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Quasi-relativistic harmonic oscillator bound states

Omar Mustafa and Maen Odeh

Department of Physics, Eastern Mediterranean University, G Magusa, North Cyprus, Mersin 10, Turkey

E-mail: omustafa.as@mozart.emu.edu.tr

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Abstract. The quasi-relativistic harmonic oscillator bound states constructed by Znojil (1996 *J. Phys. A: Math. Gen.* **29** 2905) are investigated via a new methodical proposal. Compared with those obtained by an anonymous referee (from a direct numerical integration method) of Znojil's paper, our results appear to be more favourable than those obtained by Znojil via quasi-perturbative, variational, Hill-determinant and Riccati–Padé methods. Bound states with larger angular momenta, l, are also constructed.

Among exactly soluble Hamiltonians exists the harmonic oscillator (HO) Hamiltonian

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

The equidistant form of its spectrum has attracted attention in quantum control theory [1] and represents, in the view of [2], the 'long sought-after dream' of 'steering wavepackets into desired states'. Moreover, it fits, as proved by experimental observations, vibrational excitations of molecules and some low-lying energy levels in atomic nuclei.

On the other hand, a free spin-0 field fulfils the Klein-Gordon equation

$$(E^2 - H^2)\Psi = 0 \qquad H = \sqrt{c^2 p^2 + m^2 c^4}$$
(2)

or the Schrödinger formulation of it $(E - H)\Psi = 0$. Of course, there exist two admissible solutions for a given momentum p, i.e. positive and/or negative energy solutions. However, we devote our work to the positive solution in the Schrödinger-formulated Klein–Gordon equation. With the minimal coupling, a Lorentz four-vector HO potential is coupled as the zero component of the four-vector potential, i.e. $E \longrightarrow E - eA_0$ with $eA_0 = m\omega^2 r^2/2$. Hence, a fully relativistic description of $H^{(HO)}$ leads to the emergence of a quasi-relativistic harmonic oscillator (QHO) Hamiltonian:

$$H^{(QHO)} = \sqrt{m^2 c^4 + p^2 c^2} + \frac{1}{2}m\omega^2 r^2$$
(3)

which, in momentum representation, implies the one-dimensional Schrödinger equation

$$\frac{1}{2}m\hbar^2\omega^2 \left[-\frac{d^2}{dp^2} + \frac{l(l+1)}{p^2} \right] \Psi(p) + \left[\sqrt{m^2c^4 + p^2c^2} - mc^2 \right] \Psi(p) = \acute{E}\Psi(p) \tag{4}$$

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where $r^2 = -\hbar^2 \Delta_p$, $p \in (0, \infty)$, \acute{E} is the binding energy and l = 0, 1, ... denotes the angular momentum quantum number. Of course, on asymptotically physical grounds, the wavefunction $\Psi(p)$ satisfies the boundary conditions [3]

$$\Psi(p) \approx \begin{cases} p^{l+1} & \text{for } |p| \ll 1\\ \exp(-\nu p^{3/2}) & \nu = \sqrt{\frac{8c}{9m}} (\hbar\omega)^{-1} & \text{for } |p| \gg 1. \end{cases}$$

A rescale of the variable p through $p = \sqrt{m\hbar\omega q}$ would, in turn, lead to a transparent form of the Schrödinger equation [3]. Strictly,

$$\left[-\frac{1}{2}\frac{d^2}{dq^2} + \frac{l(l+1)}{2q^2} + V(q)\right]\Psi_{n_r,l}(q) = \varepsilon_{n_r,l}\Psi_{n_r,l}(q)^{(5)}$$
(5)

where $\varepsilon_{n_r,l} = 2\acute{E}_{n_r,l}/(\hbar\omega)$,

$$V(q) = \frac{1}{\alpha^2} (V_{SRAO}(q) - 1)$$
(6)

$$V_{SRAO}(q) = \sqrt{1 + \alpha^2 q^2} \tag{7}$$

 $\alpha^2 = \hbar \omega / (mc^2)$, and the square-root anharmonic oscillator potential (7) simulates a quasirelativistic squeezing of the HO spectrum.

The transition from the parabolic HO well, in standard coordinate representation, to the hyperbolic shape $V_{SRAO}(q)$, in momentum representation, is claimed to prove phenomenologically useful and methodically challenging. Znojil [3] has, therefore, investigated several eligible (namely, perturbative, variational, Hill-determinant, and Riccati–Padé) methods to construct its bound states. With the permission of an anonymous referee of his paper, Znojil also reported (in table 2 of [3]) the referee's results from direct numerical integrations (DNI).

Whilst using a quasi-perturbation prescription (equation (11) in [3]), a loss of precision occurred at 'large' $\alpha = \frac{1}{2}$ (table 1(*b*) in [3]), upon which the anonymous referee remarked that it may also cause a loss of the upper-bound character of the quasi-perturbation prescription. In accordance with a second referee's remark, being curable by a Padé-type resummation, the loss of boundedness phenomenon may emerge at any α .

To the best of our knowledge, the paper of Znojil [3] is the only one available in the literature considering the QHO and, therefore, merits further consideration.

In this paper we formulate a new method to solve the Fourier-transformed Schrödinger equation (4), with V(q) represented by (6). Our method consists of using $1/\overline{l}$ as an expansion parameter, where $\overline{l} = l - \beta$, l is a quantum number, and β is a suitable shift introduced with the main aim of avoiding the trivial case, l = 0. The spiritual soundness of 'textbook' perturbation theory is therefore engaged. Hence the method should be called the pseudoperturbative shifted-l expansion technique (PSLET).

With the noninteger (irrational) orbital angular momentum \bar{l} , equation (5) reads

$$\left\{-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}q^2} + \tilde{V}(q)\right\}\Psi_{n_r,l}(q) = \varepsilon_{n_r,l}\Psi_{n_r,l}(q) \tag{8}$$

$$\tilde{V}(q) = \frac{\bar{l}^2 + (2\beta + 1)\bar{l} + \beta(\beta + 1)}{2q^2} + \frac{\bar{l}^2}{Q}V(q)$$
(9)

where Q is a constant that scales the potential V(q) at the large-l limit and is set, for any specific choice of l and n_r , equal to \bar{l}^2 at the end of the calculations [4–9]. β is determined in the following.

Our systematic procedure begins by shifting the origin of the coordinate through

$$x = \bar{l}^{1/2} (q - q_o) / q_o \tag{10}$$

where q_o is currently an arbitrary point given to perform Taylor expansions about, with its particular value to be determined. Expansions about this point yield

$$\frac{1}{q^2} = \sum_{n=0}^{\infty} (-1)^n \frac{(n+1)}{q_o^2} x^n \bar{l}^{-n/2}$$
(11)

$$V(x(q)) = \sum_{n=0}^{\infty} \left(\frac{d^n V(q_o)}{dq_o^n}\right) \frac{(q_o x)^n}{n!} \bar{l}^{-n/2}.$$
(12)

It should be mentioned here that the scaled coordinate, equation (10), has no effect on the energy eigenvalues, which are coordinate independent. It merely facilitates the calculations of both the energy eigenvalues and eigenfunctions. It is also convenient to expand $\varepsilon_{n_r,l}$ as

$$\varepsilon_{n_r,l} = \sum_{n=-2}^{\infty} \varepsilon_{n_r,l}^{(n)} \bar{l}^{-n}.$$
(13)

Equation (8) thus becomes

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + \frac{q_o^2}{\bar{l}}\tilde{V}(x(q))\right]\Psi_{n_r,l}(x) = \frac{q_o^2}{\bar{l}}\varepsilon_{n_r,l}\Psi_{n_r,l}(x)$$
(14)

with

$$\frac{q_o^2}{\bar{l}}\tilde{V}(x(q)) = q_o^2 \bar{l} \left[\frac{1}{2q_o^2} + \frac{V(q_o)}{Q} \right] + \bar{l}^{1/2} \left[-x + \frac{V'(q_o)q_o^3 x}{Q} \right] \\
+ \left[\frac{3}{2} x^2 + \frac{V''(q_o)q_o^4 x^2}{2Q} \right] + (2\beta + 1) \sum_{n=1}^{\infty} (-1)^n \frac{(n+1)}{2} x^n \bar{l}^{-n/2} \\
+ q_o^2 \sum_{n=3}^{\infty} \left[(-1)^n \frac{(n+1)}{2q_o^2} x^n + \left(\frac{d^n V(q_o)}{dq_o^n} \right) \frac{(q_o x)^n}{n! Q} \right] \bar{l}^{-(n-2)/2} \\
+ \beta(\beta + 1) \sum_{n=0}^{\infty} (-1)^n \frac{(n+1)}{2} x^n \bar{l}^{-(n+2)/2} + \frac{(2\beta + 1)}{2} \tag{15}$$

where the prime of $V(q_o)$ denotes the derivative with respect to q_o . Equation (14) is the exact Schrödinger-type equation for a one-dimensional anharmonic oscillator

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + \frac{1}{2}\Omega^2 x^2 + \Lambda_o + P(x)\right] X_{n_r}(x) = \lambda_{n_r} X_{n_r}(x)$$
(16)

where P(x) is a perturbation-like term and Λ_o is a constant. A simple comparison between equations (14)–(16) implies

$$\Lambda_{o} = \bar{l} \left[\frac{1}{2} + \frac{q_{o}^{2} V(q_{o})}{Q} \right] + \frac{2\beta + 1}{2} + \frac{\beta(\beta + 1)}{2\bar{l}}$$
(17)

$$\lambda_{n_r} = \bar{l} \left[\frac{1}{2} + \frac{q_o^2 V(q_o)}{Q} \right] + \left[\frac{2\beta + 1}{2} + \left(n_r + \frac{1}{2} \right) \Omega \right] + \frac{1}{\bar{l}} \left[\frac{\beta(\beta + 1)}{2} + \lambda_{n_r}^{(0)} \right] + \sum_{n=2}^{\infty} \lambda_{n_r}^{(n-1)} \bar{l}^{-n}$$
(18)

and

$$\lambda_{n_r} = q_o^2 \sum_{n=-2}^{\infty} \varepsilon_{n_r,l}^{(n)} \bar{l}^{-(n+1)}.$$
(19)

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Equations (18) and (19) yield

$$\varepsilon_{n_r,l}^{(-2)} = \frac{1}{2q_o^2} + \frac{V(q_o)}{Q}$$
(20)

$$\varepsilon_{n_r,l}^{(-1)} = \frac{1}{q_o^2} \left[\frac{2\beta + 1}{2} + \left(n_r + \frac{1}{2} \right) \Omega \right]$$
(21)

$$\varepsilon_{n_r,l}^{(0)} = \frac{1}{q_o^2} \left[\frac{\beta(\beta+1)}{2} + \lambda_{n_r}^{(0)} \right]$$
(22)

$$\varepsilon_{n_r,l}^{(n)} = \lambda_{n_r}^{(n)} / q_o^2 \qquad n \ge 1.$$
(23)

Here q_o is chosen to minimize $\varepsilon_{n_r,l}^{(-2)}$, i.e.

$$\frac{\mathrm{d}\varepsilon_{n_r,l}^{(-2)}}{\mathrm{d}q_o} = 0 \qquad \text{and} \qquad \frac{\mathrm{d}^2\varepsilon_{n_r,l}^{(-2)}}{\mathrm{d}q_o^2} > 0 \tag{24}$$

which in turn gives, with $\bar{l} = \sqrt{Q}$,

$$l - \beta = \sqrt{q_o^3 V'(q_o)}.$$
(25)

Consequently, the second term in equation (15) vanishes and the first term adds a constant to the energy eigenvalues.

The next leading correction to the energy series, $\bar{l}\varepsilon_{n_r,l}^{(-1)}$, consists of a constant term and the exact eigenvalues of the unperturbed HO potential $\Omega^2 x^2/2$. The shifting parameter β is determined by choosing $\bar{l}\varepsilon_{n_r,l}^{(-1)} = 0$. Hence

$$\beta = -\left[\frac{1}{2} + (n_r + \frac{1}{2})\Omega\right]$$
(26)

where

$$\Omega = \sqrt{3 + \frac{q_o V''(q_o)}{V'(q_o)}}.$$
(27)

Then equation (15) reduces to

$$\frac{q_o^2}{\bar{l}}\tilde{V}(x(q)) = q_o^2 \bar{l} \left[\frac{1}{2q_o^2} + \frac{V(q_o)}{Q} \right] + \sum_{n=0}^{\infty} v^{(n)}(x) \bar{l}^{-n/2}$$
(28)

where

$$v^{(0)}(x) = \frac{1}{2}\Omega^2 x^2 + \frac{2\beta + 1}{2}$$
(29)

$$v^{(1)}(x) = -(2\beta + 1)x - 2x^3 + \frac{q_o^5 V^{'''}(q_o)}{6Q} x^3$$
(30)

and for $n \ge 2$

$$v^{(n)}(x) = (-1)^{n} (2\beta + 1) \frac{(n+1)}{2} x^{n} + (-1)^{n} \frac{\beta(\beta+1)}{2} (n-1) x^{(n-2)} + \left[(-1)^{n} \frac{(n+3)}{2} + \frac{q_{o}^{(n+4)}}{Q(n+2)!} \frac{d^{n+2}V(q_{o})}{dq_{o}^{n+2}} \right] x^{n+2}.$$
(31)

Equation (14) thus becomes

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{n=0}^{\infty} v^{(n)}\bar{l}^{-n/2}\right]\Psi_{n_r,l}(x) = \left[\frac{1}{\bar{l}}\left(\frac{\beta(\beta+1)}{2} + \lambda_{n_r}^{(0)}\right) + \sum_{n=2}^{\infty}\lambda_{n_r}^{(n-1)}\bar{l}^{-n}\right]\Psi_{n_r,l}(x).$$
(32)

When setting the nodeless, $n_r = 0$, wavefunctions as

$$\Psi_{0,l}(x(q)) = \exp(U_{0,l}(x))$$

equation (32) is readily transformed into the following Riccati equation:

$$-\frac{1}{2}[U^{''}(x) + U^{'}(x)U^{'}(x)] + \sum_{n=0}^{\infty} v^{(n)}(x)\bar{l}^{-n/2} = \frac{1}{\bar{l}}\left(\frac{\beta(\beta+1)}{2} + \lambda_{0}^{(0)}\right) + \sum_{n=2}^{\infty}\lambda_{0}^{(n-1)}\bar{l}^{-n}.$$
 (34)

Hereafter, we use U(x) instead of $U_{0,l}(x)$ for simplicity, and the prime of U(x) denotes the derivative with respect to x. It is evident that this equation has as solution of the form

$$U'(x) = \sum_{n=0}^{\infty} U^{(n)}(x)\bar{l}^{-n/2} + \sum_{n=0}^{\infty} G^{(n)}(x)\bar{l}^{-(n+1)/2}$$
(35)

where

$$U^{(n)}(x) = \sum_{m=0}^{n+1} D_{m,n} x^{2m-1} \qquad D_{0,n} = 0$$
(36)

$$G^{(n)}(x) = \sum_{m=0}^{n+1} C_{m,n} x^{2m}.$$
(37)

Substituting equations (35)–(37) into (34) implies

$$-\frac{1}{2}\sum_{n=0}^{\infty} [U^{(n)'}\bar{l}^{-n/2} + G^{(n)'}\bar{l}^{-(n+1)/2}] \\ -\frac{1}{2}\sum_{n=0}^{\infty}\sum_{p=0}^{\infty} [U^{(n)}U^{(p)}\bar{l}^{-(n+p)/2} + G^{(n)}G^{(p)}\bar{l}^{-(n+p+2)/2} + 2U^{(n)}G^{(p)}\bar{l}^{-(n+p+1)/2}] \\ +\sum_{n=0}^{\infty}v^{(n)}\bar{l}^{-n/2} = \frac{1}{\bar{l}}\left(\frac{\beta(\beta+1)}{2} + \lambda_0^{(0)}\right) + \sum_{n=2}^{\infty}\lambda_0^{(n-1)}\bar{l}^{-n}$$
(38)

where the primes of $U^{(n)}(x)$ and $G^{(n)}(x)$ denote derivatives with respect to x. Equating the coefficients of the same powers of \overline{l} and x, respectively (of course, the reverse would work equally well), one obtains

$$-\frac{1}{2}U^{(0)'} - \frac{1}{2}U^{(0)}U^{(0)} + v^{(0)} = 0$$
(39)

$$U^{(0)'}(x) = D_{1,0} \qquad D_{1,0} = -\Omega$$
 (40)

and integration over dx yields

$$U^{(0)}(x) = -\Omega x. \tag{41}$$

Similarly,

$$-\frac{1}{2}[U^{(1)'} + G^{(0)'}] - U^{(0)}U^{(1)} - U^{(0)}G^{(0)} + v^{(1)} = 0$$

$$U^{(1)}(x) = 0$$
(42)
(43)

$$U^{(1)}(x) = 0$$

$$G^{(0)}(x) = C_{0,0} + C_{1,0}x^{2}$$
(43)
(44)

$$C_{1,0} = -\frac{B_1}{B_1}$$
(45)

$$C_{1,0} = -\frac{1}{\Omega}$$
(45)

$$C_{0,0} = \frac{1}{\Omega} (C_{1,0} + 2\beta + 1) \tag{46}$$

$$B_1 = -2 + \frac{q_o^5}{6Q} \frac{\mathrm{d}^3 V(q_o)}{\mathrm{d}q_o^3} \tag{47}$$

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(33)

$$-\frac{1}{2}[U^{(2)'} + G^{(1)'}] - \frac{1}{2}\sum_{n=0}^{2}U^{(n)}U^{(2-n)} - \frac{1}{2}G^{(0)}G^{(0)} - \sum_{n=0}^{1}U^{(n)}G^{(1-n)} + v^{(2)}$$
$$= \frac{\beta(\beta+1)}{2} + \lambda_{0}^{(0)}$$
(48)

$$U^{(2)}(x) = D_{1,2}x + D_{2,2}x^3$$
(49)

$$G^{(1)}(x) = 0$$
(50)
$$1 \left(C_{1,0}^{2} \right)$$

$$D_{2,2} = \frac{1}{\Omega} \left(\frac{1}{2} - B_2 \right)$$
(51)

$$D_{1,2} = \frac{1}{\Omega} \left(\frac{3}{2} D_{2,2} + C_{0,0} C_{1,0} - \frac{3}{2} (2\beta + 1) \right)$$
(52)

$$B_2 = \frac{5}{2} + \frac{q_o^6}{24Q} \frac{d^4 V(q_o)}{dq_o^4}$$
(53)

$$\lambda_0^{(0)} = -\frac{1}{2}(D_{1,2} + C_{0,0}^2) \tag{54}$$

etc. Thus, one can calculate the energy eigenvalue and the eigenfunctions, from the knowledge of $C_{m,n}$ and $D_{m,n}$, in a hierarchical manner. Nevertheless, the procedure just described is suitable for systematic calculations using software packages (such as MATHEMATICA, MAPLE, or REDUCE) to determine the energy eigenvalue and eigenfunction corrections up to any order of the pseudoperturbation series.

It should be mentioned that the energy series, equation (13), could appear as convergent, divergent or asymptotic. However, one can still calculate the eigenenergies to a very good level of accuracy by forming the sophisticated Padé approximants to the energy series [11]. The energy series, equation (13), is calculated up to $\varepsilon_{0,l}^{(8)}/\bar{l}^8$ by

$$\varepsilon_{0,l} = \bar{l}^2 \varepsilon_{0,l}^{(-2)} + \varepsilon_{0,l}^{(0)} + \dots + \varepsilon_{0,l}^{(8)} / \bar{l}^8 + \mathcal{O}(1/\bar{l}^9)$$
(55)

and with the $P_N^N(1/\overline{l})$ and $P_N^{N+1}(1/\overline{l})$ Padé approximants it becomes

$$\varepsilon_{0,l}[N,N] = \bar{l}^2 \varepsilon_{0,l}^{(-2)} + P_N^N(1/\bar{l})$$
(56)

and

$$\varepsilon_{0,l}[N, N+1] = \bar{l}^2 \varepsilon_{0,l}^{(-2)} + P_N^{N+1}(1/\bar{l}).$$
(57)

Our strategy and prescription are therefore clear.

Let us now consider the Fourier transform of equation (4), with the rescaled variable $p = \sqrt{m\hbar\omega q}$, represented by equations (5)–(7). The substitution of equation (6) in (26), for $n_r = 0$, implies

$$\beta = -\frac{1}{2}(1+\Omega) \qquad \Omega = \sqrt{\frac{4+3\alpha^2 q_o^2}{1+\alpha^2 q_o^2}}.$$
(58)

Equation (25) thus reads

$$l + \frac{1}{2}(1+\Omega) = q_o^2 \sqrt{\frac{1}{\sqrt{1+\alpha^2 q_o^2}}}.$$
(59)

Equation (59) is explicit in q_o and evidently a closed-form solution for q_o is hard to find, although not impossible. However, numerical solutions are feasible. Once q_o is determined the coefficients $C_{m,n}$ and $D_{m,n}$ are obtained in a sequential manner. Consequently, the eigenvalues, equation (55), and eigenfunctions, equations (35)–(37), are calculated in the same batch for each value of α and l.

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Table 1. PSLET results for ground-state energies $\varepsilon_{0,0}$, where *K* represents the first *K* terms of equation (54) and exact DNI results from [3].

| K | $\alpha = \frac{1}{100}$ | $\alpha = \frac{1}{20}$ | $\alpha = \frac{1}{10}$ | $\alpha = \frac{1}{5}$ |
|--|---|--|---|---|
| 1 | 2.999 906 257 850 8 | 2.997 661 14 471 | 2.990 702 721 | 2.963 706 98 |
| 2 | 2.999 906 259 959 4 | 2.997 662 45 159 | 2.990723092 | 2.964 001 14 |
| 3 | 2.999 906 259 959 1 | 2.997 662 44 641 | 2.990722775 | 2.963 984 17 |
| 4 | 2.999 906 259 959 1 | 2.997 662 44 644 | 2.990722783 | 2.963 985 58 |
| 5 | 2.999 906 259 959 1 | 2.997 662 44 644 | 2.990722782 | 2.963 985 42 |
| 6 | 2.999 906 259 959 1 | 2.997 662 44 644 | 2.990722782 | 2.963 985 45 |
| 7 | 2.999 906 259 959 1 | 2.997 662 44 631 | 2.990722775 | 2.963 985 06 |
| 8 | 2.999 906 259 959 1 | 2.997 662 44 635 | 2.990722777 | 2.963 985 17 |
| 9 | 2.999 906 259 959 1 | 2.997 662 44 635 | 2.990722777 | 2.963 985 17 |
| 10 | 2.999 906 259 959 1 | 2.997 662 44 634 | 2.990722776 | 2.963 985 14 |
| DNI | _ | 2.997 662 44 644 | 2.990 722 782 | 2.963 985 44 |
| | 1 | 1 | 1 | |
| | $\alpha = \frac{1}{4}$ | $\alpha = \frac{1}{3}$ | $\alpha = \frac{1}{2}$ | $\alpha = 2$ |
| 1 | $\alpha = \frac{1}{4}$ 2.944 289 62 | $\alpha = \frac{1}{3}$ 2.904 543 | $\alpha = \frac{1}{2}$ 2.804 82 | $\frac{\alpha = 2}{1.9189}$ |
| 1 2 | $\alpha = \frac{1}{4}$ 2.944 289 62 2.944 955 82 | $\alpha = \frac{1}{3}$ 2.904 543 2.906 342 | $\alpha = \frac{1}{2}$ 2.804 82 2.810 83 | $\alpha = 2$ 1.9189 1.9331 |
| 1 2 3 | $\alpha = \frac{1}{4}$ 2.944 289 62 2.944 955 82 2.944 899 04 | $\alpha = \frac{1}{3}$ 2.904 543 2.906 342 2.906 100 | $\alpha = \frac{1}{2}$ 2.804 82 2.810 83 2.809 51 | $\alpha = 2$ 1.9189 1.9331 1.9334 |
| 1 2 3 4 | $\alpha = \frac{1}{4}$ 2.944 289 62 2.944 955 82 2.944 899 04 2.944 905 92 | $\alpha = \frac{1}{3}$ 2.904 543 2.906 342 2.906 100 2.906 145 | $\alpha = \frac{1}{2}$ 2.804 82 2.810 83 2.809 51 2.809 87 | $\alpha = 2$ 1.9189 1.9331 1.9334 1.9323 |
| 1 2 3 4 5 | $\alpha = \frac{1}{4}$ 2.944 289 62 2.944 955 82 2.944 899 04 2.944 905 92 2.944 904 81 | $\alpha = \frac{1}{3}$ 2.904 543 2.906 342 2.906 100 2.906 145 2.906 135 | $\alpha = \frac{1}{2}$ 2.804 82 2.810 83 2.809 51 2.809 87 2.809 77 | $ \begin{array}{c} \alpha = 2 \\ \hline 1.9189 \\ 1.9331 \\ 1.9334 \\ 1.9323 \\ 1.9319 \\ \end{array} $ |
| 1 2 3 4 5 6 | $\alpha = \frac{1}{4}$ 2.944 289 62 2.944 955 82 2.944 899 04 2.944 905 92 2.944 904 81 2.944 905 03 | $\alpha = \frac{1}{3}$ 2.904 543 2.906 342 2.906 100 2.906 145 2.906 135 2.906 138 | $\alpha = \frac{1}{2}$ 2.804 82 2.810 83 2.809 51 2.809 87 2.809 77 2.809 79 | $\alpha = 2$ 1.9189 1.9331 1.9334 1.9323 1.9319 1.9322 |
| 1 2 3 4 5 6 7 | $\alpha = \frac{1}{4}$ 2.944 289 62 2.944 955 82 2.944 899 04 2.944 905 92 2.944 904 81 2.944 905 03 2.944 903 79 | $\alpha = \frac{1}{3}$ 2.904 543 2.906 342 2.906 100 2.906 145 2.906 135 2.906 138 2.906 132 | $\alpha = \frac{1}{2}$ 2.804 82 2.810 83 2.809 51 2.809 87 2.809 77 2.809 79 2.809 78 | $\alpha = 2$ 1.9189 1.9331 1.9334 1.9323 1.9319 1.9322 1.9328 |
| 1 2 3 4 5 6 7 8 | $\alpha = \frac{1}{4}$ 2.944 289 62 2.944 955 82 2.944 899 04 2.944 905 92 2.944 904 81 2.944 905 03 2.944 903 79 2.944 904 11 | $\alpha = \frac{1}{3}$ 2.904 543 2.906 342 2.906 100 2.906 145 2.906 135 2.906 138 2.906 132 2.906 134 | $\alpha = \frac{1}{2}$ 2.804 82 2.810 83 2.809 51 2.809 87 2.809 77 2.809 79 2.809 78 2.809 78 2.809 77 | $\alpha = 2$ 1.9189 1.9331 1.9334 1.9323 1.9319 1.9322 1.9328 1.9328 1.9329 |
| 1 2 3 4 5 6 7 8 9 | $\alpha = \frac{1}{4}$ 2.944 289 62 2.944 955 82 2.944 899 04 2.944 905 92 2.944 904 81 2.944 905 03 2.944 903 79 2.944 904 11 2.944 904 11 | $\alpha = \frac{1}{3}$ 2.904 543 2.906 342 2.906 100 2.906 145 2.906 135 2.906 138 2.906 132 2.906 134 2.906 134 | $\alpha = \frac{1}{2}$ 2.804 82 2.810 83 2.809 51 2.809 87 2.809 77 2.809 79 2.809 78 2.809 77 2.809 77 2.809 77 | $\alpha = 2$ 1.9189 1.9331 1.9334 1.9323 1.9319 1.9322 1.9328 1.9329 1.9329 |
| 1 2 3 4 5 6 7 8 9 10 | $\alpha = \frac{1}{4}$ 2.944 289 62 2.944 955 82 2.944 899 04 2.944 905 92 2.944 904 81 2.944 905 03 2.944 903 79 2.944 904 11 2.944 904 11 2.944 904 03 | $\alpha = \frac{1}{3}$ 2.904 543 2.906 342 2.906 100 2.906 145 2.906 135 2.906 135 2.906 138 2.906 132 2.906 134 2.906 134 2.906 133 | $\alpha = \frac{1}{2}$ 2.804 82 2.810 83 2.809 51 2.809 87 2.809 77 2.809 77 2.809 78 2.809 77 2.809 77 2.809 77 2.809 77 2.809 77 2.809 75 | $\alpha = 2$ 1.9189 1.9331 1.9334 1.9323 1.9319 1.9322 1.9328 1.9329 1.9329 1.9315 |
| 1 2 3 4 5 6 7 8 9 10 DNI | $\alpha = \frac{1}{4}$ 2.944 289 62 2.944 955 82 2.944 905 92 2.944 905 92 2.944 904 81 2.944 905 03 2.944 903 79 2.944 904 11 2.944 904 11 2.944 904 03 2.944 904 99 | $\alpha = \frac{1}{3}$ 2.904 543 2.906 342 2.906 100 2.906 145 2.906 135 2.906 135 2.906 138 2.906 132 2.906 134 2.906 134 2.906 133 2.906 136 | $\alpha = \frac{1}{2}$ 2.804 82 2.810 83 2.809 51 2.809 87 2.809 77 2.809 79 2.809 78 2.809 77 2.809 77 2.809 77 2.809 77 2.809 75 2.809 78 | $\alpha = 2$ 1.9189 1.9331 1.9334 1.9323 1.9319 1.9322 1.9328 1.9329 1.9329 1.9329 1.9315 1.932 334 |

In order to make remediable analysis of our results we have calculated the first ten terms of the energy series. The effect of each term has been taken into account. We have also computed the Padé approximants $\varepsilon_{0,l}[N, M]$ for N = 2, 3, 4 and M = 2, 3, 4, 5. Therefore, the stability of the energy series and that of the sequence of Padé approximants are in point.

Table 1 shows PSLET results for the ground-state energies $\varepsilon_{0,0}$, covering a wide range of the anharmonicity α , along with the exact results from the DNI method, carried out by the anonymous referee of [3]. To avoid exhaustive numbers of tables we do not list Znojil's results. However, we do refer to them when required. A comparison between PSLET and DNI results implies excellent agreement. The nice trend of stability in the energy series (55) (i.e. a signal of nice course of convergence.) is well pronounced. The effect of the higher-order corrections on the first few terms of the energy series bears this out.

In contrast with Znojil's results (table 1(*b*) in [3]) for 'large' $\alpha = \frac{1}{3}$ and $\alpha = \frac{1}{2}$, via a quasi-perturbative prescription (equation (11) in [3]), there is no indication that our series will blow up at higher orders and, by and large, our expansion parameter $(1/\overline{l})$ is less than one for all values of α reported in the text. Of course, there is always the contribution from the (K + 1) term, but so far our prescription has performed well. Whilst Znojil's prescription marks nice stability for small α , severe oscillations of his series occur at low order, especially for 'large' $\alpha = \frac{1}{2}$, causing, in effect, a breakdown in the bounded character of his prescription. Although this phenomenon is curable by resummation tools such as the sophisticated Padé approximants, as suggested by the second referee of [3]; however, in our opinion, this will not dramatically cure the loss of precision in Znojil's results (table 1(*b*) in [3]), as documented in the following.

Table 2. The effect of the angular momentum quantum number *l* on convergence and precision for $\alpha = \frac{1}{2}$.

| K | l = 1 | l = 5 | l = 10 | l = 20 |
|----|-----------|--------------|----------------|--------------------|
| 1 | 4.569 573 | 10.977 406 1 | 17.963 301 722 | 29.948 955 412 735 |
| 2 | 4.575 998 | 10.981 520 1 | 17.965 505 044 | 29.949 880 189 612 |
| 3 | 4.575 031 | 10.981 360 3 | 17.965 487 822 | 29.949 881 669 238 |
| 4 | 4.575 173 | 10.981 349 8 | 17.965 484 484 | 29.949 881 347 421 |
| 5 | 4.575 167 | 10.981 352 9 | 17.965 484 566 | 29.949 881 340 115 |
| 6 | 4.575 155 | 10.981 352 8 | 17.965 484 596 | 29.949 881 340 512 |
| 7 | 4.575 164 | 10.981 352 7 | 17.965 484 595 | 29.949 881 340 559 |
| 8 | 4.575 161 | 10.981 352 7 | 17.965 484 595 | 29.949 881 340 559 |
| 9 | 4.575 161 | 10.981 352 7 | 17.965 484 595 | 29.949 881 340 559 |
| 10 | 4.575 162 | 10.981 352 7 | 17.965 484 595 | 29.949 881 340 559 |

Table 3. The effect of Padé approximants on convergence and precision.

| $\varepsilon_{0,0}[N,M]$ | $\alpha = \frac{1}{100}$ | $\alpha = \frac{1}{10}$ | $\alpha = \frac{1}{3}$ | $\alpha = 2$ |
|--------------------------|--------------------------|-------------------------|------------------------|--------------|
| $\varepsilon_{0,0}[2,2]$ | 2.999 906 259 959 1 | 2.99072278 | 2.906 14 | 1.9319 |
| $\varepsilon_{0,0}[2,3]$ | 2.999 906 259 959 1 | 2.990 722 78 | 2.906 14 | 1.9323 |
| $\varepsilon_{0,0}[3,3]$ | 2.999 906 259 959 1 | 2.990 722 78 | 2.906 14 | 1.9334 |
| $\varepsilon_{0,0}[3,4]$ | 2.999 906 259 959 1 | 2.990 722 78 | 2.906 14 | 1.9325 |
| $\varepsilon_{0,0}[4,4]$ | 2.999 906 259 959 1 | 2.990 722 78 | 2.906 13 | 1.9326 |
| $\varepsilon_{0,0}[4,5]$ | 2.999 906 259 959 1 | 2.990 722 78 | 2.906 13 | 1.9326 |

Switching to alternative methods to provide independent checks of his numerical predictions, Znojil used the Hill-determinant and Riccati–Padé methods. As a result of his work using the Hill determinant, an onset of convergence is clearly manifested (table 3 in [3]), but larger dimensions and/or an improved elementary convergence factor would be necessary to reach the domain of more satisfactory numerical precision. Moreover, as a result of his work using a slightly more complicated (compared with the Hill determinant) Riccati–Padé method, the 11-dimensional Töplitz determinants offered very satisfactory precision (table 4 in [3]). However, a typical bizarre characteristic of the Riccati–Padé method is well documented [3, 12]. Namely, it leads to a number of clustered solutions, for a given value of the coupling α , resulting from the existence of several eligible physical roots of the Hankel [12] or Töplitz [3] determinants. Yet the ambiguity of these roots increases with the dimensional growth of the determinants. Although clustering is a good indication that one is close to a physical root, one has to make a decision on which of these roots is the best. So far, to the best of our knowledge, a general method of establishing this property has not been found.

The effect of the angular momentum quantum number l on the stability, and hence on convergence and precision, is reported in table 2 for $\alpha = \frac{1}{2}$. Confidently, one concludes that better convergence and more precise numerical results are obtained as l increases. A similar effect should be expected for the nodal quantum number n_r ; l and n_r have almost identical effects on our pseudoperturbative expansion parameter \overline{l} .

The stability of the sequence of Padé approximants (table 3) is fascinating. Although there is no indicator that our series will blow up (table 1 reflects this fact), the effect of the Padé approximants on precision is limited. For fixed α , say $\frac{1}{2}$, more precision is obtained via Padé approximants as *l* increases (table 4). Adhering to the conventional practice of perturbative calculations (i.e. only a few terms of a 'most useful' perturbation series reveal the important features of the solution before a state of exhaustion is reached), we list PSLET results (table 5)

| $\varepsilon_{0,l}[N,M]$ | l = 0 | l = 1 | l = 3 |
|---|--|---|---|
| $\varepsilon_{0,l}[2,2]$ | 2.809788 | 4.575 157 | 7.893 680 |
| $\varepsilon_{0,l}[2,3]$ | 2.809 826 | 4.575 161 | 7.893 681 |
| $\varepsilon_{0,l}[3,3]$ | 2.809783 | 4.575 161 | 7.893 681 |
| $\varepsilon_{0,l}[3, 4]$ | 2.809767 | 4.575 161 | 7.893 681 |
| $\varepsilon_{0,l}[4, 4]$ | 2.809 790 | 4.575 161 | 7.893 681 |
| $\varepsilon_{0,l}[4,5]$ | 2.809 797 | 4.575 161 | 7.893 681 |
| | | | |
| | l = 5 | l = 10 | l = 20 |
| $\frac{1}{\varepsilon_{0,l}[2,2]}$ | l = 5 10.981 352 490 | l = 10 17.965 484 570 | l = 20 29.949 881 340 088 |
| $\overline{\varepsilon_{0,l}[2,2]}$ $\varepsilon_{0,l}[2,3]$ | l = 5 10.981 352 490 10.981 352 767 | l = 10 17.965 484 570 17.965 484 596 | l = 20 29.949 881 340 088 29.949 881 340 530 |
| $ \frac{\overline{\varepsilon_{0,l}[2,2]}}{\varepsilon_{0,l}[2,3]} \\ \frac{\varepsilon_{0,l}[2,3]}{\varepsilon_{0,l}[3,3]} $ | l = 5 10.981 352 490 10.981 352 767 10.981 352 715 | l = 10 17.965 484 570 17.965 484 596 17.965 484 595 | <i>l</i> = 20 29.949 881 340 088 29.949 881 340 530 29.949 881 340 562 |
| $ \overline{ \varepsilon_{0,l}[2,2]} \\ \varepsilon_{0,l}[2,3] \\ \varepsilon_{0,l}[3,3] \\ \varepsilon_{0,l}[3,4] $ | l = 5 10.981 352 490 10.981 352 767 10.981 352 715 10.981 352 712 | l = 10 17.965 484 570 17.965 484 596 17.965 484 595 17.965 484 587 | l = 20 29.949 881 340 088 29.949 881 340 530 29.949 881 340 562 29.949 881 340 559 |
| $ \frac{\varepsilon_{0,l}[2,2]}{\varepsilon_{0,l}[2,3]} \\ \varepsilon_{0,l}[3,3] \\ \varepsilon_{0,l}[3,4] \\ \varepsilon_{0,l}[4,4] $ | l = 5 10.981 352 490 10.981 352 767 10.981 352 715 10.981 352 712 10.981 352 712 | l = 10 17.965 484 570 17.965 484 596 17.965 484 595 17.965 484 587 17.965 484 587 | l = 20 29.949 881 340 088 29.949 881 340 530 29.949 881 340 562 29.949 881 340 559 29.949 881 340 559 |

Table 4. The effect of *l* and Padé approximants on convergence and precision for $\alpha = \frac{1}{2}$.

Table 5. Comparison between PSLET, collecting the first six terms of the energy series, the $\varepsilon_{0,0}[3,3]$ Padé approximant and the results from DNI [3].

| α | K = 6 | $\varepsilon_{0,0}[3,3]$ | DNI [3] |
|--|---|---|--|
| $ \frac{\frac{1}{100}}{\frac{1}{20}} \\ \frac{1}{10} \\ \frac{1}{5} \\ \frac{1}{4} $ | 2.999 906 259 959 1 2.997 662 44 644 2.990 722 78 231 2.963 985 445 2.944 905 033 | 2.999 906 2 599 591 2.997 662 44 644 2.990 722 78 231 2.963 985 441 2.944 904 983 | |
| $\frac{1}{3}$ $\frac{1}{2}$ 2 | 2.906 137 610 2.809 786 91 1.932 185 | 2.906 136 824 2.809 783 442 1.933 444 | 2.906 136 36 892 2.809 786 32 134 1.932 334 34 201 |

of the first six terms of our energy series with the $\varepsilon_{0,0}[3, 3]$ Padé approximant. Compared with those from DNI, our results are readily satisfactory.

To summarize, we have used a new methodical proposal to investigate the bound states of the QHO. Using the perturbation expansion parameter $1/\overline{l}$, we have demonstrated that our apparently artificial perturbation recipe, PSLET, is convincingly powerful and methodically practical.

Perhaps it should be noted that for each entry in tables 1–5 one can construct the wavefunction from the knowledge of $C_{m,n}$ and $D_{m,n}$. However, such a study lies beyond the scope of our methodical proposal.

In addition to Znojil's interpretation of the QHO Hamiltonian (3), that it leads, in effect, to the formally correct relativistic Dirac equation, we have shown that it could also represent a Klein–Gordon particle in a parabolic well. Precisely, the four-vector potential $eA_0 = -Ze^2(3 - r^2/a)/2a$, or in short $eA_0 = A + Br^2$, which represents an improved approximation for a realistic pionic atom, hence the Hamiltonian in equation (3) addresses the Klein–Gordon Hamiltonian for the potential of a homogeneously charged sphere [13].

The applicability of our recipe extends beyond the present QHO model and its application to other areas such as the following is in order: the eigenstates of a hydrogenic impurity in a spherical quantum dot (QD) [14]; quasi-two-dimensional QD helium [15]; two-electron QD in

a magnetic field [16]; excitons in a harmonic QD [17]; hydrogenic impurity or heavy excitons in an arbitrary magnetic field [18, 19] etc.

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