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Harmonic oscillations in a quasi-relativistic regime

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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 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

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

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

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

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

addresses just this point [3]. Unfortunately, in the pragmatical experimental fits based on the anharmonic model $H^{(AHO)}$, a "mathematically unacceptable" (namely, negative) value of the resulting asymptotically dominant coupling h may reflect a decrease of 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 (cf. [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

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

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

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

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

One encounters no particular conceptual difficulties – after the standard quantization replacement of $\vec{p}^2$ by the Laplace operator, the ensuing necessity of a mathematically rigorous specification of the square-rooted operator $T = T(\vec{p}^2)$ with $\vec{p}^2 = -\hbar^2\triangle_{\vec{r}}$ 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, $H^{(AHO)} \Longleftrightarrow H^{(PHO)}$, $\vec{r}^2 \Longleftrightarrow \vec{p}^2$, we shall study, instead, the dispersive Schrödinger equation itself.

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

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

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 as stemming from the relativistic kinematics.

2 Methods

Our main purpose is a study of the QHO model in more detail. Preliminarily, let us re-scale 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 re-write 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 accord with standard monographs [9], our Schrödinger equation may be re-written as a nonlinear Riccati equation for the ratio of functions $f(x) = -\psi'(x)/\psi(x)$. Via an Ansatz

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

we get

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

As long as, near the origin,

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

we may try to postulate

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

On physical grounds, we have to pick up $F_{-1} = -\ell - 1$ (cf. (2)) while, after appropriate insertions, all the further coefficients become 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 eq. (6) reads

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

and inspires an alternative asymptotic Ansatz for 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 $G_{-1} = \sqrt{2/\lambda} > 0$ (cf. (3)), this gives the second recurrent definition,

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

$$k = 2, 3, \dots, \qquad n = 1, 2, \dots$$

with zero $G_0 = 0$, initial $G_1 = -(\lambda^{-2} + \varepsilon/2)/\sqrt{2/\lambda}$ and nonzero $G_2 = 1/4$. We may conclude that the formal algebraic construction of wavefunctions is completed: The integration in eq. (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 – however small – violation of the rigorous boundary conditions. In practice, therefore, the energies are often being determined by an independent (say, perturbative or variational) method.

2.2 Energy ε as an external parameter

The high-lying nonrelativistic HO spectrum (so called Rydberg states) may become a target of a methodically motivated attention, e.g., in quantum many-body theory

[10]. In similar contexts, a perturbative form of relativity may acquire a straight relevance. In comparison, say, with the $H^{(PHO)}$ model, the structure of Hamiltonian $H^{(QHO)} = \sum_0^\infty \lambda^k H_k$ 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 eq. (1) and, once we truncate series (6), we may immediately write down the first-order perturbative result,

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

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 $\langle n,\ell|H^{(QHO)}|n',\ell\rangle$ 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,

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

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

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

with respect to the parameter τ and in the limit $\tau \to 1$ (cf. formula 8.432.8 in ref. [11]). 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 a smooth character of the integrands, even the 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 $\varepsilon \approx \langle 0,0|H^{(QHO)}|0,0\rangle \approx \varepsilon_0 + \tilde{\varepsilon}_1(\mathcal{K})$ may be re-interpreted as a quasi-perturbative prescription. With the explicit form of

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

it provides a really useful estimate of energy (cf. Table 1). At the "sufficiently small" parameters λ (cf. Table 1a), 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 a little bit disappointing to notice that the energies (11) diverge, in the limit $\mathcal{K} \to \infty$, at all the nonzero λ. Indeed, expansion (11) of the corresponding integral (10) coincides with the hypergeometric series ${}_2F_0(3/2, -1/2; -\lambda^2)$ 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 the non-negligible practical computational difficulties (cf. Table 1b). One must proceed more carefully, switching to an alternative method for an independent check of numerical predictions whenever necessary.

In accord with the remark of an anonymous referee of this paper, the loss of precision in Table 1b 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" $\lambda = 1/2$. Of course, the phenomenon may emerge at any λ, being curable, in accord with the second referee's remark, by a Padé-type re-summation 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., $x_0 = \pm i/\lambda$). There exist several ways how to deal with similar situations.

For the sake of simplicity, let us return, for the time being, from the nonlinear

Riccati equation to its ordinary linear predecessor (1). In accord with ref. [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 ($s(\pm i/\lambda) \to \infty$). For the re-scaled wavefunctions

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

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,

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

$$+\frac{\ell(\ell+1)(2-s)^{-2}}{s^2(1-s)^2} - \frac{3\,(2-s)^{-2}}{4\,s^2} - \frac{3\,(2-s)^{-1}}{4\,s}.$$

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

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

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 (cf. eq. (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,

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

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,

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

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 a symbolic notation, it may be re-written as recurrences or in a quasi-matrix form

$$\left(\begin{array}{cccccc} Q_{00} & Q_{01} & 0 & \ldots & & \\ Q_{10} & Q_{11} & Q_{12} & 0 & \ldots & \\ & & \ldots & & & \end{array}\right)\left(\begin{array}{c} h_0 \\ h_1 \\ \ldots \end{array}\right) = 0 \qquad (17)$$

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

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

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

We must underline that, unexpectedly, the discrete Hessenberg-Schrödinger equation (18) is solved exactly. This is its main merit. At the same time, 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 approximative finite-dimensional (i.e., square-matrix) linear algebraic system of equations. In accord with the available theory [18] and under certain very nontrivial constraints (cf., 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 need not necessarily prove 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., 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 the quoted literature [18, 19].

After we pre-multiply the original differential eq. (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 nonzero diagonals, $Q_{i+7,i} = Q_{i+8,i} = \ldots = 0$. Moreover, its s-wave and, say, $\lambda = 2$ example

$$\tilde{Q} = \left(\begin{array}{ccccc} -15+2\varepsilon & 24 & 0 & \ldots & \\ 121-12\varepsilon & -764+8\varepsilon & 320 & 0 & \ldots \\ 372+16\varepsilon & 8388-48\varepsilon & -8944+32\varepsilon & \ldots & \\ -3120 & -21976+32\varepsilon & 48200-96\varepsilon & \ldots & \\ & & \ldots & & \end{array} \right) \qquad (20)$$

illustrates that the energy dependence in $\tilde{Q}$ involves just three central diagonals. By the direct computations 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 a routine work. A few specific hints for an 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 manifested but, as already mentioned, larger dimensions and/or improved $\xi(s)$'s would be necessary for us to reach the domain of a 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 $\varepsilon = 3.65339100868$ [12].

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 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 in a single Padé approximant. In the present example, we may assume that

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

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,

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

and near infinity,

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

may be re-written as a set of the $4K + 8$ algebraic equations

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

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

relations

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

with $a_{-1} = a_{-2} = \dots = 0$ and $b_1 = b_0 = b_{-1} = \dots = 0$ 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 accord with the Riccati-Padé matching prescription of refs. [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 $N = 2K + L + 5$.

At small L's, 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 eq. (24) forms a homogeneous linear equation which defines the b's,

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

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 nonzero elements are $\mathcal{M}^{(F)}_{2K+L+4,4+4j} = \mathcal{M}^{(F)}_{2K+L+3,3+4j} = \dots = F_{2K+1-2j}$, $j = 0, 1, \dots, K + 1$ and $\mathcal{M}^{(G)}_{1,2K-L+2+i} = \mathcal{M}^{(G)}_{2,2K-L+3+i} = \dots = G_{-1+i}$, $i = 0, 2, 3, \dots, 2L + 2$. 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

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

Their numerical sample is displayed in our final 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 a 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 mutual small differences just set, in a way, an upper bound upon their common numerical precision.

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

In a way paralleling the older experience with the Riccati-Padé method [24], we may extrapolate the validity of equation (27) to its $\mathcal{M}^{(G)} \equiv 0$ extreme. Our final Table 6 shows that the resulting "extrapolative" algorithm still keeps working. An apparent paradox (the strict eq. (3) seems 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 $L \geq -2$. The overall number n_r of the (in general, complex) energy roots drops to 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 $N^{(\mathrm{dim.})} \leq 6$, a reliable approximation is obtained for the ground as well as the first excited states. The Table 6 provides a 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

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" (viz., a square-root-type complex-plane singularity at $x = \pm i/\lambda$) 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 nonrelativistic 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 aplications in the 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 remained open. First of all, one would like to see a genuine more- and many-particle generalizations of our elementary combination of the kinetic "minimal relativity" with the standard solvable spacial interaction. The significant simplification of technicalities (viz., Schrödinger in place of the Dirac equation) will 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 encounter its natural (both memory- and time-related) limitations.

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References

[1] Kime K 1993 Appl. Math. Lett. 6 11

[2] Rabitz H 1995 in "Few-Body Problems in Physics", Gross F (ed) (New York: AIP Conference Proceedings 334), p. 160

[3] Bishop R F, Flynn M F, Boscá M C and Guardiola R 1989 Phys. Rev. A 40 6154

Adhikari R, Dutt R and Varshni Y P 1991 J. Math. Phys. 32 447

[4] Flügge S 1971 Practical Quantum Mechanics I (Berlin: Springer)

[5] Cooper F, Khare A and Sukhatme U 1995 Phys. Rep. 251 267

[6] Znojil M 1995 Phys. Lett. A 203 1

[7] Znojil M 1981 Phys. Rev. D 24 903

[8] Bjorken J D and Drell S D 1964 Relativistic Quantum Mechanics (New York: McGraw-Hill)

Messiah A 1961 Quantum Mechanics I, II (Amsterdam: North Holland)

[9] Ince E L 1956 Ordinary Differential Equations (New York: Dover)

[10] Van Assche W, Yáñez R J and Dehesa J S 1995 J. Math. Phys. 36 4106

[11] Gradshteyn I S and Ryzhik I M 1971 Tables of Integrals, Sums, Series and Products (Moscow: Nauka), in Russian.

[12] A comparison suggested and numbers computed by an anonymous referee.

[13] Fernández F M 1991 Phys. Lett. A 160 116 and Phys. Rev. A 44 3336

[14] Newton R G 1982 Scattering Theory of Waves and Particles (New York: McGraw-Hill)

[15] Char B W et al 1991 Maple V (New York: Springer)

[16] Biswas S N, Datta K, Saxena R P, Srivastava P K and Varma V S 1971 Phys. Rev. D 4 3617

[17] Killingbeck J P 1991 Microcomputer Algorithms (Bristol: Hilger)

[18] Hautot A 1986 Phys. Rev. D 33 437

[19] Znojil M 1994 J. Phys. A: Math. Gen. 27 4945

[20] Tater M 1987 J. Phys. A: Math. Gen. 20 2483

[21] Witwit M R M 1992 Phys. Lett. A 169 229

[22] Znojil M 1981 Lett. Math. Phys. 5 405 and 1989 J. Math. Phys. 30 413

and in Beauwens R and de Groen P P N (eds) 1992 "Iterative Methods in Linear Algebra" (Amsterdam: North Holland) p. 430

Drozdov A N 1995 J. Phys. A: Math. Gen. 28 445

[23] Baker G A Jr. 1975 Essentials of Padé Approximants (New York: Academic)

[24] Fernández F M, Ma Q and Tipping R H 1989 Phys. Rev. A 40 6149

Estrín D A, Fernández F M and Castro E A 1990 J. Phys. A: Math. Gen. 23 2395

Fernández F M 1995 J. Phys. A: Math. Gen. 28 4043

[25] Fernández F M and Guardiola R 1993 J. Phys. A: Math. Gen. 26 7169

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

Znojil M, J. Phys. A: Math. Gen., to appear

[27] Quigg C and Rosner J L 1979 Phys. Rep. 56 167

[28] Serot B D and Walecka J D 1986 in Advances in Nuclear Physics, vol. 16, Negele J W and Vogt E (eds) (New York: Plenum)

Table 1. The estimates of energies $\varepsilon \approx \langle 0,0|H^{(QHO)}|0,0\rangle \approx \varepsilon_0 + \tilde{\varepsilon}_1(\mathcal{K})$ from the truncated eq. (11).

a. Satisfactory convergence at the "sufficiently small" λ's.

$\mathcal{K}$	$\lambda = 1/5$	$\lambda = 1/10$	$\lambda = 1/20$	$\lambda = 1/100$
0	3.000000000	3.000000000	3.000000000	3.000000000
1	2.962500000	2.990625000	2.997656250	2.999906250
2	2.965125000	2.990789063	2.997666504	2.999906266
3	2.964829688	2.990784448	2.997666432	2.999906266
4	2.964875166	2.990784626	2.997666433	2.999906266
5	2.964866297	2.990784617	2.997666432	2.999906266
6	2.964868388	2.990784618	2.997666432	2.999906266
7	2.964867810	2.990784618	2.997666432	2.999906266
8	2.964867993	2.990784618	2.997666432	2.999906266
9	2.964867928	2.990784618	2.997666432	2.999906266
10	2.964867954	2.990784618	2.997666432	2.999906266
11	2.964867942	2.990784618	2.997666432	2.999906266
12	2.964867948	2.990784618	2.997666432	2.999906266

. Table 1 continued.

b. The asymptotic-series $\mathcal{K}$-dependence of deviations $\triangle_\varepsilon \equiv \varepsilon(\mathcal{K}) - \varepsilon(\mathcal{K}-1)$.

	$\lambda = 1/2$		$\lambda = 1/3$		$\lambda = 1/4$	
$\mathcal{K}$	ε	$10^2 \times \triangle_\varepsilon$	ε	$10^4 \times \triangle_\varepsilon$	ε	$10^6 \times \triangle_\varepsilon$
1	2.765625	−23.0	2.895833	−1000.	2.941406	−59000.
2	2.868164	10.0	2.916088	200.0	2.947815	6400.0
3	2.796066	−7.2	2.909758	−63.0	2.946688	−1100.0
4	2.865460	6.9	2.912466	27.0	2.946959	270.0
5	2.780886	−8.5	2.910999	−15.0	2.946877	−83.0
6	2.905482	12.0	2.911960	9.6	2.946907	30.0
7	2.690360	−22.0	2.911223	−7.4	2.946894	−13.0
8	3.116123	43.0	2.911871	6.5	2.946901	6.5
9	2.166139	−95.0	2.911228	−6.4	2.946897	−3.6
10	4.524905	240.0	2.911938	7.1	2.946899	2.2
11	−1.924846	−640.0	2.911075	−8.6	2.946898	−1.5
12	17.33138	1900.0	2.912219	11.0	2.946899	1.1

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

$\lambda = 1/2$	energy
1/20	2.99766244644
1/10	2.99072278232
1/5	2.96398544193
1/4	2.94490499229
1/3	2.90613636892
1/2	2.80978632134
2	1.93233434201

. Table 3. The first two energy levels $\varepsilon = \varepsilon_{n,\ell}(\lambda)$

. in the Hill-determinat 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

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

λ	lower bound	ambiguity interval : eligible roots			upper bound
1/2	2.015497482	2.815969135	2.827091751	2.846464154	8.088381579
1/3	2.551846250	2.906984688	2.908118779	2.909505823	7.525268269
1/4	2.743918171	2.945086629	2.945299792	2.945528177	7.305961115
1/5	2.834598527	2.964037724	2.964095041	2.964152718	7.199301467
1/10	2.958044622	2.990723717	2.990724643	2.990725500	7.051102755
1/20	2.989468027	2.997662462	2.997662476	2.997662489	7.012861455

. Table 5. The results at negative L's.

λ	truncations			energy roots		
	L	K	N	lower	correct	upper
1/5	−2	3	8	2.834598527	2.964037724	7.199301467
	−1	3	9	2.834598527	2.964037724	7.199301467
	−2	5	12	2.963639029	2.963985588	3.551237591
	−1	5	13	2.963639029	2.963985588	3.551237591
1/10	−2	3	8	2.958044622	2.990723717	7.051102755
	−1	3	9	2.958044622	2.990723717	7.051102755
	−2	5	12	2.990717361	2.990722783	3.073985738
	−1	5	13	2.990717361	2.990722783	3.073985738

Table 6. The extrapolative Töplitz-determinant example.

. a. The ground-state roots: $0 < \varepsilon \leq 6$.

λ	K	ε				
1/5	3				2.96413	
	5		1.55	2.962935	2.96398572	
	7			2.9639827	2.963985443	2.96902
	9	1.66	2.943	2.963985429	2.963985442	2.964002
1/10	3				2.9907252	
	5		1.55	2.9907087	2.990722783	
	7			2.990722779	2.990722782	2.990773
	9	1.62	2.990580	2.990722782	2.990722782	2.990722796

. b. The first excited state: $6 < \varepsilon \leq 10$.

λ	K	ε		
1/5	5		6.8287	
	7	6.785	6.8249829	
	9	6.824815	6.824971199	7.16
1/10	5		6.954022	
	7	6.95349	6.953963780	
	9	6.953963609	6.953963765	6.9562