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Schrödinger equation as recurrences: II. General solutions and their physical asymptotics

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Abstract. The general Schrödinger equation is converted into equivalent $(2t+1)$-term recurrences by the generalised Lanczos construction of the basis. Then, the exact bound states are given by the t-parametric determinantal formula. Finally, the values of the free parameters are shown to follow from the Hill type normalisability requirement.

1. Introduction and contents

In a preceding paper I (Znojil 1983a), we have described the algebraic construction of the approximate effective Hamiltonians H^{eff} by means of solving certain nonlinear algebraic equations for their matrix elements. This was based on a very weak 'smoothness' assumption concerning the original Hamiltonian H, with systematic improvements to be done in the spirit of the standard perturbation methods.

One of the possible techniques of the related perturbation-type expansions was described recently (Znojil 1983b) in a somewhat different context. The underlying fixed-point formalism is merely a generalisation of the expansion (or convergence theory, Znojil 1980a) applicable to the analytic continued fractions.

Unfortunately, the fixed-point algebra and formulae seem to be rather complicated. In the present paper, an alternative approach will, therefore, be described.

In essence, we shall merely reverse the direction in the recurrences of I. This will simplify the algebraic formalism—the corresponding details are given in § 2. Of course, the formal symmetry between the original and reversed recurrences may also be partially recovered—via analogy with the respective Jost and regular solutions to the differential equations, this is illustrated in § 2.3.

From the physical point of view, only the normalisable solutions are relevant. Preserving the above analogy, a part of the results of I may, therefore, be used here after a due re-interpretation. First of all, the original variational truncation of constant chain initialisations re-appears here as the physical asymptotic boundary conditions. Precisely, they will also fix the physical values of the present initialisations. In this way, our algebraic eigenvalue method becomes independent of its variational background and it acquires the fully rigorous, mathematically independent foundations (§ 3).

The first two examples of application of the present method are investigated in more detail in § 4. For the anharmonic power law (§ 4.1) as well as some other (§ 4.2)

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oscillators, the rate of convergence and asymptotics are obtained even without recourse to the numerical computations.

In both paper I and here, our attention is paid to the Schrödinger eigenvalue problem

$$\sum_{n=1}^{\infty} \langle m|(H-E)|n\rangle\langle n|\psi\rangle = 0, \qquad m = 1, 2, \ldots, \qquad \|\psi\| < \infty \tag{1.1}$$

such that $\langle m|H|n\rangle = 0$ for $|m-n| > t = \text{constant}$. For the general Hamiltonian, this is to be understood either as a new, infinite-dimensional type of the solvable truncation (cf I) or, without any approximations, as the exact and universal formulation of the Schrödinger eigenvalue problem written in the generalised Lanczos (1950) basis $|n\rangle$ (§ 2.1, see also Znojil 1980b). This is discussed and summarised in § 5.

2. Closed form of the wavefunctions

2.1. Generalised Lanczos basis

With the first non-trivial parameter $t = 1$ in (1.1), the matrix H becomes tridiagonal. Such a form is considered 'trivial' from the purely numerical point of view—most of the numerical eigenvalue algorithms contain a transition to an equivalent tridiagonal matrix as a preparatory step (Wilkinson 1965).

Such a transition corresponds to a unitary transformation of the whole basis. It represents of course a serious complication in the infinite-dimensional cases. The solution of this problem was given by Lanczos (1950)—we may choose only the first basis state $|1\rangle$ *a priori*. Then, we must generate the next ones, $|2\rangle, |3\rangle, \ldots$ as the orthonormalised parts of $H|1\rangle, H|2\rangle, \ldots$, respectively. Thus, the operator H will be represented by the tridiagonal matrix in this 'Lanczos' basis, as a consequence of the related algebra. By using the biorthogonal sets of bra and kets, we may treat even the non-Hermitian operators in the same way—see Wilkinson (1965) for further details.

In Znojil (1980b), such a procedure was generalised in an obvious way—we may choose t arbitrary states $|1\rangle, |2\rangle, \ldots, |t\rangle$ and then generate the next ones in an analogous way. In detail, the (orthonormalised) states $|kt+i\rangle$, $i = 1, 2, \ldots, t$ will be generated by the action of the operator H on the preceding t-plet $|(k-1)t+j\rangle$, $j = 1, 2, \ldots, t$. Thus, in full analogy with the $t = 1$ special Lanczos case, we obtain H in the required band-matrix form without any approximations.

2.2. General algebraic solution of the (2t+1)-term recurrences by the determinantal formula

The infinite set of the linear algebraic equations (1.1), i.e.,

$$\sum_{\substack{n=m-t \\ n\geqslant 1}}^{m+t} \mathscr{H}_{mn}(E) z_n = 0, \qquad \mathscr{H}_{mm+t} \neq 0, \qquad m = 1, 2, \ldots, \tag{2.1}$$

represents, irrespective of its interpretation, the algebraic set of recurrences. In particular, we may pick up t values $z_1, z_2, \ldots, z_t$ and express the remaining z_n, $n > t$, as their linear superpositions.

Theorem 1. The general solution of (2.1) is given by the formula

$$z_{n+t} = \sum_{m=1}^{t} z_m \frac{(-1)^n}{c_1^{(0)} c_2^{(0)} \ldots c_n^{(0)}} \det Q_{(n)}^{(m)}, \qquad n \geqslant 1 \tag{2.2}$$

where

$$Q_{(n)}^{(m)} = \begin{pmatrix} c_1^{(1)} & c_1^{(0)} & 0 & \cdots & & 0 \\ c_2^{(2)} & c_2^{(1)} & c_2^{(0)} & 0 & \cdots & 0 \\ & \cdots & & & & \\ 0 & \cdots & 0 & c_n^{(2t)} & c_n^{(2t-1)} & \cdots \quad c_n^{(1)} \end{pmatrix} \tag{2.3}$$

and

$$\begin{aligned} c_k^{(k)} &= \mathscr{H}_{km}, & & k = 1, 2, \ldots, \min(n, t+m) \\ c_k^{(i)} &= \mathscr{H}_{kk+t-i}, & & i = 0, 1, \ldots, \min(k-1, 2t),\ k = 1, 2, \ldots, n. \end{aligned} \tag{2.4}$$

Proof. We have to guarantee that (2.2)–(2.4) represent the solution of (2.1) for any set of parameters z_m, $0 < m \leqslant t$. Formally, we may, therefore, choose a fixed m and put $z_n = 0$, $0 < n \leqslant t$, $n \neq m$. This converts (2.1) into the simpler relation

$$Q_{(\infty)}^{(m)} \begin{pmatrix} z_m \\ z_{t+1} \\ z_{t+2} \\ \cdots \end{pmatrix} = 0$$

and the solution (2.2) becomes obvious and/or verifiable by the mathematical induction with respect to n.

A priori, the input parameters $z_1, z_2, \ldots, z_t$ in (2.2) are completely free. Indeed, the nth row of (2.1) defines the component z_{t+n} of the solution (2.2) in an unambiguous way. In the various physical interpretations of (2.1), such a freedom is usually removed—e.g., in the eigenvalue problem (1.1), the bound states are defined by the series $\Sigma\, |n\rangle z_n$ and the condition

$$\|\psi\| \left(= \left(\sum_{n=1}^{\infty} z_n^2 \right)^{1/2} \right) < \infty \tag{2.5}$$

is strong enough to fix not only the binding energy, but also the projections z_m, $m \leqslant t$ (up to the degenerate levels of course).

It is interesting to notice that the standard truncation method fixes the projections $z_1, z_2, \ldots, z_t$. We shall see below how the other eigenvalue methods may be based on theorem 1.

2.3. The $t = 1$ example—an s-wave Schrödinger equation in the finite-difference approximation scheme

As an example of (2.1) with an origin different from (1.1), we may again consider the Schrödinger equation

$$[-\mathrm{d}^2/\mathrm{d}r^2 + V(r)]\psi(r) = E\psi(r), \qquad r \geqslant 0. \tag{2.6}$$

Contrary to (1.1), we merely replace its second derivative by the approximate formula

$$d^2\psi(r)/dr^2 = h^{-2}[\psi(r+h)-2\psi(r)+\psi(r-h)], \qquad h \approx 0, \tag{2.7}$$

and consider the values $\psi(r_i)$ on the discrete mesh of coordinates $r_1 = h$ and $r_i = r_{i-1} + h$, $i = 2, 3, \ldots$.

In the limit $h \to 0$, the explicit solution (2.2) of the resulting approximate tridiagonal form

$$\begin{pmatrix} V(r_1)-E+2/h^2, & -1/h^2, & 0, & \ldots \\ -1/h^2, & V(r_2)-E+2/h^2, & -1/h^2, & 0, \quad \ldots \\ & \ldots & & \end{pmatrix} \begin{pmatrix} \psi(r_1) \\ \psi(r_2) \\ \ldots \end{pmatrix} = 0 \tag{2.8}$$

of (2.6), coincides with the so called regular solution $\psi = \psi_R$. Indeed, being initialised by $\psi_R(0) = 0$, $\psi_R'(0) = 1$ or $\psi_R(0) = 1$, $\psi_R'(0) = 0$ for odd or even parity (Newton 1965), it enables us to put $\psi_R(r_1) = h$ or $\psi_R(r_1) = 1$ in (2.8), respectively.

For the reasonable potentials $V(r)$, the physical and/or non-physical asymptotic behaviour of ψ_R is known. Hence, an elimination of the latter is easy and, reflecting the physical requirement analogous to (2.5), it fixes the binding energy. In the computational practice, this is a standard technique.

A similar construction may be developed also for the so called Jost solutions $\psi_J(r)$ defined by their physical behaviour at $r \to \infty$ (Newton 1965). It is more complicated—in contrast to $r = 0$, the point $r = \infty$ is usually an essential singularity of (2.6). Hence, to transform (2.6) into a Jost analogue of (2.8), additional information about the physical asymptotics must be employed since the derivatives $\psi_J'(\infty)$ do not exist at all.

For the differential equations of the general order $2t$, $t > 1$, the same approximative finite-difference scheme based on (2.7) may be used again—we have

$$\frac{d^{2t}}{dr^{2t}}\psi(r_i) \doteq \sum_{k=-t}^{t} \frac{(-1)^{k+t}}{h^{2t}} \binom{2t}{t+k} \psi(r_{i+k}), \qquad h \approx 0 \tag{2.9}$$

so that it is easy to generalise (2.8) to its $(2t+1)$-diagonal forms. The Jost type approach encounters again its specific difficulties. In the present context, some of them will be discussed later.

3. The physical boundary conditions for recurrences at $n \to \infty$

Provided that the series $|\psi\rangle = \Sigma\, |n\rangle z_n$ diverges, no wavefunction $\psi(r)$ corresponds to the infinite-dimensional algebraic solution (2.2) of (1.1) at the non-physical energies and *vice versa* the convergence of $\|\psi\| = \Sigma\, z_n^2$ implies that the wavefunction $\psi(r)$ exists. Thus, an adequate form of the convergence criterion may be postulated as the $n \to \infty$ boundary condition in (2.2). It should be sufficient to eliminate all the unphysical t-parametric ambiguity from (2.2), i.e., to fix $z_2, z_3, \ldots, z_t$ and E.

Its choice will depend on the properties of $\mathscr{H}$. In accordance with I, we shall restrict our attention to the simplest class of the asymptotically smooth Hamiltonians.

3.1. Hamiltonians pertaining to the quickly convergent norm of ψ

Let us consider the real and symmetric asymptotically smooth ones. In accordance

with § 4 of I, they have the property

$$\mathscr{H}_{M+mM+n} = \gamma \times \left\{ \left[\prod_{i=1}^{t} I_{(+)}(\alpha_i) \right] \times \prod_{j=1}^{t} I_{(+)}^{\mathrm{T}}(\alpha_j) \right\}_{mn}$$
$$\gamma = \text{constant}(M)/(\alpha_1 \alpha_2 \ldots \alpha_t) \times (1 + \mathrm{O}(1/M)), \qquad M \gg 1 \tag{3.1}$$

where α_i are complex numbers in general, and

$$I_{(+)}(\alpha) = \begin{pmatrix} 1 & \alpha & & \\ & 1 & \alpha & \\ & & 1 & \alpha \\ & & & \ldots \end{pmatrix}, \qquad I_{(+)}^{\mathrm{T}}(\alpha) = \begin{pmatrix} 1 & & & \\ \alpha & 1 & & \\ & \alpha & 1 & \\ & & & \ldots \end{pmatrix}. \tag{3.2}$$

As a typical illustration, we may recall the doubly anharmonic oscillators (DAHO) with

$$H = p^{2t} + g_1 p^{2t-2} + \ldots + h_1 r^{2t-2} + r^{2t}$$

as defined in § 4.3 of I.

In the light of theorem 2 of I, formula (3.1) is symmetric with respect to the change $\alpha_i \to 1/\alpha_i$. Provided that $\alpha_i \neq 1$ are real for $i = 1, 2, \ldots, t$, theorem 3 of I removes this ambiguity by the requirement $\|z\| < \infty$, i.e.,

$$\alpha = |z_{N+i+1}/z_{N+i}| = \max_i |\alpha_i| < 1, \qquad i = 1, 2, \ldots, t. \tag{3.3}$$

This is precisely the set of the boundary conditions which guarantees the convergence of ψ in the norm. In the DAHO example, (3.3) may be achieved for $t \leqslant 4$ at least.

Let us introduce an auxiliary variable $\tilde{z}_\infty \sim z_{N+t}$, $N \gg 1$. Then, we may insert the explicit determinantal definitions (2.2) into (3.3) and get the linear relations

$$\begin{pmatrix} d_{11} & d_{12} & \ldots & d_{1t} & 1 \\ d_{21} & d_{22} & \ldots & d_{2t} & \alpha \\ & \ldots & & & \\ d_{t1} & d_{t2} & \ldots & d_{tt} & \alpha^{t-1} \\ d_{t+11} & d_{t+12} & \ldots & d_{t+1t} & \alpha^t \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \\ \ldots \\ z_t \\ \tilde{z}_\infty \end{pmatrix} = 0, \tag{3.4}$$
$$d_{ij} = (-1)^i \det Q_{N+t}^{(j)}, \qquad N \gg 1.$$

Again, they are valid whenever $\alpha = \max|\alpha_i| < 1$ in the leading-order approximation.

In (3.4), the last row and column may be expected to be negligible since $c_N^{(0)} = 1 + \mathrm{O}(1/N)$ and $z_N = \mathrm{O}(\alpha^N)$. Omitting them, we get an equivalent of the truncated set of equations (2.1),

$$\sum_{j=1}^{t} d_{ij} z_j = 0, \qquad i = 1, 2, \ldots, t. \tag{3.5}$$

In practical applications, the use of (3.4) or (3.5) may suffer from the various numerical ill conditioning problems. Nevertheless, in the purely algebraic setting, these equations should determine completely both the energy parameter E and all the initial wavefunction projections z_m, $0 < m \leqslant t$. Hence, we may interpret (3.3) as an 'asymptotic boundary condition' pertaining to the general 'regular-type' solution (2.2) of our 'Schrödinger-type' eigenvalue problem (2.1) and (2.5).

The above principle of the eigenvalue determination contains non-trivial information about the structure of $\mathscr{H}$ and z_N, $N \gg 1$. We may expect that (3.4) will be more powerful than the truncation technique in practice, provided that $\mathscr{H}$ is smooth enough.

4. Examples

4.1. Anharmonic oscillators

In the light of I, the particular anharmonic oscillator (AHO) example

$$(p^2+r^2+\lambda_1 r^4+\ldots+\lambda_m r^{2m+2})\psi = E\psi, \qquad \lambda_m > 0, \qquad m = t-1 \geqslant 1 \tag{4.1}$$

may be written exactly in the band matrix form (2.1). Consulting, e.g., Graffi and Grecchi (1975) for details, we may use the standard harmonic oscillator basis $|n\rangle$.

Explicit formulae (2.2)–(2.4) may be used without any problems. At the same time, theorem 3 of I gives the explicit solution immediately—we get $\alpha = 1$ in (3.3). This makes our derivation of (3.4) invalid. Hence, we must take the next corrections into account—the leading-order asymptotic estimate of the ratio z_N/z_{N-1} appears to be insufficient to 'quantise' equation (1.1) in an algebraic way.

Of course, inclusion of the higher-order corrections is feasible in a direct way. Nevertheless, even without this (essentially non-numerical) procedure, we may conclude that the convergence of ψ in the norm will be slow. Moreover, we see that $z_N = -z_{N-1}\,(1+O(1/N))$ is a sequence with changing signs, i.e., wavefunctions may converge well in the coordinate representation. All this may be confirmed by the numerical studies (Graffi and Grecchi 1975 etc).

Our approach also permits the following analysis of the asymptotics. We take (4.1) in the form (2.1) or (1.1) and omit the first M rows, $M \geqslant 1$, as irrelevant from the present point of view. Then, in the leading-order asymptotic approximation, we get

$$[I_{(+)}(1)]^{2t}\begin{pmatrix} z_{M+1} \\ z_{M+2} \\ \ldots \end{pmatrix} = 0 \tag{4.2}$$

(see I). This immediately clarifies the general $2t$-parametric character of the initialisations in infinity.

Lemma 1. In the leading-order approximation, the AHO recurrences (4.2) admit the general solution

$$\begin{pmatrix} z_{M+1} \\ z_{M+2} \\ z_{M+3} \\ \ldots \end{pmatrix} = \sum_{j=0}^{2t-1} (-1)^j c_{2t-1-j} \begin{pmatrix} \binom{0}{j} \\ -\binom{1}{j} \\ +\binom{2}{j} \\ \ldots \end{pmatrix}, \tag{4.3}$$

where $\binom{n}{j} = 0$ for $n < j$. This solution possesses an infinite norm $(\Sigma_n z_n^2)^{1/2}$ whenever $c_{j_0} \neq 0$, $j_0 \neq 2t-1$.

Proof. First, let us notice that an infinite and homogeneous set of the linear algebraic equations

$$I_{(+)}(\beta)\begin{pmatrix} y_1 \\ y_2 \\ \ldots \end{pmatrix} = 0 \tag{4.4}$$

has no finite-dimensional non-trivial solution since $\det I_{(+)} = 1$. Indeed, an assumption $y_{N+i} = 0$, $i \geq 1$ implies that $y_0 = y_1 = \ldots = y_N = 0$. Nevertheless, it admits a class of the non-trivial infinite-dimensional solutions

$$y_{k+1} = \left(-\frac{1}{\beta}\right) y_k \tag{4.5}$$

initialised by any non-zero $y_1 \neq 0$. When we put $\beta = 1$, we have, therefore,

$$[I_{(+)}(1)]^{2t-1} \begin{pmatrix} z_{M+1} \\ z_{M+2} \\ \cdots \end{pmatrix} = c_0 \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \\ \cdots \end{pmatrix}$$

$$\cdots$$

$$\begin{pmatrix} z_{M+1} \\ z_{M+2} \\ \cdots \end{pmatrix} = \sum_{j=0}^{2t-1} (-1)^j c_{2t-j-1} \begin{pmatrix} +\binom{0}{j} \\ -\binom{1}{j} \\ +\binom{2}{j} \\ \cdots \end{pmatrix}.$$

Concerning the norm, we have

$$\|z\|^2 = \sum_{k=1}^{\infty} z_n^2 > \sum_{k=k_1}^{\infty} c_{j_0}^2 \binom{k}{2t-1-j_0}^2 \left(1 + O\left(\frac{1}{k_1}\right)\right)$$

$$= O\left[\sum_{k=k_1}^{\infty} k^{2(2t-j_0-1)} \left(1 + O\left(\frac{1}{k_1}\right)\right)\right], \qquad k_1 \gg 1$$

which is infinite whenever $c_0 = c_1 = \ldots = c_{j_0-1} = 0$ and $c_{j_0} \neq 0$ with $j_0 < 2t-1$. The higher-order corrections influence its value and may cause convergence only when $j_0 = 2t-1$.

4.2. Example with the slowly convergent norm—fractionally anharmonic oscillator

In the harmonic oscillator basis, the one-body Schrödinger equation (2.6) with the potential

$$V(r) \equiv r^2 + \lambda r^2/(1+gr^2) \tag{4.6}$$

has a general matrix form. Putting $\mathscr{H}(E) = (1+gr^2)(H-E)$ it may easily be re-written in the tridiagonal $t=1$ form (2.1) (Whitehead *et al* 1982). Of course, the solution may then be given the form (2.2). As far as $t=1$, the only unknown projection z_1 is merely an irrelevant normalisation.

The matrix $\mathscr{H}(E)$ is asymptotically smooth and satisfies (3.1) with $\alpha = 1$. Hence, theorem 3 of I is not applicable. A thorough analysis (Znojil 1983c) reveals its adequate modification (employing the d'Alembert criterion in place of (3.3)) and confirms again the validity of the secular equation (3.5),

$$z_N = 0, \qquad N \to \infty. \tag{4.7}$$

This condition resembles strongly the standard Hill-determinant techniques (Ginsburg 1982, etc).

Numerically, we may treat (4.7) in various ways. In a specific recurrent formulation directly resembling (3.3), this Hill-type approach has already been tested and gives almost correct energies even for the extremely low indices N (see, e.g., columns A1 in table 1 of Znojil 1983c).

5. Summary

In this paper, an emphasis has been laid upon the fact that the general Schrödinger equation has a form of the forward-running $(2t+1)$-term recurrences in the generalised Lanczos basis. Hence, it may be treated by purely algebraic means, which has the following merits.

(i) The explicit determinantal formula may be used. It defines the general solution in a compact form, as a function of some t free parameters. Thus, we are constructing a 'regular' solution in a way parallelling the theory of ordinary differential equations.

(ii) The results of I have specified the physical boundary conditions to be imposed in the $n \to \infty$ asymptotic region. This fixes all the free parameters and defines the physical energies and projections of the wavefunctions.

(iii) The construction is mathematically rigorous—no variational-type assumptions are needed.

(iv) In the computations, various eigenvalue algorithms 'without truncation' may be based on the present Hill-type equations (3.4).

(v) A systematic inclusion of the higher-order asymptotic corrections is possible on a purely algebraic level. In particular, we believe that this will enable us to consider the convergence problems in a non-numerical setting in the future.

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