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Perturbation method with triangular propagators and anharmonicities of intermediate strength

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We propose a new, very flexible version of the Rayleigh–Schrödinger perturbation method which admits a lower triangular matrix in place of the usual diagonal unperturbed propagator. The technique and its enhanced efficiency are illustrated on rational anharmonicities $V^{(1)}(x) = \beta \times \text{polynomial}(x)/\text{polynomial}(x)$. They are shown tractable, in the intermediate coupling regime, as $\mathcal{O}(\beta - \beta^{(0)})$ perturbations of exact states at non-vanishing $\beta^{(0)} \neq 0$. In this sense our method bridges the gap between the current weak- and strong-coupling expansions.

KEY WORDS: perturbation method, triangular propagators, anharmonicity

1. Introduction

Schrödinger equations with anharmonic potentials $\omega^2 x^2 + \beta V^{(1)}(x)$ are often solved perturbatively. It is well known that many practical implementations of this approach are full of contradictions, well illustrated by the popular quartic example with $V^{(1)}(x) = x^4$. Its weak-coupling energy estimates $E(\beta) \approx E(0) + \beta E_{(1)} + \cdots + \beta^N E_{(N)}$ are easily generated via recursion relations [1] but this approximation diverges in the limit $N \to \infty$ at *any* nonzero coupling constant β [2]. An alternative, strong-coupling series in powers of $\beta^{-2/3}$ exists and converges for the sufficiently large $|\beta|$ [3]. Unfortunately, the explicit evaluation of its coefficients is by far not easy [4]. In the literature many people have advocated, therefore, a replacement of the traditional quartic model by a *non-polynomial* anharmonicity

$$V^{(1)}(x) = \frac{x^2}{1 + Bx^2} \equiv \frac{1}{B}\left(1 - \frac{1}{1 + Bx^2}\right), \quad B > 0. \tag{1}$$

Its merits belong to the two separate categories. Firstly, its bounded character enables us to avoid the divergence of the weak-coupling series. This has been emphasized by several authors [5]. Secondly, the existence of a few elementary solutions at certain exceptional couplings $\beta = \beta^{(0)}$ [6] enables us to contemplate their perturbations, say,

$$E(\beta) = E(\beta^{(0)}) + \lambda E^{(1)} + \lambda^2 E^{(2)} + \cdots, \quad \lambda = \beta - \beta^{(0)}, \tag{2}$$

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in anharmonic regime, near any solvable $\beta^{(0)} \neq 0$ [7]. An exceptional character of the latter intermediate-coupling expansion was its shortcoming. Its feasibility relied on a replacement of the traditional unperturbed spectrum by certain auxiliary continued fractions and did not seem amenable to any sufficiently efficient generalization [8].

In the present paper we shall consider the whole class of the Padé-like potentials

$$V(\beta, x) = \omega^2 x^2 + \beta \left(\sum_{d=0}^{t} B_d x^{2d} \right)^{-1} \sum_{n=0}^{t-1} A_n x^{2n}, \quad B_t \neq 0. \tag{3}$$

An innovative construction of their perturbation solutions of the type (2) will be proposed and described in detail. We shall demonstrate that the current and usual "weak-coupling" and "strong-coupling" perturbation studies may be complemented by the broad variety of the "medium" expansions using $0 < \beta^{(0)} < \infty$. We shall show that near many non-vanishing "intermediate" couplings $\beta^{(0)}$, the perturbative treatment of the models (3) may remain feasible and unexpectedly easy. In this way, our innovation could inspire an improvement of the current situation in perturbation calculations where people often decide to work just with the respective zero-order couplings $\beta^{(0)} = 0$ or $\beta^{(0)} = \infty$. Of course, these "traditional" approaches are quite often able to achieve a satisfactory convergence just in an immediate vicinity of these two extreme values of β.

Our "intermediate-coupling" project opens several technical questions. Firstly, at any $t \geqslant 1$, the zero-order solutions must be constructed in anharmonic regime. A representative sample of these reference systems is described thoroughly in section 2. It underlines the real phenomenological appeal of equation (3) in comparison with the more popular polynomial models.

At a particular anharmonic $\beta^{(0)} \neq 0$ the usual construction of a complete unperturbed basis is prohibitively complicated. After a return to harmonic basis, numerical integration is needed for evaluation of the necessary matrix elements of $V^{(1)}(x)$ and the computation of corrections is difficult even in the lowest order Rayleigh–Schrödinger approximation [9]. Section 3 offers the remedy. Schrödinger equation is represented in a non-orthogonal basis. Its resulting $(2t + 1)$-diagonal matrix form is then much better accessible to a purely numerical matrix-inversion perturbative treatment.

In our main section 4 we deny the latter numerical "brute force" philosophy and intend to soften it significantly. Re-installing the more traditional recurrent interpretation of perturbation algorithms we describe a new approach to the Schrödinger-like families of equations with a banded-matrix form of their Hamiltonians. Our main idea is amply illustrated by its application to anharmonicities (1). Its core is a maximal simplification of the unperturbed propagator $\mathcal{R}$. In contrast to its general-matrix form in older methods [10] we shall be able to reduce it to the mere "half-filled", triangular matrix.

Section 5 is the summary showing how our new approach opens a way towards a broader variability of shapes of the theoretical and/or phenomenological interaction models. With due attention paid to the non-hermiticity of our (quasi-)Hamiltonian matrices (cf. also appendix), our new version of perturbation recipe seems well prepared for its extensions as well as further practical computational applications.

2. Solvable oscillators with $\beta^{(0)} \neq 0$

2.1. The simplest model with $t = 1$

Non-polynomial equation (3) with $t = 1$ is often recalled as one of the simplest unsolvable anharmonic models in one dimension [11]. In place of using the differential form of its Schrödinger equation, wave functions $\psi(\beta, x) \in L_2(-\infty, \infty)$ are expanded in the harmonic (i.e., Hermite or Laguerre) polynomial basis $\{|n\rangle\}_{n=0}^{\infty}$. The ansatz $\psi(\beta, x) = (1 + Bx^2) \sum_{n=0}^{\infty} \langle x|n\rangle h_n$ and scaling $\omega \to 1$ then give [12] the three-term recurrences

$$\begin{pmatrix} a_0 & d_0 & & \\ c_1 & a_1 & d_1 & \\ & c_2 & a_2 & \ddots \\ & & \ddots & \ddots \end{pmatrix} \begin{pmatrix} h_0 \\ h_1 \\ h_2 \\ \vdots \end{pmatrix} = 0, \tag{4}$$

$$a_n = \beta + (1 + B\alpha_n)(\varepsilon_n - E), \quad \alpha_n = \varepsilon_n/2 = \langle n|r^2|n\rangle = 2n + \ell + 3/2,$$
$$d_n = B\beta_n(\varepsilon_n - E), \quad \beta_n = \langle n|r^2|n+1\rangle = \left[(n+1)(n+\ell+3/2)\right]^{1/2},$$
$$c_n = B\beta_{n-1}(\varepsilon_n - E), \quad n = 0, 1, \ldots.$$

Marginally, let us note that the parity $(-1)^{\ell+1}$ of the wave functions with $\ell = -1, 0$ admits an immediate re-interpretation as angular momentum $\ell = 0, 1, \ldots$ in three dimensions with the regularity $\psi(\beta, r) \sim r^{\ell+1}$ of the radial wave functions near the origin [13].

2.1.1. Termination conditions and exact solutions

The existence of the terminating exact solutions of equation (4) is well known [6]. Let us mark them by a superscript $^{(0)}$. With normalization $h_q^{(0)} \neq 0$ their termination

Table 1
Low-lying spectra in the four deepest solvable double wells (1).

$\beta^{(0)}$	q	Energies			
81.88	3	18.999999996	19.	22.765764732	22.765764788
		26.526337990	26.526338492	30.281295324	30.281297900
64.89	3	17.	17.000000131	20.733677525	20.733679219
		24.459570379	24.459582299	28.176801248	28.176862466
52.05	3	15.301693677	15.301695784	18.999974785	19.
		22.686594466	22.686760593	26.359595371	26.360391029
49.91	2	14.999996593	15.	18.690932465	18.690972685
		22.369232872	22.369494489	26.032568100	26.033806209
39.12	3	13.356890687	13.356934267	17.	17.000474393
		20.621974574	20.624839279	24.215073151	24.227701473

property

$$h^{(0)}_{q+1} = h^{(0)}_{q+2} = \cdots = 0 \tag{5}$$

requires that $c^{(0)}_{q+1} = 0$. This means that $E^{(0)} = 4q + 2\ell + 7 \equiv \varepsilon_{q+1}$. The related energy is not arbitrary. Vice versa, bound states $\psi(\beta, x)$ with $E \neq E^{(0)}$ have to be defined by infinite series [14]. In one dimension a sample of their spectrum is given in table 1. It indicates that with a growth of the barrier the low-lying energies merge in almost degenerate doublets with opposite parities. According to figure 1 a very good fit of these numerical values $E = E(\beta)$ is provided by parabolas. One may expect that besides our ansatz (2) a useful methodical alternative could be also sought in perturbative expansions of couplings $\beta = \beta(E)$ and of the related Sturmian wave functions [12,15].

Even for the terminating bound states with $E = E^{(0)}$ we have to guarantee that the secular determinants vanish. Up to $q = 3$ the latter condition is non-numerical. For illustration we may fix $B = B^{(0)} = 1$ and choose the even parity $\ell = -1$. Then we get the elementary implicit polynomial definitions

$$\begin{gathered} y - 6 = 0, \qquad q = 0, \\ y^2 - 26y + 152 = 0, \qquad q = 1, \\ y^3 - 68y^2 + 1372y - 8304, \qquad q = 2, \\ y^4 - 140y^3 + 6588y^2 - 123216y + 777600 = 0, \qquad q = 3, \end{gathered} \tag{6}$$

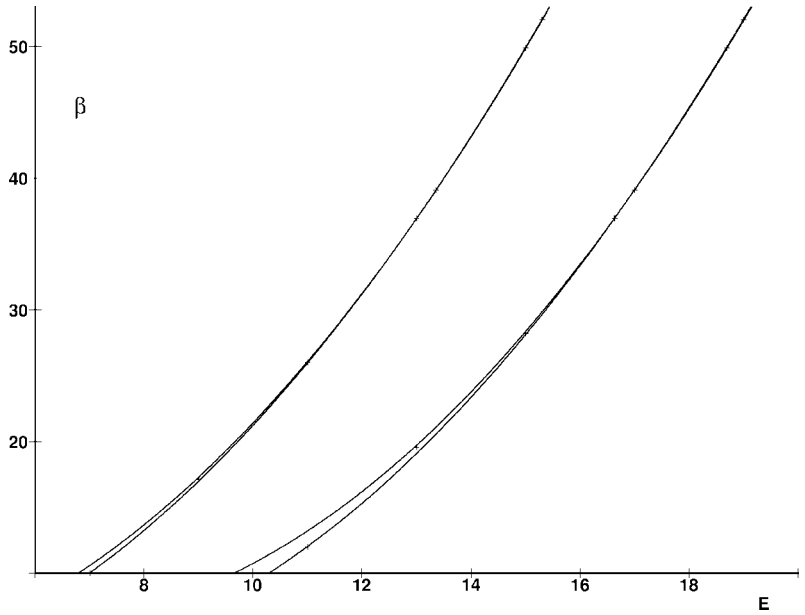

Figure 1. Coupling β vs. energy E for the first four bound states in potential (1) with $B = 1$.

Table 2
Complete list of the $t = 1$ roots $\beta^{(0)}$.

q	Parity	$\beta^{(0)}$	Excitation	$E^{(0)}$
0	even	6.	ground state	5.
	odd	10.	ground state	7.
1	even	8.8768943744	first	9.
		17.123105626	ground state	9.
	odd	12.	first	11.
		26.	ground state	11.
2	even	11.490856174	second	13.
		19.556337712	first	13.
		36.952806114	ground state	13.
	odd	13.874580313	second	15.
		28.206711029	first	15.
		49.918708658	ground state	15.
3	even	13.816182739	third	17.
		22.170398699	second	17.
		39.118906994	first	17.
		64.894511568	ground state	17.
	odd	15.630566921	third	19.
		30.443898070	second	19.
		52.049183356	first	19.
		81.876351653	ground state	19.

of the partially solvable couplings $y = y(q) \equiv \beta^{(0)}$. Besides their $q = 0$ (linear), $q = 1$ (quadratic) and $q = 2$ (Cardano) explicit solutions we may write down all the four exact $q = 3$ roots

$$\beta^{(0)} = 35 + \varepsilon_1\sqrt{127 - 2\sqrt{6821}\cos\left(\frac{1}{3}\Theta + \frac{\pi}{6}\right)} + \varepsilon_2\sqrt{127 + 2\sqrt{6821}\sin\left(\frac{1}{3}\Theta + \frac{\pi}{3}\right)} + \varepsilon_3\sqrt{127 - 2\sqrt{6821}\sin\frac{1}{3}\Theta}, \quad \Theta = \operatorname{arctg}\frac{9\sqrt{63908723442661575155}}{45902084710}$$

with $(\varepsilon_1, \varepsilon_2, \varepsilon_3) = (-,-,+), (-,+,-), (+,-,-)$ and $(+,+,+)$.

All our termination-compatible $q \leqslant 3$ values of the coupling $\beta^{(0)}$ remain real (cf. their list in table 2). All the related potentials acquire a double well shape since all our roots satisfy its sufficient condition $\beta^{(0)} > 1$.

2.2. *Unperturbed solutions with $t = 2$*

The $t = 2$ option in (3) gives the "first nontrivial" potential

$$V(x) = x^2 + \frac{\mu x^2 + \nu}{(1 - gx^2)^2 + fx^2}. \tag{7}$$

Mutatis mutandis, equation (4) becomes replaced by the $q+3$ relations

$$\begin{pmatrix} a_0 & d_0^{[1]} & d_0^{[2]} & & & \\ c_1^{[1]} & a_1 & d_1^{[1]} & d_1^{[2]} & & \\ c_2^{[2]} & c_2^{[1]} & a_2 & d_2^{[1]} & d_2^{[2]} & \\ & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & c_{q-1}^{[2]} & c_{q-1}^{[1]} & a_{q-1} & d_{q-1}^{[1]} \\ & & & c_q^{[2]} & c_q^{[1]} & a_q \\ & & & & c_{q+1}^{[2]} & c_{q+1}^{[1]} \\ & & & & & c_{q+2}^{[2]} \end{pmatrix} \begin{pmatrix} h_0{}^{(0)} \\ h_1{}^{(0)} \\ \vdots \\ h_q{}^{(0)} \end{pmatrix} = 0. \tag{8}$$

The last row implies that $c_{q+2}^{[2]} = 0$ and fixes the energy $E^{(0)} = 4q+2\ell+11$. The coupled rest remains over-determinate and defines the $q+1$ unknown coefficients (normalized, say, to $h_q^{(0)} = 1$) and two coupling constants. At $q = 0$ we have

$$\nu^{(0)} = (4\ell+6)(f-2g)+8, \qquad \mu^{(0)} = (8\ell+20)g^2 + 4f - 8g, \qquad q = 0. \tag{9}$$

These couplings are real for all the parameters f, g and ℓ.

For the sake of brevity, let us put $f = g = 1$ from now on. With option $\ell = 0$ (in one or three dimensions) and degree $q = 1$ our conditions (8) degenerate to the cubic equation $\nu^3 + 48\nu - 360 = 0$. Its only real Cardano root

$$\nu^{(0)} = \left(4\sqrt{2281}+180\right)^{1/3} - \left(4\sqrt{2281}-180\right)^{1/3} \approx 4.95914661133166 \tag{10}$$

with $\mu^{(0)} \approx 14.941997536546$ and normalization $h_1^{(0)} = 1$ leads to the exact

$$h_0^{(0)} = -\left(\frac{\sqrt{13686}}{108} + \frac{653\sqrt{6}}{486}\right)^{1/3} - \left(\frac{653\sqrt{6}}{486} - \frac{\sqrt{13686}}{108}\right)^{1/3} - \frac{2\sqrt{6}}{9}, \tag{11}$$

i.e., $h_0^{(0)} \approx -3.48195017221496$. The related energy $E^{(0)} = 15$ corresponds to the first excited state in s-wave. Its ground state predecessor does not terminate, $q \to \infty$. For it, the Runge–Kutta integration gives $E_{gs} \approx 10.943408413$.

At the next choice of $q = 2$ with the quasi-harmonic energy $E^{(0)} = 19$ and with the same convenient normalization $h_2^{(0)} = 1$ equation (8) reads

$$\begin{pmatrix} \frac{3}{2}\mu+\nu-52 & \frac{\sqrt{6}}{2}\mu - 32\sqrt{6} & -8\sqrt{30} \\ \frac{\sqrt{6}}{2}\mu - 24\sqrt{6} & \frac{7}{2}\mu+\nu-195 & \sqrt{5}\mu - 96\sqrt{5} \\ -4\sqrt{30} & \sqrt{5}\mu - 64\sqrt{5} & \frac{11}{2}\mu+\nu-330 \\ 0 & -2\sqrt{210} & \frac{\sqrt{42}}{2}\mu - 24\sqrt{42} \end{pmatrix} \begin{pmatrix} h_0^{(0)} \\ h_1^{(0)} \\ h_2^{(0)} \end{pmatrix} = 0. \tag{12}$$

In an ascending order of its rows we eliminate

$$\mu = 4\left(\sqrt{5}h_1^{(0)} + 12\right), \qquad \nu = 2\left[2\sqrt{30}h_0^{(0)} - 10\left(h_1^{(0)}\right)^2 + 3\left(11 - \sqrt{5}h_1^{(0)}\right)\right]$$

Table 3
s-wave roots $\mu^{(0)}$ and $\nu^{(0)}$ for potentials (7) with $f = g = 1$ and $q \leqslant 3$.

	Couplings		Coefficients			
q	$\mu^{(0)}$	$\nu^{(0)}$	$h_0^{(0)}$	$h_1^{(0)}$	$h_2^{(0)}$	$h_3^{(0)}$
0	16	2	1	0	0	0
1	14.9420	4.95915	−3.48195	1	0	0
2	14.0340	7.91914	8.18810	−3.79751	1	0
2	64.3015	−2.40610	1.02613	1.82256	1	0
3	13.2932	10.8801	−15.7092	9.19559	−3.91211	1
3	62.7170	0.883427	−1.93699	−2.48533	−0.0989786	1

and

$$h_0^{(0)} = \sqrt{30}\big(20\big(h_1^{(0)}\big)^3 - 8\sqrt{5}\big(h_1^{(0)}\big)^2 - 59h_1^{(0)} + 48\sqrt{5}\big)/\big(180h_1^{(0)}\big).$$

With $h_1^{(0)} = y\sqrt{5}$ our problem degenerates to the single sextic polynomial equation with integer coefficients,

$$2500y^6 + 1000y^5 - 7125y^4 + 100y^3 + 5065y^2 - 264y - 1152 = 0.$$

Its two real roots are easily localized numerically, $y_1 \approx -1.69830$ and $y_2 \approx 0.815078$. A close analogy with $t = 1$ is preserved. With the same ease we may generate the two $t = 2$ oscillators from a tenth-degree polynomial at $q = 3$ (see table 3) etc. The related energies were evaluated numerically. Their sample is given in table 4. They safely stabilize at cut-off $M = 15$.

2.3. $t = 3$ *and more*

At any $t > 1$ the requirement (5) leads to the $(t + q + 1) \times (q + 1)$-dimensional generalization of equation (8). Its last, decoupled condition $c_{q+t}^{[t]} = 0$ is satisfied if and only if $E^{(0)} = 4t + 4q + 2\ell + 3$. The remaining $t + q$ coupled equations

$$\begin{pmatrix} a_0 & d_0^{[1]} & \dots & d_0^{[t]} & 0 & \dots & 0 \\ c_1^{[1]} & a_1 & \dots & d_1^{[t-1]} & d_1^{[t]} & \dots & 0 \\ & & \dots & & & & \\ 0 & & \dots & 0 & c_{t+q-2}^{[t]} & c_{t+q-2}^{[t-1]} & c_{t+q-2}^{[t-2]} \\ 0 & & \dots & 0 & 0 & c_{t+q-1}^{[t]} & c_{t+q-1}^{[t-1]} \end{pmatrix} \begin{pmatrix} {h_0}^{(0)} \\ {h_1}^{(0)} \\ \vdots \\ {h_q}^{(0)} \end{pmatrix} = 0 \qquad (13)$$

determine all the q normalized projections $h_j^{(0)}$ plus t parameters in potential itself. With the growth of t the selfconsistent search for these exact solutions becomes less and less straightforward. Due to the implicit nonlinearity of equation (13) we must verify that its solutions keep the potentials real and non-singular. Both these properties have to be verified *a posteriori*.

It is useful to notice that at $q = 0$ the explicit solutions remain elementary at any index $t \geqslant 1$. At $t = 3$ the purely non-numerical solutions still exist at $q > 0$. This is

Table 4
$M \to \infty$ convergence of s-wave energies for couplings (10) in (7).

M	Low lying spectrum						
0	11.422198	–	–	–	–	–	–
1	10.672913	15.	–	–	–	–	–
2	10.945092	15.	16.2817	–	–	–	–
3	10.944852	15.	–	–	–	–	–
4	10.944169	15.	18.5146	–	–	–	–
5	10.943697	15.	18.2954	20.8470	–	–	–
6	10.943435	15.	18.1857	20.2068	24.0949	–	–
7	10.943317	15.	18.1222	20.0166	23.6752	28.065	–
8	10.943284	15.	18.0876	19.9294	23.5621	27.5340	34.6709
9	10.943292	15.	18.0717	19.8889	23.5096	27.4129	31.3782
10	10.943316	15.	18.0670	19.8730	23.4838	27.3538	31.2387
11	10.943343	15.	18.0682	19.8704	23.4725	27.3221	31.1673
12	10.943366	15.	18.0718	19.8743	23.4696	27.3063	31.1255
13	10.943383	15.	18.0761	19.8806	23.4711	27.3002	31.1020
14	10.943395	15.	18.0798	19.8871	23.4745	27.2999	31.0907
15	10.943402	15.	18.0828	19.8928	23.4785	27.3027	31.0874
16	10.943406	15.	18.0849	19.8971	23.4822	27.3068	31.0889
17	10.943408	15.	18.0863	19.9002	23.4851	27.3110	31.0929
18	10.943408	15.	18.0872	19.9022	23.4874	27.3147	31.0977
19	10.943408	15.	18.0876	19.9034	23.4889	27.3177	31.1023
20	10.943408	15.	18.0878	19.9040	23.4899	27.3198	31.1083

slightly unexpected. For illustration, let us employ the quartic-over-sextic model

$$V\big(\beta^{(0)}, r\big) = x^2 + \frac{u^{(0)} + v^{(0)}x^2 + w^{(0)}x^4}{1 + x^6}. \tag{14}$$

In a search for its symmetric bound states in one dimension ($\ell = -1$) the "first nontrivial" choice of $q = 1$ gives $E^{(0)} = 17$. The abbreviation $h_0^{(0)} = a$ and the eliminations guided by our previous experience re-parametrize the couplings,

$$w^{(0)} = 2\big(\sqrt{2}a + 27\big), \qquad v^{(0)} = -\sqrt{2}\big(\sqrt{2}a^2 + 11a - 6\sqrt{2}\big),$$
$$u^{(0)} = \sqrt{2}\big(2a^3 + 10\sqrt{2}a^2 - 23a + 18\sqrt{2}\big)/2.$$

The whole algebra degenerates to the single equation in $y = \sqrt{2}a$,

$$y^4 + 9y^3 - 33y^2 + 27y - 12 = 0, \quad \ell = -1,\ q = 1,\ t = 3.$$

Two of its roots are complex, $y_{3,4} = 0.451 \pm 0.534\mathrm{i}$, and the real doublet is given by the expression

$$y_{1,2} = -\frac{9}{4} - \sqrt{\frac{169}{16} - \sqrt[3]{\frac{\sqrt{25057} + 161}{16}} - \sqrt[3]{\frac{161 - \sqrt{25057}}{16}}} \pm Y_a,$$

Table 5
$t = 3$ roots $u^{(0)}$, $v^{(0)}$ and $w^{(0)}$ for even parity, $q \leqslant 2$ and potentials (14).

Auxiliary root	Couplings			Coefficients	
z	$w^{(0)}$	$v^{(0)}$	$u^{(0)}$	$h_0^{(0)}$	$h_1^{(0)}$
–	30.	0.	12.	1.	0.
2.0534020780474	58.107	−14.804	19.797	1.452	1.
−11.95601933076	30.088	0.5698	15.691	−8.454	1.
3.9105205273467	93.642	−33.229	33.945	1.091	2.258
2.1316238057633	86.526	29.646	15.572	0.578	1.231
−4.8208818863125	58.716	−15.324	23.422	−6.313	−2.783
−11.9379718900079	30.248	1.295	19.381	33.908	−6.892

where

$$Y_a = \sqrt{\frac{169}{8} + \sqrt[3]{\frac{\sqrt{25057}+161}{16}} + \sqrt[3]{\frac{161-\sqrt{25057}}{16}} + |Y_b|}.$$

The last item is a positive square root of another sum,

$$\begin{aligned}(Y_b)^2 = {} & \frac{28177}{64} + \sqrt[3]{\frac{161\sqrt{25057}+25489}{128}} + \sqrt[3]{\frac{25489-161\sqrt{25057}}{128}} \\ & + \sqrt[3]{\frac{4347\sqrt{25057}+688203}{128}} + \sqrt[3]{\frac{688203-4347\sqrt{25057}}{128}} \\ & + \sqrt[3]{\frac{4826809\sqrt{25057}+777116249}{1024}} + \sqrt[3]{\frac{777116249-4826809\sqrt{25057}}{1024}}.\end{aligned}$$

In the second illustration with $q = 2$, $E^{(0)} = 21$ and abbreviations $h_0^{(0)} = a = y/\sqrt{6}$, $h_1^{(0)} = b = z/\sqrt{3}$ and $h_2^{(0)} = 1$ the eliminations

$$\begin{aligned} w^{(0)} &= 2\sqrt{3}\big(2b + 13\sqrt{3}\big), \qquad v^{(0)} = 2\sqrt{3}\big(2\sqrt{2}a - 2\sqrt{3}b^2 - 7b + 12\sqrt{3}\big), \\ u^{(0)} &= -3a\big(6\sqrt{2}b + 4\sqrt{6} - 4\sqrt{3}b^3 - 4b^2 + 31\sqrt{3}b - 64\big), \\ y &= \frac{24z^5 + 4z^4 - 674z^3 + 1437z^2 + 1355z - 5292}{2(20z^3 + 47z^2 - 117z - 604)} \end{aligned}$$

generate the tenth-degree polynomial in z possessing the four real roots. These results are summarized in table 5.

3. Perturbations

Any family of phenomenological potentials may be supposed approximated by an asymptotically harmonic Padé approximant (3) of a suitable degree t. Up to the Kth order a consistency of its subsequent perturbative treatment is guaranteed whenever the

remainder is kept sufficiently small, $V^{(\text{phenomenological})}(x) - V^{(\text{Padé})}(x) = \mathcal{O}(\lambda_{\min}^{K+1}) = \mathcal{O}(\lambda_{\max}^{K+1})$. The stability of approximation requires that the more or less random poles in $V^{(\text{Padé})}(x)$ are under firm control. In the case of our class of potentials (3) this is most easily achieved by their unique [16] partial-fraction re-arrangement

$$V(\beta, x) = \omega^2 x^2 + \sum_{m=1}^{M_1} \sum_{j=1}^{J(m)} \frac{\sigma_{mj}}{(1 + e_m x^2)^j} + \sum_{n=1}^{N_2} \sum_{k=1}^{K(n)} \frac{\mu_{nk} x^2 + \nu_{nk}}{[1 + (f_n - 2g_n)x^2 + g_n^2 x^4]^k}. \quad (15)$$

An instructive illustration is offered by the $t = 2$ example (7). The maximal admissible range of perturbation of its couplings must be restricted by the condition of positivity of the denominator. This means that we must have $f = f(\lambda) > 0$ or $f(\lambda) = 0$ and $g = g(\lambda) \leqslant 0$ or $0 > f(\lambda) > 4g(\lambda)$ for $\lambda \in (\lambda_{\min}, \lambda_{\max})$.

We shall expand the perturbed wave functions in the same modified oscillator basis as above,

$$\psi(\lambda, r) = \mathcal{B}(r) \sum_{n=0}^{\infty} h_n(\lambda) \langle r|n\rangle \equiv \sum_{n=0}^{\infty} h_n(\lambda) \langle r|\Xi_n\rangle, \quad \mathcal{B}(r) = \sum_{d=0}^{t} B_d x^{2d}. \quad (16)$$

This leads to the infinite-dimensional Schrödinger equation

$$\big[\mathcal{H}(\lambda) - E(\lambda)\mathcal{D}(\lambda)\big]\vec{h}(\lambda) = 0. \quad (17)$$

It degenerates back to the finite-dimensional problems of preceding section in the unperturbed limit $\beta \to \beta^{(0)}$.

3.1. *Phenomenological appeal of Padé oscillators*

The degree t in equation (3) specifies also a half-bandwidth of our $(2t + 1)$-diagonal quasi-Hamiltonians $[\mathcal{H}(\lambda) - E(\lambda)\mathcal{D}(\lambda)]$. This $t = t[J(1), \ldots, J(M_1), K(1), \ldots, K(N_2)]$ grows rather quickly with all its arguments. Vice versa, the very first t's already offer a rich variety of possible shapes of the phenomenological potential (cf. figures 2 and 3).

In the simplest $t = 1$ example (1) the numerically calculated λ- or β-dependence of energies exhibits a roughly quadratic shape, $\beta \sim (E + \text{const})^2 + \text{const}$. For the four lowest states this is illustrated by figures 1 and 4. The exceptional exact energies (marked by crosses) are scattered all over the coupling-energy plane. These quasi-harmonic points may be inter-connected by auxiliary lines (cf. figures 5 and 6 and ref. [17]). In a way, these lines generalize the harmonic spectrum to $\beta^{(0)} \neq 0$. Their distinguished feature seems to be an asymptotically almost equidistant and almost linear shape, resembling strongly their harmonic predecessor.

Only the first few energies exhibit in fact a pronounced non-equidistant spacing. The onset of the almost equidistant behaviour moves only slowly up with the growth of $\beta^{(0)}$. The approximate linearity of dependence of the nth energy level E_n on the value of the coupling β is remarkable. We may expect that the first-order perturbation formulae

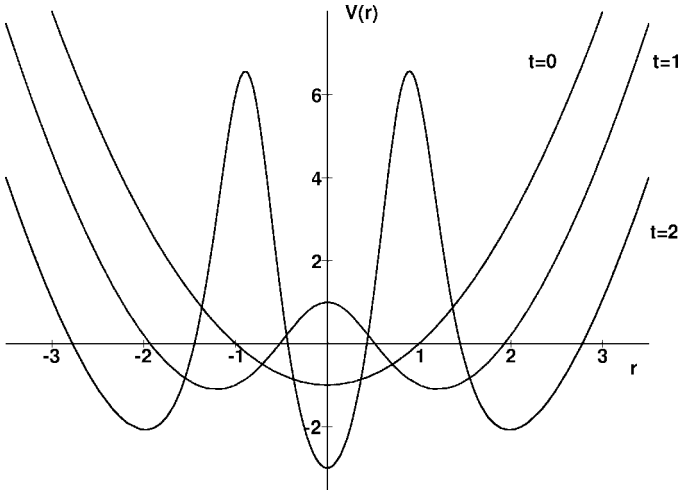

Figure 2. Three potentials (3) supporting the exact ground state at zero energy.

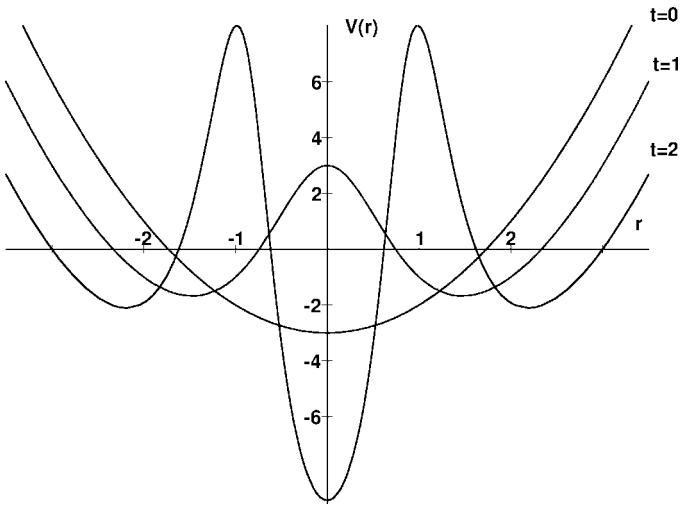

Figure 3. Three potentials (3) supporting the exact first excited state at zero energy.

will reproduce the $t = 1$ energies $E(\lambda)$ with decent precision in a broad interval of their λ-dependence.

It is well known that in the context of studies of double wells one of the big challenges to perturbation theory is posed by the related approximate degeneracy between the even and odd states. An explicit illustration of this phenomenon is provided by table 1. It indicates that the long-lasting puzzle of perturbations of the quasi-degenerate spectra in the deep double wells may find one of its very natural resolutions in the present language since our formalism treats the states with different parity as perturbations of different systems. For example, in between the first two couplings of the table [i.e.,

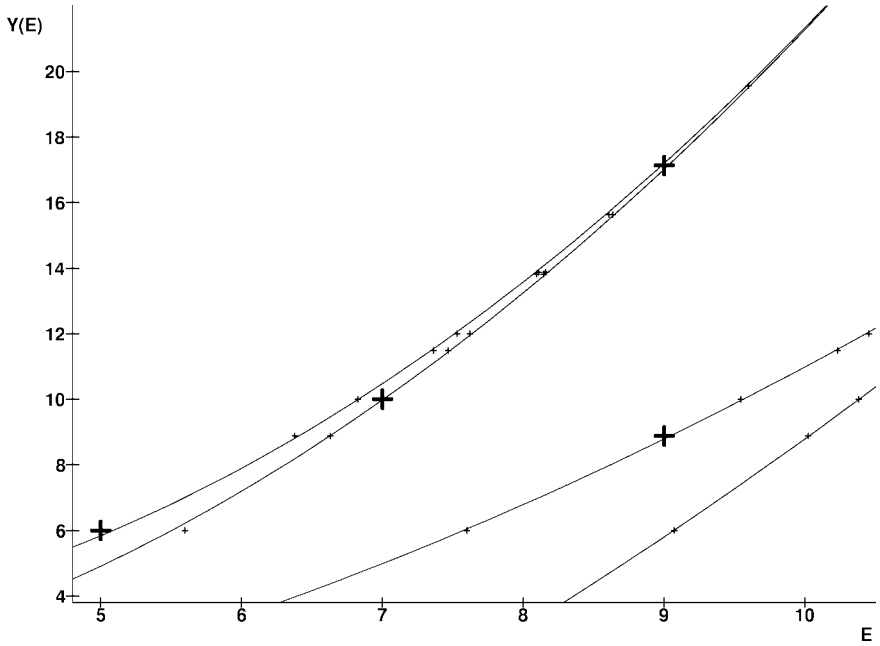

Figure 4. An empirical fit $Y(E) = a + bE + cE^2$ of the couplings $\beta = \beta(E)$. The thin and thick crosses denote the respective numerical and non-numerical levels at various $\beta^{(0)}$.

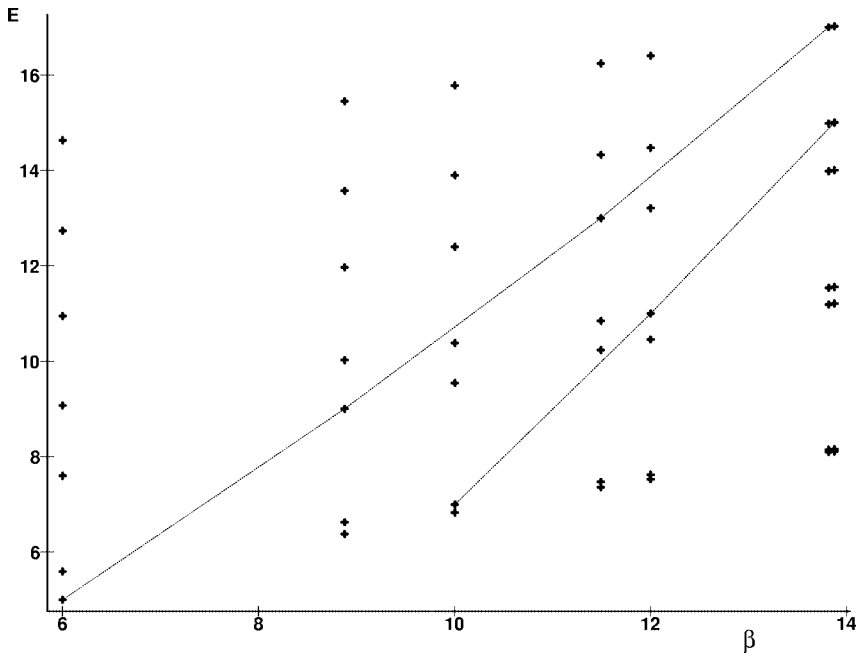

Figure 5. The seven lowest energies for the seven lowest barriers $\beta^{(0)}$ in (1). The auxiliary "Gallas" lines connect the symmetric (upper curve) and asymmetric (lower curve) exact levels with growing q.

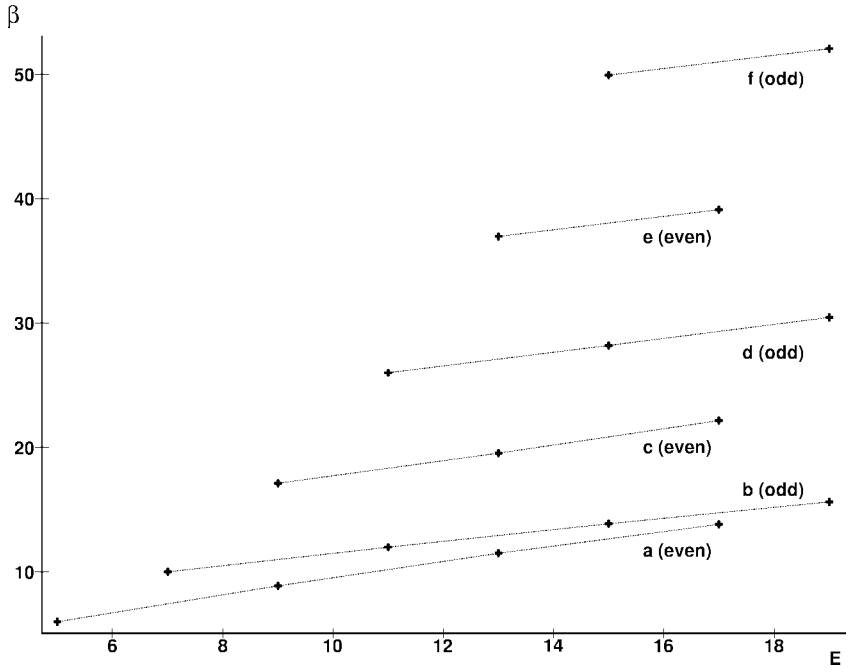

Figure 6. Several "Gallas" lines in a bigger part of the $E-\beta$ plane.

for $\beta \in (64.89\ldots, 81.88\ldots)$] one should calculate the ground state energies as perturbations of $E^{(0)} = 17$ while the very close first excitations should be perturbations of $E^{(0)} = 19$ in another potential. In low orders the split of energies will probably remain disguised by errors of their separate perturbative determinations but the related quasi-degenerate eigenfunctions themselves become clearly distinguished by their parity.

3.2. Rayleigh–Schrödinger expansions near $\beta^{(0)}$

The measure $\lambda = \beta - \beta^{(0)}$ of deviation of our perturbed Schrödinger equation from its zero-order form should be sufficiently small in the Kato's sense [18]. Then, any analytic λ-dependence of the matrices

$$\mathcal{D}(\lambda) = \mathcal{D}(0)+\lambda\mathcal{D}^{(1)}+\lambda^2\mathcal{D}^{(2)}+\cdots, \qquad \mathcal{H}(\lambda) = \mathcal{H}(0)+\lambda\mathcal{H}^{(1)}+\lambda^2\mathcal{H}^{(2)}+\cdots, \quad (18)$$

may be expected to imply the validity of the energy series (2) and of its wave function counterpart

$$h_j = h_j(\lambda) = h_j(0) + \lambda h_j^{(1)} + \lambda^2 h_j^{(2)} + \cdots. \quad (19)$$

This transforms our λ-dependent Schrödinger equation into a set of its separate $\mathcal{O}(\lambda^k)$ components. At $k = 0$, the unperturbed problem $[\mathcal{H}(0) - E(0)\mathcal{D}(0)]\vec{h}(0) = 0$ of preceding section is re-obtained. Next we get its $\mathcal{O}(\lambda)$ descendant

$$\left[\mathcal{H}(0) - E^{(0)}\mathcal{D}(0)\right]\vec{h}^{(1)} = \left[E^{(0)}\mathcal{D}^{(1)} - \mathcal{H}^{(1)}\right]\vec{h}(0) + E^{(1)}\mathcal{D}(0)\vec{h}(0). \quad (20)$$

In compact notation with abbreviations $\vec{\tau}^{(0)} \equiv [E^{(0)}\mathcal{D}^{(1)} - \mathcal{H}^{(1)}]\vec{h}(0)$, $\vec{\rho}^{\{0\}} \equiv \mathcal{D}(0)\vec{h}(0)$ and $\mathcal{M} = \mathcal{H}(0) - E(0)\mathcal{D}(0)$ this equation shares its form with all the subsequent $\mathcal{O}(\lambda^k)$ equations

$$\mathcal{M}\vec{h}^{(k)} = \vec{\tau}^{(k-1)} + E^{(k)}\vec{\rho}^{\{0\}} \tag{21}$$

requiring only the further abbreviation

$$\vec{\tau}^{(1)} = \left[E^{(0)}\mathcal{D}^{(2)} + E^{(1)}\mathcal{D}^{(1)} - \mathcal{H}^{(2)}\right]\vec{h}(0) + \left[E^{(0)}\mathcal{D}^{(1)} + E^{(1)}\mathcal{D}(0) - \mathcal{H}^{(1)}\right]\vec{h}^{(1)}$$

and, in general,

$$\vec{\tau}^{(k-1)} = \left[\sum_{j=0}^{k-1} E^{(j)}\mathcal{D}^{(k-j)} - \mathcal{H}^{(k)}\right]\vec{h}(0) + \sum_{m=1}^{k-1}\left[\sum_{i=0}^{k-m-1} E^{(i)}\mathcal{D}^{(k-m-i)} + E^{(k-m)}\mathcal{D}(0) - \mathcal{H}^{(k-m)}\right]\vec{h}^{(m)}. \tag{22}$$

As long as $\det\mathcal{M} = 0$ each particular solution $\vec{h}^{(k)}$ may contain an arbitrarily large admixture of the zero-order column vector $\vec{h}(0)$. This is the well known renormalization freedom of perturbative wave functions in quantum mechanics. We get rid of it by the normalization $h_q^{(k)} = 0$ in each perturbation order $k > 0$. Such a convention differs from the standard textbook recommendations but serves the same purpose and makes the solutions of our key equation (21) well defined.

3.3. *Example: tridiagonal $\mathcal{M}$*

Let us choose $t = 1$, fix the nodal count q and accept an exact solution at $\beta = \beta^{(0)}$ as our illustrative $^{(0)}$-superscripted zero-order approximation. The perturbed couplings $\beta = \beta^{(0)}+\lambda$ and $B = B^{(0)}+\lambda B^{(1)}+\cdots$ with a small measure of perturbation $\lambda \neq 0$ enter the infinite dimensional Schrödinger equation (4) or (17). After appropriate insertions we get the $t = 1$ set of equations (21),

$$\begin{pmatrix} a_0^{(0)} & d_0^{(0)} & & \\ c_1^{(0)} & a_1^{(0)} & d_1^{(0)} & \\ & c_2^{(0)} & a_2^{(0)} & \ddots \\ & & \ddots & \ddots \end{pmatrix}\begin{pmatrix} h_0^{(k)} \\ h_1^{(k)} \\ h_2^{(k)} \\ \vdots \end{pmatrix} = E^{(k)}\begin{pmatrix} \rho_0^{(0)} \\ \rho_1^{(0)} \\ \rho_2^{(0)} \\ \vdots \end{pmatrix} + \begin{pmatrix} \tau_0^{(k-1)} \\ \tau_1^{(k-1)} \\ \tau_2^{(k-1)} \\ \vdots \end{pmatrix}. \tag{23}$$

Only the first $q+2$ components of $\vec{\rho}^{(0)} = \mathcal{D}^{(0)}\vec{h}^{(0)}$ are nonzero since

$$\begin{pmatrix} \rho_0^{(0)} \\ \rho_1^{(0)} \\ \rho_2^{(0)} \\ \vdots \end{pmatrix} = \begin{pmatrix} a_0^{\{kin\}} & d_0^{\{kin\}} & & \\ c_1^{\{kin\}} & a_1^{\{kin\}} & d_1^{\{kin\}} & \\ & c_2^{\{kin\}} & a_2^{\{kin\}} & \ddots \\ & & \ddots & \ddots \end{pmatrix}\begin{pmatrix} h_0^{(0)} \\ h_1^{(0)} \\ h_2^{(0)} \\ \vdots \end{pmatrix}, \tag{24}$$

$$a_n^{\{kin\}} = (1 + f^{(0)}\alpha_n), \qquad d_n^{\{kin\}} = f^{(0)}\beta_n, \qquad c_n^{\{kin\}} = f^{(0)}\beta_{n-1}.$$

In contrast, the compressed previous-order (i.e., already known) corrections $\tau_j^{(k-1)}$ only terminate in the first order, at $k = 1$.

3.3.1. Ground-state illustration

In the $k = 1$ and $q = 0$ exemplification of equation (23)

$$\left(\begin{array}{cc|ccc} 0 & d_0^{(0)} & 0 & \dots & \\ 0 & a_1^{(0)} & 0 & 0 & \dots \\ \hline 0 & c_2^{(0)} & a_2^{(0)} & d_2^{(0)} & \dots \\ 0 & 0 & c_3^{(0)} & a_3^{(0)} & \dots \\ \vdots & & & \ddots & \ddots \end{array}\right) \left(\begin{array}{c} 0 \\ h_1^{(1)} \\ \hline h_2^{(1)} \\ h_3^{(1)} \\ \vdots \end{array}\right) = \left(\begin{array}{c} \tau_0^{(0)} \\ 0 \\ \hline 0 \\ 0 \\ \vdots \end{array}\right) + E^{(1)} \left(\begin{array}{c} \rho_0^{\{0\}} \\ \rho_1^{\{0\}} \\ \hline 0 \\ 0 \\ \vdots \end{array}\right) \tag{25}$$

the first two energy-dependent rows decouple from the rest. For the even-parity $\ell = -1$ they read

$$-2\sqrt{2}h_1^{(1)} = -\beta^{(1)} + 3E^{(1)}/2,$$
$$\beta^{(0)}h_1^{(1)} = E^{(1)}/\sqrt{2}.$$

As long as $\beta^{(0)} = 6$ and $\beta^{(1)} = 1$ their solution reproduces the current textbook first-order overlap formula for the energy,

$$E^{(1)} = \frac{\int_{-\infty}^{\infty} \exp(-x^2)(1 + x^2)\,\mathrm{d}x}{\int_{-\infty}^{\infty} \exp(-x^2)(1 + x^2)^2\,\mathrm{d}x} = \frac{6}{11}\,. \tag{26}$$

This test demonstrates the user-friendliness of our non-Hermitian recipe.

3.3.2. The first excitation

In our preceding illustration we did not mark the cut-off M in $\mathcal{M}$. For the next, $q = 1$ state with $M = 6$ (chosen small for paedagogical purposes) we have to solve the set

$$\left(\begin{array}{ccc|cccc} a_0 & 0 & 0 & 0 & 0 & 0 & 0 \\ c_1 & 0 & d_1 & 0 & 0 & 0 & 0 \\ 0 & 0 & a_2 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & c_3 & a_3 & d_3 & 0 & 0 \\ 0 & 0 & 0 & c_4 & a_4 & d_4 & 0 \\ 0 & 0 & 0 & 0 & c_5 & a_5 & d_5 \\ 0 & 0 & 0 & 0 & 0 & c_6 & a_6 \end{array}\right) \left(\begin{array}{c} h_0^{(k)} \\ 0 \\ h_2^{(k)} \\ \hline h_3^{(k)} \\ h_4^{(k)} \\ h_5^{(k)} \\ h_6^{(k)} \end{array}\right) = \left(\begin{array}{c} \tau_0^{(k-1)} \\ \tau_1^{(k-1)} \\ \tau_2^{(k-1)} \\ \hline \tau_3^{(k-1)} \\ \tau_4^{(k-1)} \\ \tau_5^{(k-1)} \\ \tau_6^{(k-1)} \end{array}\right) + E^{(k)} \left(\begin{array}{c} \rho_0^{\{0\}} \\ \rho_1^{\{0\}} \\ \rho_2^{\{0\}} \\ \hline 0 \\ 0 \\ 0 \\ 0 \end{array}\right). \tag{27}$$

The upper part of this equation (separated by the inset lines) stays decoupled. We can underline that in contrast to the current textbook recipe we do not need any left eigenvector

of $\mathcal{M}$ and still can define the kth energy correction via the finite, $(q+t+1)$-dimensional matrix inversion

$$\begin{pmatrix} a_0 & \rho_0^{\{0\}} & 0 \\ c_1 & \rho_1^{\{0\}} & d_1 \\ 0 & \rho_2^{\{0\}} & a_2 \end{pmatrix} \begin{pmatrix} h_0^{(k)} \\ -E^{(k)} \\ h_2^{(k)} \end{pmatrix} = \begin{pmatrix} \tau_0^{(k-1)} \\ \tau_1^{(k-1)} \\ \tau_2^{(k-1)} \end{pmatrix}. \tag{28}$$

In the second, lower part of equation (27) the cut-off M should grow to infinity in principle. The matrix-inversion evaluation of the remaining wave function components $h_{q+t+1}^{(k)}, h_{q+t+2}^{(k)}, \ldots$ is much more difficult and acquires a purely numerical character. In a schematic representation $\vec{h}^{(k)} \sim \mathcal{R}\vec{\tau}^{(k-1)} + \cdots$ the "unperturbed propagator" $\mathcal{R}$ is a general, *fully non-diagonal* matrix.

3.3.3. The higher excitations

The size of the upper part of equation (23) grows with q (cf. (25) and (27)). Only its last, $(q+1)$-subscripted line remains trivial. As long as $c_{q+1}^{(0)} = 0$, $d_{q+1}^{(0)} = 0$ and $a_{q+1}^{(0)} = g^{(0)} > 0$, it degenerates to an explicit definition of the $(q+1)$-st coefficient in terms of the not yet specified energy,

$$h_{q+1}^{(k)} = \frac{E^{(k)}\rho_{q+1}^{(0)} + \tau_{q+1}^{(k-1)}}{g^{(0)}}. \tag{29}$$

Thus, in practice, our equation (23) decays in the two equally difficult subsystems at the larger q. Its upper $q+1$ rows are, fortunately, not as complicated as they look. Firstly, an immediate elimination of energies may help for $q \gg 1$. It proves unexpectedly easy since the array $\vec{\rho}^{(0)}$ is a left eigenvector of our non-Hermitian quasi-Hamiltonian $\mathcal{M}$. The left action of this vector on equation (21) eliminates all $h_n^{(k)}$'s and defines the kth energy correction at any t,

$$E^{(k)} = -\frac{\sum_{m=0}^{q+t} \rho_m^{(0)} \tau_m^{(k-1)}}{\sum_{n=0}^{q+t} \left(\rho_n^{(0)}\right)^2}. \tag{30}$$

With this knowledge, equation (29) determines $h_{q+1}^{(k)}$. At the exact energy (30) an abbreviated right-had-side vector $\widetilde{\tau}_m^{(k-1)} \equiv \tau_m^{(k-1)} + E^{(k)}\rho_m^{(0)}$, $m = 0, 1, \ldots$ enters the equation (23) whose first $q+1$ separate rows become linearly dependent. We omit the very first one as redundant. Simultaneously, our normalization $h_q^{(k)} = 0$ annihilates a column in $\mathcal{M}$ and we get the reduced equation

$$\begin{pmatrix} c_1^{(0)} & a_1^{(0)} & d_1^{(0)} & & & \\ & c_2^{(0)} & a_2^{(0)} & d_2^{(0)} & & \\ & & \ddots & \ddots & \ddots & \\ & & & c_{q-1}^{(0)} & a_{q-1}^{(0)} & \\ & & & & c_q^{(0)} & \end{pmatrix} \begin{pmatrix} h_0^{(k)} \\ h_1^{(k)} \\ \vdots \\ h_{q-2}^{(k)} \\ h_{q-1}^{(k)} \end{pmatrix} = \begin{pmatrix} \widetilde{\tau}_1^{(k-1)} \\ \widetilde{\tau}_2^{(k-1)} \\ \vdots \\ \widetilde{\tau}_{q-1}^{(k-1)} \\ \widetilde{\tau}_q^{(k-1)} \end{pmatrix}. \tag{31}$$

This gives a non-diagonal, upper triangular generalization

$$\begin{pmatrix} h_0^{(k)} \\ h_1^{(k)} \\ \vdots \\ h_{q-2}^{(k)} \\ h_{q-1}^{(k)} \end{pmatrix} = \begin{pmatrix} 1/c_1^{(0)} & \mathcal{R}_{12} & \dots & & \mathcal{R}_{1q} \\ & 1/c_2^{(0)} & \mathcal{R}_{23} & \dots & \mathcal{R}_{2q} \\ & & \ddots & \ddots & \vdots \\ & & & 1/c_{q-1}^{(0)} & \mathcal{R}_{q-1q} \\ & & & & 1/c_q^{(0)} \end{pmatrix} \begin{pmatrix} \widetilde{\tau}_1^{(k-1)} \\ \widetilde{\tau}_2^{(k-1)} \\ \vdots \\ \widetilde{\tau}_{q-1}^{(k-1)} \\ \widetilde{\tau}_q^{(k-1)} \end{pmatrix} \tag{32}$$

of the current rule based on a diagonal unperturbed propagator. Unfortunately, any extension of the latter trick fails. For all $t > 1$ a different approach is needed.

4. New recipe using triangular propagators

Previous examples clarified an exceptional role of the $(q+t)$th row in $\mathcal{M}$ where $c_{q+t} = d_{q+t} = 0$. The trick is not fully transferable to $t > 1$ [8]. At the higher t's, one is usually expected to simplify the matrix $\mathcal{M}$ by a brute force diagonalization. This would be a purely numerical step of course. In what follows we are going to describe a more analytic approach. It will lie somewhere in between the fully analytic (schematically, $t = 0$) and purely numerical (i.e., pre-diagonalization) extremes: Our unperturbed propagators $\mathcal{R}$ will be constructed as sparse, triangular matrices.

The presentation of this material will be split in three parts. Firstly, using just $t = 1$ for simplicity, section 4.1 explains the idea of constructing $\mathcal{R}$ in the upper triangular form. Secondly, section 4.2 employs the next, $t = 2$ example and explains the alternative approach using the lower triangular unperturbed propagators.

We believe that this gives a clear guide to the general t's. Still, an abstract and detailed description of our innovated perturbation theory (with any t) is offered in the appendix. The reason is that, building on the reader's experience with our previous examples, we may introduce a less transparent but much more compact notation. Moreover, we also relax there the immediate connection of our technique to some peculiarities (e.g., one-dimensional nature) of our illustrative example (3).

4.1. Upper triangular propagators: $t = 1$ example

We have split our equation (23) into the separate rule (29), the upper part (31) with solution (32) and the lower part

$$\begin{pmatrix} a_{q+2}^{(0)} & d_{q+2}^{(0)} & & & \\ c_{q+3}^{(0)} & a_{q+3}^{(0)} & d_{q+3}^{(0)} & & \\ & c_{q+4}^{(0)} & a_{q+4}^{(0)} & \ddots & \\ & & \ddots & \ddots & d_{M-1}^{(0)} \\ & & & c_M^{(0)} & a_M^{(0)} \end{pmatrix} \begin{pmatrix} h_{q+2}^{(k)} \\ h_{q+3}^{(k)} \\ h_{q+2}^{(k)} \\ \vdots \\ h_M^{(k)} \end{pmatrix} = \begin{pmatrix} \widetilde{\tau}_{q+2}^{(k-1)\star} \\ \widetilde{\tau}_{q+3}^{(k-1)} \\ \widetilde{\tau}_{q+4}^{(k-1)} \\ \vdots \\ \widetilde{\tau}_M^{(k-1)} \end{pmatrix} \tag{33}$$

truncated at certain $M \gg q+2$ and containing, on its right-hand side, a re-defined, *-superscripted known quantity $\widetilde{\tau}_{q+2}^{(k-1)\star} = \widetilde{\tau}_{q+2}^{(k-1)} - c_{q+2}^{(0)} h_{q+1}^{(k)}$.

For a clear explanation of our main idea let us now drop the superscripts and choose $q = 1$ and $M = 6$ again. This returns us back to our pedagogical example (27) re-written now in a re-partitioned, equivalent square-matrix form

$$\left(\begin{array}{c|ccccc} c_3 & a_3 & d_3 & & & \\ \hline & c_4 & a_4 & d_4 & & \\ & & c_5 & a_5 & d_5 & \\ & & & c_6 & a_6 & \\ & & & & c_7 & \end{array}\right) \left(\begin{array}{c} h_2 \\ \hline h_3 \\ h_4 \\ h_5 \\ h_6 \end{array}\right) = \left(\begin{array}{c} \widetilde{\tau}_3 \\ \widetilde{\tau}_4 \\ \widetilde{\tau}_5 \\ \widetilde{\tau}_6 \\ c_7 h_6 \end{array}\right), \tag{34}$$

where h_2 is already known and a trivial last row $c_7 h_6 = c_7 h_6$ has been added. The trick is that we may now remove the cut-off completely. The infinite-dimensional left-hand-side matrix

$$\mathcal{Z}^{-1} = \begin{pmatrix} c_{q+2}^{(0)} & a_{q+2}^{(0)} & d_{q+2}^{(0)} & & \\ & c_{q+3}^{(0)} & a_{q+3}^{(0)} & d_{q+3}^{(0)} & \\ & & c_{q+4}^{(0)} & a_{q+4}^{(0)} & \ddots \\ & & & \ddots & \ddots \end{pmatrix} \tag{35}$$

is regular. It may be inverted in an algebraic, non-numerical and cut-off-independent manner, "forgetting" our use of the vectors with $M = 6$, i.e., $\widetilde{\tau}_7 = c_7 h_6$ and $h_{6+j} = 0$ and $\widetilde{\tau}_{7+j} = 0$ for all $j = 1, 2, \ldots$. We may conclude that once we know our upper triangular propagator matrix $\mathcal{Z}$ we may pre-multiply by it equation (34) from the left and get the final wave function defined by the formula

$$h_{q+m}^{(k)} = \mu_{q+m}^{(k-1)} + h_M^{(k)} c_{M+1} \nu_{q+m}^{(0)}, \quad m = 1, 2, \ldots, M-q-1, \tag{36}$$

at any cut-off $M \gg q+1$. Both its components have just an elementary form

$$\begin{pmatrix} \mu_{q+1}^{(k-1)} \\ \mu_{q+2}^{(k-1)} \\ \vdots \\ \mu_{M-2}^{(k-1)} \\ \mu_{M-1}^{(k-1)} \end{pmatrix} = \mathcal{Z} \begin{pmatrix} \widetilde{\tau}_{q+2}^{(k-1)} \\ \widetilde{\tau}_{q+3}^{(k-1)} \\ \vdots \\ \widetilde{\tau}_{M-1}^{(k-1)} \\ \widetilde{\tau}_M^{(k-1)} \end{pmatrix}, \qquad \begin{pmatrix} \nu_{q+1}^{(0)} \\ \nu_{q+2}^{(0)} \\ \vdots \\ \nu_{M-2}^{(0)} \\ \nu_{M-1}^{(0)} \end{pmatrix} = \begin{pmatrix} \mathcal{Z}_{1,M-q} \\ \mathcal{Z}_{2,M-q} \\ \vdots \\ \mathcal{Z}_{M-q-2,M-q} \\ \mathcal{Z}_{M-q-1,M-q} \end{pmatrix}. \tag{37}$$

This is a key point of our considerations. Starting from the first omitted index $m = M-q$ our equation (36) is an identity. At the first *admitted* (and exceptional) index $m = 1$ this equation defines, paradoxically, the right-hand side quantity h_M itself. Indeed, the pertaining left-hand side value h_{q+1} is already known.

In equation (37) an *ascending* recurrent evaluations may be recommended as giving, step by step, $\mu_{M-1}^{(k-1)} = \widetilde{\tau}_M^{(k-1)} / c_M^{(0)}$ etc. Our recipe is complete. We may summarize: In a deeply anharmonic double well regime, the partial solvability of our unperturbed

system *and* the reducibility of its propagator to a triangular matrix implies the feasibility of an innovated perturbation construction with propagator $\mathcal{R}$ of an upper triangular matrix form.

An additional, marginal remark is due. If needed, the recurrences (37) may be solved in a closed form

$$\mu^{(k-1)}_{M-m-1} = \frac{(-1)^m}{c^{(0)}_M c^{(0)}_{M-1}\cdots c^{(0)}_{M-m}} F, \tag{38}$$

where

$$F = \det \begin{pmatrix} a^{(0)}_{M-m} & d^{(0)}_{M-m} & 0 & \dots & 0 & \tilde\tau^{(k-1)}_{M-m} \\ c^{(0)}_{M-m+1} & a^{(0)}_{M-m+1} & d^{(0)}_{M-m+1} & \dots & \dots & \tilde\tau^{(k-1)}_{M-m+1} \\ 0 & \ddots & \ddots & \ddots & & \vdots \\ \vdots & \ddots & & & & \\ 0 & \dots & 0 & c^{(0)}_{M-1} & a^{(0)}_{M-1} & \tilde\tau^{(k-1)}_{M-1} \\ 0 & \dots & & 0 & c^{(0)}_M & \tilde\tau^{(k-1)}_M \end{pmatrix} \tag{39}$$

due to the Kramer's rule.

4.2. *Lower triangular propagators: $t = 2$ example*

Let us consider the pentadiagonal version of equation (21),

$$\left(\begin{array}{cccccc|c} a_0 & d^{[1]}_0 & d^{[2]}_0 & 0 & 0 & 0 & \dots \\ c^{[1]}_1 & a_1 & d^{[1]}_1 & d^{[2]}_1 & 0 & 0 & \dots \\ c^{[2]}_2 & c^{[1]}_2 & a_2 & d^{[1]}_2 & 0 & 0 & \dots \\ \hline 0 & c^{[2]}_3 & c^{[1]}_3 & a_3 & d^{[1]}_3 & d^{[2]}_3 & \dots \\ \hline 0 & 0 & c^{[2]}_4 & c^{[1]}_4 & a_4 & d^{[1]}_4 & \dots \\ \vdots & & & \ddots & \ddots & \ddots & \ddots \end{array}\right) \left(\begin{array}{c} h^{(k)}_0 \\ (h^{(k)}_1) \\ h^{(k)}_2 \\ h^{(k)}_3 \\ h^{(k)}_4 \\ \vdots \end{array}\right) = \left(\begin{array}{c} \tau^{(k-1)}_0 \\ \tau^{(k-1)}_1 \\ \hline \tau^{(k-1)}_2 \\ \hline \tau^{(k-1)}_3 \\ \hline \tau^{(k-1)}_4 \\ \vdots \end{array}\right) + E^{(k)} \left(\begin{array}{c} \rho^{\{0\}}_0 \\ \rho^{\{0\}}_1 \\ \hline \rho^{\{0\}}_2 \\ \hline \rho^{\{0\}}_3 \\ \hline \rho^{\{0\}}_4 \\ \vdots \end{array}\right)$$

with, say, $q = 1$, i.e., $c^{[2]}_3 = d^{[2]}_3 = 0$ and $\rho^{\{0\}}_4 = \rho^{\{0\}}_5 = \cdots = 0$. After the insertion of energy (30) we sum the two right hand side vectors in one, $\tau^{(k-1)}_j + E^{(k)}\rho^{\{0\}}_j \equiv \tilde\tau^{(k-1)}_j$, and omit the $_3$-subscripted row (between lines). Simultaneously our normalization $h^{(k)}_q = 0$ (in parenthesis) annihilates the second column in $\mathcal{M}$.

Moving further the first $t - 1$ (i.e., one) plus one (exceptional, $(q + t)$th) columns of $\mathcal{M}$ to the right hand side and dropping the redundant superscripts $^{(k)}$ and $^{(k-1)}$ we get

the equivalent equation

$$\mathcal{Z}^{-1}\left(\begin{array}{c} h_2\\ h_3\\ h_4\\ \hline h_6\\ \vdots\\ h_{M+2}\\ \hline 0\\ \vdots \end{array}\right)=\left(\begin{array}{c} \widetilde{\tau}_0\\ \widetilde{\tau}_1\\ \widetilde{\tau}_2\\ \hline \widetilde{\tau}_4\\ \vdots\\ \widetilde{\tau}_M\\ \hline \widetilde{\tau}^{\star}_{M+1}\\ \vdots \end{array}\right)-h_0\left(\begin{array}{c} \rho_0^{\{1\}}\\ \rho_1^{\{1\}}\\ \rho_2^{\{1\}}\\ \hline \rho_4^{\{1\}}\\ \vdots\\ \rho_M^{\{1\}}\\ \vdots\\ \vdots \end{array}\right)-h_5\left(\begin{array}{c} \rho_0^{\{2\}}\\ \rho_1^{\{2\}}\\ \rho_2^{\{2\}}\\ \hline \rho_4^{\{2\}}\\ \vdots\\ \rho_M^{\{2\}}\\ \vdots\\ \vdots \end{array}\right) \tag{40}$$

with the appropriate auxiliary $\widetilde{\tau}^{\star}_{M+1}=c^{[2]}_{M+1}h_{M-1}+c^{[1]}_{M+1}h_M$ and $\widetilde{\tau}^{\star}_{M+2}=c^{[2]}_{M+2}h_M$ (while $\widetilde{\tau}^{\star}_{M+3}=\widetilde{\tau}^{\star}_{M+4}=\cdots=0$), with $\rho_0^{\{1\}}=a_0$ etc., $\rho_4^{\{2\}}=d_4^{[1]}$ etc. and with the lower triangular and infinite matrix

$$\mathcal{Z}^{-1}=\left(\begin{array}{ccc|c} d_0^{[2]} & & & \\ d_1^{[1]} & d_1^{[2]} & & \\ a_2 & d_2^{[1]} & d_2^{[2]} & \\ \hline c_4^{[2]} & c_4^{[1]} & a_4 & d_4^{[2]} \\ 0 & c_5^{[2]} & c_5^{[1]} & d_5^{[1]}\ d_5^{[2]} \\ \vdots & \ddots & \ddots & \ddots\ \ddots\ \ddots \end{array}\right).$$

This pentadiagonal matrix is easily invertible since its main diagonal is all non-zero. Indeed, by construction, $n\neq t+q$ in $d_n^{[t]}=B_t[\varepsilon_n-\varepsilon_{t+q}]\langle n|r^{2t}|n+t\rangle$. The action of $\mathcal{Z}$ upon equation (40) from the left gives our final wave functions

$$\left(\begin{array}{c} h_2\\ h_3\\ h_4\\ \hline h_6\\ \vdots\\ h_{M+2} \end{array}\right)=\mathcal{Z}\left(\begin{array}{c} \widetilde{\tau}_0\\ \widetilde{\tau}_1\\ \widetilde{\tau}_2\\ \hline \widetilde{\tau}_4\\ \vdots\\ \widetilde{\tau}_M \end{array}\right)-h_0\,\mathcal{Z}\left(\begin{array}{c} \rho_0^{\{1\}}\\ \rho_1^{\{1\}}\\ \rho_2^{\{1\}}\\ \hline \rho_4^{\{1\}}\\ \vdots\\ \rho_M^{\{1\}} \end{array}\right)-h_5\,\mathcal{Z}\left(\begin{array}{c} \rho_0^{\{2\}}\\ \rho_1^{\{2\}}\\ \rho_2^{\{2\}}\\ \hline \rho_4^{\{2\}}\\ \vdots\\ \rho_M^{\{2\}} \end{array}\right). \tag{41}$$

The seemingly redundant last two rows form in fact a core of the whole construction: With the well known left-hand side values of $h_{M+1}=h_{M+2}=0$ they must be read as the two necessary linear algebraic equations needed to determine the two "input parameters" h_0 and h_5.

Table 6
Double test: Interpolation (42) between the two solvable potentials.

"Large" coupling	$\lambda = 1$	$\delta = 1 - \lambda = 1$
	Ground state	First excitation
unperturbed energy	11.0000	15.0000
the first correction	−0.0449	−0.0985
$k = 1$ approximation	10.9551	14.9015
Runge Kutta value	10.9434	14.6332

4.2.1. An illustration

A straightforward transition to the general t's does not require any new ideas but merely an appropriate "shorthand" notation. Its explicit description may be found in the appendix. A nontrivial advantage of its more abstract language is that one can immediately work with a much more general class of Hamiltonians, say, with their non-Hermiticity and asymmetry related to the phenomenological absorption, etc. At the same time, even our simple Padé oscillators may provide a number of useful applications.

Flexibility of our fairly weak assumptions may lead to a few non-standard constructions. Imagine just an *interpolation* between two zero-oder models. Thus, our previous $t \geqslant 2$ solvable model (7) may be re-interpreted as the new potential

$$V_{[b]}(\delta, r) = r^2 + \frac{[16 + (1-\delta)\mu^{(1)}]r^2 + [2 + (1-\delta)\nu^{(1)}]}{1 - r^2 + r^4} \tag{42}$$

also solvable at $\delta = 0$. With a new "small" parameter $\delta = 1 - \lambda$ and the new couplings

$$\mu^{(1)} = 14.941997\ldots - 16 \approx 1.05800, \qquad \nu^{(1)} = 4.959146\ldots - 2 \approx 2.95915$$

this leads to a methodically appealing *linear* interpolation between the two solvable cases.

This may serve as a test of our method. In table 6 the first-order precision compares well with the purely numerical exact energies. In a way paralleling our above $t = 1$ test (26) the usual evaluation of the $t = 2$ overlap integrals is much more tedious of course. Although the integrators in MAPLE [19] still manage and offer their evaluation, the immediate algebraic solution of our linear algebraic three-by-three equations proves, definitely, much preferable.

5. Summary

Our present recipe treats a phenomenological Schrödinger equation in three steps. In the preliminary one we choose the potential in its Padé (or perturbed Padé) asymptotically harmonic representation (3). In the next preparatory stage the rational potential with $2t + 1$ free parameters is assigned a suitable solvable zero-order approximant with as many as $t + 1$ free parameters. We pick up the parity (or angular momentum) ℓ and

degree q of the unperturbed wave function and determine, algebraically, all the parameters which are constrained by the solvability. In the third step we finally apply our modified or innovated Rayleigh–Schrödinger perturbation algorithm. In each order we

- compress our knowledge of preceding corrections (say, in an auxiliary vector $\vec{\tau}$ given by formula (22)) and, if needed,
- define immediately the new energy (by equation (30));
- construct another auxiliary array (in general, vector $\vec{\theta}$ defined by recurrences (48) in the appendix);
- choose a cut-off $M \gg 1$;
- satisfy the M-dependent model-space constraints (i.e., $t+1$ linear equations (50) + (51) in general);
- evaluate all the missing components of the wave function corrections (their general form is given by equation (46) below).

As a comfortable methodical alternative to the current prescriptions our innovated procedure admits a non-diagonality of unperturbed Hamiltonians and avoids the necessity of their pre-diagonalization at $\lambda = 0$. Its computational efficiency stems from its consequently recurrent character.

For practical puposes, it is promising that our recipe is reducible, basically, just to a single recurrence relation per each perturbation order. This lowers the common danger of a possible undetected numerical loss of precision, further suppressed here (and especially in the context of non-linear algebra in the zero-order constructions) by the high-precision computer arithmetics and programming in MAPLE [19].

Originally, our choice of the illustrative rational potentials (3) has been motivated, mathematically, by a comparative smallness of their short-range perturbations. *A posteriori*, numerical tests clarified their phenomenological appeal. The flexibility of their shapes proved paralleled by the "fairly dense" occurrence of their partially solvable bound states. Indeed, their observables (e.g., energies) exhibit often an almost linear or quadratic coupling-dependence. In a way extending the $t = 1$ observations by Gallas [17] this supports a very good precision of perturbative predictions over a major part of the coupling space. We may expect a facilitated tractability of potentials with less common (e.g., multiple well) shapes. The frequent physical need of analysis of large variations of realistic models seems to have found here an adequate computational tool.

Appendix. Perturbation construction without left eigenvectors

The main mathematical starting point of all our previous considerations was the linear algebraic zero-order Schrödinger equation $\mathcal{M}(E^{(0)})\vec{h}^{(0)} = 0$ with elements such that

$$\mathcal{M}_{m,m+t+j} = 0, \quad m = 0, 1, \ldots, \ j = 1, 2, \ldots,$$

$$\mathcal{M}_{n,n+t} = d_n^{[t]} > 1/D > 0, \quad n = 0, 1, \ldots, \ n \neq n_0 = t + q, \tag{43}$$

$$\mathcal{M}_{n_0,n_0+t} = d_{n_0}^{[t]} = 1/D, \quad 1/D \to 0.$$

Let us now forget about any one-dimensional interpretation or Padé-oscillator origin of these matrices which are, by assumption, non-Hermitian. In such a case, it is natural to suppose that the left eigenvector of $\mathcal{M}$ is infinite-dimensional and ceases to be available. This appendix will show that (and how) our formalism remains applicable even without this auxiliary array.

A. Notation

The mathematical importance of the upper-diagonal dominance (43) in $\mathcal{M}$ lies in its relevance for recurrences. Up to the exceptional $n = n_0$, each (i.e., the nth) row of our equation (21) may be read as an explicit recurrent definition of its "leftmost" unknown $h_n^{(k)}$. The exception is unpleasant and its naive *-superscripted regularization

$$d_n^{[t]*} = \begin{cases} D \neq 0, & \text{for } n = n_0 = t + q, \\ d_n^{[t]}, & \text{otherwise}, \end{cases} \tag{44}$$

would produce a wrong value of $h_{2t+q}^{(k}$ without the limiting transition $D \to \infty$. A slightly more sophisticated recipe must be used. For its general formulation, the energy $E^{(k)}$ and elements $\vec{h}^{(k)}$ will be split in a pair of arrays $\vec{\zeta}$ and $\vec{\xi}$. The former vector will be finite, containing just the $t + 1$ "difficult" components: energy $E^{(k)} \equiv \zeta_0$, initial values $h_j^{(k)} \equiv -\zeta_j$, $j = 1, 2, \ldots, t - 1$ (let us now prefer $h_0^{(k)} = 0$ for normalization) and the exempted $h_{2t+q}^{(k)} \equiv -\zeta_t$. All the remaining unknowns will lie in the infinite-dimensional vector $\vec{\xi}$ such that $\xi_j = h_{j+t}^{(k)}$, $j = 0, 1, \ldots, \ j \neq q$ (notice that $j = q$ would double-count the exceptional $h_{2t+q}^{(k)}$).

For the time being, let us leave the undetermined component of the new vector $\vec{\xi}$ free. The presence of this new temporary variable $z \equiv \xi_{t+q}$ opens the possibility of a straightforward elimination of the vectors $\vec{\xi}$ as functions of the *finite* number of unknowns in $\vec{\zeta}$. Indeed, with an index j out of the interval $j = 1, 2, \ldots, t - 1$ we may abbreviate all the jth (i.e., leftmost) columns of our zero-order matrix $\mathcal{M}$ as respective vectors $\vec{\rho}^{\{j\}}$ distinguished by the braced superscript. We move them all to the right-hand side of equation (21). This will reduce the left-hand side matrix $\mathcal{M}$ (acting on a vector) to the mere triangular submatrix denoted as $\mathcal{Z}$ from now on (and acting on a subvector). After the above simple-minded replacement (44) giving

$$\mathcal{Z} \to \mathcal{Z}^* = \begin{pmatrix} d_0^{[t]*} & 0 & 0 & 0 & \ldots \\ d_1^{[t-1]} & d_1^{[t]*} & 0 & 0 & \ldots \\ d_2^{[t-2]} & d_2^{[t-1]} & d_2^{[t]*} & 0 & \ldots \\ & & \ldots & & \end{pmatrix}$$

we may re-write our fundamental equation (21) in the alternative, regularized form

$$\mathcal{Z}^* \begin{pmatrix} \xi_0 \\ \xi_1 \\ \xi_2 \\ \vdots \end{pmatrix} = \begin{pmatrix} \tau_0^{(k-1)} \\ \tau_1^{(k-1)} \\ \tau_2^{(k-1)} \\ \vdots \end{pmatrix} + \sum_{j=0}^{t} \zeta_j \begin{pmatrix} \rho_0^{\{j\}} \\ \rho_1^{\{j\}} \\ \rho_2^{\{j\}} \\ \vdots \end{pmatrix}. \tag{45}$$

The last column vector $\vec{\rho}^{\{t\}}$ on the right hand side is defined as the irregular, $(2t+q)$th column of $\mathcal{M}$ without asterisk. The D-dependent matrix

$$\mathcal{Z}^* = \begin{pmatrix} d_0^{[t]} & 0 & \dots & & & \\ d_1^{[t-1]} & \ddots & 0 & \dots & & \\ d_2^{[t-2]} & \ddots & d_{t+q-1}^{[t]} & 0 & \dots & \\ \vdots & \ddots & d_{t+q}^{[t-1]} & D & 0 & \dots \\ & \ddots & d_{t+q+1}^{[t-2]} & \ddots & d_{t+q+1}^{[t]} & \ddots \\ & & \vdots & \ddots & \ddots & \ddots \end{pmatrix}$$

is manifestly regular and invertible at any choice of $D > 0$. It defines the unique value of $z = z(D)$ as well as the rest of the left-hand-side vector

$$\begin{pmatrix} \xi_0 \\ \vdots \\ \xi_{t+q-1} \\ z \\ \xi_{t+q+1} \\ \vdots \end{pmatrix}.$$

Let us summarize: We have achieved a completely recurrent solvability of our infinite-dimensional equation (45). Indeed, its first row defines $\xi_0 = h_t^{(k)}$ etc. This is the key computational benefit of our new recipe. Of course, two auxiliary parameters (viz., D and z) were introduced so that the results carry more information than before. It easily follows from our construction that at any $D \neq 0$ our new equation remains *precisely* equivalent to its predecessor (21) *if and only if* the second variable z vanishes, $z = 0$. Let us now pay attention to this condition.

B. Reduction to a model space

As long as, by construction, $\det \mathcal{Z}^* \neq 0$, equation (45) could be solved by an immediate matrix inversion at an arbitrary t, D and z, $\vec{\xi} = (\mathcal{Z}^*)^{-1}\big(\vec{\tau}^{(k-1)} + \sum_{j=0}^{t} \vec{\rho}^{\{j\}}\big)$.

This would specify the infinite-dimensional left-hand side vector $\vec{\xi}$ as a finite sum,

$$\begin{pmatrix} \xi_0 \\ \xi_1 \\ \vdots \end{pmatrix} = \begin{pmatrix} \theta_0^{(k-1)} \\ \theta_1^{(k-1)} \\ \vdots \end{pmatrix} + \sum_{j=0}^{t} \zeta_j \begin{pmatrix} \eta_0^{\{j\}} \\ \eta_1^{\{j\}} \\ \vdots \end{pmatrix}. \tag{46}$$

Accepting this idea, we may even try to determine each of the right-hand side components separately. This would be a tremendous simplification of the algorithm since the last $t+1$ individual recurrences are order-independent,

$$\begin{pmatrix} d_0^{[t]*} & 0 & 0 & \dots \\ d_1^{[t-1]} & d_1^{[t]*} & 0 & \dots \\ & & \dots & \end{pmatrix} \begin{pmatrix} \eta_0^{\{j\}} \\ \eta_1^{\{j\}} \\ \vdots \end{pmatrix} = \begin{pmatrix} \rho_0^{\{j\}} \\ \rho_1^{\{j\}} \\ \vdots \end{pmatrix}, \quad j = 0, 1, \dots, t. \tag{47}$$

They just "reparametrize" a part of our zero-order Hamiltonian. Only the very first definition will vary with the order k,

$$\begin{pmatrix} d_0^{[t]*} & 0 & 0 & \dots \\ d_1^{[t-1]} & d_1^{[t]*} & 0 & \dots \\ & & \dots & \end{pmatrix} \begin{pmatrix} \theta_0^{(k-1)} \\ \theta_1^{(k-1)} \\ \vdots \end{pmatrix} = \begin{pmatrix} \tau_0^{(k-1)} \\ \tau_1^{(k-1)} \\ \vdots \end{pmatrix}. \tag{48}$$

Still, it depends neither on the unknown energy $E^{(k)}$ nor on the unknown coefficients $\vec{h}^{(k)}$. We may say that it "compactifies" the previous, known results $E^{(k-1)}$, $\vec{h}^{(k-1)}$, $E^{(k-2)}, \dots$, and "compresses" them into a new input vector $\vec{\theta}^{(k-1)} = (\mathcal{Z}^*)^{-1}\,\vec{\tau}^{(k-1)}$.

It remains for us to find the values of the $t+1$ unknown parameters ζ_j. For this purpose we return to the "forgotten" truncation conditions

$$\xi_{M+1} = \xi_{M+2} = \dots = \xi_{M+t} = 0. \tag{49}$$

In the present notation these requirements read

$$\begin{aligned} \theta_{M+1}^{(k-1)} + \sum_{j=0}^{t} \eta_{M+1}^{\{j\}} \zeta_j &= 0, \\ \theta_{M+2}^{(k-1)} + \sum_{j=0}^{t} \eta_{M+2}^{\{j\}} \zeta_j &= 0, \\ &\dots \\ \theta_{M+t}^{(k-1)} + \sum_{j=0}^{t} \eta_{M+t}^{\{j\}} \zeta_j &= 0, \end{aligned} \tag{50}$$

and suppress the variability of parameters $\vec{\zeta}$. By construction, all these equations still depend on our auxiliary and, generically, nonvanishing variable z. Vice versa, the va-

lidity condition $z = 0$ may only be re-introduced as an additional, explicit requirement $\xi_{t+q} = 0$, i.e., as the $(t+1)$-st equation

$$\theta^{(k-1)}_{t+q} + \sum_{j=0}^{t} \eta^{\{j\}}_{t+q} \zeta_j = 0. \tag{51}$$

The concatenated system (51) + (50) of $t+1$ conditions is our final model-space-like formula. It defines all the $t+1$ parameters collected in the array $\vec{\zeta}$.

At the correct value of energy (30) our auxiliary regularization variable z becomes identically equal to zero and the redundant equation (51) may be omitted. Our model-space-like boundary conditions then degenerate to the mere t equations (50).

C. Illustrations

In the real fixed-point arithmetics an accumulation of errors may make the numerical value of z (i.e., the right-hand side of equation (51)) still slightly different from zero. Nevertheless, as long as the components of the latter equation itself are all of the order $\mathcal{O}(D^{-1})$ for large $D \gg 1$ (cf. equation (54)) the errors accumulate in the product Dz rather than in the quantity z itself. The choice of a sufficiently large $D \to \infty$ settles the problem of errors.

C.1. $t = 1$

After we return to $t = 1$ for illustration, the last line of equation (28) will represent our $z = 0$ constraint (51). Similarly, the last line of equation (27) plays the role of the second constraint (50). Once we define the auxiliary two-column matrix η,

$$\vec{\eta}^{\{0\}} = (\mathcal{Z}^*)^{-1} \begin{pmatrix} \rho^{\{0\}}_0 \\ \rho^{\{0\}}_1 \\ \vdots \\ \rho^{\{0\}}_{q+1} \end{pmatrix}, \qquad \vec{\eta}^{\{1\}} = (\mathcal{Z}^*)^{-1} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ a_{q+2}(0) \\ c_{q+3}(0) \end{pmatrix}$$

the inverse matrix in the pair of equations (51) and (50) remains triangular,

$$\begin{pmatrix} -E^{(k)} \\ h^{(k)}_{q+2} \end{pmatrix} = \begin{pmatrix} \eta^{\{0\}}_{q+1} & 0 \\ \eta^{\{0\}}_{M+1} & \eta^{\{1\}}_{M+1} \end{pmatrix}^{-1} \begin{pmatrix} \theta^{(k-1)}_{q+1} \\ \theta^{(k-1)}_{M+1} \end{pmatrix}, \quad M \gg q \geqslant 0,\ t = 1. \tag{52}$$

This means that in any order k and at an arbitrary termination q and/or cut-off $M < \infty$ the definition of energies $E^{(k)}$ remains finite-dimensional.

C.2. $t = 2$

Above, we have already chosen $q = 1$ and $M = 6$ for illustration at $t = 2$. Here, this gives the triangular regularized submatrix $\mathcal{Z}^*$ which has the ordinary square-matrix form

$$\mathcal{Z}^* = \left(\begin{array}{ccc|c|ccc} d_0^{[2]} & 0 & 0 & 0 & 0 & 0 & 0 \\ d_1^{[1]} & d_1^{[2]} & 0 & 0 & 0 & 0 & 0 \\ a_2 & d_2^{[1]} & d_2^{[2]} & 0 & 0 & 0 & 0 \\ \hline c_3^{[1]} & a_3 & d_3^{[1]} & D & 0 & 0 & 0 \\ \hline c_4^{[2]} & c_4^{[1]} & a_4 & d_4^{[1]} & d_4^{[2]} & 0 & 0 \\ 0 & c_5^{[2]} & c_5^{[1]} & a_5 & d_5^{[1]} & d_5^{[2]\star} & 0 \\ 0 & 0 & c_6^{[2]} & c_6^{[1]} & a_6 & d_6^{[1]\star} & d_6^{[2]\star} \end{array}\right), \quad t = 2.$$

Its elements marked by the superscript* are in fact arbitrary but, wherever possible, we shall keep them strictly equal to their nonzero unmarked values. Such a convention (with $d_5^{[2]\star} = d_5^{[2]}$, $d_6^{[2]\star} = d_6^{[2]}$ and $d_6^{[1]\star} = d_6^{[1]}$) makes our construction less cut-off-dependent. Only the single element $d_3^{[2]\star} \equiv D \neq 0$ remains really indeterminate.

C.3. $D \approx 0$

Whenever the value of D vanishes in a "correct" limit $D \to 0$, matrix $\mathcal{Z}$ drops its asterisk and equation (21) acquires its non-recurrent, pseudo-inversion form,

$$\mathcal{Z}\left(\begin{array}{c} h_2^{(k)} \\ h_3^{(k)} \\ h_4^{(k)} \\ \hline 0 \\ \hline h_6^{(k)} \\ h_7^{(k)\star} \\ h_8^{(k)\star} \end{array}\right) = \left(\begin{array}{c} \tau_0^{(k-1)} \\ \tau_1^{(k-1)} \\ \tau_2^{(k-1)} \\ \hline \tau_3^{(k-1)} \\ \hline \tau_4^{(k-1)} \\ \tau_5^{(k-1)} \\ \tau_6^{(k-1)} \end{array}\right) + E^{(k)} \left(\begin{array}{c} \rho_0^{\{0\}} \\ \rho_1^{\{0\}} \\ \rho_2^{\{0\}} \\ \hline \rho_3^{\{0\}} \\ \hline 0 \\ 0 \\ 0 \end{array}\right) - h_1^{(k)} \left(\begin{array}{c} d_0^{[1]} \\ a_1 \\ c_2^{[1]} \\ \hline 0 \\ \hline 0 \\ 0 \\ 0 \end{array}\right) - h_5^{(k)} \left(\begin{array}{c} 0 \\ 0 \\ 0 \\ \hline 0 \\ \hline d_4^{[1]} \\ a_5 \\ c_6^{[1]} \end{array}\right). \qquad (53)$$

Step by step, it defines the "upper" coefficients $h_2^{(k)}$, $h_3^{(k)}$ and $h_4^{(k)}$ as functions of the energy *and* of another undetermined parameter $h_1^{(k)}$. Similarly, the first "lower" nonzero coefficient $h_6^{(k)}$ is specified as a quantity which depends on all the "upper" coefficients *plus* on a new parameter $h_5^{(k)}$. At the end, the correct values of our three unknown variables should be fixed by the "forgotten" fourth row and by the two truncation conditions $h_7^{(k)\star} = h_8^{(k)\star} = 0$.

C.4. $D \gg 1$

In the example (53), the regularization $\mathcal{Z}(D=0) \to \mathcal{Z}^*(D \neq 0)$ leads to the equivalent equation (45) if and only if the contributions proportional to z vanish, $z \to 0$. The situation remains virtually unchanged when we admit a growth of q. We may invert, in partitioned notation,

$$\left(\mathcal{Z}^*\right)^{-1} = \left(\begin{array}{c|c|c} \mathcal{Z}_1 & 0 & 0 \\ \hline u^{\mathrm{T}} & D & 0 \\ \hline \mathcal{Z}_3 & w & \mathcal{Z}_2 \end{array}\right)^{-1} = \left(\begin{array}{c|c|c} \mathcal{Z}_1^{-1} & 0 & 0 \\ \hline -D^{-1}u^{\mathrm{T}}\mathcal{Z}_1^{-1} & D^{-1} & 0 \\ \hline \mathcal{Z}_2^{-1}\mathcal{C}\mathcal{Z}_1^{-1} & -\mathcal{Z}_2^{-1}wD^{-1} & \mathcal{Z}_2^{-1} \end{array}\right) \tag{54}$$

(with $\mathcal{C} = -\mathcal{Z}_3 + D^{-1}wu^T$) and define the three order-independent and infinite-dimensional vectors

$$\left(\vec{\eta}^{\{0\}},\ \vec{\eta}^{\{1\}},\ \vec{\eta}^{\{2\}}\right) = \left(\mathcal{Z}^*\right)^{-1} \left[\begin{pmatrix} \rho_0^{\{0\}} \\ \vdots \\ \rho_{q+1}^{\{0\}} \\ \rho_{q+2}^{\{0\}} \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} d_0^{[1]} \\ \vdots \\ c_3^{[2]} \\ 0 \\ \vdots \\ \vdots \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ \vdots \\ \vdots \\ 0 \\ d_{q+3}^{[1]} \\ \vdots \\ c_{q+6}^{[2]} \end{pmatrix} \right]. \tag{55}$$

It is easy to show that the D-dependence of these components of the wavefunction corrections (cf. equations (45) and (54)) implies their linear z-dependence. We may choose $D \gg 1$ and get the small numerical span of $z = \mathcal{O}(D^{-1})$, i.e., only a small spuriosity in our tentative $z \neq 0$ wavefunctions, $h_j^{(k)}(z) = h_j^{(k)}(0) + \mathcal{O}(z)$. In the limit $D \to \infty$ we just return to the formulae studied above. Nevertheless, also any time *before* such a limiting transition, equations (51) and (50) define our last unknown parameters $\vec{\zeta}$ in terms of the vectors (55), via the three-dimensional matrix inversion

$$\begin{pmatrix} -E^{(k)} \\ h_1^{(k)} \\ h_{q+4}^{(k)} \end{pmatrix} = \begin{pmatrix} \eta_{q+2}^{\{0\}} & \eta_{q+2}^{\{1\}} & 0 \\ \eta_{M+1}^{\{0\}} & \eta_{M+1}^{\{1\}} & \eta_{M+1}^{\{2\}} \\ \eta_{M+2}^{\{0\}} & \eta_{M+2}^{\{1\}} & \eta_{M+2}^{\{2\}} \end{pmatrix}^{-1} \begin{pmatrix} \theta_{q+2}^{(k-1)} \\ \theta_{M+1}^{(k-1)} \\ \theta_{M+2}^{(k-1)} \end{pmatrix}, \quad M \gg q \geqslant 0. \tag{56}$$

The occurrence of a zero matrix element is a peculiarity of the scheme (cf. equation (55)).

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