数理解析研究所講究録 1424 巻 2005 年 240-253

The method of Hill determinants in PT-symmetric quantum mechanics

Miloslav Znojil

Ústav jaderné fyziky AV ČR, 250 68 Řež, Czech Republic

Abstract

Hill-determinant method is described and shown applicable within the so called PT-symmetric quantum mechanics. We demonstrate that in a way paralleling its traditional Hermitian applications and proofs the method guarantees the necessary asymptotic decrease of wave functions $\psi(x)$ as resulting from a fine-tuned mutual cancellation of their asymptotically growing exponential components. Technically, the rigorous proof is needed/offered that in a quasi-variational spirit the method allows us to work, in its numerical implementations, with a sequence of truncated forms of the rigorous Hill-determinant power series for the normalizable bound states $\psi(x)$.

PACS 03.65.Ge, 03.65.Fd

1 Introduction

One of the key sources of an enormous popularity of one-dimensional anharmonic-oscillator Schrödinger equations

$$\left(-\frac{d^2}{dx^2}+V(x)\right)\,\psi(x)=E\,\psi(x),\qquad x\in(-\infty,\infty) \tag{1}$$

with polynomial potentials, say, of the quartic form

$$V(x)=a\,x^4+b\,x^3+c\,x^2+d\,x,\qquad a=1 \tag{2}$$

lies, definitely, in their methodically illuminating role of apparently "next-to-solvable" examples in quantum theory.

Thirty five years ago one of the characteristic results in this direction has been obtained by Bender and Wu [1] who made a highly nontrivial observation that in some models of such a type, *all* the pertaining bound-state energies E_n may be understood as values of a *single* analytic function when evaluated on its different Riemann sheets. This observation (made at $b = d = 0$) was a real breakthrough in the intensive contemporary perturbative analysis of eq. (1) + (2). Later on, it has been complemented by the alternative semi-classical [2] and quasi-variational [3] sophisticated treatments of eq. (2). In this sense, the model provided an extremely useful insight in the possible structures encountered within relativistic quantum field theory [4].

The hypotheses of ref. [1] have also been explicitly verified in the phenomenologically equally important cubic-oscillator limit $a \to 0$ [5]. In parallel, the closely interrelated semi-classical and quasi-variational (often called Hill-determinant, HD) constructions of bound states were subsequently generalized to virtually all polynomials $V(x)$. In the former semi-classical setting, an updated sample of references is offered by these proceedings. In contrast, the parallel HD approach to polynomial $V(x)$ [6] seems "forgotten" at present, in spite of its extremely useful capability of complementing the perturbative and semi-classical constructions. This is one of the reasons why the forthcoming text has been written for the same proceedings.

A nice illustration of the HD – semi-classical complementarity of the corresponding algorithms has been thoroughly described in ref. [7] (here, we shall skip this illustration referring to the original paper containing a few numerical tables and further references).

The HD method emphasizes certain important non-perturbative features of the energies. Again we would like to recollect an elementary illustrative two-dimensional example of ref. [8], or a more extensive one-dimensional sextic-oscillator study [9] where the HD-type energies have been specified as roots of a convergent continued fraction. Unfortunately, in the contemporary literature at least, the acceptance and credibility of the HD approach to polynomial $V(x)$ has been marred, in the quasi-variational context as well as in perturbation theory, by a few unfortunate misunderstandings concerning the related mathematics.

For a sketchy explanation of the latter point the reader should consult the twenty years old Hautot's concise review [10]. A more thorough account of the problem may be found in my own long and unpublished dissertation [11] including references to the misleading papers (responsible for the unfortunate continuation of the whole misunderstanding up to these days) as well as a detailed account and an exhaustive specification of the domain of validity of the HD techniques in Hermitian cases with polynomial potentials.

The present updated HD review is going to move one step further. The reason is that in the light of some most recent semi-classical analyses of anharmonic oscillators, another important motivation for a renewal of interest in HD philosophy might be found in the formal parallels between these two techniques, both having to deal with complexified coordinates and both being based on the infinite-series expansions of the energies E and of the related wave functions $\psi(x)$, respectively. It is also worth a marginal note that in both of them a different role is played by certain exponentially suppressed small contributions.

2 $\mathcal{PT}-$symmetric quantum mechanics

Within the framework of the pure quantum physics, the idea of a complexification of the couplings or coordinates is in fact neither too popular nor formally welcome. A characteristic comment has been made by the author of [4] whose historical remarks clarified the situation in the seventies when people imagined that the convergence of perturbation series would imply that the "observables" may be well defined even when the Hamiltonians themselves become manifestly non-Hermitian.

For this reason, perhaps, Carl Bender needed almost thirty years more to return to the complexified models in the two pioneering papers [12] where the two new versions of eq. (2) have been studied with the purely imaginary couplings $b = i\beta$ and $d = i\delta$. The emphasis has been laid upon quite amazing an observation that the spectrum remains real *in spite* of the obvious fact that $H \neq H^{\dagger}$. In the light of the possible applications of such an approach in Quantum Mechanics, the authors characterized the underlying specific non-Hermiticity as a "weakened Hermiticity" or "$\mathcal{PT}$ symmetry" of the Hamiltonian. Indeed, in their most elementary models the operators $\mathcal{P}$ and $\mathcal{T}$ denoted the parity and the time reversal (i.e., in effect, the Hermitian conjugation), respectively.

The methods they used were mainly perturbative and semi-classical. In what follows, we intend to answer the question whether some models of $\mathcal{PT}-$symmetric quantum mechanics could admit the constructive solution of their Schrödinger equations by the techniques of the HD type. For the sake of definiteness and in a way employing our recent results in [13], we shall mainly review the results concerning the above-mentioned quartic problem

$$\left(-\frac{d^2}{dx^2}+x^4+i\,\beta\,x^3+c\,x^2+i\,\delta\,x\right)\,\psi(x)=E\,\psi(x),\qquad x\in(-\infty,\infty)\tag{3}$$

again, with the real values of β, c and δ and, therefore, with the manifestly non-Hermitian, $\mathcal{PT}-$symmetric form of the Hamiltonian.

Before getting in more details, let us only add that during the rapid development of the field (summarized, e.g., in the proceedings of the recent Workshop which have to appear in the October issue of Czechoslovak Journal of Physics this year), the "parity" $\mathcal{P}$ should be understood, in a broader sense, as an arbitrary (Hermitian and invertible) operator of a pseudo-metric $\eta_{(pseudo)}$ in Hilbert space [14]. Similarly, the symbol $\mathcal{T}$ should be understood as an antilinear operator mediating the Hermitian conjugation of H [15].

In the context of physical applications, the concept of the "parity" itself becomes insufficient and must be complemented by a "quasi-parity" operator $\mathcal{Q}$ [16] which makes the scalar products (between eigenstates of $H \neq H^\dagger$) positively definite [17]. This means that we must perform a highly nontrivial transition from the non-singular and, by assumption, indeterminate original pseudo-metric $\mathcal{P}=\eta_{(pseudo)}=\eta^\dagger_{(pseudo)}$ to some other, positively definite "true" metric $\mathcal{QP}=\eta_+>0$, the knowledge of which allows us to call our Hamiltonians $H\neq H^\dagger$ "quasi-Hermitian" and "physical" again (cf. the reviews [18] for more details). In the other words, only the change of the metric $\mathcal{P}\to\mathcal{QP}=\eta_{(quasi)}=\eta^\dagger_{(quasi)}$ (where, at present, the name "charge" for $\mathcal{Q}\equiv\mathcal{C}$ is being preferred [19]) makes the non-Hermitian $\mathcal{PT}-$symmetric models with real spectrum fully compatible with the probabilistic interpretation and other postulates of quantum mechanics in a way illustrated very recently on the non-Hermitian square well [20, 21].

3 HD construction

The wave functions $\psi(x)$ defined by eq. (3) are analytic at all the complex $x\in C$. In the asymptotic region of the large $|x|\gg 1$ the semi-classical analysis reveals that

$$\psi^{(AHO)}(x)\sim\left\{\begin{array}{ll} c_{phys}e^{-x^3/3}+c_{unphys}e^{+x^3/3}, & 0\le|\,\mathrm{Im}\,(x)|\ll+\mathrm{Re}\,(x)/\sqrt{3},\\ d_{phys}e^{+x^3/3}+d_{unphys}e^{-x^3/3}, & 0\le|\,\mathrm{Im}\,(x)|\ll-\mathrm{Re}\,(x)/\sqrt{3}.\end{array}\right.\tag{4}$$

The HD method proceeds, traditionally, in an opposite direction and employs the power-series formulae for $\psi(x)$ near the origin. Thus, in the $\mathcal{PT}$−symmetric manner we write

$$\psi^{(ansatz)}(x) = e^{-sx^2} \sum_{n=0}^{\infty} h_n \, (ix)^n \,, \qquad x \in (-\infty, \infty) \tag{5}$$

with a suitable (optional) value of s. The key reason may be seen in the success of such a strategy in the harmonic-oscillator case where such an ansatz converts the differential Schrödinger equation (3) into solvable recurrences. Here, of course, the resulting recurrent rule

$$A_n \, h_{n+2} + C_n \, h_n + \delta \, h_{n-1} + \theta \, h_{n-2} - \beta \, h_{n-3} + h_{n-4} = 0 \tag{6}$$

$$A_n = (n+1)(n+2), \quad C_n = 4sn + 2s - E, \quad \theta = 4s^2 - c$$

is not solvable in closed form. At all the parameters (including also the unconstrained, variable energy E), it only defines the coefficients h_n as superpositions

$$h_n = h_0 \sigma_n + h_1 \omega_n, \qquad \sigma_0 = \omega_1 = 1, \quad \sigma_1 = \omega_0 = 0 \tag{7}$$

where all the three sequences h_n, σ_n and ω_n satisfy the same recurrences with different initial conditions. Still, we may write the latter two funtions of n in a very compact determinantal form

$$\sigma_{n+1} = (-1)^n \frac{\det \Sigma_{n-1}}{n!(n+1)!}, \qquad \omega_{n+1} = (-1)^n \frac{\det \Omega_{n-1}}{n!(n+1)!}, \qquad n = 1, 2, \ldots$$

with $(m+1)$−dimensional matrices

$$\Sigma_m = \left(\begin{array}{ccccccc} C_0 & A_0 & & & & & \\ \delta & 0 & A_1 & & & & \\ \vdots & C_2 & 0 & A_2 & & & \\ 1 & \vdots & C_3 & \ddots & \ddots & & \\ 0 & -\beta & \ddots & \ddots & 0 & A_{m-2} & \\ \vdots & 1 & \ddots & \delta & C_{m-1} & 0 & A_{m-1} \\ & & \ddots & \ldots & \delta & C_m & 0 \end{array} \right) \tag{8}$$

(note: the second column of the matrix of the linear system (6) is omitted here since $\sigma_1 = 0$) and

$$\Omega_m = \begin{pmatrix} 0 & A_0 & & & & & \\ C_1 & 0 & A_1 & & & & \\ \delta & C_2 & 0 & A_2 & & & \\ \vdots & \delta & C_3 & \ddots & \ddots & & \\ 1 & \vdots & \delta & \ddots & 0 & A_{m-2} & \\ & \ddots & \vdots & \ddots & C_{m-1} & 0 & A_{m-1} \\ & & 1 & \dots & \delta & C_m & 0 \end{pmatrix} \tag{9}$$

(now the first column is omitted in the light of our choice of $\omega_0 = 0$).

It remains for us to specify the norm $\rho = \sqrt{h_0^2 + h_1^2}$, the ratio $h_1/h_0 \equiv \tan\zeta$ and the physical energy E which enters the $(m+1)$−dimensional matrices (8) and (9). In the other words, our wave functions $\psi(x)$ must be made "physical" via the standard boundary conditions

$$\psi^{(ansatz)}(X_R) = 0 = \psi^{(ansatz)}(-X_L)\,, \qquad X_R \gg 1, \;\; X_L \gg 1\,. \tag{10}$$

These conditions play, obviously, the role of an implicit definition of the above free parameters. Nevertheless, our ambitions are higher and in the HD approach people usually try to replace eq. (10) by a quasi-variational finite-matrix truncation of eq. (6) [10], i.e., equivalently, by innovated difference-equation boundary conditions

$$h_N = h_{N+1} = 0\,, \qquad N \gg 1\,. \tag{11}$$

with a much simpler numerical implementation. Of course, such a replacement of eq. (10) by eq. (11) is not always well founded [10] so that in each particular construction its validity must be based on a rigorous mathematical proof, in a way illustrated in what follows.

4 The proof

4.1 The s−dependence of the asymptotics of h_n

In the first step of the proof, the recurrences (6) should be read as a linear difference equation of the sixth order. The sextuplet of its independent asymptotic solutions

h_n may be found by the standard techniques. Thus, the leading-order solution may be extracted from eq. (6) by its reduction to its two-term dominant form of relation between h_{n+2} and h_{n-4}. Thus, we put

$$h_n(p) = \frac{\lambda^n(p)\, g_n(p)}{(3^{1/3})^n\, \Gamma(1+n/3)} \tag{12}$$

where the integer $p = 1, 2, \ldots, 6$ numbers the six independent solutions and where $\lambda(p) = \exp[i(2p-1)\pi/6]$. The new coefficients $g_n = g_n(p)$ vary more slowly with n. Thus, our first conclusion is that at the large indices n, all solutions decrease as $h_n \sim \mathcal{O}(n^{-n/3})$ at least. This means that in a way confirming our expectations the radius of convergence of our Taylor series (5) is always infinite.

On this level of precision the size of our six independent solutions remains asymptotically the same. In order to remove this degeneracy we amend equation (6) and having temporarily dropped the p's we get

$$g_{n+2} - g_{n-4} = \frac{4s\lambda^4}{n^{1/3}}\, g_n - \frac{\beta\,\lambda}{n^{1/3}}\, g_{n-3} + \mathcal{O}\left(\frac{g_n}{n^{2/3}}\right). \tag{13}$$

The smallness of $1/n^{1/3}$ in the asymptotic region of $n \gg 1$ enables us to infer that

$$g_n = e^{\gamma\, n^{2/3} + \mathcal{O}(n^{1/3})}, \qquad \gamma = \gamma(p) = s\lambda^4(p) - \beta\,\lambda(p)/4, \tag{14}$$

i.e.,

$$\text{Re}\ \gamma(1) = \text{Re}\ \gamma(6) = -\frac{\sqrt{3}}{8}\beta - \frac{s}{2}, \qquad \text{Re}\ \gamma(2) = \text{Re}\ \gamma(5) = s,$$
$$\text{Re}\ \gamma(3) = \text{Re}\ \gamma(4) = \frac{\sqrt{3}}{8}\beta - \frac{s}{2}. \tag{15}$$

We may conclude that whenever we satisfy the condition

$$s > \frac{|\beta|}{4\sqrt{3}} \tag{16}$$

the general, six-parametric form of the Taylor coefficients

$$h_n = \sum_{p=1}^{6} G_p\, h_n(p) \tag{17}$$

will be equivalent to the two-term formula in the leading order,

$$h_n = G_2\, h_n(2) + G_5\, h_n(5), \qquad n \gg 1, \tag{18}$$

i.e., only its two dominant components remain asymptotically relevant while, in the leading order, we may simply put $G_1 = G_3 = G_4 = G_6 = 0$ in eq. (17) at $n \gg 1$.

The same argument implies that for

$$s < \frac{|\beta|}{4\sqrt{3}} \tag{19}$$

we get

$$h_n = \begin{cases} G_3\, h_n(3) + G_4\, h_n(4), & \beta > 0,\ n \gg 1, \\ G_1\, h_n(1) + G_6\, h_n(6), & \beta < 0,\ n \gg 1. \end{cases} \tag{20}$$

while the degeneracy of more than two solutions survives at $\beta = 0$ or at $s = \frac{|\beta|}{4\sqrt{3}} > 0$.

4.2 Single-term dominant exponentials in $\psi^{(ansatz)}(x)$

We know that the shape of the function $\psi^{(ansatz)}(x)$ is determined by the energy E and by the not yet fully specified choice of the two coefficients h_0 and h_1. In the language of the preceding section, each choice of the energy E and of the initial h_0 and h_1 will generate a different, $x-$ and $n-$independent pair of the coefficients G_2 and G_5 in h_n at the sufficiently large s (the discussion of the smaller s will be omitted for the sake of brevity).

As long as our aim is a completion of the proof of the validity of the replacement of the standard boundary conditions (10) (containing infinite sums) by the more natural HD truncation of recurrences due to eq. (11), we just have to parallel the Hermitian considerations of ref. [22]. Firstly, we remind the reader that at an arbitrary finite precision we always have $E \neq E(physical)$. This means that our infinite series $\psi^{(ansatz)}(x)$ as defined by equation (5) will *always* exhibit an exponential asymptotic growth in a certain wedge-shaped vicinity of the real line [12].

The main point of the HD proof is that due to the standard oscillation theorems the last (left as well as right) nodal zeros will move *towards* their (left and right) infinities with the decrease of $E > E(physical)$ (say, at a fixed pair $h_{0,1}$). In the language of coordinates this means that the values of $\psi^{(ansatz)}(x)$ (both at some $x > X_R$ and at another $x < X_L$) will change sign for E somewhere in between the (smaller) $E(physical)$ and (larger) $E(numerical)$. Such a simultaneous change of the sign of $\psi^{(ansatz)}(x)$ at any sufficiently large absolute value of the coordinate $|x| \gg 1$ should be understood as resulting from our appropriate asymptotic estimate of $\psi^{(ansatz)}(x)$.

Although this sounds like a paradox, this estimate will *always* lead to an asymptotic growth (since $E \neq E_{physical}$ with probability one) so that it cannot be changed by the (key) omission of any *finite* number N of the exponentially small components $\sim \exp[-sx^2 + \mathcal{O}(\ln x)]$. They may be safely ignored as irrelevant. This means that we may choose $N \gg 1$ so that just the asymptotically dominant coefficients will play the role. Inserting (12) and (18) in $\psi^{(ansatz)}(x) \sim \exp(-sx^2)\sum_{n=N+1}^{\infty} h_n\,(ix)^n$ we finally get

$$\psi^{(ansatz)}(x) \sim e^{-sx^2} \sum_{n=N+1}^{\infty} \frac{G_2\lambda^n(2)\,g_n(2) + G_5\lambda^n(5)\,g_n(5)}{(3^{1/3})^n\,\Gamma(1+n/3)}\,(ix)^n, \qquad |x| \gg 1.$$

The validity of this formula is a strict consequence of the specific constraint (16) imposed (say, from now on) upon the admissible quasi-variational parameter s.

Once we split $\psi^{(ansatz)}(x) = \psi^{(ansatz)}(G_2, G_5, x)$ in its two components

$$\psi^{(ansatz)}(G_2, 0, x) \sim G_2\, e^{-sx^2} \sum_{n=N+1}^{\infty} \frac{(-x)^n \exp\left[\gamma(2)\, n^{2/3} + \mathcal{O}(n^{1/3})\right]}{(3^{1/3})^n\,\Gamma(1+n/3)},$$

$$\psi^{(ansatz)}(0, G_5, x) \sim G_5\, e^{-sx^2} \sum_{n=N+1}^{\infty} \frac{x^n \exp\left[\gamma(5)\, n^{2/3} + \mathcal{O}(n^{1/3})\right]}{(3^{1/3})^n\,\Gamma(1+n/3)},$$

we may apply the rule $e^z \sim (1+z/t)^t,\ t \gg 1$ in the error term and get

$$\frac{\psi^{(ansatz)}(G_2, 0, -y)}{\exp(-sy^2)} \sim G_2 \sum_{n=N+1}^{\infty} \frac{1}{(3^{1/3})^n\,\Gamma(1+n/3)} \left\{y \cdot \left[1 + \mathcal{O}\left(\frac{1}{N^{1/3}}\right)\right]\right\}^n$$

and

$$\frac{\psi^{(ansatz)}(0, G_5, y)}{\exp(-sy^2)} \sim G_5 \sum_{n=N+1}^{\infty} \frac{1}{(3^{1/3})^n\,\Gamma(1+n/3)} \left\{y \cdot \left[1 + \mathcal{O}\left(\frac{1}{N^{1/3}}\right)\right]\right\}^n.$$

This is valid at all the large arguments y. Along the *positive* semi-axis $y \gg 1$, both the right-hand-side summands are real and positive. They sum up to the same function $\exp[y^3/3 + \mathcal{O}(y^2)]$. This is a consequence of the approximation of the sum by an integral and its subsequent evaluation by means of the saddle-point method. The same trick was used by Hautot, in similar context, for the $\mathcal{P}-$symmetric and Hermitian anharmonic oscillators [10].

In contrast to the Hautot's resulting one-term estimates of ψ, the present asymmetric, $\mathcal{PT}-$invariant construction leads to the more general two-term asymptotic estimate

$$\psi^{(ansatz)}(G_2, G_5, x) \sim G_2\, \exp[-x^3/3 + \mathcal{O}(x^2)] + G_5\, \exp[x^3/3 + \mathcal{O}(x^2)], \qquad |x| \gg 1.$$

As long as we deal with the holomorphic function of x, this estimate may be analytically continued off the real axis of x. Near both the ends of the real line and within the asymptotic wedges $|\text{Im } x|/|\text{Re } x| < \tan \pi/6$ we simply have the rules

$$\psi^{(ansatz)}(G_2, G_5, x) \sim G_2 \exp[-x^3/3 + \mathcal{O}(x^2)], \quad \text{Re } x < -X_L \ll -1 \tag{21}$$

and

$$\psi^{(ansatz)}(G_2, G_5, x) \sim G_5 \exp[x^3/3 + \mathcal{O}(x^2)], \quad 1 \ll X_R < \text{Re } x. \tag{22}$$

They are fully compatible with our *a priori* expectations and represent in fact the main step towards our forthcoming completion of the rigorous proof of the validity of the HD matrix truncation (11).

4.3 The changes of sign of $\psi^{(ansatz)}(x)$ at $|x| \gg 1$

Our complex differential Schrödinger equation (3) becomes asymptotically real, in the leading-order approximation at least. In a suitable normalization the wave functions $\psi^{(ansatz)}(x)$ may be made asymptotically real as well. Near infinity they will obey the standard Sturm Liouville oscillation theorems. As we explained, after a small decrease of the tentative energy parameter $E > E(physical)$ the asymptotic nodal zero X_R or $-X_L$ originating in one of our boundary conditions (10) will move towards infinity. This may be re-read as a doublet of conditions

$$G_2 = G_2(E_0, \zeta_0) = 0, \qquad G_5 = G_5(E_0, \zeta_0) = 0 \tag{23}$$

using an assumption that $\zeta_0 \approx \zeta(physical)$ in the suitable parametrization of $h_0 = \rho \cos\zeta$ and $h_1 = \rho \sin\zeta$ with $\zeta \in (0, 2\pi)$ at a convenient normalization $\rho = 1$.

In the limit $N \to \infty$ the two requirements (23) may be interpreted as equivalent to the truncation recipe (11). Indeed, at a fixed $N \gg 1$ we may re-scale

$$f_p = G_p \frac{\lambda^N(p) \exp[\gamma(p) N^{2/3}]}{(3^{1/3})^N \Gamma(1 + N/3)}, \qquad p = 2, 5$$

where $f_p(E, \zeta_0) \approx F_p \cdot (E - E_0)$. This enables us to write

$$h_N \approx (F_2 + F_5)(E - E_0) + \mathcal{O}[(E - E_0)^2],$$
$$(N+3)^{1/3} h_{N+1} \approx [F_2 \lambda(2) + F_5 \lambda(5)](E - E_0) + \mathcal{O}[(E - E_0)^2]$$

due to equation (12). We see that the two functions G_2, G_5 are connected with the Taylor coefficients $h_N = h_N(E_0, \zeta_0)$ and $h_{N+1} = h_{N+1}(E_0, \zeta_0)$ near the physical E_0

and ζ_0 by an easily invertible regular mapping. This means that the implicit algebraic boundary conditions (23) are strictly equivalent to the fully explicit requirements

$$h_N(E_0, \zeta_0) = 0, \qquad h_{N+1}(E_0, \zeta_0) = 0, \qquad N \gg 1. \tag{24}$$

This completes our proof.

5 Discussion

5.1 Truncated secular Hill determinants

By construction, our present result may be re-read as a demonstration that the intuitive quasi-variational square-matrix truncation of our recurrences represents in fact a mathematically well founded approximation recipe. The evaluation of both the energies and wave functions may be started at any approximative cut-off $N < \infty$ and the solution of the linear algebraic problem

$$\left(\begin{array}{cccccccc} C_0 & 0 & A_0 & & & & \\ \delta & C_1 & 0 & A_1 & & & \\ \theta & \delta & \ddots & \ddots & \ddots & & \\ -\beta & \theta & \ddots & & & & \\ 1 & -\beta & \ddots & & & \ddots & A_{N-3} \\ & \ddots & \ddots & \ddots & \ddots & \ddots & 0 \\ & & 1 & -\beta & \theta & \delta & C_{N-1} \end{array} \right) \left(\begin{array}{c} h_0 \\ h_1 \\ h_2 \\ \ldots \\ h_{N-3} \\ h_{N-2} \\ h_{N-1} \end{array} \right) = 0 \tag{25}$$

must only be completed by the limiting transition $N \to \infty$. As long as the energy only enters the main diagonal, $C_n = 4sn + 2s - E$, we may determine all the approximate low-lying spectrum by the routine $N \times N-$dimensional asymmetric-matrix diagonalization. With $s = 2$ and $a = c = \beta = \delta = 1$, Table 1 illustrates the practical implementation as well as the highly satisfactory rate of convergence of the numerical HD algorithm.

5.2 Outlook

We have re-confirmed that the HD methods bridge a gap between the brute-force variational algorithms and sophisticated analytic semi-classical constructions. In the present context, we emphasized that the HD techniques may be combined not only with the complexification of the variables (characteristic for the latter approach) but also with the requirements of a numerical efficiency (pursued, usually, in the former setting).

In the conclusion we may note that another link connects also the HD and perturbative techniques. In the latter, semi-analytic type of considerations, an indispensable role is played by asymptotic expansions, say, of the power-series form

$$Z(\lambda) = \sum_{k=0}^{M} \lambda^k z_k + R_M(\lambda) \tag{26}$$

where λ represents a - presumably, "sufficiently" small - coupling constant while the typical example of the observable $Z(\lambda)$ is a bound-state energy. In the present HD setting we employed a similar ansatz (26) where the variable λ denoted the coordinate x while the function $Z(\lambda)$ represented the wave function.

Currently, a numerical credibility of the similar perturbative (and also semi-classical) constructions is being enhanced via an improved treatment of the error term $R_M(\lambda)$. In general, this does not seem to be the case in the present HD context. The reason is that although for the bound states the exponentially growing right-hand sum must be identically zero, we are still not interested in the explicit evaluation of the exponentially suppressed remainder $R_M(\lambda)$ (which would be hopeless) but merely in the bracketing property of the wave-function sum $\sum_{k=0}^{M} \lambda^k z_k \neq 0$ evaluated *slightly below and slightly above* the actual physical energy.

In this sense, we may summarize that the HD "trick" is different and enables us to pay a more detailed attention to the new perspectives opened by the consequent complexification of λ. Here, such a perspective enabled us to extend the standard mathematical background of the Hill-determinant constructions of bound states. We have seen that the old principles stay at work, making use of the same mechanism as in the standard Hermitian cases, viz, the constructively employed asymptotic cancellation of the growing exponentials in the exponentially decreasing wave functions $\psi(x)$.

Acknowledgements

Work partially supported by RIMS, Kyoto, and by the AS CR grant Nr. A 1048302.

Table

Table 1. The convergence of HD energies.

	energies E_n				
n / N	0	1	2	3	4
15	1.69347	5.106	9.152	13.043	17.82
20	1.691638	5.1256	9.2800	14.050	19.24
25	1.691579	5.12344	9.2581	13.869	18.79
30	1.691590	5.12361	9.2617	13.883	18.89
35	1.691590	5.12358	9.2615	13.879	18.88

References

[1] C. M. Bender and T. T. Wu, Phys. Rev. Lett. 21 (1968) 406 and Phys. Rev. 184 (1969) 1231.

[2] A. Voros, Ann. Inst. Henri Poincaré A 39 (1983) 211 and J. Phys. A: Math. Gen. 27 (1994) 4653.

[3] S. N. Biswas, K. Datta, R. P. Saxena, P. K. Srivastava and V. S. Varma, J. Math. Phys. 14 (1973) 1190; F. T. Hioe, D. MacMillan and E. W. Montroll, Phys. Rep. 43 (1978) 305.

[4] B. Simon, Int. J. Quant. Chem. 21 (1982) 3.

[5] E. Caliceti, S. Graffi and M. Maioli, Commun. Math. Phys. 75 (1980) 51.

[6] M. Znojil, Lett. Math. Phys. 5, 405 (1981) and J. Math. Phys. 29 (1988) 139.

[7] F. M. Fernández, R. Guardiola and M. Znojil, Phys. Rev. A 48 (1993) 4170.

[8] M. Znojil, J. Phys. A: Math. Gen. 31 (1998) 3349.

[9] V. Singh, S. N. Biswas and K. Data, Phys. Rev. D 18 (1978) 1901.

[10] A. Hautot, Phys. Rev. D 33 (1986) 437.

[11] M. Znojil, Non-variational Matrix Methods in Quantum Theory, INP AS CR Řež, 1993, unpublished.

[12] C. M. Bender and S. Boettcher, Phys. Rev. Lett. 24 (1998) 5243 and J. Phys. A: Math. Gen. 31 (1998) L273.

[13] M. Znojil, J. Phys. A: Math. Gen. 32 (1999) 7419.

[14] M. Znojil, Rendiconti del Circ. Mat. di Palermo, Ser. II, Suppl. 72 (2004) 211 (math-ph/0104012).

[15] C. M. Bender, D. C. Brody and H. F. Jones, Phys. Rev. Lett. 92 (2004) 119902 (erratum).

[16] M. Znojil, Phys. Lett. A 259 (1999) 220.

[17] B. Bagchi, C. Quesne and M. Znojil, Mod. Phys. Letters A 16 (2001) 2047 (quant-ph/0108096).

[18] P. A. M. Dirac, Proc. Roy. Soc. London A 180 (1942) 1; W. Pauli, Rev. Mod. Phys., 15 (1943) 175;

H. Feshbach and F. Villars, Rev. Mod. Phys., **30** (1958) 24; E. P. Wigner, J. Math. Phys. 1 (1960) 409; F. G. Scholtz, H. B. Geyer and F. J. W. Hahne, Ann. Phys. 213 (1992) 74; A. Mostafazadeh, J. Math. Phys. 43 (2002) 2814 and 3944.

[19] C. M. Bender, D. C. Brody and H. F. Jones, Phys. Rev. Lett. 89 (2002) 270401.

[20] M. Znojil, Phys. Lett. A 285 (2001) 7 (quant-ph/0101131).

[21] A. Mostafazadeh and A. Batal, Physical Aspects of Pseudo-Hermitian and PT-symmetric Quantum Mechanics, quant-ph/0408132.

[22] D. A. Estrin, F. M. Fernandez and E. A. Castro, Phys. Lett. A 130, 330 (1988); M. Znojil, J. Math. Phys. 33 (1992) 213 and J. Phys. A: Math. Gen. 27 (1994) 4945.