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Harmonic oscillations in a quasi-relativistic regime

Miloslav Znojil†
Ústav jaderné fyziky AV ČR, 250 68 Řež, Czech Republic

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Abstract. A square-root anharmonic oscillator potential $V(r) = \sqrt{A + B\,r^2}$ is analysed as a model which simulates a quasi-relativistic squeezing of the harmonic oscillator spectrum. Several eligible (namely, perturbative, variational, Hill-determinant and Riccati–Padé) methods of construction of its bound states are compared.

1. Introduction

The elementary character of the energies $E_{n,\ell} = \hbar\omega\,(2n + \ell + \frac{3}{2}),\ n,\ \ell = 0, 1, \ldots$ of the exactly solvable linear harmonic oscillator (HO) Hamiltonian

$$H^{(\mathrm{HO})} = \frac{1}{2m}\,\boldsymbol{p}^2 + \frac{1}{2}m\omega^2\,\boldsymbol{r}^2$$

reflects its symmetries. Spectra of this type are often observed in experiments—at low energies, the HO model fits vibrational excitations of molecules as well as some low-lying energy levels in atomic nuclei. Recently, the HO system and, in particular, the equidistant form of its spectrum have again attracted attention (see [1]) in quantum control theory which, in the formulation of the review [2], represents 'a long sought-after dream' of 'steering wavepackets into desired states'.

In the latter context, as well as in more standard applications, deviations from the strict HO rule may remain small in a broad range of energies. The next, anharmonic oscillator (AHO) model

$$H^{(\mathrm{AHO})} = \frac{1}{2m}\boldsymbol{p}^2 + \frac{1}{2}m\omega^2\boldsymbol{r}^2 + h\boldsymbol{r}^4$$

addresses just this point [3]. Unfortunately, in the pragmatical experimental fits based on the anharmonic model $H^{(\mathrm{AHO})}$, a 'mathematically unacceptable' (namely, negative) value of the resulting asymptotically dominant coupling h may reflect a decrease in the distance between higher excitations. A different type of anharmonicity is then needed. In two-atomic systems, for example, s-wave vibrations are currently being fitted by the less easily tractable exponential Morse potential (see [4, p 182]) or by a suitable element of the so-called shape-invariant class of potentials (see, e.g., the review [5]).

Besides an alteration of interactions, a source of deformation of the HO-like spectrum might be sought in a modification of the dispersion law itself. The example

$$H^{(\mathrm{PHO})} = f\boldsymbol{p}^4 + \frac{1}{2m}\boldsymbol{p}^2 + \frac{1}{2}m\omega^2\boldsymbol{x}^2$$

† E-mail address: znojil@ujf.cas.cz

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(i.e. a momentum-space version of the anharmonic oscillator) is a realization of such a strategy. In the letter [6], we noticed that the component p^4 may facilitate numerical as well as analytic considerations. With the coefficient $f = -1/(8m^3c^2)$ where c denotes the velocity of light, it also acquires a natural kinematical (namely relativistic) physical interpretation.

In the present paper, encouraged by the latter observations, we shall try to make a next move and postulate $\boldsymbol{p}^2/2m \to T^{(\mathrm{relativistic})}(\boldsymbol{p}^2) = \sqrt{m^2c^4 + \boldsymbol{p}^2c^2} - m\,c^2$, i.e. a fully relativistic dispersion rule. For the sake of simplicity, we shall keep the HO interaction unchanged (the paper [7] may be consulted for discussion of the spatial corrections if needed) and define the quasi-relativistic harmonic oscillator (QHO) Hamiltonian

$$H^{(\mathrm{QHO})} = \sqrt{m^2c^4 + \boldsymbol{p}^2c^2} - m\,c^2 + \tfrac{1}{2}m\,\omega^2\boldsymbol{r}^2.$$

One encounters no particular conceptual difficulties: after the standard quantization replacement of $\boldsymbol{p}^2$ by the Laplace operator, the ensuing necessity of a mathematically rigorous specification of the square-rooted operator $T = T(\boldsymbol{p}^2)$ with $\boldsymbol{p}^2 = -\hbar^2\triangle_r$ would lead, in effect, to the formally correct relativistic Dirac equation. Real difficulties arise as a consequence of the unlimited asymptotic increase of the HO interaction: this makes its formal Dirac description virtually useless [8]. In a way inspired by the Fourier equivalence of the above-mentioned anharmonicities, $H^{(\mathrm{AHO})} \Longleftrightarrow H^{(\mathrm{PHO})}$, $\boldsymbol{r}^2 \Longleftrightarrow \boldsymbol{p}^2$, we shall instead study the dispersive Schrödinger equation itself.

In the momentum representation, i.e. with the 'quantized' coordinates $\boldsymbol{r}^2 = -\hbar^2\triangle_{\boldsymbol{p}}$, the partial-wave decomposition of $H^{(\mathrm{QHO})}$ leads to the second-order ordinary linear differential Schrödinger equation

$$\frac{1}{2}m\omega^2\hbar^2\left[-\frac{\mathrm{d}^2}{\mathrm{d}p^2} + \frac{\ell(\ell+1)}{p^2}\right]\psi_\ell(p) + [\sqrt{m^2c^4 + p^2c^2} - m\,c^2]\psi_\ell(p) = E_{n,\ell}\psi_\ell(p).$$

With the variable $p \in (0,\infty)$ and with the angular momenta $\ell = 0, 1, \ldots$, such a Fourier-transformed equation offers a unique non-polynomial anharmonicity stemming from the relativistic kinematics.

2. Methods

Our main purpose is a study of the QHO model in more detail. Preliminarily, let us rescale the variable p, $p \to x = \varrho p$, with $\varrho = m\hbar\omega$. In terms of a parameter $\lambda^2 = \hbar\omega/(m\,c^2) \ll 1$ and with the new energy $\varepsilon = 2E/(\hbar\omega)$, this enables us to rewrite the Schrödinger equation in a transparent form:

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\ell(\ell+1)}{x^2}\right]\psi(x) + \frac{2}{\lambda^2}\left(\sqrt{1+\lambda^2\,x^2}\ -1\right)\psi(x) = \varepsilon\psi(x). \tag{1}$$

On physical grounds, it must be complemented by the boundary conditions

$$\psi(x_0) \approx x_0^{\ell+1} \qquad |x_0| \ll 1 \tag{2}$$

$$\psi(x_\infty) \approx \exp(-\mu x_\infty^{3/2}) \qquad \mu = \frac{2\sqrt{2}}{3\sqrt{\lambda}} \qquad |x_\infty| \gg 1. \tag{3}$$

The bound states must be constructed numerically in general.

2.1. Wavefunctions in the Riccati representation

In accordance with standard monographs [9], our Schrödinger equation may be rewritten as a nonlinear Riccati equation for the ratio of functions $f(x) = -\psi'(x)/\psi(x)$. Via an ansatz

$$\psi(x) = \exp\left[-\int^x f(\tau)\,\mathrm{d}\tau\right] \tag{4}$$

we get

$$f'(x) - f^2(x) + \frac{\ell(\ell+1)}{x^2} - \varepsilon + \frac{2}{\lambda^2}\left(\sqrt{1+\lambda^2 x^2} - 1\right) = 0. \tag{5}$$

Provided the following expression holds near the origin:

$$\frac{2}{\lambda^2}\left[\sqrt{1+\lambda^2 x^2}\ -1\right] = x^2 - \frac{1}{4}\lambda^2 x^4 + \frac{1}{8}\lambda^4 x^6 - \frac{5}{64}\lambda^6 x^8 + \cdots \tag{6}$$

we may try to postulate

$$f(x) = \sum_{j=-1}^{\infty} F_j x^j \qquad x \approx 0. \tag{7}$$

On physical grounds, we have to pick up $F_{-1} = -\ell - 1$ (see equation (2)) while, after appropriate insertions, all the remaining coefficients are generated recursively:

$$(2\ell + 2k + 3)\,F_{2k+1} = \frac{2\,(2k-3)!!}{\lambda^2(2k)!!}(-\lambda^2)^k + \sum_{m=0}^{k-1} F_{2m+1}\,F_{2k-2m-1} \qquad k = 1,\ 2,\ \ldots$$

with trivial $F_{2k-2} = 0$, initial $F_1 = \varepsilon/(2\ell+3)$ and $(-1)!! = 1$.

In the strongly anharmonic regime, the large-x counterpart of (6) reads

$$\sqrt{1+\lambda^2 x^2} = \lambda\, x\,\sqrt{1 + 1/(\lambda^2 x^2)} = \lambda\, x + \frac{1}{2\lambda\, x} - \frac{1}{8\lambda^3 x^3} + \cdots \tag{8}$$

and inspires an alternative asymptotic ansatz for the Riccatian wavefunctions:

$$f(x) \sim \sum_{k=-1}^{\infty} G_k t^{-k} \qquad t = t(x) \equiv \sqrt{x} \gg 1. \tag{9}$$

With the asymptotically physical choice of $G_{-1} = \sqrt{2/\lambda} > 0$ (see equation (3)), this gives the second recurrent definition

$$2\sqrt{2/\lambda}\,G_{k+1} = \frac{2\,(-1)^{n+1}(2n-3)!!}{\lambda^{2n+1}(2n)!!}\,\delta_{k,4n-2} + \ell(\ell+1)\delta_{k,4} + (1-k/2)G_{k-2}$$

$$-\sum_{m=1}^{k-1} G_m\,G_{k-m} \qquad k = 2,\ 3,\ \ldots \quad n = 1,\ 2,\ \ldots$$

with zero $G_0 = 0$, initial $G_1 = -(\lambda^{-2}+\varepsilon/2)/\sqrt{2/\lambda}$ and non-zero $G_2 = \frac{1}{4}$. We may conclude that the formal algebraic construction of wavefunctions is complete: the integration in (4) remains trivial.

The basic practical difficulty with the Riccati-equation wavefunctions is related to the final implementation of 'missing' boundary conditions, i.e. to the asymptotic restriction (3) of the regular series (7) and/or to the threshold constraint (2) which must complement the asymptotic expansion (9).

The easiest solution of this problem may lie in its circumvention. We may shift the responsibility to an *ad hoc* variation of the energy ε. After all, the physical values of ε are numerical in most cases. Each deviation from their absolutely exact value (with infinitely

many significant digits in principle) will already imply a violation (however small) of the rigorous boundary conditions. In practice, therefore, the energies are often being determined by an independent (say, perturbative or variational) method.

2.2. The energy ε as an external parameter

The high-lying non-relativistic HO spectrum (the so-called Rydberg states) may become the object of methodically motivated attention, e.g. in quantum many-body theory [10]. In similar contexts, a perturbative form of relativity may acquire a straightforward relevance. In comparison, say, with the $H^{(\mathrm{PHO})}$ model, the structure of Hamiltonian $H^{(\mathrm{QHO})} = \sum_0^\infty \lambda^k H_k$ may induce new challenges, say, in connection with the rigorous analysis of convergence. Fortunately, we are only interested in the low-order perturbative tractability of (1) and, once we truncate the series (6), we may immediately write down the first-order perturbative result

$$\varepsilon(n,\ell) \approx \varepsilon_0 + \lambda^2\varepsilon_1 = 4n + 2\ell + 3 - \tfrac{1}{4}\lambda^2[6n^2 + (6\ell+9)n + (\ell+\tfrac{3}{2})(\ell+\tfrac{5}{2})].$$

The calculation of higher-order corrections is analogous.

In a variational setting, the same HO basis $|n,\ell\rangle,\ n,\ \ell = 0, 1, \ldots, \mathcal{N}$ may be employed non-perturbatively, in a dynamical regime with the larger λ's. Technically, one has only to evaluate matrix elements $\langle n,\ell|H^{(\mathrm{QHO})}|n',\ell\rangle$ and to diagonalize a finite submatrix of this array. It is worth noticing that the present example admits an explicit non-numerical evaluation of the input matrix elements in question,

$$\langle n,\ell|H^{(\mathrm{QHO})}|n',\ell\rangle = \sum_{m=0}^{n}\sum_{m'=0}^{n'} C_{m,m'}^{(n,n')} \int_0^\infty t^{m+m'+\ell+1/2}\,\mathrm{e}^{-t}\sqrt{1+\lambda^2 t}\;\mathrm{d}t.$$

Indeed, all the necessary integrations may be performed non-numerically, in terms of the at most $(n+n'+\ell)$th derivatives of the Bessel function

$$K_1(\frac{\tau}{2\lambda^2}) \equiv 2\,\lambda\,\tau\,\mathrm{e}^{-\tau/2\lambda^2}\int_0^\infty t^{1/2}\,\mathrm{e}^{-\tau\,t}\sqrt{1+\lambda^2 t} \tag{10}$$

with respect to the parameter τ and in the limit $\tau \to 1$ (see [11, equation 8.432.8]). Thus, nicely convergent standard expansions of the Bessel functions near zero (i.e. in the negative powers of λ) may be used. Moreover, due to the smooth character of the integrands, even direct numerical integration (e.g. via a Simpson or Chebyshev rule) would converge quickly.

In the s-wave setting and with the single trial state, $\mathcal{N} = 0$, the variational recipe approximates (or, more precisely, majorizes) the ground-state energy by the mean value of the Hamiltonian. The resulting estimate $\varepsilon \approx \langle 0,0|H^{(\mathrm{QHO})}|0,0\rangle \approx \varepsilon_0 + \tilde{\varepsilon}_1(\mathcal{K})$ may be re-interpreted as a quasi-perturbative prescription. With the explicit form of

$$\tilde{\varepsilon}_1(\mathcal{K}) = -\sum_{k=1}^{\mathcal{K}} \frac{(2k-1)!!(2k+3)!!}{(2k+2)!!}\left(-\frac{\lambda^2}{2}\right)^k \qquad \mathcal{K} > 1 \tag{11}$$

it provides a really useful estimate of energy (see table 1). At the 'sufficiently small' parameters λ (see table 1(a)), the approximation remains reliable as well as satisfactorily precise in a broad interval of the cut-offs $\mathcal{K}$.

In the light of this experience, it is rather disappointing to notice that the energies (11) diverge, in the limit $\mathcal{K} \to \infty$, at all the non-zero λ. Indeed, expansion (11) of the corresponding integral (10) coincides with the hypergeometric series ${}_2F_0(\frac{3}{2}, -\frac{1}{2}; -\lambda^2)$ which has a zero radius of convergence. In the present weakly anharmonic regime, this is just a mathematical peculiarity, pertaining to highly precise calculations. At the larger λ's, the asymptotic series character of our estimates (11) may lead to non-negligible practical

Table 1. The estimates of energies $\varepsilon \approx \langle 0,0|H^{(\mathrm{QHO})}|0,0\rangle \approx \varepsilon_0 + \tilde{\varepsilon}_1(\mathcal{K})$ from the truncated equation (11). (*a*) Satisfactory convergence at the 'sufficiently small' λ's. (*b*) The asymptotic series $\mathcal{K}$-dependence of the deviations $\triangle_\varepsilon \equiv \varepsilon(\mathcal{K}) - \varepsilon(\mathcal{K}-1)$.

(*a*)

$\mathcal{K}$	$\lambda = 1/5$	$\lambda = 1/10$	$\lambda = 1/20$	$\lambda = 1/100$
0	3.000 000 000	3.000 000 000	3.000 000 000	3.000 000 000
1	2.962 500 000	2.990 625 000	2.997 656 250	2.999 906 250
2	2.965 125 000	2.990 789 063	2.997 666 504	2.999 906 266
3	2.964 829 688	2.990 784 448	2.997 666 432	2.999 906 266
4	2.964 875 166	2.990 784 626	2.997 666 433	2.999 906 266
5	2.964 866 297	2.990 784 617	2.997 666 432	2.999 906 266
6	2.964 868 388	2.990 784 618	2.997 666 432	2.999 906 266
7	2.964 867 810	2.990 784 618	2.997 666 432	2.999 906 266
8	2.964 867 993	2.990 784 618	2.997 666 432	2.999 906 266
9	2.964 867 928	2.990 784 618	2.997 666 432	2.999 906 266
10	2.964 867 954	2.990 784 618	2.997 666 432	2.999 906 266
11	2.964 867 942	2.990 784 618	2.997 666 432	2.999 906 266
12	2.964 867 948	2.990 784 618	2.997 666 432	2.999 906 266

(*b*)

	$\lambda = 1/2$		$\lambda = 1/3$		$\lambda = 1/4$	
$\mathcal{K}$	ε	$10^2 \times \triangle_\varepsilon$	ε	$10^4 \times \triangle_\varepsilon$	ε	$10^6 \times \triangle_\varepsilon$
1	2.765 625	−23.0	2.895 833	−1000.0	2.941 406	−59 000.0
2	2.868 164	10.0	2.916 088	200.0	2.947 815	6400.0
3	2.796 066	−7.2	2.909 758	−63.0	2.946 688	−1100.0
4	2.865 460	6.9	2.912 466	27.0	2.946 959	270.0
5	2.780 886	−8.5	2.910 999	−15.0	2.946 877	−83.0
6	2.905 482	12.0	2.911 960	9.6	2.946 907	30.0
7	2.690 360	−22.0	2.911 223	−7.4	2.946 894	−13.0
8	3.116 123	43.0	2.911 871	6.5	2.946 901	6.5
9	2.166 139	−95.0	2.911 228	−6.4	2.946 897	−3.6
10	4.524 905	240.0	2.911 938	7.1	2.946 899	2.2
11	−1.924 846	−640.0	2.911 075	−8.6	2.946 898	−1.5
12	17.331 38	1900.0	2.912 219	11.0	2.946 899	1.1

Table 2. A sample of the numerically exact 'external parameters' ε [12].

$\lambda = 1/2$	Energy
1/20	2.997 662 446 44
1/10	2.990 722 782 32
1/5	2.963 985 441 93
1/4	2.944 904 992 29
1/3	2.906 136 368 92
1/2	2.809 786 321 34
2	1.932 334 342 01

computational difficulties (see table 1(*b*)). One must proceed more carefully, switching to an alternative method for an independent check of numerical predictions whenever necessary.

In accordance with the remark of an anonymous referee of this paper, the loss

of precision in table 1(b) may also cause a loss of the upper-bound character of the approximants (11). For illustration, the referee employed a direct numerical integration of our ordinary differential Schrödinger equation and produced a small sample of the numerically exact values of the energies. With his kind permission, let us recall his results (table 2) to see that the explicit loss-of-boundedness really takes place here at the 'large' $\lambda = \frac{1}{2}$. Of course, the phenomenon may emerge at any λ, being curable, in accordance with the second referee's remark, by a Padé-type resummation technique and/or, as already mentioned, by an immediate numerical integration in (10).

2.3. Transition to a finite interval

During the study of wavefunctions, one discovers an important obstacle of applicability of the power series method to our particular potential $V^{(A,B)}(x) = \sqrt{A + B\,x^2}$. The radius of convergence of all the expansions proves finite, limited by the presence of a square-root singularity in the complex plane (at all $x = x_0$ such that $A + B\,x_0^2 = 0$, i.e. $x_0 = \pm \mathrm{i}/\lambda$). Several ways of dealing with similar situations exist.

For the sake of simplicity, let us return, for the time being, from the nonlinear Riccati equation to its ordinary linear predecessor (1). In accordance with [13], the most natural treatment of the singularity problem lies, definitely, in a suitable change of variables in our differential Schrödinger equation. We may map the semi-infinite interval of momentum coordinates x upon a finite interval of variables

$$v = v(x) = \frac{1}{\sqrt{1 + \lambda^2\,x^2}} \in (0,\ 1) \tag{12}$$

or, better, of the coordinates $s = s(x) = 1 - v(x) \in (0,\ 1)$ such that $s(0) = 0$ and $s(\infty) = 1$. This moves the complex singularity of the potential out of the interior of the expected circle of convergence ($s(\pm \mathrm{i}/\lambda) \to \infty$). For the rescaled wavefunctions

$$\psi(x) \equiv v(x)^{\rho}[1 - v^2(x)]^{\nu}\,\varphi[1 - v(x)] \qquad \rho = -1 \quad \nu = -\tfrac{1}{4} \tag{13}$$

our differential Schrödinger equation (1) acquires the following new form:

$$-\frac{\mathrm{d}^2}{\mathrm{d}s^2}\varphi(s) + [W(s) - \eta]\,\varphi(s) = 0 \qquad s \in (0,\ 1). \tag{14}$$

In the compactified interval, the interaction becomes more complicated:

$$W(s) - \eta = \frac{2\,\lambda^{-4}\,(2 - s)^{-1}}{s(1 - s)^5} - \frac{(2\,\lambda^{-4} + \varepsilon\,\lambda^{-2})\,(2 - s)^{-1}}{s(1 - s)^4}$$
$$+ \frac{\ell(\ell + 1)(2 - s)^{-2}}{s^2(1 - s)^2} - \frac{3\,(2 - s)^{-2}}{4\,s^2} - \frac{3\,(2 - s)^{-1}}{4\,s}. \tag{15}$$

Nevertheless, the absence of singularities within the discs $|s| \leqslant 1$ and $|v| \leqslant 1$ may be expected to mediate or accelerate numerical convergence.

Near the origin ($s \approx 0$), the switch from the half-axis $x \in (0, \infty)$ to the compact interval $s \in (0, 1)$ still leaves the leading-order contributions reasonably transparent:

$$W(s) - \eta = \left(-\frac{3}{16} + \frac{l\,(l + 1)}{4}\right) x^{-2} + \mathrm{O}(x^{-1}).$$

As a consequence, we may easily specify an 'effective' angular momentum and postulate a general representation of wavefunctions

$$\varphi(s) = \mathrm{e}^{\xi(s)} \sum_{n=0}^{\infty} s^{n+\ell/2+3/4} h_n. \tag{16}$$

Such a replacement of coordinates $s \in (0, 1)$ by integers $n = 0, 1, \ldots$ and the related Fourier-like discrete 'change of representation' $\varphi(s) \to h(n)$ ($\equiv h_n$) will guarantee the required regularity of wavefunctions near the origin (see equation (2)). The auxiliary asymptotic regularization exponent $\xi(s)$ remains virtually arbitrary.

Marginally, it is worth noticing that a systematic and consequent optimalization of the Riccati-related 'asymptotics' $\xi(s)$ might proceed in full analogy with our previous considerations. Its basic ingredient would lie in an asymptotic re-arrangement of the interaction

$$W(1-v)-\eta = \frac{2}{\lambda^4}v^{-5} + \left(-\frac{\varepsilon}{\lambda^2} - \frac{2}{\lambda^4}\right)v^{-4} + \frac{2}{\lambda^4}v^{-3} + \left(l\,(l+1) - \frac{\varepsilon\lambda^2+2}{\lambda^4}\right)v^{-2} + \frac{2}{\lambda^4}v^{-1} - \frac{3}{2} - \frac{\varepsilon\lambda^2+2}{\lambda^4} + 2\,l\,(l+1) + \mathrm{O}(v)$$

via a Jost-solution [14] counterpart to our above transformation (16). This will not be done here; for the sake of brevity, we shall only work with the elementary convergence factor $\xi(s) = 1/(s-1)$.

A computer symbolic-manipulation language (e.g. MAPLE [15]) may be recommended to facilitate the algebra. It enables us to expand $W(s)$ in the (fairly complicated) Taylor series

$$W(s)-\eta = \left(-\frac{3}{16} + \frac{l\,(l+1)}{4}\right)s^{-2} + \left(-\frac{9}{16} - \frac{\varepsilon}{2\,\lambda^2} + \frac{3\,l\,(l+1)}{4}\right)s^{-1} + \frac{23\,l\,(l+1)}{16} - \frac{21}{64} - \frac{9\,\varepsilon}{4\,\lambda^2} + \frac{1}{\lambda^4} + \left(-\frac{3}{16} + \frac{31}{4\,\lambda^4} + \frac{9\,l\,(l+1)}{4} - \frac{5\,\varepsilon}{\lambda^2} - \frac{9\,\varepsilon\lambda^2+18}{8\,\lambda^4}\right)s + \left(\frac{191}{8\,\lambda^4} - \frac{49\,\varepsilon\lambda^2+98}{16\,\lambda^4} - \frac{10\,\varepsilon}{\lambda^2} + \frac{201\,l\,(l+1)}{64} - \frac{27}{256}\right)s^2 + \left(\frac{911}{16\,\lambda^4} - \frac{15}{256} - \frac{209\,\varepsilon\lambda^2+418}{32\,\lambda^2} - \frac{35\,\varepsilon}{2\,\lambda^2} + \frac{261\,l\,(l+1)}{64}\right)s^3 + \left(\frac{1291\,l\,(l+1)}{256} - \frac{33}{1024} + \frac{3711}{32\,\lambda^4} - \frac{769\,\varepsilon\,\lambda+1538}{64\,\lambda^4} - \frac{28\,\varepsilon}{\lambda^2}\right)s^4 + \mathrm{O}(s^5)$$

and to insert this expansion and wavefunctions (16) in the Schrödinger equation (14). A discrete difference-equation equivalent of the original differential equation is obtained. In symbolic notation, it may be rewritten as recurrences or in a quasi-matrix form as

$$\begin{pmatrix} Q_{00} & Q_{01} & 0 & \cdots & \\ Q_{10} & Q_{11} & Q_{12} & 0 & \cdots \\ & & \cdots & & \end{pmatrix}\begin{pmatrix} h_0 \\ h_1 \\ \cdots \end{pmatrix} = 0 \tag{17}$$

with an unspecified truncation. The quasi-Hamiltonian Q is a Hessenberg matrix, $Q_{i,i+2} = Q_{i,i+3} = \cdots = 0$. As a consequence, we may generate all the solutions, step by step, in a compact form

$$h_1 = \frac{h_0}{(-Q_{01})}Q_{00}, \qquad h_2 = \frac{h_0}{(-Q_{01})(-Q_{12})}\det\begin{pmatrix} Q_{00} & Q_{01} \\ Q_{10} & Q_{11} \end{pmatrix}, \ldots,$$

$$h_n = \frac{h_0}{(-Q_{01})(-Q_{12})\cdots(-Q_{n-1n})}\det\begin{pmatrix} Q_{00} & Q_{01} & 0 & \cdots & \\ Q_{10} & Q_{11} & Q_{12} & 0 & \cdots \\ & & \cdots & & \\ Q_{n-10} & Q_{n-11} & \cdots & & Q_{n-1n-1} \end{pmatrix}. \tag{18}$$

We must underline that, unexpectedly, the discrete Hessenberg–Schrödinger equation (18) is exactly solvable. This is its main merit. At the same time, the energies ε keep playing the same external-parameter role as above.

3. Numerical tests

3.1. The Hill determinant method

In the spirit of the so-called Hill determinant method [16, 17], equation (17) may be understood as an approximate finite-dimensional (i.e. square-matrix) linear algebraic system of equations. In accordance with the available theory [18] and under certain very non-trivial constraints (see, e.g., [19]), such a quasi-variational conjecture may often be made rigorous and, hence, provide a correct definition of the physical values of energies.

Computationally, the Hill-determinant method does not necessarily prove to be too efficient [18, 20]. Nevertheless, the recipe is quite robust [21] and intuitively appealing. It generates the approximate spectrum as a set of roots of the not-too-complicated secular equation

$$\det Q = 0. \tag{19}$$

The construction is non-variational and must rely on a strict mathematical analysis. Basically, it must be shown that the old asymptotic boundary condition (3) (i.e. the condition $\varphi(1) = 0$ in the new notation) is equivalent to the new condition (19). The rigorous proof of such an equivalence is usually not difficult; its technical basis may be found in [18, 19].

After pre-multiplying the original differential equation (14) by a factor $(1-s)^5(2-s)^2$ from the left, we obtain an alternative, 'tilded' quasi-Hamiltonian $\tilde{Q}$ which possesses a band-matrix Hessenberg structure with just eight non-zero diagonals, $Q_{i+7,i} = Q_{i+8,i} = \cdots = 0$. Moreover, its s-wave and, say, $\lambda = 2$ example

$$\tilde{Q} = \begin{pmatrix} -15+2\varepsilon & 24 & 0 & \cdots & \\ 121-12\varepsilon & -764+8\varepsilon & 320 & 0 & \cdots \\ 372+16\varepsilon & 8388-48\varepsilon & -8944+32\varepsilon & \cdots & \\ -3120 & -21\,976+32\varepsilon & 48\,200-96\varepsilon & \cdots & \\ & & \cdots & & \end{pmatrix} \tag{20}$$

illustrates that the energy dependence in $\tilde{Q}$ involves just three central diagonals. By direct computation in MAPLE, we have verified that numerical instabilities do not play any significant role, at the smallest dimensions N at least—the tilded eigenvalues precisely coincide with their untilded predecessors (as they must). The computation was extremely quick—an increase of precision seems to be routine work. A few specific hints for optional algebraic acceleration of convergence may be found elsewhere [17, 18, 22].

A sample of computed roots is offered here in table 3. At the smallest dimensions, this test shows that not all of the Hill-determinant roots remain real [20]. An onset of convergence is clearly manifest, but, as already mentioned, larger dimensions and/or improved $\xi(s)$'s would be necessary for us to reach the domain of more satisfactory numerical precision. The latter point must be emphasized, in particular, in an analysis and calculations of excited states: We may see that, e.g., the $n = 1$ state at $\lambda = 2$ only too slowly converges to the exact $\varepsilon = 3.653\,391\,008\,68$ [12].

Table 3. The first two energy levels $\varepsilon = \varepsilon_{n,\ell}(\lambda)$ in the Hill-determinant approach.

	$\ell = 0$						$\ell = 1$	
	$\lambda = 1/5$		$\lambda = 1/2$		$\lambda = 2$		$\lambda = 1/2$	
N	$n = 0$	$n = 1$	$n = 0$	$n = 1$	$n = 0$	$n = 1$	$n = 0$	$n = 1$
2	—	—	—	—	6.842	78.158	2.729	7.333
3	0.665	—	14.016	—	5.452	47.580	21.668	—
4	—	—	7.653	32.337	4.588	34.385	12.946	43.817
5	1.688	—	2.868	20.100	4.009	26.958	8.569	28.045
6	—	—	2.609	14.174	3.597	22.196	4.690	20.328
7	3.696	3.785	2.621	10.376	3.291	18.886	4.193	15.592
8	2.821	16.836	2.705	7.000	3.055	16.456	4.157	12.216
9	2.952	5.809	2.788	5.408	2.870	14.599	4.268	9.311
10	2.986	5.574	2.835	5.090	2.721	13.136	4.443	7.055

3.2. The Riccati–Padé method

In comparison with Hill determinants, a slighlty more complicated direct Padé [23] matching of Riccati solutions may be expected to be much more efficient. The basic idea of such a methodically consistent determination of energies [24–26] lies in the use of a two-point Padé interpolation between the pair of expansions of $f(x)$ near $x = 0$ and near $x \to \infty$. In this formalism, the information carried by the respective threshold and asymptotic expansions is being compressed into a single Padé approximant. In the present example, we may assume that

$$f(x) \approx f^{[N]}[x(t)] = \frac{a_0 + a_1 t + a_2 t^2 + \cdots + a_{N+1} t^{N+1}}{b_2 t^2 + b_3 t^3 + \cdots + b_N t^N} \qquad t = \sqrt{x} \tag{21}$$

where $b_2 \neq 0 \neq a_0$ due to the required behaviour of $f[x(t)]$ near $t = 0$ while, *mutatis mutandis*, we have $b_N \neq 0 \neq a_{N+1}$ due to analogous restrictions near infinity.

The step-by-step comparisons of the separate powers of t near the threshold

$$\begin{aligned} a_0 + a_1 t + a_2 t^2 + \cdots + a_{N+1} t^{N+1} &= (b_2 + b_3 t + \cdots + b_N t^{N-2})[F_{-1} + F_1 t^4 + F_3 t^8 + \cdots \\ &\quad + F_{2K+1} t^{4K+4} + \mathrm{O}(t^{4K+8})] \end{aligned} \tag{22}$$

and near infinity

$$\begin{aligned} a_0 t^J + a_1 t^{J+1} + \cdots + a_{N+1} r^{J+N+1} &= (b_2 t^2 + b_3 t^3 + \cdots + b_N t^N)[G_{-1} t^{J+1} + G_1 t^{J-1} + G_2 t^{J-2} + \cdots \\ &\quad + G_J + \mathrm{O}(1/t)] \end{aligned} \tag{23}$$

may be rewritten as a set of the $4K + 8$ algebraic equations

$$\begin{aligned} &a_0 = F_{-1} b_2, \qquad a_1 = F_{-1} b_3, \ \ldots \ , a_3 = F_{-1} b_5, \\ &a_4 = F_{-1} b_6 + F_1 b_2, \ \ldots \\ &\ldots \\ &a_{4K+4} = F_{-1} b_{4K+6} + F_1 b_{4K+2} + \cdots + F_{2K+1} b_2, \ \ldots \\ &a_{4K+7} = F_{-1} b_{4K+9} + F_1 b_{4K+5} + \cdots + F_{2K+1} b_5 \end{aligned} \tag{24}$$

with $a_{N+2} = a_{N+3} = \cdots = 0$ and $b_{N+1} = b_{N+2} = \cdots = 0$, complemented by the $J+2$ relations

$$\begin{aligned} a_{N+1} &= G_{-1} b_N \\ a_N &= G_0 b_N + + G_{-1} b_{N-1} \\ &\vdots \\ a_{N-J} &= G_J\, b_N + G_{J-1} b_{N-1} + \cdots + G_{-1} b_{N-J-1} \end{aligned} \tag{25}$$

with $a_{-1} = a_{-2} = \cdots = 0$ and $b_1 = b_0 = b_{-1} = \cdots = 0$ plus, incidentally, $G_0 = 0$. After a normalization, say, $b_2 = 1$, we could specify all the $2N$ Padé coefficients via the latter two sets of conditions, provided only that $2N = 4K + 8 + J + 2$. Nevertheless, in accordance with the Riccati–Padé matching prescription of [24–26], we must also define the pertaining bound state energy and fix $2N+1$ parameters. Thus, we have to put $2N+1 = 4K+8+J+2$ and the integer J must be odd, $J = 2L + 1$, giving the Padé superscript $N = 2K + L + 5$.

For small L, we employ all the $2L + 3$ rows of the second set (25) as a mere definition of the left-hand-side a's in terms of the right-hand-side b's. In the first set (24), similarly, the first $2K - L + 4$ rows define the remaining a's. The rest of (24) forms a homogeneous linear equation which defines the b's:

$$(\mathcal{M}^{(F)} + \mathcal{M}^{(G)}) \begin{pmatrix} b_2 \\ b_3 \\ \vdots \\ b_N \end{pmatrix} = 0. \tag{26}$$

It has a simple $(2K + L + 4)$-dimensional matrix structure with the Töplitz (i.e. constant-diagonal) matrices $\mathcal{M}^{(F)}$ and $\mathcal{M}^{(G)}$. They are sparse: their non-zero elements are $\mathcal{M}^{(F)}_{2K+L+4,4+4j} = \mathcal{M}^{(F)}_{2K+L+3,3+4j} = \cdots = F_{2K+1-2j}$, $j = 0, 1, \ldots, K+1$ and $\mathcal{M}^{(G)}_{1,2K-L+2+i} = \mathcal{M}^{(G)}_{2,2K-L+3+i} = \cdots = G_{-1+i}$, $i = 0, 2, 3, \ldots, 2L+2$. With the use of the recursively specified matrix elements, the unknown energies ε may finally be computed as roots of the pertaining Töplitz-determinant secular equation

$$\det(\mathcal{M}^{(F)} + \mathcal{M}^{(G)})(\varepsilon) = 0. \tag{27}$$

Table 4. The interpolative Töplitz-determinant results ($K = 3$, $L = 1$).

λ	Lower bound	Ambiguity interval: eligible roots			Upper bound
1/2	2.015 497 482	2.815 969 135	2.827 091 751	2.846 464 154	8.088 381 579
1/3	2.551 846 250	2.906 984 688	2.908 118 779	2.909 505 823	7.525 268 269
1/4	2.743 918 171	2.945 086 629	2.945 299 792	2.945 528 177	7.305 961 115
1/5	2.834 598 527	2.964 037 724	2.964 095 041	2.964 152 718	7.199 301 467
1/10	2.958 044 622	2.990 723 717	2.990 724 643	2.990 725 500	7.051 102 755
1/20	2.989 468 027	2.997 662 462	2.997 662 476	2.997 662 489	7.012 861 455

Their numerical sample is displayed in tables 4–6. In detail, table 4 illustrates the efficiency of the method. For a broad spectrum of λ's, the 11-dimensional Töplitz determinants already offer very satisfactory precision. The typical feature of the method, namely, an ambiguity of the eligible physical roots, is well documented. A comparatively large gap separates them from the clearly unphysical solutions. At a fixed dimension, on the other hand, their

Table 5. The results for negative L.

	Truncations			Energy roots		
λ	L	K	N	Lower	Correct	Upper
1/5	−2	3	8	2.834 598 527	2.964 037 724	7.199 301 467
	−1	3	9	2.834 598 527	2.964 037 724	7.199 301 467
	−2	5	12	2.963 639 029	2.963 985 588	3.551 237 591
	−1	5	13	2.963 639 029	2.963 985 588	3.551 237 591
1/10	−2	3	8	2.958 044 622	2.990 723 717	7.051 102 755
	−1	3	9	2.958 044 622	2.990 723 717	7.051 102 755
	−2	5	12	2.990 717 361	2.990 722 783	3.073 985 738
	−1	5	13	2.990 717 361	2.990 722 783	3.073 985 738

Table 6. The extrapolative Töplitz-determinant example. (*a*) The ground-state roots: $0 < \varepsilon \leqslant 6$. (*b*) The first excited state: $6 < \varepsilon \leqslant 10$.

(*a*)

λ	K	ε				
1/5	3				2.964 13	
	5		1.55	2.962 935	2.963 985 72	
	7			2.963 982 7	2.963 985 443	2.969 02
	9	1.66	2.943	2.963 985 429	2.963 985 442	2.964 002
1/10	3				2.990 725 2	
	5		1.55	2.990 708 7	2.990 722 783	
	7			2.990 722 779	2.990 722 782	2.990 773
	9	1.62	2.990 580	2.990 722 782	2.990 722 782	2.990 722 796

(*b*)

λ	K	ε		
1/5	5		6.828 7	
	7	6.785	6.824 982 9	
	9	6.824 815	6.824 971 199	7.16
1/10	5		6.954 022	
	7	6.953 49	6.953 963 780	
	9	6.953 963 609	6.953 963 765	6.956 2

mutual small differences just set, in a way, an upper bound upon their common numerical precision.

Table 5 samples the effect of a change of dimension at the smallest non-trivial L's. Via comparison of it with table 4, we may notice a rigorous coincidence of certain roots at different N's (e.g., at $N = 8$ and $N = 11$ or at $N = 12$ and $N = 13$), an artefact of the sparse structure of the Q's. Simultaneously, during the growth of dimension $N \to N+4$, an emergence of new roots increases the ambiguity in our choice of the best approximant [25].

In a way parallelling the older experience with the Riccati–Padé method [24], we may extrapolate the validity of (27) to its $\mathcal{M}^{(G)} \equiv 0$ extremum. Table 6 shows that the resulting 'extrapolative' algorithm still keeps working. An apparent paradox (the strict equation (3) appears to be violated) has the following explanation. Almost always (i.e. up to a set of

measure zero), the very assumption (21) represents a weaker constraint

$$\psi(x_\infty) \neq \exp(+\mu x_\infty^{3/2}) \qquad \mu = \frac{2\sqrt{2}}{3\sqrt{\lambda}} \qquad |x_\infty| \gg 1 \tag{28}$$

which, by itself, still suffices for suppression of the undesirable and unphysical asymptotic growth of the physical wavefunctions.

An unexpected and specific byproduct of the elimination of $\mathcal{M}^{(G)}$ lies in a decoupling of elements in $\mathcal{M}^{(G)}$. We get much smaller dimensions of the Töplitz determinants, $N^{(\mathrm{dim.})} = (K+3)/2$. In the extrapolated '$L = -3$' case, we also get rid of the degeneracy of roots which reflected the sparse structure of Q's at $L \geqslant -2$. The overall number n_r of the (in general, complex) energy roots drops to a mere $n_r = N^{(\mathrm{dim.})}(N^{(\mathrm{dim.})} - 1)$. As a consequence, good precision may already be achieved at the smallest dimensions. Thus, in table 6, with $N^{(\mathrm{dim.})} \leqslant 6$, a reliable approximation is obtained for the ground as well as the first excited states. Table 6 provides complete agreement with the numerical integration (table 2) and it also nicely illustrates the empirical rule of selecting the best approximants as roots with the weakest $N^{(\mathrm{dim.})}$-dependence [25].

4. Summary

The popularity of the quartic anharmonic oscillator is supported not only by its simplicity and phenomenological appeal but also by its methodical importance in numerical computations and perturbation theory. Our present 'next-step' model $V^{(A,B)}(x) = \sqrt{A + B\,x^2}$ seems similarly inspiring. It introduces a complicated Hamiltonian operator $H = \sum_0^\infty \lambda^k\, H_k$ in perturbation theory and exemplifies a 'minimal breakdown of analyticity' (namely a square-root-type complex-plane singularity at $x = \pm \mathrm{i}/\lambda$) for analytic considerations.

Of course, the appeal of our potential $V^{(A,B)}$ may transcend its 'minimal relativity' and/or perturbative origin. Even at the low, fully non-relativistic energies and in the standard coordinate representation, a transition from the 'parabolic' HO well to the present 'hyperbolic' shape $V^{(A,B)}(r)$ (with arbitrarily large coupling constants A and B) may prove phenomenologically useful and methodically challenging. In the physical context one might find an independent use of $V^{(A,B)}(r)$ in QCD: notice that its broadly accepted [27] linear asymptotics $V^{(A,B)}(r) \approx r \times \sqrt{B},\ r \gg 1$ are smoothly combined with the common HO limit $V^{(A,B)}(r) \approx A' + B' r^2,\ r \approx 0$. In nuclear physics, the 'minimally relativistic' compression of energies might find applications in intermediate-energy simulations [28], etc.

In our methodically oriented paper, we have emphasized that the QHO model exhibits the lowest-order perturbative as well as purely numerical good behaviour and 'smoothness'. At the same time, several important questions remain open. First of all, one would like to see genuine more- and many-particle generalizations of our elementary combination of the kinetic 'minimal relativity' with the standard solvable spatial interaction. The significant simplification of technicalities (namely the Schrödinger equation in place of the Dirac equation) also deserve a further detailed study: beyond the present one-body case, the extremely user-friendly PC implementation of the symbolic manipulation language MAPLE could easily reach its natural (both memory- and time-related) limitations.

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