Anharmonic oscillators energies via artificial perturbation method

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Abstract. A new pseudoperturbative (artificial in nature) methodical proposal [15] is used to solve for Schrödinger equation with a class of phenomenologically useful and methodically challenging anharmonic oscillator potentials $V(q) = \alpha_o q^2 + \alpha q^4$. The effect of the [4,5] Padé approximant on the leading eigenenergy term is studied. Comparison with results from numerical (exact) and several eligible (approximation) methods is made.

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1 Introduction

Quartic anharmonic interactions continue to remain a focus of attention. Their Hamiltonian

$$H = \frac{p^2}{2m} + \alpha_0 r^2 + \alpha r^4 \qquad (1)$$

forms one of the most popular theoretical laboratories for examining the validity of various approximation techniques and represents a nontrivial physics. Interest in this model Hamiltonian arises in quantum field theory and molecular physics [1–6].

Although enormous progress has been made over the years in our understanding of this Hamiltonian, questions of delicate nature inevitably arise in the process. The hardest amongst often relate to the existence of the assumed small expansion parameter and the universality of an adequately attendant powerful approximation. The implementation of Rayleigh-Schrödinger perturbation theory, or even naive perturbation series, expresses the eigenvalues as a formal power series in α which is quite often divergent, or at best asymptotic, for every $\alpha \neq 0$. One has therefore to sum up such series [7–10]. Hence, apparently artificial perturbation recipes have been devised and shown to be ways to make progress [2,3,11–16]. Without being exhaustive, several eligible methods have been used to calculate the eigenvalues and eigenfunctions for Hamiltonian (1). Long lists of these could be found in references [2,3,8–10,13,17–19].

In this paper we introduce, in Section 2, a new analytical (or, preferably, semianalytical) perturbation method for solving Schrödinger equation. The construction of which starts with the time-independent one-dimensional

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form of Schrödinger equation, in $\hbar = m = 1$ units,

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

where l is some quantum number and n_r counts the nodal zeros in $\Psi_{n_r,l}(q)$. The symmetry of an attendant problem obviously manifests the admissibility of the quantum number l: in one-dimension (1D), l specifies parity, $(-1)^{l+1}$, with the permissible values -1 and/or 0 (even and/or odd parity, respectively) where $q = x \in (-\infty,\infty)$. For two-dimensional (2D) cylindrically symmetric Schrödinger equation one sets $l = |m| - 1/2$, where m is the magnetic quantum number and $q = (x^2 + y^2)^{1/2} \in (0,\infty)$. Finally, for three-dimensional (3D) spherically symmetric Schrödinger equation, l denotes the angular momentum quantum number with $q = (x^2 + y^2 + z^2)^{1/2} \in (0,\infty)$.

We shall focus our attention, in Section 3, on 1D and 3D problems and consider, for the sake of diversity;

(i) 3D anharmonic oscillators $V(r) = r^2/2 + r^4/2$ with $n_r = 0$ and $l = 0, 1, 2, 5, 10, 50$,

(ii) 3D ground state, or equivalently 1D first excited (odd-parity) state, for anharmonic oscillators $V(q) = q^2/2 + \alpha q^4$ over a wide range of anharmonicities (i.e. $\alpha = 0.002$ to $\alpha = 20000$),

(iii) 3D single-well anharmonic oscillator ground state, or equivalently 1D double-well anharmonic oscillator first excited state, for $V(q) = -aq^2/2 + q^4/2$ at various well depths (i.e. $a = 1, 5, 10, 15, 25, 50, 100$).

For the sake of comparison, we use results from exact numerical methods reported in [2,5], the best estimation of the phase-integral method (PIM) [5], an open perturbation technique [2], and a perturbative-variational method (PVM) [6]. Section 4 is reserved for concluding remarks.

2 The method

Our methodical proposal uses $1/\bar{l}$ as a perturbation expansion parameter, where $\bar{l} = l - \beta$ and β is a suitable shift mainly introduced to avoid the trivial case $l = 0$. Hence, hereafter, it will be referred to as the pseudoperturbative (artificial in nature) shifted-l expansion technique (PSLET). Equation (2) thus becomes

$$\left\{ -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}q^2} + \tilde{V}(q) \right\} \Psi_{n_r,l}(q) = E_{n_r,l}\Psi_{n_r,l}(q), \quad (3)$$

$$\tilde{V}(q) = \frac{\bar{l}^2 + (2\beta+1)\bar{l} + \beta(\beta+1)}{2q^2} + \frac{\bar{l}^2}{Q}V(q). \quad (4)$$

Herein, it should be noted that Q is a constant that scales the potential $V(q)$ at 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 [11,16]. And, β is to be determined in the sequel.

PSLET procedure begins with shifting the origin of the coordinate through

$$x = \bar{l}^{1/2}(q - q_\mathrm{o})/q_\mathrm{o}, \quad (5)$$

where q_o is currently an arbitrary point to perform Taylor expansions about, with its particular value to be determined. Expansions about this point, $x = 0$ (*i.e.* $q = q_\mathrm{o}$), yield

$$\frac{1}{q^2} = \sum_{n=0}^{\infty}(-1)^n\frac{(n+1)}{q_\mathrm{o}^2}x^n\bar{l}^{-n/2}, \quad (6)$$

$$V(x(q)) = \sum_{n=0}^{\infty}\left(\frac{\mathrm{d}^nV(q_\mathrm{o})}{\mathrm{d}q_\mathrm{o}^n}\right)\frac{(q_\mathrm{o}x)^n}{n!}\bar{l}^{-n/2}. \quad (7)$$

Obviously, the expansions in (6, 7) center the problem at an arbitrary point q_o and the derivatives, in effect, contain information not only at q_o but also at any point on q-axis, in accordance with Taylor's theorem. Also it should be mentioned here that the scaled coordinate, equation (5), has no effect on the energy eigenvalues, which are coordinate-independent. It just facilitates the calculations of both the energy eigenvalues and eigenfunctions. It is also convenient to expand E as

$$E_{n_r,l} = \sum_{n=-2}^{\infty}E_{n_r,l}^{(n)}\bar{l}^{-n}. \quad (8)$$

Equation (3) thus becomes

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{q_\mathrm{o}^2}{\bar{l}}\tilde{V}(x(q)) \right]\Psi_{n_r,l}(x) = \frac{q_\mathrm{o}^2}{\bar{l}}E_{n_r,l}\Psi_{n_r,l}(x), \quad (9)$$

with

$$\frac{q_\mathrm{o}^2}{\bar{l}}\tilde{V}(x(q)) = q_\mathrm{o}^2\bar{l}\left[\frac{1}{2q_\mathrm{o}^2} + \frac{V(q_\mathrm{o})}{Q}\right] + \bar{l}^{1/2}\left[-x + \frac{V'(q_\mathrm{o})q_\mathrm{o}^3x}{Q}\right]$$

$$+ \left[\frac{3}{2}x^2 + \frac{V''(q_\mathrm{o})q_\mathrm{o}^4x^2}{2Q}\right] + (2\beta+1)\sum_{n=1}^{\infty}(-1)^n\frac{(n+1)}{2}x^n\bar{l}^{-n/2}$$

$$+ q_\mathrm{o}^2\sum_{n=3}^{\infty}\left[(-1)^n\frac{(n+1)}{2q_\mathrm{o}^2}x^n + \left(\frac{\mathrm{d}^nV(q_\mathrm{o})}{\mathrm{d}q_\mathrm{o}^n}\right)\frac{(q_\mathrm{o}x)^n}{n!Q}\right]\bar{l}^{-(n-2)/2}$$

$$+ \beta(\beta+1)\sum_{n=0}^{\infty}(-1)^n\frac{(n+1)}{2}x^n\bar{l}^{-(n+2)/2} + \frac{(2\beta+1)}{2}, \quad (10)$$

where the prime of $V(q_\mathrm{o})$ denotes derivative with respect to q_o. Equation (9) is exactly of the type of Schrödinger equation for one-dimensional anharmonic oscillator

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}w^2x^2 + \varepsilon_\mathrm{o} + P(x)\right]X_{n_r}(x) = \lambda_{n_r}X_{n_r}(x), \quad (11)$$

where $P(x)$ is a perturbation-like term and ε_o is a constant. A simple comparison between equations (9, 10, 11) implies

$$\varepsilon_\mathrm{o} = \bar{l}\left[\frac{1}{2} + \frac{q_\mathrm{o}^2V(q_\mathrm{o})}{Q}\right] + \frac{2\beta+1}{2} + \frac{\beta(\beta+1)}{2\bar{l}}, \quad (12)$$

$$\lambda_{n_r} = \bar{l}\left[\frac{1}{2} + \frac{q_\mathrm{o}^2V(q_\mathrm{o})}{Q}\right] + \left[\frac{2\beta+1}{2} + \left(n_r + \frac{1}{2}\right)w\right]$$

$$+ \frac{1}{\bar{l}}\left[\frac{\beta(\beta+1)}{2} + \lambda_{n_r}^{(0)}\right] + \sum_{n=2}^{\infty}\lambda_{n_r}^{(n-1)}\bar{l}^{-n}, \quad (13)$$

and

$$\lambda_{n_r} = q_\mathrm{o}^2\sum_{n=-2}^{\infty}E_{n_r,l}^{(n)}\bar{l}^{-(n+1)}. \quad (14)$$

Equations (13, 14) yield

$$E_{n_r,l}^{(-2)} = \frac{1}{2q_\mathrm{o}^2} + \frac{V(q_\mathrm{o})}{Q} \quad (15)$$

$$E_{n_r,l}^{(-1)} = \frac{1}{q_\mathrm{o}^2}\left[\frac{2\beta+1}{2} + \left(n_r + \frac{1}{2}\right)w\right] \quad (16)$$

$$E_{n_r,l}^{(0)} = \frac{1}{q_\mathrm{o}^2}\left[\frac{\beta(\beta+1)}{2} + \lambda_{n_r}^{(0)}\right] \quad (17)$$

$$E_{n_r,l}^{(n)} = \lambda_{n_r}^{(n)}/q_\mathrm{o}^2; \quad n \geq 1. \quad (18)$$

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

$$\frac{\mathrm{d}E_{n_r,l}^{(-2)}}{\mathrm{d}q_\mathrm{o}} = 0 \quad \text{and} \quad \frac{\mathrm{d}^2 E_{n_r,l}^{(-2)}}{\mathrm{d}q_\mathrm{o}^2} > 0. \tag{19}$$

Hereby, $V(q)$ is assumed to be well behaved so that $E^{(-2)}$ has a minimum q_o and there are well-defined bound-states. Equation (19) in turn gives, with $\bar{l} = \sqrt{Q}$,

$$l - \beta = \sqrt{q_\mathrm{o}^3 V'(q_\mathrm{o})}. \tag{20}$$

Consequently, the second term in equation (10) vanishes and the first term adds a constant to the energy eigenvalues. It should be noted that energy term $\bar{l}^2 E_{n_r,l}^{(-2)}$ has its counterpart in classical mechanics. It corresponds roughly to the energy of a classical particle with angular momentum $L_z = \bar{l}$ executing circular motion of radius q_o in the potential $V(q_\mathrm{o})$. This term thus identifies the leading-order approximation, to all eigenvalues, as a classical approximation and the higher-order corrections as quantum fluctuations around the minimum q_o, organized in inverse powers of $\bar{l}$. The next leading correction to the energy series, $\bar{l}E_{n_r,l}^{(-1)}$, consists of a constant term and the exact eigenvalues of the unperturbed harmonic oscillator potential $w^2 x^2/2$. The shifting parameter β is determined by choosing $\bar{l}E_{n_r,l}^{(-1)} = 0$. This choice is physically motivated. It requires not only the agreements between PSLET eigenvalues and the exact known ones for the harmonic oscillator and Coulomb potentials but also between the eigenfunctions. Hence

$$\beta = -\left[\frac{1}{2} + \left(n_r + \frac{1}{2}\right)w\right], \tag{21}$$

where

$$w = \sqrt{3 + \frac{q_\mathrm{o} V''(q_\mathrm{o})}{V'(q_\mathrm{o})}}. \tag{22}$$

Then equation (10) reduces to

$$\frac{q_\mathrm{o}^2}{\bar{l}}\tilde{V}(x(q)) = q_\mathrm{o}^2\bar{l}\left[\frac{1}{2q_\mathrm{o}^2} + \frac{V(q_\mathrm{o})}{Q}\right] + \sum_{n=0}^{\infty} v^{(n)}(x)\bar{l}^{-n/2}, \tag{23}$$

where

$$v^{(0)}(x) = \frac{1}{2}w^2 x^2 + \frac{2\beta + 1}{2}, \tag{24}$$

$$v^{(1)}(x) = -(2\beta + 1)x - 2x^3 + \frac{q_\mathrm{o}^5 V'''(q_\mathrm{o})}{6Q}x^3, \tag{25}$$

and for $n \geq 2$

$$v^{(n)}(x) = (-1)^n(2\beta + 1)\frac{(n+1)}{2}x^n$$

$$+ (-1)^n\frac{\beta(\beta + 1)}{2}(n-1)x^{(n-2)}$$

$$+ \left[(-1)^n\frac{(n+3)}{2} + \frac{q_\mathrm{o}^{(n+4)}}{Q(n+2)!}\frac{\mathrm{d}^{n+2}V(q_\mathrm{o})}{\mathrm{d}q_\mathrm{o}^{n+2}}\right]x^{n+2}. \tag{26}$$

Equation (9) thus becomes

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

$$\left[\frac{1}{\bar{l}}\left(\frac{\beta(\beta + 1)}{2} + \lambda_{n_r}^{(0)}\right) + \sum_{n=2}^{\infty} \lambda_{n_r}^{(n-1)}\bar{l}^{-n}\right]\Psi_{n_r,l}(x). \tag{27}$$

Up to this point, one would conclude that the above procedure is nothing but an imitation of the eminent shifted large-N expansion (SLNT) [12,14,16,20–22]. However, because of the limited capability of SLNT in handling large-order corrections *via* the standard Rayleigh-Schrödinger perturbation theory, only low-order corrections have been reported, sacrificing in effect its preciseness. Therefore, one should seek for an alternative and proceed by setting the nodeless, $n_r = 0$, wave functions as

$$\Psi_{0,l}(x(q)) = \exp(U_{0,l}(x)). \tag{28}$$

In turn, equation (27) readily transforms into the following Riccati equation ([2,3] and references therein):

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

$$\frac{1}{\bar{l}}\left(\frac{\beta(\beta + 1)}{2} + \lambda_0^{(0)}\right) + \sum_{n=2}^{\infty} \lambda_0^{(n-1)}\bar{l}^{-n}. \tag{29}$$

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

$$U'(x) = \sum_{n=0}^{\infty} U^{(n)}(x)\bar{l}^{-n/2} + \sum_{n=0}^{\infty} G^{(n)}(x)\bar{l}^{-(n+1)/2}, \tag{30}$$

where

$$U^{(n)}(x) = \sum_{m=0}^{n+1} D_{m,n}x^{2m-1}; \quad D_{0,n} = 0, \tag{31}$$

$$G^{(n)}(x) = \sum_{m=0}^{n+1} C_{m,n}x^{2m}. \tag{32}$$

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

$$+\sum_{n=0}^{\infty}v^{(n)}\bar{l}^{-n/2}=\frac{1}{\bar{l}}\left(\frac{\beta(\beta+1)}{2}+\lambda_0^{(0)}\right)+\sum_{n=2}^{\infty}\lambda_0^{(n-1)}\bar{l}^{-n}\quad(33)$$

Substituting equations (30–32) into equation (29) implies

see equation (33) above,

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

$$-\frac{1}{2}U^{(0)'}-\frac{1}{2}U^{(0)}U^{(0)}+v^{(0)}=0,\quad(34)$$

$$U^{(0)'}(x)=D_{1,0};\quad D_{1,0}=-w,\quad(35)$$

and integration over x yields

$$U^{(0)}(x)=-wx.\quad(36)$$

Similarly,

$$-\frac{1}{2}[U^{(1)'}+G^{(0)'}]-U^{(0)}U^{(1)}-U^{(0)}G^{(0)}+v^{(1)}=0,\quad(37)$$

$$U^{(1)}(x)=0,\quad(38)$$

$$G^{(0)}(x)=C_{0,0}+C_{1,0}x^2,\quad(39)$$

$$C_{1,0}=-\frac{B_1}{w},\quad(40)$$

$$C_{0,0}=\frac{1}{w}(C_{1,0}+2\beta+1),\quad(41)$$

$$B_1=-2+\frac{q_o^5}{6Q}\frac{\mathrm{d}^3V(q_o)}{\mathrm{d}q_o^3},\quad(42)$$

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

$$-\sum_{n=0}^{1}U^{(n)}G^{(1-n)}+v^{(2)}=\frac{\beta(\beta+1)}{2}+\lambda_0^{(0)},\quad(43)$$

$$U^{(2)}(x)=D_{1,2}x+D_{2,2}x^3,\quad(44)$$

$$G^{(1)}(x)=0,\quad(45)$$

$$D_{2,2}=\frac{1}{w}(\frac{C_{1,0}^2}{2}-B_2),\quad(46)$$

$$D_{1,2}=\frac{1}{w}\left(\frac{3}{2}D_{2,2}+C_{0,0}C_{1,0}-\frac{3}{2}(2\beta+1)\right),\quad(47)$$

$$B_2=\frac{5}{2}+\frac{q_o^6}{24Q}\frac{\mathrm{d}^4V(q_o)}{\mathrm{d}q_o^4},\quad(48)$$

$$\lambda_0^{(0)}=-\frac{1}{2}(D_{1,2}+C_{0,0}^2)\quad(49)$$

and so on. 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.

Although the energy series, equation (8), could appear divergent, or, at best, asymptotic for small $\bar{l}$, one can still calculate the eigenenergies to a very good accuracy by forming the sophisticated $[N, M+1]$ Padé approximation

$$P_N^{M+1}(1/\bar{l})=$$
$$(P_0+P_1/\bar{l}+\cdots+P_M/\bar{l}^M)/(1+q_1/\bar{l}+\cdots+q_N/\bar{l}^N)$$

to the energy series [23]. The energy series, equation (8), is calculated up to $E_{0,l}^{(8)}/\bar{l}^8$ by

$$E_{0,l}=\bar{l}^2E_{0,l}^{(-2)}+E_{0,l}^{(0)}+\cdots+E_{0,l}^{(8)}/\bar{l}^8+O(1/\bar{l}^9),\quad(50)$$

and with the $P_4^5(1/\bar{l})$ Padé approximant it becomes

$$E_{0,l}[4,5]=\bar{l}^2E_{0,l}^{(-2)}+P_4^5(1/\bar{l}).\quad(51)$$

3 Quartic anharmonic interactions

Let us consider the phenomenologically useful and methodically challenging quartic anharmonic interactions

$$V(q)=\alpha_o q^2+\alpha q^4\quad(52)$$

of Hamiltonian (1). Equation (22) then reads

$$w=\sqrt{\frac{8\alpha_o q_o+24\alpha q_o^3}{2\alpha_o q_o+4\alpha q_o^3}},\quad(53)$$

and equation (20) yields

$$l+\frac{1}{2}\left(1+\sqrt{\frac{8\alpha_o q_o+24\alpha q_o^3}{2\alpha_o q_o+4\alpha q_o^3}}\right)=q_o^2\sqrt{2\alpha_o+4\alpha q_o^2}.\quad(54)$$

In the absence of a closed form solution for q_o in (54), one should appeal to some software packages (MAPLE is used here) to resolve this issue. Of course there is always more than one root for (54). However, the symmetry of

Table 1. Eigenvalues from the fifth-order phase-integral method E_{PIM} [5], the pseudoperturbative shifted-l expansion technique E_{PSLET}, the effect of the [4,5] Padé approximant on our leading energy term $E[4,5]$, and from the exact numerical calculations [5] for the three-dimensional anharmonic oscillator $V(r) = \frac{1}{2}r^2 + \frac{1}{2}r^4$, with $n_r = 0$.

	$l = 0$	$l = 1$	$l = 2$
E_{PIM}	2.324 83	4.190 26	6.242 80
E_{PSLET}	2.324 40	4.190 17	6.242 78
$E[4,5]$	2.324 41	4.190 17	6.242 78
E_{exact}	2.324 41	4.190 17	6.242 78
	$l = 5$	$l = 10$	$l = 50$
E_{PIM}	13.264 459 9	27.092 492 362	187.529 708 014 021
E_{PSLET}	13.264 458 8	27.092 492 304	187.529 708 014 0025
$E[4,5]$	13.264 458 8	27.092 492 304	187.529 708 014 0025
E_{exact}	13.264 458 8	27.092 492 305	187.529 708 014 003

Table 2. Three-dimensional ground state energies or equivalently one-dimensional first excited state energies for $V(q) = \frac{q^2}{2} + \alpha q^4$. E_{BB} denotes Bessis and Bessis results [2] and the exact ones E_{exact}, reported therein, for different anharmonicities.

α	E_{PSLET}	$E[4,5]$	E_{BB}	E_{exact}
0.002	1.507 41940	1.507 41940	1.507 4194	1.507 41939
0.006	1.521 80570	1.521 80570	1.521 8057	1.521 80565
0.01	1.535 64844	1.535 64846	1.535 6483	1.535 64828
0.05	1.653 439	1.653 439	1.653 441	1.653 43601
0.1	1.769 512	1.769 625	1.769 529	1.769 50264
0.3	2.094 678	2.094 640	2.094 795	2.094 64199
0.5	2.324 401	2.324 407	2.324 661	2.324 40635
0.7	2.509 16	2.509 23	2.509 56	2.509 22810
1	2.737 73	2.737 91	2.738 32	2.737 89227
2	3.292 48	3.292 94	3.293 50	3.292 86782
50	8.913 21	8.916 61	8.917 41	8.915 09636
200	14.056 17	14.062 53	14.062 96	14.059 2268
1000	23.966 93	23.978 93	23.978 63	23.972 2061
8000	47.880 19	47.890 95	47.903 66	47.890 7687
20000	64.972 32	65.006 64	65.004 18	64.986 6757

Table 3. Three-dimensional ground state energies or equivalently one-dimensional first excited state energies for $V(q) = -aq^2/2 + q^4/2$. E_{PVM} represents the results from perturbative-variational method [6].

a	E_{PVM}	E_{PSLET}	$E[4,5]$
1	2.834 5	2.835 3	2.834 4
5	−3.250 68	−3.250 85	−3.250 84
10	−20.633 55	−25.633 69	−20.633 50
15	−50.841 387	−50.841 42	−50.841 42
25	−149.219 456	−149.219 454	−149.219 454
50	−615.020 090 9	−615.020 091 0	−615.020 091 0
100	−2845.867 880 34	−2485.867 880 337	−2485.867 880 337

the problem in hand along with equation (19) would single out one eligible root q_o as a minimum of $E^{(-2)}$. Once q_o is determined the coefficients $C_{m,n}$ and $D_{m,n}$ are obtained in a sequential manner. Consequently, the eigenvalues, equation (50), and eigenfunctions, equations (30–32), are calculated in the same batch for each value of α_o, α, and l.

Our results (Tabs. 1–3) are obtained from the first eleven terms of our energy series (50). Also, the effect of the [4,5] Padé approximant on the leading term $\bar{l}^2 E^{(-2)}$ is reported as $E[4,5]$. In Table 1 we list our results along with the exact numerical ones and the (best estimated) eigenvalues obtained from the fifth-order phase-integral method (PIM) reported by Lakshmanen *et al.* [5]. Obviously, our results compare excellently with the exact numerical ones and surpass those from PIM. Whilst the [4,5] Padé approximant had no dramatic effect on the energy eigenvalues for $l = 0$, it had no effect on the energy eigenvalues for $l \geq 1$. A common feature between PSLET and PIM is well pronounced here; the precession of both methods increases as l increases.

Again we proceed with the theoretical laboratory (52) and examine the validity of PSLET over a wide range of

anharmonicities for $V(q) = q^2/2 + \alpha q^4$. In Table 2 we list our results for the three-dimensional (3D) ground states energies, or equivalently for the one-dimensional (1D) first excited state energies. The results of Bessis and Bessis [2], *via* an open perturbation recipe, and the exact ones [24], using Bargman representation, are also displayed. Clearly and satisfactorily, the trend of the exact values of the energies is reproduced.

Finally, we consider the ground state energies of the 3D single-well, or equivalently the first excited state energies of the 1D double-well, potentials $V(q) = -aq^2/2 + q^4/2$. We compare our results (Tab. 3) with those obtained by Saavedra and Buendia [6] *via* a perturbative-variational method (PVM). They are in excellent agreement not only with the PVM but also with the hypervirial perturbation method [25], especially for deep wells.

4 Concluding remarks

The method (PSLET) just described is conceptually sound. It avoids troublesome questions such as those pertaining to the nature of small-parameter expansions, the trend of convergence to the exact numerical values, the utility in calculating the eigenvalues and eigenfunctions (in one batch) to sufficiently heigher-orders, and the applicability to a wide rang of potentials. Provided that the latter is analytic and give rise to one minimum of $E^{(-2)}$ and an infinite number of bound states.

On the computational and practical methodology sides, PSLET comes in quite handy and very accurate numerical results are obtained. Nevertheless, if greater accuracy is in demand, another suitable criterion for choosing the value of the shift β, reported in [13,25], is also feasible. However, one would always be interested, for practical exploratory purposes, in the conventional wisdom of perturbation prescriptions that only a few terms of a "most useful" perturbation series reveal the important features of the solution before a state of exhaustion is reached. Our method indeed belongs to this category where the results of the illustrative challenging examples used bear this out.

On the other hand, asymptotic wavefunctions emerge in our procedure from the knowledge of $C_{m,n}$ and $D_{m,n}$ to study, for example, electronic transitions and multiphoton emission occurring in atomic systems. Such studies already lie beyond the scope of our present methodical proposal.

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