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A simplified fixed-point perturbation theory: I. The method

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Abstract. For a simple potential, we propose a conversion of the standard differential radial Schrödinger equation into an infinite-dimensional matrix equation $A\varphi = 0$ and describe its systematic non-numerical solution. The results may be characterised as infinite asymptotic expansions of the wavefunctions φ and/or of the secular determinant (an inverse 'Green function') $\det A$. The inverse model-space dimension plays a role of the small perturbation parameter.

1. Introduction

Recently, a straightforward diagonalisation of complicated Hamiltonians (say, by means of the Lanczos (1950) method) appeared even in the field-theoretical calculations on the lattice (e.g. Duncan and Roskies 1985). A methodical essence of these calculations seems to lie in a consequent use of the algebraic non-numerically specified matrix elements of H. This resembles similar assumptions of the so-called fixed point perturbation theory (FPPT) (Znojil 1984a) and is also an inspiration of the present development of the FPPT approach to the matrix Schrödinger equations

$$H\psi = E\psi. \tag{1.1}$$

Methodically, FPPT may be understood as a generalisation and modification of the original Lanczos method. We assume that H is a matrix with $(2t+1)$ diagonals, $t \geqslant 1$, and notice that (1.1) may be converted into its finite 'effective' equivalent

$$H^{\text{eff}}\psi = E\psi \tag{1.2}$$

(Feshbach 1958). Here, in full analogy with an iterative (numerical) or continued-fractional (analytic) form of H^{eff} in the Lanczos algorithm (cf, e.g., Wilkinson (1965) or Akhiezer (1965), respectively), the $(t \times t)$-dimensional matrix continued fractions (MCF) may be defined and used (Graffi and Grecchi 1975). Finally, with a fixed model-space dimension $M < \infty$, we have to replace the MCF part of H^{eff} by an asymptotic FPPT series (cf also Znojil 1983). Its 'small parameter' is some quantity $\kappa = (1/M)^{\text{constant}}$. In practice, the eigenvalue/eigenvector FPPT condition (1.2) is to be solved numerically of course.

A geometric background of the MCF FPPT formalism leads to the tedious immediate applications. Their improvement has been stimulated by a detailed study of the central potentials

$$V(r) = ar^2 + \frac{b}{1+cr^2} \qquad c > 0 \tag{1.3}$$

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(Znojil 1984b) and

$$V(r) = ar^2 + br^4 \qquad b > 0 \tag{1.4}$$

(Znojil and Tater 1986). This has inspired a formal transition to the so-called vectorial continued fractions (Znojil 1983) and resulted in an alternative difference-equation formulation of the whole FPPT construction (Znojil 1984c, Znojil *et al* 1985). In the present paper, its simplified purely algebraic version will be described.

For the sake of simplicity, we shall start from a simple particular example again (see § 2 below). This will enable us to illustrate the separate steps of the FPPT construction of H^{eff} in full detail: a change of variables (§ 2.1), a conversion of the differential Schrödinger equation into its band-matrix or difference-equation equivalent

$$\sum_{n=m-l}^{m+l} A_{mn}\varphi_n = 0 \qquad m = 0, 1, \ldots \tag{1.5}$$

(§ 2.2), an explicit algebraic construction of the wavefunctions (§ 3) and, finally, a reconstruction of a numerically soluble equation of the type (1.2) (§ 4).

2. Wavefunctions

2.1. Schrödinger equation and a change of variables

The radial Schrödinger equation

$$\left(-\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} + \frac{b}{1+cr^2}\right)\psi(r) = E\psi(r)$$
$$l = 0, 1, \ldots \qquad c > 0 \qquad b < 0 \tag{2.1}$$

with a negative energy $E = -k^2$ describes a particle in a central shallow potential well. In spite of its simplicity, it does not seem to admit a closed solution. Hence, it is a good candidate for the present FPPT analysis. We shall employ it as a methodical example, which is to be generalised in paper II of the present series (Znojil 1987).

The Hamiltonian in (2.1) contains the continuous spectrum. Via a simple change of variables

$$r = x^2/2k \qquad \psi(r) = x^{1/2}\chi(x) \qquad L = 2l + \tfrac{1}{2} = \tfrac{1}{2}, \tfrac{5}{2}, \ldots \tag{2.2}$$

we shall get rid of it. Indeed, assuming that $k > 0$, we obtain a new form of (2.1):

$$\left(H_0 - \frac{\lambda x^2}{\eta^2 + x^4}\right)\chi(x) = 0 \tag{2.3}$$

where $\lambda = -4b/c > 0$, $\eta = 2k/\sqrt{c} > 0$ and

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

is the harmonic oscillator Hamiltonian, $H_0|n\rangle = (4n + 2L + 3)|n\rangle$.

Formally, equation (2.3) may again be understood as a zero-energy Schrödinger equation with a harmonic oscillator unperturbed part of the Hamiltonian. Since $\chi(x) \sim x^{L+1}$ if and only if $\psi(r) \sim r^{l+1}$, the new wavefunctions will again be regular in the origin whenever $L + 1 > -L$ and $l + 1 > -l$, i.e. for $l > -\frac{1}{2}$ and/or $L > -\frac{1}{2}$. Similarly,

in accord with the oscillation theorems (Ince 1956), the general (unphysical) asymptotics $\psi(r) \sim \pm\exp kr$, $r \gg 1$ and $\chi(x) \sim \pm\exp \frac{1}{2}x^2$, $x \gg 1$, will also become physical (change sign and remain proportional to $\exp(-kr)$) precisely at the 'physical' values of the coupling/energy parameters. This establishes an equivalence between the $k > 0$ problem (2.1) and a slightly modified form

$$[(x^2+\varepsilon)H_0(x^2-\varepsilon) - \lambda x^2]\varphi(x) = 0 \tag{2.4}$$

of (2.3) with $\varepsilon = i\eta$ and $\varphi(x) = (x^2 - i\eta)^{-1}\chi(x)$.

2.2. Recurrences

An addition of some interaction a/r in (2.1) would lead to a non-zero energy $E' = -2a/k$ in (2.3). This will be analysed in paper II of the present series. We see that (2.2) represents just a formal Coulomb-oscillator equivalence (Newton 1982). Hence, in terms of the complete set of the harmonic oscillator states $|n\rangle$, we may also expand the bound states here:

$$\varphi(x) = \sum_{n=0}^{\infty} \langle x|n\rangle \varphi_n.$$

Our knowledge of the matrix elements

$$\langle n|x^2|n\rangle = a_n \qquad \langle n|x^2|n+1\rangle = b_n$$

as simple functions of the indices $m = n \pm k$:

$$\begin{aligned} &a_m = 2n[1+(\alpha \pm k)n^{-1}] \qquad \alpha = \tfrac{1}{2}(L+\tfrac{3}{2}) = 1, 2, \ldots \\ &b_m = n[1+(1\pm k)n^{-1}]^{1/2}[1+(2\alpha \pm k)n^{-1}]^{1/2} \\ &n, k = 0, 1, \ldots \end{aligned} \tag{2.5}$$

is important. It enables us to rewrite (2.4) easily in the form (1.5)

$$\sum_{m=-2}^{2} A_{nn+m}\varphi_{n+m} = 0 \tag{2.6}$$

where $t = 2$, $\varphi_{-1} = \varphi_{-2} = 0$ and

$$\begin{aligned} &A_{nn-2} = b_{n-2}b_{n-1}a_{n-1} \qquad A_{nn+2} = b_n b_{n+1} a_{n+1} \\ &A_{nn\pm 1} = b_{n-\frac{1}{2}\pm\frac{1}{2}}(a^2_{n\pm 1} + a_n^2 \mp 2\varepsilon - \tfrac{1}{2}\lambda) \\ &A_{nn} = a_n^3 + a_{n-1}b_{n-1}^2 + a_{n+1}b_n^2 + \eta^2 a_n - \tfrac{1}{2}\lambda a_n \qquad n = 0, 1, \ldots. \end{aligned} \tag{2.7}$$

For sufficiently large indices $n \gg 1$, both the functions (2.5) and matrix elements in (2.6) may be interpreted as Taylor series in the variable $1/n$. This may be employed in converting the difference equation (2.6) into its approximate asymptotic form

$$\sum_{m=-2}^{2} \binom{4}{m+2} \left(1 + \sum_{k=1}^{L} X_{km} n^{-k} + O(n^{-L-1})\right)\varphi_{n+m} = 0 \qquad n \gg 1. \tag{2.8}$$

By means of the related tedious but straightforward algebraic manipulations, we may evaluate the separate coefficients:

$$X_{1m} = 3\alpha + \tfrac{3}{2}m$$

$$X_{2m}=\frac{(8-3|m|)\alpha^2+\alpha}{3-|m|}+\tfrac{13}{24}m^2+\tfrac{1}{3}+3m\alpha$$
$$+\tfrac{1}{24}\delta_{m0}(\lambda+4\eta^2)-\tfrac{1}{16}(\lambda+4m\varepsilon)\binom{2}{1+m} \tag{2.9}$$

$$X_{3m}=\frac{\alpha+\frac{1}{2}m}{3-|m|}[(2-|m|)\alpha^2+(1+m)\alpha+1-\tfrac{1}{4}|m|$$
$$+\tfrac{1}{2}\delta_{m0}\eta^2+2\alpha m-\tfrac{1}{4}m\varepsilon-\tfrac{1}{8}\lambda]$$

etc ($m=-2, -1, 0, 1, 2$ and $\delta_{00}=1$, $\delta_{m0}=0$ for $m\neq 0$).

3. Algebraic solution of the difference Schrödinger equation

In accord with the standard textbooks on difference equations (we have used Nörlund (1923)) a general solution of (2.6) at large n is a superposition of the four independent solutions

$$\varphi_n=g_1\varphi_n^{(1)}+g_2\varphi_n^{(2)}+g_3\varphi_n^{(3)}+g_4\varphi_n^{(4)}. \tag{3.1}$$

A construction of the dominant terms is quite straightforward (cf, e.g., Znojil 1986, Hautot 1986) and, in the present $t=2$ case, it may be expected to acquire the form

$$\varphi_n=\varphi_n^{(i)}=(-1)^n\exp(an^{3/4}+bn^{2/4}+\dots) \tag{3.2}$$

analogous to the quartic oscillator case (Znojil *et al* 1985). In (2.8), equation (3.2) will simply be used as an ansatz.

In general, the superposition (3.1) will violate our requirement

$$\varphi_{-1}=\varphi_{-2}=0 \tag{3.3}$$

i.e. the 'physical boundary conditions in the origin'. Moreover, it may also become incompatible with the normalisation condition

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

Vice versa, equations (3.3) and (3.4) should fix the physical wavefunction (3.1) uniquely.

In a constructive proof of this statement, let us fix the index n and re-normalise $\varphi_{n\pm k}\to\varphi_{n\pm k}(-1)^{n+k}$. Then, due to the smooth asymptotic behaviour of the projections φ_n, we may employ and truncate the Taylor series

$$\frac{\varphi_{n\pm k}}{\varphi_n}=1\pm k\Omega_1+\frac{k^2}{2!}\Omega_2\pm\dots$$
$$\Omega_l=\frac{1}{\varphi_n}\frac{\mathrm{d}^l}{\mathrm{d}n^l}\varphi_n. \tag{3.5}$$

When we compare (3.1) with (3.5), we may also write

$$\Omega_1=\frac{\mathrm{d}}{\mathrm{d}n}\ln\varphi_n=\tfrac{3}{4}a\rho+\tfrac{2}{4}b\rho^2+\dots=\sum_{m=1}^{\infty}c_m^{(1)}\rho^m \qquad \rho=n^{-1/4} \tag{3.6}$$

Now, step by step, the coefficients are to be determined algebraically from the asymptotic form (2.8) of our Schrödinger equation (2.6).

We may notice that

$$\frac{\mathrm{d}}{\mathrm{d}n} = -\frac{\rho^5}{4}\frac{\mathrm{d}}{\mathrm{d}\rho}$$

so that the recurrences

$$\Omega_{k+1} = \Omega_k\Omega_1 + \frac{\mathrm{d}}{\mathrm{d}n}\Omega_k = \Omega_k\Omega_1 - \frac{\rho^5}{4}\frac{\mathrm{d}}{\mathrm{d}\rho}\Omega_k \tag{3.7}$$

i.e.

$$c_m^{(k+1)} = \sum_{l=k}^{m-1} c_l^{(k)} c_{m-l}^{(1)} + (1-\tfrac{1}{4}m)c_{m-4}^{(k)} \qquad k = 1, 2, \ldots \tag{3.8}$$

in

$$\Omega_k = \sum_{m=k}^{\infty} c_m^{(k)}\rho^m \qquad c_{k-1}^{(k)} = c_{k-2}^{(k)} = \ldots = 0$$

determine the expansion (3.5) as a power series in the new variable ρ, with $\Omega_k = \mathrm{O}(\rho^k)$ for $\rho \ll 1$. In this way, we may insert (3.5) in (2.8) and, comparing the coefficients at each power of the variable ρ, obtain the identity

$$0\rho^0 + 0\rho^1 + 0\rho^2 + 0\rho^3 + \Omega_4 + \mathrm{O}(\rho^5) = 0. \tag{3.9}$$

This is a surprising conclusion—we have to put $c_1^{(1)} = 0$. As a consequence, $\Omega_k = \mathrm{O}(\rho^{2k})$.

This is an important simplification of the formulae when compared with the anharmonic oscillator case.

Due to the above result, an ordering of terms Ω_k as belonging to the ρ^{2k} contributions to the left-hand side of our equation (2.8) must be performed. Thus, in place of (3.9), we obtain a new simplified relation:

$$0\rho^0 + 0\rho^2 + 0\rho^4 + 0\rho^6 + \left(\Omega_4 + \frac{\eta^2}{n^2}\right) + \left(\frac{6\Omega_3}{n} + \frac{2\varepsilon\Omega_1}{n^2}\right)$$
$$+ \left(\tfrac{1}{6}\Omega_6 + \frac{3\alpha}{n}\Omega_4 + (-4\alpha^2 + 4\alpha + 13 + \tfrac{1}{2}\lambda)\frac{\Omega_2}{2n^2}\right) + \mathrm{O}(\rho^{14}) = 0 \tag{3.10}$$

where also the higher-order corrections may be added in the same manner. Again, due to the independence of the different powers of the variable ρ, the separate coefficients must be assigned the zero values.

From the lowest non-trivial $\mathrm{O}(\rho^8)$ contribution to the left-hand side of the equation (3.10), we obtain the requirement

$$[c_2^1]^{(4)} + \eta^2 \doteq 0. \tag{3.11}$$

It defines the dominant component of φ_n and the ansatz (3.6) proves compatible with our recurrences. All the four general solutions are generated by the formula (3.11)—we may eliminate the two unphysical (non-normalisable) components and write

$$c_2^{(1)} = (\eta/2)^{1/2}(-1 + \mathrm{i}\sigma) \qquad \sigma = \pm 1. \tag{3.12}$$

A choice of these two roots of (3.11) as coefficients in (3.6) makes our ansatz (3.2) compatible with the asymptotic boundary conditions (3.4). Any superposition of the

corresponding two wavefunctions $\varphi_n = \varphi_n^{(\sigma)}$ will therefore define the Jost solution, in full analogy with the FPPT anharmonic oscillator construction of Znojil *et al* (1985).

From the next $O(\rho^{10})$ component of (3.10), we obtain

$$c_3^{(1)} = 0 \qquad c_4^{(1)} = -\tfrac{3}{4} + \tfrac{1}{2}\mathrm{i}(c_2^{(1)})^2 = -\tfrac{3}{4} + \tfrac{1}{2}\sigma. \tag{3.13}$$

As a consequence, we may write the Jost solutions as superpositions of the components

$$\varphi_n^{(\sigma)} = (-1)^n \exp[-(2n\eta)^{1/2}] n^{(-3+2\sigma)/4} [\cos(2n\eta)^{1/2} + \mathrm{i}\sigma \sin(2n\eta)^{1/2}] f_n^{(\sigma)} \tag{3.14}$$

where, asymptotically, $f_n^{(\sigma)} = 1 + O(1/\sqrt{n})$ for $n \gg 1$.

An analysis of the higher-order corrections

$$f_n^{(\sigma)} = 1 - \sum_{m=1}^{\infty} 2m^{-1} n^{-m/2} c_{2m+4}^{(1)} \tag{3.15}$$

may proceed in precisely the same manner. Their derivation as well as the explicit formulae

$$c_6^{(1)} = \frac{(\eta/2)^{1/2}(1-\mathrm{i}\sigma)}{16\eta^2} \{\lambda + 8\alpha\eta^2 - 2\mathrm{i}\sigma\eta[\tfrac{1}{3}\eta^2 + L^2 + L + 2(\sigma - 1)]\} \tag{3.16}$$

and

$$c_8^{(1)} = \alpha(\tfrac{3}{4} - \tfrac{1}{2}\sigma) + \frac{\lambda}{\eta^2}(\sigma - \tfrac{3}{2}) + \frac{\mathrm{i}\sigma}{16\eta}(2\sigma - \eta^2 + L^2 + L - 2) \tag{3.17}$$

etc, become more and more involved. Presumably, a symbolic manipulation language like REDUCE should be employed.

4. A variable model space and binding energies

Methodically, our example (2.4) is a substitute for some 'realistic' (say, nuclear) eigenvalue problem. There, in contrast to the simple examples, the variational approximation $H^{\mathrm{eff}} = H$ converges slowly with the increasing dimension of the model space or, vice versa, we have to choose a small dim H^{eff} here. The (perturbatively) improved $H^{\mathrm{eff}} \neq H$ becomes needed.

With a limited number of rows, say, $n \leqslant M - t \geqslant 1$, our basic difference equation (2.6) involves merely the first $M+1$ components $\varphi_0, \varphi_1, \ldots, \varphi_M$ of the wavefunction and vice versa, the Feshbach $(M+1)$-dimensional relation

$$\sum_{m=0}^{M} A_{nm}^{\mathrm{eff}} \varphi_m = 0 \qquad n = 0, 1, \ldots, M \tag{4.1}$$

and eigenvalue condition

$$\det A^{\mathrm{eff}} = 0 \tag{4.2}$$

specify our solution as a function of the four unknown matrix elements

$$\begin{pmatrix} A_{M-1\,M-1}^{\mathrm{eff}} & A_{M-1\,M}^{\mathrm{eff}} \\ A_{M\,M-1}^{\mathrm{eff}} & A_{MM}^{\mathrm{eff}} \end{pmatrix} = \begin{pmatrix} h_1 & h_2 \\ h_2^* & h_3 \end{pmatrix} \tag{4.3}$$

since $A_{mn}^{\mathrm{eff}} = A_{mn}$ for $m < M-1$ or $n < M-1$.

In the present example, we may *a priori* expect that, up to the $O(\rho^8)$ corrections, our matrix (4.3) remains Hermitian, real and symmetric,

$$\begin{aligned} &h_m = h_{m0} + h_{m1}\rho^2 + h_{m2}\rho^4 + O(\rho^6) \\ &m = 1, 2, 3 \qquad h_m = h_m^* + O(\rho^8). \end{aligned} \tag{4.4}$$

The higher-order corrections, tractable along the same lines in principle, will necessitate an introduction of the complex quantities. In the present approximation, the simplified requirement of compatibility of (4.4), (4.3) and (4.1) may be postulated.

Provided that ρ (i.e. the model space dimension M) represents an independently variable quantity, we may treat (4.4) as an ansatz. After its insertion in (4.1), we obtain the relations

$$\begin{aligned} &(1+3\alpha/n)(-1+\Omega_1-\tfrac{1}{2}\Omega_2)+4[1+(3\alpha+\tfrac{3}{2})/n] \\ &\qquad + h_1(-1-\Omega_1-\tfrac{1}{2}\Omega_2)+h_2(1+2\Omega_1+2\Omega_2)=O(\rho^6) \\ &[1+(3\alpha+3)/n]+h_2(-1-\Omega_1-\tfrac{1}{2}\Omega_2)+h_3(1+2\Omega_1+2\Omega_2)=O(\rho^6) \end{aligned} \tag{4.5}$$

where

$$\begin{aligned} &\Omega_1 = \Omega_1^{(\pm)} = c_2^{(\pm)}\rho^2 + c_4^{(\pm)}\rho^4 + O(\rho^6) \\ &\Omega_2 = \Omega_2^{(\pm)} = c_2^{(\pm)2}\rho^4 + O(\rho^6). \end{aligned} \tag{4.6}$$

In the leading-order approximation, the set of equations (4.5) (on the $O(1)$ level of precision) is incomplete for a determination of the leading order part of (4.4). Thus, an inclusion of the $O(\rho^2)$ relations is needed to provide the values

$$h_{10} = 5 \qquad h_{20} = 2 \qquad h_{30} = 1. \tag{4.7}$$

Similarly, a partial $O(\rho^2)$ result

$$h_{11} = h_{21} = h_{31} \tag{4.8}$$

may be combined with the $O(\rho^4)$ requirements and gives the first non-trivial contribution

$$h_{11} = (2\eta)^{1/2} > 0. \tag{4.9}$$

An analogous generation of the higher-order contributions to the infinite asymptotic fixed-point series representation of A^{eff} may be continued, presumably by means of the symbolic manipulation algorithm on a computer. The preliminary second-order constraints

$$\begin{aligned} &h_{12} - h_{22} = 9\alpha + 6 - \eta \\ &h_{22} - h_{32} = 3\alpha + 3 - \eta \end{aligned} \tag{4.10}$$

follow already from the present $O(\rho^4)$ restriction.

5. Conclusions

The present algebraic expansion of the particular finite-dimensional (Feshbach-projected) Schrödinger equation (4.1) is to be understood, first of all, as an illustration of feasibility of the FPPT constructions. The formalism has several consequences. Its character of an asymptotic series with the small parameter $1/M^{\text{constant}}$ may prove useful not only in an acceleration of convergence of the $M \to \infty$ limiting transition, but also, at a fixed M, as an approximation including systematically the higher-order corrections.

With our particular choice of the interaction (a shallow well) there is no need to produce the numerical results—almost any method will converge here. At the same time, the non-numerical results (the four asymptotic solutions, a pair of their physical, normalisable subclass) enable one to notice the phenomena not always recovered by the numerical means (e.g. a subdominant suppression of the $\sigma = -1$ Jost solutions (not observed in the anharmonic oscillator (1.4))), or the asymptotic degeneracy of the physical and unphysical effective Hamiltonians (cf (4.7)).

An application of the present method to a large variety of more complicated potentials will be studied in the forthcoming paper II. Here, the preliminary results also deserve a few remarks.

(i) We may recall that, in spite of the standard regularity condition $l > -\frac{1}{2}$ (Newton 1982), a number of interactions may formally be considered at $l = -1$ as well. This enables one to switch to the one-dimensional analogue of the given potential. Here, a similar switch is not allowed, unfortunately. Indeed, due to a change of the scalar product, the restriction $l > -\frac{1}{2}$ becomes essential in the transformation (2.2).

(ii) From another point of view, the change of variables (2.2) pushes the one-dimensional ground state ψ out of the standard Hilbert space. Our harmonic oscillator basis $|n\rangle$ (in fact, the so-called Sturmians, cf, e.g., Whitehead *et al* (1982) for more details) necessitates a modification before being used in a one-dimensional counterpart of our three-dimensional bound-state problem (2.1).

In full analogy with the preceding results concerning the simple potentials (1.3) and (1.4), we might emphasise in the conclusion that the present approach to the band-matrix Schrödinger equations treated as difference equations exhibits a striking analogy with the standard matching method applied currently to the ordinary differential equations. We may expect also that the discrete analogues of the regular and Jost solutions will soon find applications in the various problems of an immediate physical interest.

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