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Classification of oscillators in the Hessenberg-matrix representation

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Abstract. For an arbitrary finite and not too singular (presumably, phenomenological) superposition of potentials r^δ with rational exponents we solve the old problem of conversion of the corresponding differential Schrödinger bound-state problem into its matrix equivalent with the minimalized number L of non-zero diagonals. The construction—with proofs—is performed via the standard power-series method in its non-Hermitian matrix (sometimes called Hill-determinant) version. All the simplest and (in this sense) ‘algebraizable’ interactions are then displayed up to $L = 5$. An example of application in perturbation theory is included.

1. Introduction and summary

The harmonic-oscillator Hamiltonians

$$H^{(\text{HO})} = -\frac{\hbar}{2\mu}\Delta + \frac{f}{r^2} + g_2 r^2$$

with $f > -\frac{1}{4}$ and $g_2 > 0$ and/or their ‘Schwinger’ duals $H^{(\text{Coulomb})}$ (with the force $g_2 r^2$ replaced by a Coulombic attraction $-e^2|r|^{-1}$ [1]) are exceptional. All their bound-state energies $E_{n,\ell}$ and wavefunctions $\psi_{n,\ell}(r)$ are known and are elementary functions of couplings and of the quantum numbers $\ell = 0, 1, \dots$ (angular momentum) and $n = 0, 1, \dots$. Some of their most immediate generalizations

$$H^{(\text{rational})} = -\frac{\hbar}{2\mu}\Delta + \frac{f}{r^2} + g_{\delta_1} r^{\delta_1} + g_{\delta_2} r^{\delta_2} + \dots + g_{\delta_{\max}} r^{\delta_{\max}} \quad (1)$$
$$r = |r| \quad -2 < \delta_1 < \delta_2 < \dots < \delta_{\max}$$

remain easily tractable perturbatively, due to the extreme simplicity of their zero-order harmonic or Coulombic reductions.

In what follows, we are going to study all the latter, phenomenologically extremely useful [2] oscillators (1). In a non-perturbative regime, i.e. at all the values of their couplings, we shall work within the framework of the so-called Hill-determinant method [3]. Its formulae which cannot be safely used without simple though rigorous proofs [4] have offered one of the best possible quasi-analytic descriptions for many not too complicated systems. Equation (1) provides a good as well as an important further candidate for such an application.

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Our basic motivation stems from the enormous phenomenological appeal [5] and descriptive universality, elementarity and flexibility of the power-law superpositions (1). Nevertheless, our work is also inspired formally. Indeed, the non-perturbative Hill-determinant method, being essentially non-variational, is not without specific problems itself. Seemingly highly intuitive and clear, its application requires careful mathematical foundations. Moreover, some of the problems with Hill determinants seem to have a purely psychological root: there is no other explanation why, e.g., the recent numerical study of their 'failure' [6] did not take into consideration any available *a priori* condition of their applicability as provided in virtually any of the recent reviews.

The history of contradictions started with the 15-year-old paper by Singh *et al* [7]. Its authors noticed that the quartic-plus-sextic anharmonicities and Hamiltonians

$$H^{(\text{sextic})} = -\frac{\hbar}{2\mu}\Delta + \frac{f}{r^2} + g_2r^2 + g_4r^4 + g_6r^6 \quad f > -\frac{1}{4} \quad g_6 > 0 \quad (2)$$

might be called 'next-to-solvable'. Indeed, in the context of the standard power-series method [8], these authors re-discovered (see [9]) the possibility of survival of a few elementary bound states (and explicit exact formulae for energies) in certain strongly perturbed anharmonic-oscillator cases. Moreover, they revealed and emphasized a close analogy between these harmonic-oscillator-like terminating solutions and all the remaining, non-terminating and non-elementary bound states of the given Hamiltonian.

In its time, [7] inspired a boom of papers on $H^{(\text{sextic})}$. It was immediately noticed [10] that the elementary and exact partial solvability of $H^{(\text{sextic})}$ at certain couplings may be extended to many other integer-power oscillators

$$H^{(q)} = -\frac{\hbar}{2\mu}\Delta + \frac{f}{r^2} + g_0 + g_2r^2 + g_4r^4 + \dots + g_{4q+2}r^{4q+2} \quad (3)$$

with $g_{4q+2} = \alpha^2 > 0$, to their further non-integer-power descendants with arbitrary rational exponents δ in (1) [11] and to some even more general systems (see other references as listed, say, in [12]).

The main 'next-to-solvability' hypothesis of Singh *et al* [7] was based on a Hill-determinant tridiagonal-matrix representation of all the Hamiltonians $H^{(\text{sextic})}$. Unexpectedly, it proved to be wrong—the reader may consult [4] and [13] for several alternative explanations of this puzzling phenomenon. A few years later, sextic oscillators were shown to require at least a quadridiagonal-matrix representation of $H^{(\text{sextic})}$ whenever $g_4 \leq 0$ in equation (2) [14].

Of course, any coupling-dependent split of Hamiltonians (3) into 'more' and 'less solvable' cases is highly counter-intuitive and unpleasant. Nevertheless, as far as the present author knows, there is still no complete solution of this problem. Here, therefore, we are going to settle the question—for all the forces (1), we shall describe and prove the following consequent algebraization of the underlying Schrödinger bound-state problem:

- (i) All the bound states will be determined by an infinite-dimensional matrix equation

$$Q^{[N]} \begin{pmatrix} \omega_0 \\ \omega_1 \\ \dots \\ \omega_N \end{pmatrix} = 0 \quad N \rightarrow \infty \quad (4)$$

for the Taylor-series coefficients ω of the wavefunctions (see below for more detailed general definitions and rigorous proofs).

(ii) All the binding energies subsequently become fixed by the algebraic ‘Hill-determinant’ prescription

$$\det Q^{[N]} = 0 \quad N \rightarrow \infty. \tag{5}$$

(iii) The number (say L) of non-zero diagonals in the pertaining non-variational matrix representatives $Q^{[\infty]} = Q^{[\infty]}(E)$ of Schrödinger operators $H^{(1)(q)} - EI$ (with a unit operator I) will be kept minimal.

The resulting constructive classification of all the oscillators (1) with arbitrary couplings and arbitrary rational exponents will bring the preceding developments in the field to a climax:

(i) At $L = 2$, we encounter the well known pair of the exactly solvable (i.e. two-term recurrent, harmonic and Coulombic) oscillators.

(ii) In full accord with previous results, four and only four ‘next-to-solvable’ $L = 3$ descendents exist. With the usual $f > -\frac{1}{4}$ and properly scaled-out $g_{\delta_{\max}}$ ’s, their explicit Hamiltonians read:

$$\begin{aligned} & -\frac{\hbar}{2\mu}\Delta + fr^{-2} + ar^2 + \Omega r^4 + r^6 \\ & -\frac{\hbar}{2\mu}\Delta + fr^{-2} + ar^{-1} + \Omega r + r^2 \\ & -\frac{\hbar}{2\mu}\Delta + fr^{-2} + ar^{-4/3} + br^{-2/3} + r^{2/3} \\ & -\frac{\hbar}{2\mu}\Delta + fr^{-2} + ar^{-3/2} + br^{-1} + r^{-1/2}. \end{aligned} \tag{6}$$

Their list presents their asymptotic terms $r^{\delta_{\max}}$ in descending order and the necessary ‘superconfinement’ condition of the tridiagonality of their Q ’s has the form $\Omega > 0$ (and $E < 0$ in the latter two cases, see [14, 15]).

(iii) As the next $L = 4$ set of oscillators with four-diagonal Q ’s, there emerge 19 separate ‘next-to-next-to-solvable’ Hamiltonians

$$H^{(q)} = -\frac{\hbar}{2\mu}\Delta + \frac{f}{r^2} + V(r)$$

with a centrifugal-like strongly singular core if needed, $f > -\frac{1}{4}$, and with the further, at most weakly, singular interactions $V(r)$ which are listed here in table 1.

(iv) Pentadiagonal Q ’s with $L = 5$ appear in connection with the further 35 ‘next-to-next-to-next-to-solvable’ oscillators (see table 2), etc.

We might continue our L -classification indefinitely. A few phenomenologically most appealing elements of the further group of oscillators with hexadiagonal Q ’s are sampled here in table 3. In general, for even L we get $N_L = \frac{1}{4}(11L^2 - 26L + 4)$ different potentials for the L -diagonal matrices Q with the so-called Hessenberg-matrix structure [16]. Similarly, the odd- L sets would comprise as many as $N_L = \frac{1}{4}(11L^2 - 28L + 5)$ separate potentials.

In all the tables, many Hamiltonians may be inter-related by a Liouvillean change of variables $r \rightarrow r^{\text{const}}$ in the underlying Schrödinger differential equations [17]. As a consequence of this ‘generalized Schwinger duality’ [1], we may restrict our attention to mere ‘canonical’ representatives $H^{(q)}$ (3) of all our Hamiltonians (1) with rational exponents

Table 1. The complete list of oscillators with quadriagonal Hill determinants ($\Omega > 0$).

Potential $V(r)$	Admissible energies
$ar^2 + br^4 + cr^6 + \Omega r^8 + r^{10}$	all
$ar^2 + br^4 + \Omega r^6 + r^{10}$	all
$ar^2 - \Omega r^4 + r^6$	all
$ar^2 + r^6$	all
$ar^{-1} + br + cr^2 + \Omega r^3 + r^4$	all
$ar^{-1} + br + \Omega r^2 + r^4$	all
$ar^{-4/3} + br^{-2/3} + cr^{2/3} + \Omega r^{4/3} + r^2$	all
$ar^{-1} - \Omega r + r^2$	all
$ar^{-4/3} + br^{-2/3} + \Omega r^{2/3} + r^2$	all
$ar^{-1} + r^2$	all
$ar^{-3/2} + br^{-1} + cr^{-1/2} + \Omega r^{1/2} + r$	all
$ar^{-3/2} + br^{-1} + cr^{-1/2} + r$	$E < 0$
$ar^{-4/3} + br^{-2/3} + r^{2/3}$	$E \geq 0$
$ar^{-8/5} + br^{-6/5} + cr^{-4/5} + dr^{-2/5} + r^{2/5}$	$E < 0$
$ar^{-8/5} + br^{-6/5} + cr^{-4/5} + \Omega r^{-2/5} + r^{2/5}$	$E = 0$
$ar^{-5/3} + br^{-4/3} + cr^{-1} + dr^{-2/3} + \Omega r^{-1/3}$	$E < 0$
$ar^{-3/2} + br^{-1} - \Omega r^{-1/2}$	$E < 0$
$ar^{-5/3} + br^{-4/3} + cr^{-1} + \Omega r^{-2/3}$	$E < 0$
$ar^{-3/2} + br^{-1}$	$E < 0$

8. An alternative and more concise presentation of our classification pattern may then be found in table 4.

In practice, our separate minimal matrixizations $Q(E)$ may be applied not only as certain re-summed perturbation theories (see [7] or [18]) but also, directly, in potential models of the various simple quantized systems in the atomic, nuclear or chemical physics. The multiterm sextic anharmonicities or the Coulomb plus harmonic ('harmonium') superpositions in equation (6) and table 1 are worth noticing. One of the most popular ones—the quartic anharmonic oscillator [19]—stands as the sixth, $M = 1$ row in table 1. Its double-well alternative lies on the ninth line of table 2. The well known Coulomb plus linear 'quarkonium' potential [20] enters both tables 1 and 2 at different energies. Finally, several versions of the octic or popular cubic anharmonicities may only be found among the less simple forces in table 3.

In the text, our starting point will be the power-series method (section 2.1) and the related question of the length of recurrences L (section 2.2). In section 3, we shall remind the reader of the hypergeometric-like structure of wavefunctions at large $n \gg 1$ (section 3.1) and $r \gg 1$ (section 3.2), and discuss the problem of boundary conditions (section 3.3) for all the forces in question.

Section 4 will summarize these preparatory steps and clarify the one-to-one correspondence between operators H and Hessenberg matrices Q . The maximal admissible simplicity of the secular Hill determinants $\det Q^{|\infty|}(E)$ is achieved there resulting in the related ordering or classification and hierarchization of potentials (see tables 1–4). Finally, section 5 recalls [18] and adds a few more details to the applicability of the whole scheme in a perturbative setting. We show that (and how) the standard anharmonic oscillator admits an entirely new Hill-determinant-inspired perturbative study.

2. Wavefunctions

Up to the above-mentioned (and entirely straightforward) Liouvillean changes of variables

Table 2. The complete list of oscillators with pentadiagonal Hill determinants ($\Omega > 0$).

Potential $V(r)$	Admissible energies
$ar^2 + \dots + dr^8 + er^{10} + \Omega r^{12} + r^{14}$	all
$ar^2 + br^4 + cr^6 + dr^8 + \Omega r^{10} + r^{14}$	all
$ar^2 + br^4 + cr^6 + \Omega r^8 + r^{14}$	all
$ar^2 + br^4 - \Omega r^6 + r^{10}$	all
$ar^2 + br^4 + r^{10}$	all
$ar^{-1} + \dots + dr^3 + er^4 + \Omega r^5 + r^6$	all
$ar^{-1} + br + cr^2 + dr^3 + \Omega r^4 + r^6$	all
$ar^{-1} + br + cr^2 + \Omega r^3 + r^6$	all
$ar^{-1} + br - \Omega r^2 + r^4$	all
$ar^{-1} + br + r^4$	all
$ar^{-4/3} + \dots + dr^{4/3} + er^2 + \Omega r^{8/3} + r^{10/3}$	all
$ar^{-4/3} + br^{-2/3} + cr^{2/3} + dr^{4/3} + \Omega r^2 + r^{10/3}$	all
$ar^{-4/3} + br^{-2/3} + cr^{2/3} + \Omega r^{4/3} + r^{10/3}$	all
$ar^{-3/2} + \dots + dr^{1/2} + er + \Omega r^{3/2} + r^2$	all
$ar^{-3/2} + br^{-1} + cr^{-1/2} + dr^{1/2} + \Omega r + r^2$	all
$ar^{-4/3} + br^{-2/3} - \Omega r^{2/3} + r^2$	all
$ar^{-3/2} + br^{-1} + cr^{-1/2} + \Omega r^{1/2} + r^2$	all
$ar^{-4/3} + br^{-2/3} + r^2$	all
$ar^{-8/5} + \dots + dr^{-2/5} + er^{2/5} + \Omega r^{4/5} + r^{6/5}$	all
$ar^{-8/5} + \dots + dr^{-2/5} + \Omega r^{2/5} + r^{6/5}$	all
$ar^{-8/5} + br^{-6/5} + cr^{-4/5} + dr^{-2/5} + r^{6/5}$	$E < 0$
$ar^{-3/2} + br^{-1} + cr^{-1/2} + r$	$E \geq 0$
$ar^{-5/3} + \dots + er^{-1/3} + \Omega r^{1/3} + r^{2/3}$	all
$ar^{-5/3} + \dots + dr^{-2/3} + er^{-1/3} + r^{2/3}$	$E < 0$
$ar^{-5/3} + br^{-4/3} + cr^{-1} + dr^{-2/3} + \Omega r^{-1/3} + r^{2/3}$	$E = 0$
$ar^{-8/5} + br^{-6/5} + cr^{-4/5} - \Omega r^{-2/5} + r^{2/5}$	$E = 0$
$ar^{-8/5} + br^{-6/5} + cr^{-4/5} + r^{2/5}$	$E = 0$
$ar^{-12/7} + \dots + er^{-4/7} + fr^{-2/7} + r^{2/7}$	$E < 0$
$ar^{-12/7} + \dots + er^{-4/7} + \Omega r^{-2/7} + r^{2/7}$	$E = 0$
$ar^{-12/7} + \dots + dr^{-6/7} + \Omega r^{-4/7} + r^{2/7}$	$E = 0$
$ar^{-7/4} + \dots + er^{-3/4} + fr^{-1/2} + \Omega r^{-1/4}$	$E < 0$
$ar^{-7/4} + \dots + dr^{-1} + er^{-3/4} + \Omega r^{-1/2}$	$E < 0$
$ar^{-5/3} + br^{-4/3} + cr^{-1} - \Omega r^{-2/3}$	$E < 0$
$ar^{-7/4} + dr^{-3/2} + cr^{-5/4} + dr^{-1} + \Omega r^{-3/4}$	$E < 0$
$ar^{-5/3} + br^{-4/3} + cr^{-1}$	$E < 0$

$$r = r(x) = x^\mu \tag{7}$$

$$\psi(r) \rightarrow \chi(x) = r^{\text{const}} \psi(r)$$

which preserve the power-law character of potentials

$$r^{2j} \rightarrow x^\delta \quad \delta = 2(j + 1)\mu - 2$$

we may restrict our attention to the ‘canonical’ Hamiltonians (3). Demanding that the energy term remains non-trivial (i.e. that we obtain the zero exponent $\delta = 0$ at some integer $j_0 < q + 1$) we may enumerate all the admissible Liouvillean exponents μ at each q ,

$$\mu = 1, \frac{1}{2}, \frac{1}{3}, \dots, \frac{1}{2q + 2}.$$

Then, our explicit tables 1–3 of different potentials are easily reconstructed from our final, schematic table 4.

Table 3. The sample of oscillators with hexadiagonal Hill determinants ($\Omega > 0$).

Potential $V(r)$	Admissible energies
$ar^2 + \dots + er^{10} + fr^{12} + gr^{14} + \Omega r^{16} + r^{18}$	all
\vdots	\vdots
$ar^2 + br^4 + cr^6 + dr^8 + \Omega r^{10} + r^{18}$	all
$ar^2 + br^4 + cr^6 - \Omega r^8 + r^{14}$	all
$ar^2 + br^4 + cr^6 + r^{14}$	all
$ar^2 + br^4 + cr^6 - \Omega r^8 + r^{10}$	all
$ar^{-1} + \dots + er^4 + fr^5 + gr^6 + \Omega r^7 + r^8$	all
$ar^{-1} + \dots + dr^3 + er^4 + fr^5 + \Omega r^6 + r^8$	all
\vdots	\vdots
$ar^{-1} + br + cr^2 + dr^3 + \Omega r^4 + r^8$	all
$ar^{-1} + br + cr^2 - \Omega r^3 + r^6$	all
$ar^{-1} + br + cr^2 + r^6$	all
\vdots	\vdots
$ar^{-1} + br + cr^2 - \Omega r^3 + r^4$	all
\vdots	\vdots
$ar^{-3/2} + \dots + fr^{3/2} + gr^2 + \Omega r^{5/2} + r^3$	all
$ar^{-3/2} + \dots + fr^{3/2} + \Omega r^2 + r^3$	all
\vdots	\vdots
$ar^{-3/2} + br^{-1} + cr^{-1/2} + dr^{1/2} + \Omega r + r^3$	all
$ar^{-8/5} + \dots + fr^{4/5} + gr^{6/5} + \Omega r^{8/5} + r^2$	all
$ar^{-4/3} + br^{-2/3} + cr^{2/3} - \Omega r^{4/3} + r^2$	all
$ar^{-8/5} + \dots + er^{2/5} + fr^{4/5} + \Omega r^{6/5} + r^2$	all
$ar^{-8/5} + \dots + dr^{-2/5} + er^{2/5} + \Omega r^{4/5} + r^2$	all
$ar^{-3/2} + br^{-1} + cr^{-1/2} - \Omega r^{1/2} + r^2$	all
$ar^{-8/5} + br^{-6/5} + cr^{-4/5} + dr^{-2/5} + \Omega r^{2/5} + r^2$	all
$ar^{-3/2} + br^{-1} + cr^{-1/2} + r^2$	all
$ar^{-5/3} + \dots + dr^{-2/3} + er^{-1/3} + \Omega r + r^{4/3}$	$E < 0$
\vdots	\vdots
$ar^{-5/3} + \dots + dr^{-2/3} + er^{-1/3} + r^{4/3}$	$E < 0$
$ar^{-8/5} + br^{-6/5} + cr^{-4/5} + dr^{-2/5} + r^{6/5}$	$E \geq 0$
$ar^{-3/2} + br^{-1} + cr^{-1/2} - \Omega r^{1/2} + r$	all
$ar^{-7/4} + \dots + dr^{-1} + \dots + gr^{-1/4} + \Omega r^{1/4} + r^{1/2}$	all
$ar^{-7/4} + \dots + dr^{-1} + \dots + gr^{-1/4} + r^{1/2}$	$E < 0$
$ar^{-7/4} + \dots + er^{-3/4} + fr^{-1/2} + \Omega r^{-1/4} + r^{1/2}$	$E = 0$
$ar^{-7/4} + \dots + dr^{-1} + er^{-3/4} + \Omega r^{-1/2} + r^{1/2}$	$E = 0$
$ar^{-8/5} + br^{-6/5} + cr^{-4/5} + dr^{-2/5} + r^{2/5}$	$E > 0$
\vdots	\vdots
$ar^{-16/9} + \dots + er^{-8/9} + \Omega r^{-2/3} + r^{2/9}$	$E = 0$
$ar^{-9/5} + \dots + gr^{-3/5} + hr^{-2/5} + r^{-1/5}$	$E < 0$
$ar^{-9/5} + \dots + gr^{-3/5} + r^{-2/5}$	$E < 0$
$ar^{-9/5} + \dots + fr^{-4/5} + r^{-3/5}$	$E < 0$
$ar^{-5/3} + br^{-4/3} + cr^{-1} + dr^{-2/3} - r^{-1/3}$	$E < 0$
$ar^{-7/4} + br^{-3/2} + cr^{-5/4} + dr^{-1} - r^{-3/4}$	$E < 0$
$ar^{-9/5} + br^{-8/5} + cr^{-7/5} + dr^{-6/5} + er^{-1} + r^{-4/5}$	$E < 0$
$ar^{-7/4} + br^{-3/2} + cr^{-5/4} + dr^{-1}$	$E < 0$

Table 4. The complete list of polynomial oscillators with L diagonal Q 's.

Parameters			Constraints					
L	q	t	sign g_{4q}	sign g_{4q-2}	sign g_{4q-4}	sign g_{4q-6}	sign g_{4q-8}	sign g_{4q-10}
(a) $L \leq 6$								
2	0	0	—					
3	1	1	1					
4	1	0	-1 or 0					
4	2	2	1					
4	2	2	0	1				
5	2	1	0	-1 or 0				
5	3	3	1					
5	3	3	0	1				
5	3	3	0	0	1			
6	2	0	-1					
6	3	2	0	0	-1 or 0			
6	4	4	1					
6	4	4	0	1				
6	4	4	0	0	1			
6	4	4	0	0	0	1		
(b) $L = 7$ and $L = 8$								
7	3	1	0	-1				
7	4	3	0	0	0	-1 or 0		
7	5	5	1					
7	5	5	0	1				
7	5	5	0	0	1			
7	5	5	0	0	0	1		
7	5	5	0	0	0	0	1	
8	3	0	-1					
8	4	2	0	0	-1			
8	5	4	0	0	0	0	-1 or 0	
8	6	6	1					
8	6	6	0	1				
8	6	6	0	0	1			
8	6	6	0	0	0	1		
8	6	6	0	0	0	0	1	
8	6	6	0	0	0	0	0	1

2.1. The power-series method

In our canonical, radial ($\ell = 0, 1, \dots$) differential Schrödinger equation

$$\left[-\frac{d^2}{dr^2} + \frac{\ell(\ell + 1) + f}{r^2} + g_0 + g_2r^2 + g_4r^4 + \dots + g_{4q+2}r^{4q+2} \right] \psi(r) = E\psi(r) \tag{8}$$

we may re-parametrize the regular part of the interaction:

$$\begin{aligned} V(r) &= u^{(q)}(r) + r^2[w^{(q)}(r)]^2 \\ u^{(q)}(r) &= (c_0+)c_1r^2 + c_2r^4 + \dots + c_qr^{2q} \\ w^{(q)}(r) &= d_1 + d_2r^2 + \dots + d_{q+1}r^{2q} \\ d_{q+1} &= \sqrt{g_{4q+2}} \equiv \alpha > 0. \end{aligned} \tag{9}$$

This is a useful technicality—via an obvious recurrent definition of the new coupling constants, $d_q = g_{4q}/(2\alpha), \dots$ (or, *vice versa*, $g_{4q} = 2, d_q, d_{q+1}, \dots$), we immediately arrive at the compact asymptotic estimates of the wavefunctions,

$$\begin{aligned}\psi^{(\text{physical})}(r) &\approx e^{-G(r)} & r \gg 1 \\ \psi^{(\text{unphysical})}(r) &\approx e^{+G(r)} & r \gg 1\end{aligned}\quad (10)$$

with

$$G(r) = G_{\text{WKB}}(r) = \frac{1}{2}d_1 r^2 + \frac{1}{4}d_2 r^4 + \dots + \frac{1}{2q+2}d_{q+1} r^{2q+2}.$$

In terms of a re-parametrization $l(l+1) = \ell(\ell+1) + f$ of the angular momentum, $l > -\frac{1}{2}$, we may distinguish between the physical (regular) and unphysical (irregular) solutions in the origin,

$$\begin{aligned}\psi^{(\text{regular})}(r) &\approx r^{l+1} & r \ll 1 \\ \psi^{(\text{unphysical})}(r) &\approx r^{-l} & r \ll 1.\end{aligned}$$

In accord with Hautot [4], we may now build the wavefunctions from a most flexible and regular power-series ansatz

$$\psi(r) \equiv \psi^{(\text{regular})}(r) = r^{l+1} e^{-G_{\text{Hautot}}(r)} \sum_{n=0}^{\infty} \omega_n r^{2n} \quad (11)$$

where the $q+1$ free parameters β in the exponent

$$G_{\text{Hautot}}(r) = \frac{1}{2}\beta_1 r^2 + \frac{1}{4}\beta_2 r^4 + \dots + \frac{1}{2q+2}\beta_{q+1} r^{2q+2} \quad (12)$$

generalize their above-mentioned WKB predecessors and may be arbitrary. In a purely numerical context, their values may *a priori* be very easily optimized by means of Hautot's very elegant quasi-variational recipe [4].

The insertion of ansatz (11) converts the radial differential Schrödinger equation (8) + (9) in $2q+3$ -term recurrences [8],

$$\begin{aligned}B_n \omega_{n+1} &= C_n^{(0)} \omega_n + C_n^{(1)} \omega_{n-1} + \dots + C_n^{(q)} \omega_{n-q} + \\ &+ D^{(1)} \omega_{n-q-1} + \dots + D^{(q)} \omega_{n-2q} + D^{(q+1)} \omega_{n-2q-1} \quad n = 0, 1, \dots\end{aligned}\quad (13)$$

where

$$\begin{aligned}B_n &= (2n+2)(2n+2l+3) \\ C_n^{(j)} &= 4n\beta_{j+1} + O(1) \quad j = 0, 1, \dots, q \\ D^{(q+1)} &= (d_{q+1} + \beta_{q+1})(d_{q+1} - \beta_{q+1}) \\ D^{(q)} &= (d_{q+1} + \beta_{q+1})(d_q - \beta_q) + (d_q + \beta_q)(d_{q+1} - \beta_{q+1}) \\ D^{(1)} &= (d_{q+1} + \beta_{q+1})(d_1 - \beta_1) + \dots + (d_1 + \beta_1)(d_{q+1} - \beta_{q+1}).\end{aligned}$$

These recurrences are readily solvable:

$$\omega_{n+1} = \frac{\omega_0}{\prod_{k=1}^n B_k} \det Q^{[n]} \quad n = 0, 1, \dots \tag{14}$$

Here, matrices

$$Q^{[n]} = \begin{pmatrix} C_0^{(0)} & -B_0 & & & & \\ C_1^{(1)} & C_1^{(0)} & -B_1 & & & \\ C_2^{(2)} & C_2^{(1)} & C_2^{(0)} & -B_2 & & \\ & & & & \ddots & \\ & D_n^{(q)} & D_n^{(q-1)} & \dots & C_n^{(1)} & C_n^{(0)} \end{pmatrix}$$

are finite-dimensional. As long as $Q_{m,n} = 0$ for all $n > m + 1$, these matrices possess the so-called Hessenberg structure [16].

We may summarize: in terms of the free parameters β and undetermined physical energy E , all our bound-state wavefunctions are explicitly defined by the closed formulae (11) and (14). At $q = 0$, equation (14) degenerates to an elementary product. Of course, no similar degeneracy occurs at non-zero q 's.

2.2. Lowering the number L of non-zero diagonals

Let us choose a non-negative integer $t \leq q$ and demand that $\beta_{q+1} = d_{q+1}$, $\beta_q = d_q, \dots, \beta_{q+1-t} = d_{q-t+1}$ in equation (11). As a consequence, the first $t + 1$ rightmost coefficients D drop out of our recurrences (13). In other words, each subsequent WKB-like choice of the $(t + 1)$ th asymptotically dominant coefficient β will lower the length of our recurrences to $L = 2q + 2 - t$ and the order of our difference Schrödinger equation (13) to $L - 1 = 2q + 1 - t$.

In accord with the above-mentioned particular studies of the example $q = 1$, unexpected difficulties may arise at any such choice with $t \geq 0$. Hence, besides the fully WKB case with $t = q$ and Singh-like exponentials (10), we may need the partially WKB or transitional exponents

$$G^{(t)}(r) = \frac{1}{2}\beta_1 r^2 + \frac{1}{4}\beta_2 r^4 + \dots + \frac{1}{2q - 2t}\beta_{q-t} r^{2q-2t} + \frac{1}{2q - 2t + 2}d_{q-t+1} r^{2q-2t+2} + \dots + \frac{1}{2q + 2}d_{q+1} r^{2q+2} \tag{15}$$

with all the non-negative integers $t \leq q$.

The maximally WKB choice of $G^{(t)}(r)$ with $t = q > 1$ and with the most compact matrization ($L = q + 2$) was first proposed and tested in a letter [21]. In [15], the related construction of equation (4) with L -diagonal quasi-Hamiltonians $Q(E)$ was then complemented by its rigorous proof and by the necessary and sufficient 'superconfinement' condition of its validity. Briefly, whenever we define a maximal non-negative integer $M \leq q$ such that

$$d_{q-M+1} = d_{q-M+2} = \dots = d_{q-1} = d_q = 0 \tag{16}$$

(cf equation (9)—we put $M = 0$ for $d_q \neq 0$), the latter superconfinement condition reads, simply, as

$$d_{q-M} > 0 \quad M < q. \tag{17}$$

We may immediately trace it in equation (6) and in all the minimal-length $L = q + 2$ sub-items of our tables where equation (17) appears disguised as a requirement $\Omega > 0$ or, sometimes, $E < 0$.

Arbitrary external and independent (say, numerical or variational) specification of the sufficiently precise $E^{(\text{physical})}$ enables one always to choose $t = q$ (i.e. minimize $L = q + 2$) and use equation (11) as an approximate wavefunction, without any recourse to its secular equation companion (5). Nevertheless, we need the Hill-determinant matricization conditions (17) and (5) whenever we intend to replace recurrences (13) by their specific truncation (4). Indeed, unless we have it, we are not permitted to construct Green's functions in terms of (generalized) continued fractions [7, 15], and we also lose the possibility of applying any form of the related perturbation theories [18, 22]. For these reasons, the explicit Hill-determinant-like matricization (4) as well as its L -minimalization and rigorous proof remain highly desirable.

In the literature, the consequent and systematic minimalization of L 's has not yet been studied at all. Hautot's universal prescription (12) even keeps the length of recurrences at its *maximum* (!) $L = 2q + 3$. Even our preceding study of Hill determinants [22] only offered an insignificant improvement. With mere leading-order-WKB exponentials ($G^{(t)}$ with $t = 0$ in the present language), its choice of $d_{q+1} = \beta_{q+1}$ only lowered Hautot's L by one unit in general, to $L = 2q + 2$.

Now, we are going to cover all the WKB $t \leq q$ matricizations and to propose and prove the universal, unrestricted construction of quasi-Hamiltonians $Q(E)$ which contain the lowest possible number of non-zero diagonals $L = 2q + 2 - t$.

3. The difference Schrödinger equation

A missing link between the standard numerical boundary conditions

$$\psi^{(\text{regular})}(R) = 0 \quad R \gg 1 \quad (18)$$

(where the nodal zero R moves to infinity in principle) and their present Hill-determinant equivalent (5) or, in the light of equation (14), numerical analogue

$$\omega_{N+1} = 0 \quad N \gg 1 \quad (19)$$

lies obviously in an analysis of the asymptotic behaviour of Taylor coefficients ω_n themselves. Unfortunately, it can hardly be inferred from the explicit Hill determinants (14) since it becomes more and more difficult to evaluate them with increasing n 's. A return to recurrences is called for. As a byproduct, it will recover another parallelism between the $q = 0$ ('solvable') and $q > 0$ ('unsolvable') interactions.

3.1. Asymptotics in $n \gg 1$

In accord with [22] and for all the non-negative q 's, the new change of variables

$$\omega_{n+1} = \lambda^n \frac{\Gamma\left(1 + \frac{n+q}{q+1}\right)}{\Gamma\left(1 + \frac{n+1}{q+1}\right) \Gamma\left(1 + \frac{n+1+3/2}{q+1}\right)} p_n \quad (20)$$

i.e. $\omega_{n+1} \rightarrow p_n$, with

$$\eta = \frac{1}{4} \left(2l + 3 - 2q + \frac{c_q + d_q}{\alpha} \right)$$

and with the (in general, complex) parameter

$$\lambda = \lambda_{(k)} = \left| \left(\frac{\beta_{q+1}}{q+1} \right)^{1/(q+1)} \right| \exp \left(i \frac{2k\pi}{q+1} \right) \tag{21}$$

is ambiguous and has to be further specified by the choice of index $k = 0, 1, \dots, q$. For each of these choices, our difference Schrödinger equation (13) acquires the same new and much more transparent form

$$p_N - p_{N-q-1} = (F_q p_{N-q} + F_{2q+1} p_{N-2q-1}) + (F_{q-1} p_{N-q+1} + F_{2q} p_{N-2q}) + \dots + (F_1 p_{N-1} + F_{q+2} p_{N-q-2}) \tag{22}$$

where all the coefficients are N - and k -dependent, $F_i = F_i(N, k)$.

By definition, equation (13) and equations (22) with all the possible different k 's are mutually equivalent. In the asymptotic region, the coefficients F may be simplified, namely

$$F_{q-m} = \lambda_{(k)}^{m-q} \frac{\beta_{q-m}}{q+1} \left(\frac{N}{q+1} \right)^{-(m+1)/(q+1)} [1 + O(1/N)]$$

and

$$F_{2q+1-m} = \lambda_{(k)}^{m-q} \frac{D^{(q-m)}}{4\beta_{q+1}(q+1)} \left(\frac{N}{q+1} \right)^{-(m+1)/(q+1)} [1 + O(1/N)].$$

Due to the asymptotic smallness of these F 's, all the difference Schrödinger equations (22) with different k 's and q 's become identical at large N ,

$$p_N - p_{N-q-1} = 0 \quad N \gg 1. \tag{23}$$

The $q + 1$ leading-order asymptotic components of our Taylor coefficients may now be written as numbered by the index $k = 0, 1, \dots, q$ as well,

$$\omega_N^{(k)} \approx \tilde{\omega}_N^{(k)} \equiv \lambda_{(k)}^{N-1} \frac{\Gamma \left(1 + \frac{N+\eta-1}{q+1} \right)}{\Gamma \left(1 + \frac{N}{q+1} \right) \Gamma \left(1 + \frac{N+l+1/2}{q+1} \right)} \quad N \gg 1. \tag{24}$$

In the fully WKB regime with $t = q$, this set of solutions is complete and the general $n \gg 1$ solution equals to their superposition,

$$\omega_N \approx \sum_{k=0}^q c_k \tilde{\omega}_N^{(k)}. \tag{25}$$

This asymptotic formula complements the small- n determinantal prescription (14).

Whenever we choose a $t < q$ at a non-zero q , a few additional independent components of ω must exist in principle. Nevertheless, in accord with [22], all these $k > q$ components remain asymptotically negligible and may be ignored. Thus, the above explicit equations (24) and (25) and the common 'hypergeometric-function-like' asymptotic structure of coefficients ω_N link the $q = 0$ and $q > 0$ cases and remain t -independent.

3.2. The compatibility with asymptotics in $r \gg 1$

At almost all (i.e. unphysical) energies E , the exponential asymptotics of the regular solutions remain unphysical,

$$\psi^{(\text{regular})}(r) \approx \exp\left(+\frac{d_{q+1}}{2q+2}r^{2q+2}\right) \quad r \gg 1 \quad E \neq E^{(\text{exact})}. \quad (26)$$

Vice versa, the normalizable bound states in equation (10) may be interpreted as mere limits of solutions (26) constrained by the standard asymptotic boundary condition (18). This only defines the energies $E^{(\text{physical})}$ as roots $E^{(\text{approximate})}(R)$ of equation (18) in a double (i.e. Taylor-series and $R \rightarrow \infty$) and purely numerical limit. A further analysis is needed.

3.2.1. The $q = 0$ guide. In the trivial harmonic-oscillator example with $q = 0$ and $E \neq E^{(\text{exact})}$, the Taylor series (11) does not terminate. For an estimate of its $r \approx R \gg 1$ asymptotics, we may ignore the exponentially small corrections in equation (11),

$$\psi^{(\text{regular})}(R) \approx \sum_{n=N+1}^{\infty} \dots \quad N \gg 1$$

approximate the summation by an integration,

$$\psi^{(\text{regular})}(R) \approx \omega_{N+1} \int_{N+1}^{\infty} \dots$$

and, due to the non-negativity of the integrand, recall the so-called saddle-point method (see, e.g., [4] or [22] for more details).

Of course, the resulting formula

$$\psi^{(\text{regular})}(R) \approx \omega_{N+1} \exp\left(+\frac{1}{2}R^2\right) \quad R \gg 1 \quad (27)$$

is dominated by a single exponential and, hence, cannot coexist with boundary conditions (18) at any E . As a consequence, in accord with the textbooks, the whole series must terminate. It is worth noticing that even the truncated $q = 0$ secular equation (5) or, equivalently, (19) is in fact exact and defines precisely the first $N + 2$ lowest harmonic-oscillator (or Coulombic) bound-state energies. This feature may (and, up to a few exceptional couplings and energies [10], will) be lost for $q > 0$.

3.2.2. The assumption of one-term dominance for $q > 0$. Our leading-order knowledge (24) and (25) of Taylor coefficients ω_n at large n suffices for a straight generalization of the $q = 0$ saddle-point estimates. Indeed, we may always split the regular wavefunctions into separate components generated by the different λ 's as numbered by k 's in equation (21),

$$\psi^{(\text{regular})}(r) \approx \sum_{k=0}^q c_k \psi^{(k)}(r) \quad (28)$$

$$\psi^{(k)}(r) \approx \exp[-G(r)] \sum_{n=N+1}^{\infty} \omega_n^{(k)} r^{2n+l+1} \quad r \gg 1.$$

Each of the latter sub-sums may be replaced by an integral. Their subsequent saddle-point estimates lead to the set of $q + 1$ formulae

$$\psi^{(k)}(r) \approx \omega_{N+1}^{(k)} \exp\left(+\frac{d_{q+1}}{2q+2} R^{2q+2}\right) \tag{29}$$

which are all similar to their single $q = 0$ predecessor.

At $q > 0$, we encounter a qualitatively new situation. First, the single equation (19) cannot be interpreted as a termination requirement for all the $q + 1$ independent sub-sums—we would need $q + 1$ independent algebraic conditions as well [10]. Second, even at $q = 1$, an interplay of the $q + 1$ separate exponentials (29) is complicated. An analysis of their mutual asymptotic cancellation at physical energies is a difficult task unless one of them clearly asymptotically dominates. This is our basic idea, to be further developed in what follows.

4. Hamiltonians in the Hessenberg-matrix representation

Guided by the $q = 1$ example, we shall try to satisfy boundary conditions (18) in a maximal analogy to harmonic oscillators: In the asymptotic domain of coordinates $r \gg 1$, we shall simply postulate that just one exponential (29) (i.e. the k_0 th) dominates the superposition (28).

Once we replace this superposition by its single exponential component, our explicit knowledge of it immediately reduces our exponential-dominance postulate to mere requirement of dominance of a single Taylor coefficient, i.e. $\omega_{N+1} \approx \omega_{N+1}^{(0)}$, $N \gg 1$, or

$$|\omega_{N+1}^{(0)}| \gg |\omega_{N+1}^{(k)}| \quad k \neq 0 \quad N \gg 1. \tag{30}$$

With, for the sake of definiteness, $k_0 = 0$, this is suitable for further analysis. At $t = 0$, the idea has been followed in [22]. Now, we are going to extend it to all other eligible positive integers $t \leq q$.

4.1. The consequences of one-term dominance

For the time being, let us assume that condition (30) holds. As its consequence, we have

$$\psi^{(\text{regular})}(r) \approx \psi^{(0)}(r) \approx \omega_{N+1}^{(0)} \exp(\dots)$$

and see that, in a partial analogy to harmonic oscillators, the only way of meeting the boundary-condition requirement (18) leads through the existence of a zero in the coefficient $\omega_{N+1}^{(0)} \approx \omega_{N+1}$ itself,

$$\text{sign}[\psi^{(\text{regular})}(R)(\pm\text{corrections})] \approx \text{sign}[\omega_{N+1}(\pm\text{corrections})].$$

Thus, in the appropriate limits, the nodal coincidence

$$\omega_{N+1} = 0 \quad \text{iff} \quad \psi^{(\text{regular})}(R) = 0$$

represents precisely the necessary background and proof of the validity of secular equations (19) or (5). Hence, the correctness of the non-variational and non-Hermitean Hessenberg-matrix matrixizations (4) of our Schrödinger bound-state problem for all the q 's would simply follow from the validity of our single-term dominance postulate (30).

4.2. The guarantee of one-term dominance

The desired asymptotic suppression of all the $k \neq 0$ coefficients $\omega_n^{(k)}$ is to be achieved now by an appropriate choice for Hautot's free parameters β .

In the underlying sufficient condition (30), the explicit first-order asymptotical estimate (24) of ω_n 's gives no hint. In the leading-order approximation and at all the k 's, the magnitude of all the complex $\omega^{(k)}$'s remains the same.

The second-order asymptotic solution of our difference Schrödinger equation (22) is not difficult. Its construction is simplified by the harmonic-oscillator-like two-term form of recurrences

$$B_n \omega_{n+1} - C_n^{(q)} \omega_{n-q} = \text{small.}$$

Indeed, we may use the old leading-order solutions (20) to define the new, non-zero and explicit right-hand-side expression. The idea may be applied iteratively and the exact difference Schrödinger equation (22) may be solved with higher and higher precision if needed.

In the first step with an input $p_n^{(k)} \approx$ a constant we get the output

$$p_N = \exp \left[\frac{\beta_q + (D^{(q)}/4\beta_{q+1})}{q\lambda^q} \left(\frac{N}{q+1} \right)^{q/q+1} \right] \quad N \gg 1$$

which may already remove the degeneracy. Indeed, with the k -dependence hidden in the (complex) parameter λ (cf equation (21)) and, hence, in the factor $\lambda_{(k)}^{-q}$, we get

$$p_N^{(k)} = f(N, k) \exp \left[\frac{\beta_q + (D^{(q)}/4\beta_{q+1})}{q|(\beta_{q+1}/(q+1))^{q/(q+1)}|} \left(\frac{N}{q+1} \right)^{q/q+1} \cos \left(\frac{2kq\pi}{q+1} \right) \right] \quad (31)$$

where

$$f(N, k) \approx \exp \left[-i \frac{\beta_q + (D^{(q)}/4\beta_{q+1})}{q|(\beta_{q+1}/(q+1))^{q/(q+1)}|} \left(\frac{N}{q+1} \right)^{q/q+1} \sin \left(\frac{2kq\pi}{q+1} \right) \right] \quad N \gg 1.$$

Now, as long as the norm of $f(N, k)$ still remains asymptotically equal to one, we may satisfy the asymptotic inequality (30) whenever our choice of β_q makes the argument in the exponential (31) positive, i.e. whenever

$$\beta_q > -\frac{D^{(q)}}{4\beta_{q+1}}. \quad (32)$$

This is our simplest sufficient condition. It demonstrates that there exists a non-empty class of parameters (here: β_q restricted by equation (32)) which guarantees the validity of the Hill-determinant secular equation (5).

4.3. The guarantee of one-term dominance at a minimal integer L

Among all the matricization-permitting parametrizations β and ansätze $\psi^{(\text{regular})}(r)$ it is still possible and quite natural to search for those which lead to the minimal length $L = 2q + 2 - t$ of recurrences (13). In other words, once we assign several exponents $G^{(t)}(r)$ to a given

potential $V^{(q)}(r)$, the maximal permissible WKB precision t will minimize the L 's as required.

Our above result (32) only indicates the tactics. Indeed, after further insertions, it may be deciphered as a condition

$$\beta_q + d_q > 0 \tag{33}$$

which is only compatible with the $t > 0$ WKB requirement $\beta_q = d_q$ at the positive d_q 's (i.e. $g_{4q} > 0$, i.e. equation (17) with $M = 0$). *Vice versa*, we may say that equation (32) leads to our final, minimal possible L if and only if the inequality $g_{4q} < 0$ characterizes the least favourable case with only a minimally WKB admissible ansatz and $t = 0$. The length of recurrences $L = 2q + 2$ is then still quite large, anyway (see tables 1–4 for a few samples). In all the other cases, our preceding proof must be extended, basically, to all the integers $M \neq 0$ in equation (16).

In a routine manner we then get

$$p_N = p_N^{(k)[M]} = \exp \left[\frac{\beta_{q-M} + (D^{(q-M)}/4\beta_{q+1})}{(q-M)\lambda_{(k)}^{q-M}} \left(\frac{N}{q+1} \right)^{(q-M/q+1)} \right] \tag{34}$$

and, for further discussion, we have to distinguish between the subdominantly attractive and subdominantly repulsive forces with the positive and negative couplings $g_{4q-2M} > 0$ and $g_{4q-2M} < 0$, respectively.

4.3.1. *The subdominantly attractive cases with $M < q$.* In full analogy to our preceding $M = 0$ discussion, we may derive the multiplet of independent dominant solutions for any M ,

$$p_N \approx p_N^{(k)[M]} = \exp \left[\frac{\beta_{q-M}}{(q-M)\lambda_{(k)}^{q-M}} \left(\frac{N}{q+1} \right)^{(q-M/q+1)} \right].$$

Obviously, its $k = 0$ component remains dominant if and only if we require that $\beta_{q-M} > 0$ for $M < q$. *Vice versa*, once the 'decisive' coupling g_{4q-2M} at some $M < q$ happens to be positive, we are free to put all the β 's equal to their WKB values d . Thus, the optimal choice of the maximal $t = q$ is admissible, and the recurrences remain the shortest possible ones, with length $L = q + 2$. As its particular $q = t$ items, table 4 enumerates the corresponding subdominantly attractive potentials $V^{(q)}(r)$ up to $q = 6$.

4.3.2. *The subdominantly repulsive cases with $M < q$.* In all the subdominantly repulsive cases—with the exclusion of $M \geq q$ —we may still achieve a partial shortening of recurrences via the trivial WKB choice of

$$\beta_{q-M+1} = \beta_{q-M+2} = \dots = \beta_q = 0.$$

Next, we have to recall formula (34) once more. The sufficient condition of applicability of our formalism (namely, the dominance of the $k = 0$ term in equation (30)) will obviously follow from the presence and arrangement of the powers of the complex and unimodular quantities $\lambda_{(k)}$ in the exponent again. *Mutatis mutandis*, we derive the corresponding sufficient condition for general M

$$\beta_{q-M} + \frac{D^{(q-M)}}{4\beta_{q+1}} = \frac{1}{2}(\beta_{q-M} + d_{q-M}) > 0 \quad M < q. \tag{35}$$

Our discussion comes to its end—the latter prescription has a form of restriction

$$\beta_{q-M} > -d_{q-M} \geq 0 \quad M < q \tag{36}$$

imposed upon our choice of β_{q-M} in the ansatz (15). In the non-attractive regime with

$$0 < \beta_{q-M} \neq d_{q-M} < 0$$

it implies the incompletely WKB character of our ansatz. The necessity as well as optimality of the choice of $t = M < q$ is obvious, and the validity of the Hill-determinant secular equation (5) is guaranteed by equation (36). By construction, the WKB violation remains minimal. Thus, all the subdominantly repulsive potentials $V^{(q)}(r)$ (3) with $M < q$ may be assigned recurrences of the minimal matricization-compatible length $L = 2q + 2 - M$. Up to $L = 8$, the complete list of these potentials is provided by all the negative-coupling items in table 4.

4.3.3. *All the remaining cases (with $M = q$).* At $M \geq q$ or rather $M = q$, we again arrive at equation (36). Formally, we put $d_0 = 0$ and choose $\beta_1 > 0$. In this way, we obtain the repulsive-like value of the number $L = q + 3$ irrespectively of the sign of the next non-zero couplings if any (cf all the ' $M = q = t + 1$ ' items in table 4).

5. A few remarks on applications

5.1. Perturbation theory

5.1.1. *A variation of couplings.* Our optimal Hessenberg non-diagonal Q 's carry much more compressed information about the system in question (with, e.g., 4–6 diagonals at $q = 2$) than the standard-matrix Hamiltonians (say, in a harmonic-oscillator basis, with 11 non-zero diagonals at $q = 2$). In the applications and computations, one of the most important immediate merits of this compression lies in the existence of explicit determinantal formulae (14) and asymptotics (e.g. (31)) for an immediate semi-numerical evaluation of wavefunctions.

Another immediate application of the compressed Q 's may be found in perturbative constructions (cf [18] for more details). Indeed, whenever we have to analyse a variable coupling in equation (1),

$$g\delta = g\delta_{(0)} + \lambda g\delta_{(1)} + \lambda^2 g\delta_{(2)} + \dots \quad |\lambda| \ll 1 \tag{37}$$

the Rayleigh–Schrödinger ansätze

$$E = E_{(0)} + \lambda E_{(1)} + \lambda^2 E_{(2)} + \dots \tag{38}$$

$$\omega_j = \omega_{(0)j} + \lambda \omega_{(1)j} + \lambda^2 \omega_{(2)j} + \dots$$

and

$$Q(E) = Q_{(0)}(E_{(0)}) + \lambda Q_{(1)}(E_{(0)}, E_{(1)}) + \lambda^2 Q_{(2)}(E_{(0)}, E_{(1)}, E_{(2)}) + \dots \tag{39}$$

will enable us to reconstruct the energies by perturbative techniques, i.e. via a systematic step-by-step construction of corrections to energies and wavefunctions in the spirit of the textbook. The use of minimal L 's will just simplify the formulae.

An important technical ingredient in similar recipes lies in an optimal choice of the zero-order approximant $Q_{(0)}(E_{(0)})$. Its adequacy is vital for the feasibility of perturbative computations as well as for their convergence. Besides this, the construction of a simplified, finite-dimensional $Q_{(0)}(E_{(0)})$ may also be interpreted as the final missing part of our preceding considerations.

5.1.2. *An example: Quartic oscillators.* Our ‘hierarchization’ of potentials (tables 1–4) exhibits a few seemingly counter-intuitive features:

- (i) it misses a variational background;
- (ii) it depends on the signs of some couplings and energies; and
- (iii) it presents the popular [19] phenomenological quartic anharmonic oscillator (i.e. in general, the $q = 2$ and $L \geq 4$ Hamiltonian

$$H^{(\text{quartic})} = -\frac{\hbar}{2\mu} \Delta + \frac{f}{r^2} + \frac{e}{r} + ar + br^2 + cr^3 + dr^4 \tag{40}$$

with an admissible centrifugal-like term $f > -\frac{1}{4}$, Coulombic coupling e , polynomial corrections a, b, c and the asymptotically dominant, confining $d > 0$) as a system more complicated than its sextic partner $H^{(\text{sextic})}$ (equation (2)).

The quartic equation (40) requires a non-trivial Liouvillean change of variables (7) with $\mu = \frac{1}{2}$, and the underlying $q = q^{(\text{quartic})} = 2$ Hamiltonians become transformed into manifestly asymmetric Hessenberg matrices with $L \geq 4$. This proves both challenging and useful for illustration purposes.

Our classification distinguishes between the following five domains of couplings:

- (D1) $c > 0$ (i.e. $M = 0$ and $L = 4$, see table 1, row 5 or table 4, row 4);
- (D2) $c = 0$ and $b > 0$ (i.e. $M = 1$ and $L = 4$, see table 1, row 6 or table 4, row 5);
- (D3) $c = 0$ and $b = 0$ (i.e. $a = \text{arbitrary}$, $M = 2$ and $L = 5$, see table 2, row 10 or table 4, row 6);
- (D4) $c = 0$ and $b < 0$ (i.e. $M = 1$ and $L = 5$, see table 2, row 9 or table 4, row 6), and
- (D5) $c < 0$ (i.e. $M = 0$ and $L = 6$, see table 3, row 14 or table 4, row 10).

As long as the physical and unphysical asymptotic behaviour (10) of the quartic wavefunctions is well known,

$$G(r) = G_{\text{WKB}}(r) = \frac{1}{3}\alpha_{\text{WKB}}r^3 + \frac{1}{2}\beta_{\text{WKB}}r^2 + \gamma_{\text{WKB}}r$$

$$\alpha_{\text{WKB}} = \sqrt{d} > 0 \quad \beta_{\text{WKB}} = c/2\alpha_{\text{WKB}} \quad \gamma_{\text{WKB}} = (b - \beta_{\text{WKB}}^2)/2\alpha_{\text{WKB}} \tag{41}$$

we may immediately recall our general results and postulate

$$\psi(r) = \exp(-\frac{1}{3}\alpha_{\text{WKB}}r^3 - \frac{1}{2}\beta r^2 - \gamma r) \sum_{n=0}^{\infty} \omega_n r^{n+l+1}. \tag{42}$$

Here the non-negative angular momentum ℓ is modified into a quantity $l > -\frac{1}{2}$ defined by the quadratic equation $l(l+1) = \ell(\ell+1) + f$. The remaining parameters β and γ are free (cf equation (11)).

Being guided by section 4.3.1, we may now choose the optimal $\beta = \beta_{\text{WKB}} (\geq 0)$ and $\gamma = \gamma_{\text{WKB}}$ in the domains (D1) and (D2). The related matrix Schrödinger equation

$$Q^{(L, \text{quartic})} \begin{pmatrix} \omega_0 \\ \omega_1 \\ \vdots \end{pmatrix} = 0 \tag{43}$$

will contain just four non-zero diagonals ($L = 4$),

$$\begin{aligned} Q_{n, n+1}^{(4, \text{quartic})} &= -(n+1)(n+2l+2) \\ Q_{n, n}^{(4, \text{quartic})} &= 2\gamma_{\text{WKB}}(n+l+1) + e \\ Q_{n+1, n}^{(4, \text{quartic})} &= 2\beta_{\text{WKB}}(n+l+3/2) - \gamma_{\text{WKB}}^2 - E \\ Q_{n+2, n}^{(4, \text{quartic})} &= 2\alpha_{\text{WKB}}(n+l+2) - 2\beta_{\text{WKB}}\gamma_{\text{WKB}} + a \end{aligned} \tag{44}$$

where $n = 0, 1, \dots$. In the subsequent two domains (D3) and (D4) the respective analyses of sections 4.3.3. and 4.3.2 with $\beta = \beta_{\text{WKB}} = 0$ impose a WKB-breaking $\gamma > -\gamma_{\text{WKB}} \geq 0$. The pentadiagonality of equation (43) results in

$$\begin{aligned} Q_{n,n+1}^{(5, \text{quartic})} &= -(n+1)(n+2l+2) \\ Q_{n,n}^{(5, \text{quartic})} &= 2\gamma(n+l+1) + e \\ Q_{n+1,n}^{(5, \text{quartic})} &= -\gamma^2 - E \\ Q_{n+2,n}^{(5, \text{quartic})} &= 2\alpha_{\text{WKB}}(n+l+2) + a \\ Q_{n+3,n}^{(5, \text{quartic})} &= 2\alpha(\gamma_{\text{WKB}} - \gamma). \end{aligned} \quad (45)$$

In accord with section 4.3.2, the last domain (D5) necessitates $\beta > -\beta_{\text{WKB}} (> 0)$ and six diagonals:

$$\begin{aligned} Q_{n,n+1}^{(6, \text{quartic})} &= -(n+1)(n+2l+2) \\ Q_{n,n}^{(6, \text{quartic})} &= 2\gamma(n+l+1) + e \\ Q_{n+1,n}^{(6, \text{quartic})} &= 2\beta(n+l+3/2) - \gamma^2 - E \\ Q_{n+2,n}^{(6, \text{quartic})} &= 2\alpha_{\text{WKB}}(n+l+2) - 2\beta\gamma + a \\ Q_{n+3,n}^{(6, \text{quartic})} &= 2\alpha_{\text{WKB}}(\gamma_{\text{WKB}} - \gamma) + \beta_{\text{WKB}}^2 - \beta^2 \\ Q_{n+4,n}^{(6, \text{quartic})} &= 2\alpha_{\text{WKB}}(\beta_{\text{WKB}} - \beta). \end{aligned} \quad (46)$$

Here, the value of γ remains arbitrary and may be fixed, e.g., on the purely numerical grounds.

Besides the above-mentioned perturbative constructions, our infinite-dimensional Hessenberg Schrödinger (43) may also immediately be solved numerically. The details of realization of an appropriate algorithm may be found elsewhere: reference [21] simplifies $a = c = e = 0$ and pays attention to the various possibilities of an acceleration of convergence.

5.2. The finite-dimensional Hessenberg Hamiltonians

5.2.1. The $N+1$ -dimensional zero-order $\omega_{(0)}$'s and Magyari equations. The tacit non-degeneracy assumption $\omega_n \neq 0$, $n \gg 1$ in the preceding sections is known to fail at a few exceptional energies and couplings [10]. With the above zero-order perturbative motivation, we may (and shall) restrict our attention just to these exceptional finite-dimensional vectors $\omega_{(0)}$,

$$\omega_{N(0)} \neq 0 \quad \omega_{N+1(0)} = \dots = \omega_{N+q(0)} = 0 \quad (47)$$

and related matrices $Q_{(0)}(E_{(0)})$.

Obviously, the termination requirements (47) cannot be satisfied unless we employ the WKB form of exponents $G(r)$ (41). *Vice versa*, under the assumption (47) the fully WKB choice of these exponents guarantees a trivial normalizability of the wavefunctions in any domain (D1–D5).

Moreover, once we replace the coefficients h in equation (47) by Hill determinants (14), we obtain a coupled set of nonlinear (polynomial, determinantal, ‘Magyari’) algebraic equations. These equations define (at most a few) exceptional ‘Magyari’ couplings and energies. As a consequence, our above WKB-compatible domains (D1) and (D2) may be complemented by the resulting set of roots (DM) in principle.

Our specific $q = 2$ definition of potentials (40) and ansatz (42) convert the corresponding radial differential ‘homework’ Coulomb + quartic equation into the purely algebraic quasi-linear equation

$$\begin{pmatrix} C_0 & D_0 & 0 & \dots & & 0 \\ B_1 & C_1 & D_1 & 0 & \dots & 0 \\ A_2 & B_2 & C_2 & D_2 & 0 & \dots \\ 0 & A_3 & B_3 & C_3 & D_3 & \dots \\ \dots & & & & & \\ 0 & \dots & 0 & A_N & B_N & C_N \\ 0 & \dots & & 0 & A_{N+1} & B_{N+1} \\ 0 & \dots & & 0 & 0 & A_{N+2} \end{pmatrix} \begin{pmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \\ \dots \\ \omega_{N-1} \\ \omega_N \end{pmatrix} = 0 \tag{48}$$

where the last row removes just one degree of freedom,

$$a = a(N) = -2\alpha(N + l + 2) + 2\beta\gamma \quad A_n = 2\alpha(n - 2 - N) \tag{49}$$

and the non-square matrix remainder with

$$\begin{aligned} B_n &= X_n + x & X_n &= 2\beta(n + L + \frac{1}{2}) & x &= -\gamma^2 - E \\ C_n &= Y_n + e & Y_n &= 2\gamma(n + L + 1) \\ D_n &= -(n + 1)(n + 2L + 2) & n &= 0, 1, \dots, N + 1 \end{aligned} \tag{50}$$

forms an overcomplete system of $N + 2$ equations for $N + 1$ Taylor coefficients ω_n and has to fix another pair of free parameters in principle.

One of the most natural numerical forms of the necessary conditions of existence of the non-trivial solutions of equation (48) is the—mutually coupled—pair of eigenvalue conditions

$$\det \begin{pmatrix} e + Y_0 & D_0 & 0 & \dots & & 0 \\ B_1(x) & e + Y_1 & D_1 & 0 & \dots & 0 \\ \dots & & & & & \\ 0 & \dots & 0 & A_N & B_N(x) & e + Y_N \end{pmatrix} = 0 \tag{51}$$

and

$$\det \begin{pmatrix} x + X_1 & C_1(e) & D_1 & 0 & \dots & 0 \\ A_2 & x + X_2 & C_2(e) & D_2 & 0 & \dots \\ \dots & & & & & \\ 0 & \dots & 0 & A_N & x + X_N & C_N(e) \\ 0 & 0 & \dots & 0 & A_{N+1} & x + X_{N+1} \end{pmatrix} = 0 \tag{52}$$

for $e = e(x)$ and $x = x(e)$. Their numerical solution is sampled here in table 5—it only remains trivial at $N = 0$ [10].

Table 5. A sample of roots of Magyar equations: (a) s-wave ($l = 0$), $b = 1$, $c = 0.1$, $d = 0.01$; (b) $b = 1$, $c = 0$, $d = 1$.

N		0	2	4	6	8	10
(a)	a	3.35	2.95	2.55	2.15	1.75	1.35
	e	-7.50	-7.22	-6.95	-6.66	-6.38	-6.09
	E	-12.56	-11.64	-10.76	-9.91	-9.09	-8.31
		s-wave ($l = 0$)		p-wave ($l = 1$)			
N		3	6	3	6		
(b)	a	-10.00	-16.00	-12.00	-18.00		
	e	-1.60	-2.09	-2.75	-3.39		
	E	-0.298	-0.350	-0.267	-0.289		

5.2.2. An ambiguity of non-numerical constructions: $N = 1$. The s-wave ($l = 0$) Magyar equations (48) with $N = 1$ seem fairly clear. They imply that

$$\det \begin{pmatrix} x + 3\beta & 4\gamma + e \\ -2\alpha & x + 5\beta \end{pmatrix} = 0 \tag{53}$$

and

$$\det \begin{pmatrix} 2\gamma + e & -2 \\ x + 3\beta & 4\gamma + e \end{pmatrix} = 0. \tag{54}$$

An elimination of the variable $e = e(x)$ from the first equation (53) and its insertion in the latter equation (54) gives

$$x^4 + 16\beta x^3 + 2x^2(2\alpha\gamma + 47\beta^2) + 8x(4\alpha\beta\gamma + \alpha^2 + 30\beta^3) + 60\alpha\beta^2\gamma + 24\alpha^2\beta + 225\beta^4 = 0. \tag{55}$$

Unexpectedly, the degree of this equation may easily be lowered. Once we replace, say, equation (53) by its alternative

$$\det \begin{pmatrix} 2\gamma + e & -2 \\ -2\alpha & x + 5\beta cr \end{pmatrix} = 0 \tag{56}$$

the same elimination leads to a mere cubic secular equation

$$x^3 + 13\beta x^2 + x(4\alpha\gamma + 55\beta^2) + 20\alpha\beta\gamma + 8\alpha^2 + 75\beta^3 = 0. \tag{57}$$

It coincides with equation (55) divided by the factor $(x + 3\beta)$.

5.2.3. The feasibility of non-numerical constructions: $N = 2$ and $N = 3$. Let us return to an arbitrary partial wave $\theta = 2l + 1 > 0$, re-scale $g_4 = 1$ (i.e. $\alpha = 1$), shift the energies in such a way that $x = -\beta^2 - E = 0$ and suppress one degree of freedom by the postulate $\gamma = 2\alpha(b - \beta^2) = 0$. Then, Magyar equations (48) become significantly simplified:

$$\begin{pmatrix} e & -(\theta + 1) & 0 & 0 & \dots & 0 \\ \beta(\theta + 2) & e & -2(\theta + 2) & 0 & \dots & 0 \\ -2N & \beta(\theta + 4) & e & -3(\theta + 3) & \dots & 0 \\ \dots & & & & & \\ 0 & \dots & -6 & \beta(\theta + 2N - 2) & e & -N(\theta + N) \\ 0 & \dots & 0 & -4 & \beta(\theta + 2N) & e \\ 0 & \dots & 0 & 0 & -2 & \beta(\theta + 2N + 2) \end{pmatrix} \begin{pmatrix} \omega_0 \\ \omega_1 \\ \dots \\ \omega_N \end{pmatrix} = 0 \tag{58}$$

and remain solvable non-numerically. Their explicit $N = 2$ formulation

$$\det \begin{pmatrix} e & -(\theta + 1) & 0 \\ -4 & \beta(\theta + 4) & e \\ 0 & -2 & \beta(\theta + 6) \end{pmatrix} = 0 \tag{59}$$

and

$$\det \begin{pmatrix} e & -(\theta + 1) & 0 \\ \beta(\theta + 2) & e & -2(\theta + 2) \\ 0 & -2 & \beta(\theta + 6) \end{pmatrix} = 0 \tag{60}$$

and a change of variable $z = \beta e$ leads to the coupled pair of nonlinear equations

$$\begin{aligned} z^2(\theta + 4)(\theta + 6) - 4z(\theta + 1)(\theta + 6) + 2e^3 &= 0 \\ z^2(\theta + 1)(\theta + 2)(\theta + 6) + e^3z(\theta + 6) - 4e^3(\theta + 2) &= 0. \end{aligned} \tag{61}$$

Subsequently, the replacement $e = (tz^2)^{1/3}$ makes these equations linear in z or in t (though not in both of these variables at the same time—it contains their products).

The elimination of z is slightly simpler. It leads to the single quadratic equation in the third variable $w = 2t/(\theta + 6)$,

$$2w^2 - w(3 + \theta + 8/(\theta + 2)) - (\theta + 1)(\theta + 4) = 0. \tag{62}$$

The pair of its roots

$$w_{\pm} = \frac{1}{4(\theta + 2)} (\theta^2 + 5\theta + 14 \pm \sqrt{\Delta}) \quad \Delta = 9\theta^4 + 82\theta^3 + 277\theta^2 + 428\theta + 324 \tag{63}$$

may easily be analysed in both the limits $\theta \rightarrow 0$ and $\theta \rightarrow \infty$.

Insertions give the final couplings

$$e_{\pm} = \left[32(\theta + 1)^2(\theta + 2)(\theta + 6)(\pm\sqrt{\Delta} + \theta^2 + 5\theta + 14)/(\pm\sqrt{\Delta} + 5\theta^2 + 29\theta + 46)^2 \right]^{1/3} \tag{64}$$

as well as the related parameter

$$\begin{aligned} \beta_{\pm} = \left\{ 128(\theta + 1)(\theta + 2)^2 / \left[(\pm\sqrt{\Delta} + 5\theta^2 + 29\theta + 46) \right. \right. \\ \left. \left. \times (\pm\sqrt{\Delta} + \theta^2 + 5\theta + 14)(\theta + 6) \right] \right\}^{1/3}. \end{aligned} \tag{65}$$

The same change of variables $(\beta, e) \Rightarrow (z, t)$ also works in the $N = 3$ case—in the s-wave, we eliminate

$$t = 12(9z - 22)/z(8 - 3z) \tag{66}$$

and derive

$$315z^3 - 3252z^2 + 10384z - 10560 = 0 \tag{67}$$

or, alternatively, eliminate the second variable first,

$$z = 6(34t - 63)/t(2t + 63) \tag{68}$$

and obtain the slightly simpler final secular equation

$$40t^3 - 52t^2 + 126t + 19845 = 0. \tag{69}$$

The unique and exact real root of this equation may still be written in a closed and compact form:

$$\begin{aligned} t = -(63\sqrt{155793}/100 + 3356959/13500)^{1/3} \\ + (63\sqrt{155793}/100 - 3356959/13500)^{1/3} + 13/30. \end{aligned} \tag{70}$$

5.2.4. *Further simplifications and non-numerical constructions: $N = 4$ and $N = 5$.* At $N = 4$ and $l = 0$, the change of variables $\beta = z/e$ and $e = (tz^2)^{1/3}$ still enables us to eliminate

$$z = 576(8t^2 + 671t + 7623)/(232t^3 + 1476t^2 + 100386t + 1029105) \quad (71)$$

or, alternatively,

$$t = -33(501z^2 - 3944z + 7424)/(363z^3 - 3582z^2 + 8048z + 3712). \quad (72)$$

The insertions of the functions $z = z(t)$ or $t = t(z)$ in complementary equations prove inequivalent, and the division of the resulting polynomial equations by the respective spurious factors $58t + 693$ and $2t + 99$ leads to the final secular equation

$$\begin{aligned} & -26912t^6 - 3(648464t^5 + 10430160t^4 + 27009576t^3 + 606623094t^2 \\ & + 686001393t - 47069204490) = 0 \end{aligned} \quad (73)$$

(as well as to its t -alternative) of mere sixth order.

The next, $N = 5$ s-wave choice of determinants

$$\begin{aligned} 0 = & 46332\beta^4 e + \beta^3(1287e^3 - 216216) - 7776\beta^2 e^2 \\ & + 2\beta e(35e^3 - 8952) - 384e^3 + 28800 \end{aligned} \quad (74)$$

$$0 = 72072\beta^4 + 17160\beta^3 e^2 + 11\beta^2 e(13e^3 - 12360) + 800\beta(156 - e^3) + 2e^2(e^3 - 696)$$

requires the application of some new tricks: we remove z^3 by subtraction, denote z^2 as w and insert it back, whenever applicable, into one of the original equations. The result becomes linear in z and we may eliminate

$$\begin{aligned} z = & 1200t(16392t^4 + 42652t^3 + 1352650t^2 - 51615135t - 753647895)/D \\ D = & 317952t^6 + 15508704t^5 + 3858016t^4 + 66109560t^3 - 21056323860t^2 \\ & - 237039654852t + 522277991235 \end{aligned} \quad (75)$$

necessarily by symbolic manipulations on a computer. The result—a 13th-order equation—has a real root $t = 4.126607$.

In practice, several alternative unperturbed Q 's may be used. In particular, when we assume that $\beta = 0$ vanishes while $x \neq 0$ (i.e. the energy itself remains unrestricted), we may recall [23] and simplify $\gamma = 0$. This enables us to reduce the Magyari equations to a polynomial of a low degree, namely linear at $N = 1$, quadratic at $N = 2$, cubic at $N = 3$ and of the seventh degree at $N = 4$. Here, in our final example, let us fix $N = 5$,

$$\begin{pmatrix} e & -2 & 0 & 0 & 0 & 0 \\ x & e & -6 & 0 & 0 & 0 \\ -10 & x & e & -12 & 0 & 0 \\ 0 & -8 & x & e & -20 & 0 \\ 0 & 0 & -6 & x & e & -30 \\ 0 & 0 & 0 & -4 & x & e \\ 0 & 0 & 0 & 0 & -2 & x \end{pmatrix} \begin{pmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \\ \omega_3 \\ \omega_4 \\ \omega_5 \end{pmatrix} = 0. \quad (76)$$

Again, an omission of (the third and fourth) rows gives a pair of determinantal equations which, after the changes of variable $x = (y z^2)^{1/3}$ and $e = (z/y)^{1/3}$, acquire the form

$$y^2(8z^3 - 264z^2) + y(z^3 - 24z^2 - 2928z + 28800) + 6z^2 - 384z = 0$$

$$24z^2y^3 + y^2(20z^2 - 1288z + 9600) + y(z^2 - 40z - 1392) + 2z = 0. \tag{77}$$

We may use the first line in order to remove the third power of y in the second line. Then, we subtract the new pair of equations (after having normalized to one the coefficients at, unusually, y^0) and obtain a linear equation and formula

$$y = -2 \frac{z^4 - 204z^3 + 11\,424z^2 - 97\,488z - 3\,934\,656}{43z^4 - 8364z^3 + 534\,144z^2 - 12\,900\,096z + 77\,414\,400} \tag{78}$$

for $y = y(x)$. Its insertion converts the remaining quadratic equation into the final single-variable secular equation of the eleventh degree,

$$z^{11} - 617z^{10} + 158\,632z^9 - 22\,585\,440z^8 + 1\,981\,730\,304z^7 - 112\,514\,572\,800z^6$$

$$+ 4\,222\,916\,388\,864z^5 - 105\,488\,581\,091\,328z^4 + 1\,750\,679\,680\,057\,344z^3$$

$$- 18\,938\,384\,468\,213\,760z^2 + 121\,740\,048\,728\,064\,000z$$

$$- 324\,905\,635\,676\,160\,000 = 0. \tag{79}$$

Its numerical solution is standard, giving the (unique) approximate real root $z = 6.487\,94$. The related variable $y = 0.591\,66$ and approximate ‘physical’—real—quantities $x = -E = 2.9203$ and $e = 2.221\,66$ follow.

It is worth emphasizing that the direct use of the original variables in [23] would only enable us to generate an analogue of the present equation (79) with some 18th-degree polynomial.

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