smaller than $M-p$. The $N$ dependence of the solutions of (3.9) comes just from the $p^2$ matrix elements

$$G_{ij} = A^{\text{eff}}_{M+i-p-1,M+j-p-1} \qquad i, j = 1, 2, \ldots, p. \tag{3.11}$$

This simplifies the discussion—in particular, we may put $N = M$ and choose tentatively $A^{\text{eff}} = PAP$ (truncate $A$) for the sufficiently large dimensions $M$.

In the latter approximation, we may treat (3.9) as a matching of a regular solution to a trivial (zero-order) FPPT approximant $\varphi^{(\text{Jost})}_{n_i} = 0$ at $p$ points $n_i = M, M+1, \ldots, M+p-1$. Here, we intend to search for the higher-order corrections in (3.11), keeping in mind that the truncation acquires a rigorous meaning in the $M \to \infty$ limit only.

Our main idea is simple. We assume that (2.8) represents a sufficiently reliable definition of the set of solutions (3.5) for the indices $n \geqslant n_0 \gg 1$. In this way, (2.6) holds for $m \geqslant n_0 + p$ and represents a recurrent definition of $\varphi_{n_0-k}$ for $m = n_0 + p - k$ and $k = 1, 2, \ldots, n_0$. The first $p$ rows of it are not satisfied by the general Jost solution, so that the non-zero part of $A\varphi^{(\text{Jost})} = \lambda$

$$\lambda^{(\sigma)}_{m+1} = \sum_{n=0}^{m+p} A_{mn}\varphi^{(\sigma)}_n \neq 0 \qquad \sigma > 0,\ m = 0, 1, \ldots, p-1 \tag{3.12}$$

is a $p$-dimensional vector with respect to the lower index, or a matrix which specifies just the physical coefficients in the superposition (3.5),

$$\sum_{\sigma=1}^{p} \lambda^{(\sigma)}_{m+1} g^{(\sigma)} = 0 \qquad m = 0, 1, \ldots, p-1. \tag{3.13}$$

We see from (3.12) that the physical coefficients $g^{(\sigma)}$, $\sigma > 0$, are functions of the first few matrix elements of $A$, so that any effective truncated form of the Schrödinger equation (3.9) must be satisfied asymptotically for an arbitrary Jost solution. When we recall the corresponding definitions, this statement leads to the set of $p^2$ relations (the last $p$ rows of (3.9))

$$FY + GX = 0 \tag{3.14}$$

where each column corresponds to one Jost solution

$$F_{ij} = A_{M-p-1+i,\,M-2p-1+j},\ Y_{ij} = \varphi^{(j)}_{M-2p-1+i},\ X_{ij} = \varphi^{(j)}_{M-p-1+i},\ i, j = 1, 2, \ldots, p.$$

Now, assuming that $\det X \neq 0$, we may evaluate immediately the matrix $G$ (3.11)—its FPPT expansion is simply a combination of (2.8) and (3.14) with $n_0 \leq M-2p$,

$$G = -FYX^{-1}. \tag{3.15}$$

This is our main result—a knowledge of $p$ independent Jost solutions enables us to write immediately all the missing maxtrix elements (3.11) in the eigenvalue condition (3.9). Hence, in the standard way, we may identify the binding energies with the roots of the transcendental equation

$$\det A^{\text{eff}} = 0 \tag{3.16}$$

which must be solved numerically of course (cf, e.g., Killingbeck 1985).

## 4. Potentials with $p = 2$

We have seen that in the Padé+Coulombic Schrödinger equation (1.1), both the implicit energies and explicit wavefunctions may be written immediately in terms of the FPPT coefficients $d_m$. Now let us illustrate their construction on the first few simplest potentials $V(r)$.

We shall omit the $p = 1$ case. It has often been studied in the literature (e.g. Mitra 1978) and its matrix $A^{\text{eff}}$ may be constructed semi-numerically in terms of the analytic continued fractions (Znojil 1983a). It has already been described also within the present FPPT framework (Znojil 1984b). In the latter paper, the numerical efficiency of the eigenvalue conditions of the type (3.16) has also been thoroughly illustrated and tested.

For the 'first non-trivial' equation (2.2) with $p = 2$ and $\varepsilon = -2a/k$,

$$\left(H_0 + \frac{x^2}{k^2}\,\frac{b_0 + b_1 x^2/2k}{1 + c_1 x^2/2k + c_2 x^4/4k^2}\right)\chi = \varepsilon\chi \qquad c_1 > -2\sqrt{c_2} \tag{4.1}$$

we may recall the existence of the exceptional (exact and elementary) solutions for some particular couplings (Znojil 1983b). We introduce a slightly modified notation (2.3):

$$\left(H_0 + \frac{G_0 + G_1 x^2}{(x^2+U)(x^2+V)}\right)\chi(x) = E\chi(x) \tag{4.2}$$

where

$$\begin{aligned} E &= -\frac{2}{kc_2}(ac_2 + b_1) & G_0 &= -\frac{8kb_1}{c_2^2} \\ G_1 &= \frac{4}{c_2^2}(b_0 c_2 - b_1 c_1) & U,\, V &= \frac{k}{c_2}[c_1 \pm (c_1^2 - 4c_2)^{1/2}]. \end{aligned} \tag{4.3}$$

With $a = b_1 = c_1 = G_0 = E = 0$, $G_1 < 0$ and purely imaginary $U = -V$, (4.2) degenerates to the methodical example of I. In the present general case, we merely assume that $U, V \notin (-\infty, 0\rangle$ are complex, and arrive at our final Schrödinger equation (2.6) with the matrix

$$A = (x^2+U)(H_0 - E)(x^2+V) + G_0 + G_1 x^2 \tag{4.4}$$

pentadiagonal in the standard harmonic oscillator basis (I).

At some large and fixed $n$, our equation (2.6) may be written in the form

$$\frac{1}{n^2}\left(A_{nn-2}\frac{\varphi_{n-2}}{\varphi_n}+A_{nn-1}\frac{\varphi_{n-1}}{\varphi_n}+\ldots+A_{nn+2}\frac{\varphi_{n+2}}{\varphi_n}\right)=0 \tag{4.5}$$

where the renormalised wavefunctions $\varphi_{n\pm k}/\varphi_n$ may be replaced by their Taylor series expansions (I). Via the FPPT ansatz (2.9), this converts (4.5) into a power-series asymptotic requirement of the implicit form

$$0=\sum_{m=0}^{K} D_m(L, G_0, G_1, U, V, E)\rho^m+O(\rho^{K+1}) \qquad \rho=1/n^{1/4}\ll 1. \tag{4.6}$$

This holds if and only if

$$D_m(L, G_0, G_1, U, V, E)=0 \qquad m=0, 1, \ldots. \tag{4.7}$$

The latter relations form a coupled set of non-linear algebraic equations for the unknown coefficients $d_1, d_2, \ldots$. In the leading-order approximation with $K=0$, they are satisfied identically since the leading-order solution $\varphi_n\ (-1)^n\approx 1$ has already been incorporated into our ansatz (2.8). Further items of (4.7) with $m=1$-3 reflect the degeneracy of the leading-order solution—the first non-trivial $p=2$ result

$$d_1=0 \tag{4.8}$$

follows from the $m=4$ row in (4.7).

Equation (4.8) does not remove the degeneracy—the $m=5$-7 conditions (4.7) become trivial again. At $m=8$, we get the requirement

$$(d_2^2-U)(d_2^2-V)=0. \tag{4.9}$$

For $U\neq 0$ and $V\neq 0$, it removes the degeneracy completely and we obtain

$$d_2^{(1)}=\sqrt{U} \qquad d_2^{(2)}=\sqrt{V}. \tag{4.10}$$

With the square root signs chosen such that $\mathrm{Re}\ d_2^{(1,2)}<0$, this coincides with a definition of a pair of the physical or Jost $\sigma>0$ $d_m=d_m^{(\sigma)}$ coefficients and asymptotics (2.8).

The $m=9$ requirement (4.7) becomes

$$d_2d_3(U+V-2d_2^2)=0. \tag{4.11}$$

This is satisfied identically for $U=V$. With a new independent assumption that $U\neq V$, it implies that

$$d_3=0. \tag{4.12}$$

Equation (4.7) with $m=10$ has a form which depends on our choice of $d_2$ (4.10). We obtain a pair of different values

$$d_4^{(1)}=-\tfrac{5}{4} \qquad d_4^{(2)}=-\tfrac{1}{4} \tag{4.13}$$

which reflects the $U\leftrightarrow V$ asymmetry of our original wavefunctions

$$\psi(r)\sim x^{1/2}(x^2+V)\varphi(x) \qquad x=(2kr)^{1/2}.$$

By means of the computer symbolic manipulations in the language REDUCE, it is possible and easy to verify that

$$d_5=0$$

$$d_6^{(1)}=\frac{d_2^{(1)}}{8U(U-V)}[-G_0+G_1U-\tfrac{1}{3}U^3+(\tfrac{1}{3}V-4\alpha)U^2$$

$$+4\alpha(V+\alpha-1)U-\tfrac{29}{4}U-4(\alpha^2-\alpha)V-\tfrac{3}{4}V]$$

and

$$d_6^{(2)}=\frac{d_2^{(2)}}{8V(V-U)}\left[-G_0+G_1V-\tfrac{1}{3}V^3+(\tfrac{1}{3}U-4\alpha)V^2\right.$$
$$\left.+4\alpha(V-\alpha+1)U-\tfrac{3}{4}U+4(\alpha^2-\alpha)V+\tfrac{3}{4}V\right] \tag{4.14}$$

$$d_7=0$$

etc. These results follow from the subsequent items $m=11$, 12, 13, etc, of (4.7), respectively. The assumption $U\neq V$ is important here.

In the particular example of I, we have obtained the results compatible with the present ones. In contrast, our computer manipulations verified a possibility of using the simplified ansatz here, with all $d_{n=\text{odd}}=0$.

The solution (4.10) does not remove the degeneracy of asymptotics $\varphi_n$, $n\gg 1$ in the special case with $U=V$. Moreover, the $m=10$ condition (4.7) does not imply the definition (4.13) but merely gives the zero coefficient (4.12). This is an interesting difference from the old $U\neq V$ case, underlined even more by the $m=11$ triviality and by a delayed removal of $\varphi_n$ degeneracy at $m=12$ in (4.7),

$$d_4^2+d_4+\tfrac{1}{16}(G_0/U+3-G_1)=0. \tag{4.15}$$

The physical Jost asymptotics and coefficients will now be given by the $U=V$ prescription

$$d_2^{(1)}=d_2^{(2)}=d \qquad d^2=U=V \qquad \operatorname{Re} d<0$$
$$d_4^{(1,2)}=-\tfrac{1}{2}\pm\tfrac{1}{4}(1+G_1-G_0/U)^{1/2}. \tag{4.16}$$

In principle, we must assume again that $G_0\neq(1+G_1)U$ or analyse the degeneracy $d_4^{(1)}=d_4^{(2)}$ in the third independent branch of the $m>12$ solution. This will not be done here.

## 5. Potentials with $p=3$

The $p=3$ screened Coulombic potential

$$V(r)=\frac{a}{r}+\frac{b_0+b_1r+b_2r^2}{1+c_1r+c_2r^2+c_3r^3} \qquad c_3>0 \tag{5.1}$$

or its equivalent fractionally anharmonic force

$$\tilde{W}(x)=x^2+\frac{G_0+G_1x^2+G_2x^4}{(x^2+U)(x^2+V)(x^2+W)} \tag{5.2}$$

leads to the Schrödinger equation (2.6) with a heptadiagonal matrix $A$. For example, we may choose

$$A=(x^2+U)(x^2+V)(H_0-E)(x^2+W)+G_0+G_1x^2+G_2x^4 \tag{5.3}$$

or

$$A=(x^2+U)(H_0-E)(x^2+V)(x^2+W)+G_0+G_1x^2+G_2x^4 \tag{5.4}$$

as the two possible extensions of (4.4).

In both these cases, the FPPT technique and ansatz (2.9) with $\rho = 1/n^{1/6}$ lead to the non-linear algebraic set of equations of the implicit form

$$D_m(L, G_0, G_1, G_2, U, V, W, E) = 0 \qquad m = 0, 1, \ldots \tag{5.5}$$

analogous to (4.7).

Up to the $m = 6$ and $m = 12$ conditions giving

$$d_1 = 0 \qquad d_2 = 0 \tag{5.6}$$

the first 18 conditions (5.5) are identities. The first non-trivial $m = 18$ item

$$(d_3^2 - U)(d_3^2 - V)(d_3^2 - W) = 0 \tag{5.7}$$

becomes an analogue of (4.9), and the $m = 19$ condition

$$0 = d_3 d_4[-3d_3^4 + 2d_3^2(U + V + W) - (UV + UW + VW)] \tag{5.8}$$

replaces (4.11) here. Again, it is necessary to distinguish between the separate special cases.

With a complete absence of coincidences, $U \neq V \neq W$, the square roots

$$d_3^{(1)} = \sqrt{U} \qquad d_3^{(2)} = \sqrt{V} \qquad d_3^{(3)} = \sqrt{W} \tag{5.9}$$

with the negative real parts specify the non-degenerate physical $K = 3$ asymptotics $\varphi_n^{(\sigma)}$ (2.8) of the Jost type. We also get

$$d_4 = 0 \qquad d_5 = 0 \tag{5.10}$$

from (5.8) and from its $m = 20$ successor.

An exhaustive solution of the $m = 21$ equation (5.5) starts to depend on our choice of $d_3^{(\sigma)}$. For example, the choice of $\sigma = 1$ leads to

$$\begin{aligned} d_6^{(1)} &= \tfrac{1}{4}[3d_3^{(1)^4} - \ldots]^{-1}[-11d_3^{(1)^4} + \ldots] \\ &= -\tfrac{5}{4} \end{aligned} \tag{5.11}$$

for $A$ from (5.3), and to the same value

$$\begin{aligned} d_6^{(1)} &= \tfrac{1}{4}(3d_3^{(1)^4} - \ldots)^{-1} \times (-7d_3^{(1)^4} + \ldots) \\ &= -\tfrac{5}{4} \end{aligned} \tag{5.12}$$

for $A$ from (5.4), etc.

The $U = V = W$ confluence modifies the above picture in a way similar to the preceding $p = 2$ case. Now, besides the trivially satisfied equations $D_{19} = 0$, $D_{20} = 0$ and also $D_{22} = 0$ and $D_{23} = 0$, we obtain

$$d_4 = 0 \tag{5.13}$$

from $D_{21} = 0$. The $m = 24$ requirement (5.5) has an explicit cubic non-linear form

$$(d_5^{(\sigma)})^3 = \tfrac{1}{32}d_3(G_2 - G_1/U + G_0/U^2) \qquad \sigma = 1, 2, 3 \tag{5.14}$$

which removes the degeneracy in general.

From the forthcoming $m > 24$ items of (5.5), we obtain

$$d_6 = -\tfrac{7}{12}$$

$$d_7^{(\sigma)} = \frac{1}{96 d_5^{(\sigma)}} \left( \frac{13}{9} + \frac{5}{2} G_2 - \frac{1}{2} \frac{G_1}{U} - \frac{3}{2} \frac{G_0}{U^2} \right) \tag{5.15}$$

or

$$d_6 = -\tfrac{1}{4}$$

$$d_7^{(\sigma)} = \frac{1}{96 d_5^{(\sigma)}} \left( \frac{16}{9} + \frac{5}{2} G_2 - \frac{1}{2} \frac{G_1}{U} - \frac{3}{2} \frac{G_0}{U^2} \right) \tag{5.16}$$

etc, from the matrix $A$ in (5.3) or (5.4), respectively.

## 6. Summary

In its original formulation, the FPPT formalism has been based on a complicated solution of quadratic equations for $(p \times p)$-dimensional matrices (Znojil 1984c). This inspired its later conversion into a more numerically oriented method (cf, e.g., Znojil *et al* 1985). In its present description, we have re-established it as an algebraic power-series expansion technique again.

In brief, our FPPT procedure starts from a certain asymptotic wavefunction ansatz, and its essence lies in an immediate algebraic reconstruction of the effective Hamiltonians. Its core, namely a solution of a system of the coupled and non-linear algebraic equations, proved to have an almost elementary character. In fact, all the examples considered here as illustrations of the general technique lead to a trivial decoupling of these equations. In a recurrent way, we were able to determine the new higher-order perturbative contributions as functions of the old ones.

The leading-order non-linear FPPT equations have a simple interpretation as conditions removing the asymptotic degeneracy of wavefunctions. In a few 'confluent' cases with some mutually interrelated couplings, this non-linearity and removal of degeneracy may move to the higher orders but, in general, we simply obtain the linear definitions of the higher-order corrections. This makes the FPPT structure and formulae very similar to the traditional, say, Rayleigh-Schrödinger ones.

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