Part of the *D*-dimensional spiked harmonic oscillator spectra

2000 J. Phys. A: Math. Gen. 33 5207

(http://iopscience.iop.org/0305-4470/33/29/305)

J. Phys. A: Math. Gen. **33** (2000) 5207–5217. Printed in the UK PII: S0305-4470(00)12335-2

Part of the D-dimensional spiked harmonic oscillator spectra

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

Received 3 March 2000, in final form 26 May 2000

Abstract. The pseudoperturbative shifted-l expansion technique (PSLET) is generalized for states with an arbitrary number of nodal zeros. Interdimensional degeneracies, emerging from the isomorphism between the angular momentum and the dimensionality of the central force Schrödinger equation, are used to construct part of the D-dimensional spiked harmonic oscillator bound-state spectra. PSLET results are found to compare excellently with those from direct numerical integration and generalized variational methods.

1. Introduction

The simplest model of realistic interaction potentials in atomic, molecular and nuclear physics is provided by the spiked harmonic oscillator

$$V(q) = c_1 q^2 + c_2 q^{-b} \qquad c_1, c_2, b > 0 \qquad q \in (0, \infty). \tag{1}$$

The construction of its bound states has attracted attention over the last few years [1–9]. It is an interesting model not only because of being a singular potential representing a repulsive core in realistic interactions, but also because of its intrinsic properties in view of mathematical physics [10–16]. However, most of the studies on this model potential (1) have been devoted to one spatial dimension (1D, the hyperquantum limit in view of Herschbach [17, 18]). It was just very recently, to the best of our knowledge, that Hall and Saad generalized their variational analysis (see the first reference of [1]) and smooth transformation [2] methods, VAM and STM, respectively, to the D-dimensional case and studied its bound states. They have also used direct numerical integration (DNI) for the purposes of comparison. It is therefore interesting to carry out systematic studies of the bound-state spectra generated by this interesting class of singular potentials (1).

On the other hand, results from exactly solvable potentials (an interesting field of mathematical physics in itself) are essential ingredients for the description of realistic physical problems [1–5, 19]. The solutions of these can be used in perturbation and pseudoperturbation theories, or they can be combined with numerical calculations. Nevertheless, in the simplest case, analytical calculations can aid numerical studies in areas where numerical techniques might not be safely controlled. For example, when bound-state wavefunctions with arbitrary nodal zeros are required for certain singular potentials (a next level of complexity), analytical solutions can supply a basis for numerical calculations. Moreover, in many problems the Hamiltonian does not contain any physical parameter suitable for a perturbation expansion

0305-4470/00/295207+11$30.00

treatment. More often, the Hamiltonian contains physical parameters, but, typically, zeroth-order solutions for special values of these are not tractable or good starting approximations. One therefore resorts to variational calculations [1], pseudoperturbation expansions (artificial in nature) [5, 18–26], etc.

Recently, we have introduced a pseudoperturbative shifted-l (l is the angular momentum quantum number) expansion technique (PSLET) to solve for nodeless states of the Schrödinger equation. It simply consists of using $1/\bar{l}$ as a pseudoperturbation parameter, where $\bar{l} = l - \beta$ and β is a suitable shift. The shift β is vital as it removes the poles that would emerge, at lowest orbital states with $l = 0$, in our proposed expansions below. Our analytical, or often semianalytical, methodical proposal PSLET has been successfully applied to the quasi-relativistic harmonic oscillator [20], spiked harmonic oscillator [5], anharmonic oscillators [21] and to the two-dimensional (*flatland*, in view of Godson and López- Cabrera in [17]) hydrogenic atom in an arbitrary magnetic field [22].

Encouraged by its satisfactory performance in handling nodeless states, we generalize the PSLET recipe (in section 2) for states with an arbitrary number of nodal zeros, $k \geqslant 0$. Moreover, in the underlying 'radical' time-independent radial Schrödinger equation, in $\hbar = m = 1$ units

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

the isomorphism between the orbital angular momentum l and the dimensionality D invites interdimensional degeneracies [17]. Which, in effect, allows us to generate the ladder of excited states for any given k and non-zero l from the $l = 0$ result, with that k, by the transcription $D \longrightarrow D + 2l$. That is, if $E_{k,l}(D)$ is the eigenvalue in D dimensions, then

$$E_{k,l}(2) \equiv E_{k,l-1}(4) \equiv \cdots \equiv E_{k,1}(2l) \equiv E_{k,0}(2l+2) \tag{3}$$

for even D, and

$$E_{k,l}(3) \equiv E_{k,l-1}(5) \equiv \cdots \equiv E_{k,1}(2l+1) \equiv E_{k,0}(2l+3) \tag{4}$$

for odd D. For more details the reader may refer to [17, 18, 27]. We therefore calculate, in section 3, the energies for $D = 2$ and 3 spiked harmonic oscillators, for a given number of nodes k and different values of l, and construct part of its D-dimensional bound-state spectra. We compare our results with those reported by Hall and Saad via generalized variational analysis VAM, and direct numerical integration methods [1, 2]. Section 4 is devoted to concluding remarks.

2. The generalization of PSLET

With the shifted angular momentum, equation (2) reads

$$\left\{-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}q^2} + \frac{\bar{l}^{\,2} + (2\beta+1)\bar{l} + \beta(\beta+1)}{2q^2} + \frac{\bar{l}^{\,2}}{Q}V(q)\right\}\Psi_{k,l}(q) = E_{k,l}\Psi_{k,l}(q) \tag{5}$$

where Q is a constant that scales the potential $V(q)$ at large-l_D limit (the pseudoclassical limit [17]) and is set, for any specific choice of l_D and k, equal to $\bar{l}^{\,2}$ at the end of the calculations. Here $l_D = l + (D-3)/2$, to incorporate the interdimensional degeneracies associated with the isomorphism between the angular momentum and the dimensionality D. Hence, $\bar{l} \longrightarrow \bar{l} = l_D - \beta$ throughout this paper. Next, we shift the origin of the coordinate system through $x = \bar{l}^{\,1/2}(q - q_0)/q_0$, where q_0 is currently an arbitrary point to be determined

below. Expansions about this point (see the appendix for more details), $x = 0$ (i.e. $q = q_0$), obviously localize the problem at an arbitrary point q_0 and the derivatives, in effect, contain information not only at q_0 but also at any point on the q-axis, in accordance with Taylor's theorem. It is then convenient to expand $E_{k,l}$ as

$$E_{k,l} = \sum_{n=-2}^{\infty} E_{k,l}^{(n)}\, \bar{l}^{\,-n}. \tag{6}$$

Equation (5) thus becomes

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{n=0}^{\infty} v^{(n)} \bar{l}^{\,-n/2}\right] \Psi_{k,l}(x) = \left[\sum_{n=1}^{\infty} q_0^2 E_{k,l}^{(n-1)} \bar{l}^{\,-n}\right] \Psi_{k,l}(x). \tag{7}$$

Up to this point, one would conclude that the above procedure is nothing but an imitation of the eminent shifted large-N expansion (SLNT) [25, 26, 28–30]. 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, in effect sacrificing its preciseness. Therefore, one should seek for an alternative and proceed by setting the wavefunctions with any number of nodes as

$$\Psi_{k,l}(x(q)) = F_{k,l}(x) \exp(U_{k,l}(x)). \tag{8}$$

In turn, equation (7) readily transforms into the following Riccati equation:

$$F_{k,l}(x)\left[-\tfrac{1}{2}\left(U_{k,l}^{\prime\prime}(x) + U_{k,l}^{\prime}(x)U_{k,l}^{\prime}(x)\right) + \sum_{n=0}^{\infty} v^{(n)}(x)\bar{l}^{\,-n/2} - \sum_{n=1}^{\infty} q_0^2 E_{k,l}^{(n-1)} \bar{l}^{\,-n}\right]$$
$$-F_{k,l}^{\prime}(x)U_{k,l}^{\prime}(x) - \tfrac{1}{2}F_{k,l}^{\prime\prime}(x) = 0 \tag{9}$$

where the primes denote derivatives with respect to x. It is evident that this equation admits solution of the form

$$U_{k,l}^{\prime}(x) = \sum_{n=0}^{\infty} U_k^{(n)}(x)\, \bar{l}^{\,-n/2} + \sum_{n=0}^{\infty} G_k^{(n)}(x)\, \bar{l}^{\,-(n+1)/2} \tag{10}$$

$$F_{k,l}(x) = x^k + \sum_{n=0}^{\infty}\sum_{p=0}^{k-1} a_{p,k}^{(n)}\, x^p\, \bar{l}^{\,-n/2} \tag{11}$$

where

$$U_k^{(n)}(x) = \sum_{m=0}^{n+1} D_{m,n,k}\, x^{2m-1} \qquad D_{0,n,k} = 0 \tag{12}$$

$$G_k^{(n)}(x) = \sum_{m=0}^{n+1} C_{m,n,k}\, x^{2m}. \tag{13}$$

Substituting equations (10)–(13) into equation (9) implies

$$F_{k,l}(x)\left[-\tfrac{1}{2}\sum_{n=0}^{\infty}\left(U_k^{(n)^{\prime}} \bar{l}^{\,-n/2} + G_k^{(n)^{\prime}} \bar{l}^{\,-(n+1)/2}\right)\right.$$
$$\left.-\tfrac{1}{2}\sum_{n=0}^{\infty}\sum_{m=0}^{n}\left(U_k^{(m)}U_k^{(n-m)}\bar{l}^{\,-n/2} + G_k^{(m)}G_k^{(n-m)}\bar{l}^{\,-(n+2)/2} + 2U_k^{(m)}G_k^{(n-m)}\bar{l}^{\,-(n+1)/2}\right)\right.$$

$$+\sum_{n=0}^{\infty} v^{(n)}\bar{l}^{\,-n/2} - \sum_{n=1}^{\infty} q_0^2 E_{k,l}^{(n-1)}\bar{l}^{\,-n}\Bigg]$$

$$-F'_{k,l}(x)\left[\sum_{n=0}^{\infty}\left(U_k^{(n)}\bar{l}^{\,-n/2} + G_k^{(n)}\bar{l}^{\,-(n+1)/2}\right)\right] - \tfrac{1}{2}F''_{k,l}(x) = 0. \tag{14}$$

The above procedure obviously reduces to that described by Mustafa and Odeh [5, 20–22], for $k = 0$. Moreover, the solution of equation (14) follows from the uniqueness of the power-series representation. Therefore, for a given k we equate the coefficients of the same powers of $\bar{l}$ and x, respectively. For example, when $k = 1$ one obtains

$$D_{1,0,1} = -w \qquad U_1^{(0)}(x) = -wx \tag{15}$$

$$C_{1,0,1} = -\frac{B_3}{w} \qquad a_{0,1}^{(1)} = -\frac{C_{0,0,1}}{w} \tag{16}$$

$$C_{0,0,1} = \frac{1}{w}\left(2C_{1,0,1} + 2\beta + 1\right) \tag{17}$$

$$D_{2,2,1} = \frac{1}{w}\left(\tfrac{1}{2}C_{1,0,1}^2 - B_4\right) \tag{18}$$

$$D_{1,2,1} = \frac{1}{w}\left(\tfrac{5}{2}\,D_{2,2,1} + C_{0,0,1}\,C_{1,0,1} - \tfrac{3}{2}(2\beta + 1)\right) \tag{19}$$

$$E_{1,l}^{(0)} = \frac{1}{q_0^2}\left(\tfrac{1}{2}\beta(\beta+1) + a_{0,1}^{(1)}\,C_{1,0,1} - \tfrac{3}{2}D_{1,2,1} - \tfrac{1}{2}C_{0,0,1}^2\right) \tag{20}$$

etc. Here, we reported the non-zero coefficients only and give the definitions of the related parameters in the appendix. One can then calculate the energy eigenvalues and eigenfunctions from knowledge of $C_{m,n,k}$, $D_{m,n,k}$ and $a_{p,k}^{(n)}$ in a hierarchical manner. Nevertheless, the procedure just described is suitable for a software package such as *Maple* to determine the energy eigenvalue and eigenfunction corrections up to any order of the pseudoperturbation series (6).

Although the energy series, equation (6), 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 $[N, M]$ Padé approximation [24]

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

to the energy series (6). The energy series (6) is calculated up to $E_{k,l}^{(8)}/\bar{l}^{\,8}$ by

$$E_{k,l} = \bar{l}^{\,2}E_{k,l}^{(-2)} + E_{k,l}^{(0)} + \cdots + E_{k,l}^{(8)}/\bar{l}^{\,8} + \mathrm{O}(1/\bar{l}^{\,9}) \tag{21}$$

and with the $P_4^4(1/\bar{l})$ Padé approximant it becomes

$$E_{k,l}[4,4] = \bar{l}^{\,2}E_{k,l}^{(-2)} + P_4^4(1/\bar{l}). \tag{22}$$

Our recipe is therefore well prescribed.

3. *D*-spiked harmonic oscillator spectra

In this section we consider the spiked harmonic oscillator potential (1) and illustrate the above-mentioned procedure. The substitution of equation (1) in (A16), for $k \geqslant 0$, implies

$$w = \sqrt{\frac{8c_1q_0 + bc_2(b-2)q_0^{-(b+1)}}{2c_1q_0 - bc_2q_0^{-(b+1)}}} \qquad \beta = -\tfrac{1}{2}(1 + [2k+1]w). \tag{23}$$

Equation (A15), in turn, reads

$$l_D + \frac{1}{2}\left(1 + [2k+1]\sqrt{\frac{8c_1q_0 + bc_2(b-2)q_0^{-(b+1)}}{2c_1q_0 - bc_2q_0^{-(b+1)}}}\right) = q_0^2\sqrt{c_1 - \tfrac{1}{2}bc_2q_0^{-(b+2)}} \tag{24}$$

which is explicit in q_0. However, in the absence of a closed-form solution for q_0, which is often the case (hence the notion that PSLET is often semianalytical), numerical solutions of (24) could resolve this issue. Once q_0 is determined the coefficients $C_{m,n,k}$, $D_{m,n,k}$ and $a_{p,k}^{(n)}$ are determined in a sequential manner. Hence, the eigenvalues, equation (21), and eigenfunctions, equations (10)–(13), are calculated in the same batch for each value of k, D, l, c_1, c_2 and b.

Table 1 shows PSLET results for the ground-state energies, covering a wide range of the coupling c_2 when $b = 2.5$, along with those reported by Hall and Saad ([1], first reference), via a generalized variational analysis and direct numerical integration methods. Using the

Table 1. 3D ground-state energies, in $\hbar = m = 1$ units, for $V(q) = (q^2 + c_2/q^{5/2})/2$, where E_{P} represents PSLET results, equation (21), and $\bar{l}^2E^{(-2)}$ is its zeroth-order approximation. $E[4,4]$ shows the effect of the $P_4^4(1/\bar{l})$ Padé approximant, equation (22). E_{VAM} from VAM, and E_{DNI} from DNI [1], first reference.

c_2	$\bar{l}^2E^{(-2)}$	E_{P}	$E[4,4]$	E_{VAM}	E_{DNI}
1000	44.003 142	44.955 4848	44.955 4848	44.955 485	44.955 485
100	16.666 664	17.541 890	17.541 890	17.541 890	17.541 890
10	7.001 49	7.735 15	7.735 10	7.735 11	7.735 11
1	3.847 71	4.315 78	4.314 13	4.323 26	4.317 31
0.1	3.111 32	3.269 84	3.266 33	3.296 02	3.266 87
0.01	3.011 6	3.034 1	3.034 4	3.039 2	3.036 7
0.001	3.001 2	3.003 5	3.004 0	3.004 1	3.004 0

Table 2. $D = 2, \ldots, 10$ ground-state energies, in $\hbar = m = 1$ units, for the potential $V(q) = (q^2 + 10/q^{1.9})/2$, where E_{P} represents PSLET results, equation (21), and $\bar{l}^2E^{(-2)}$ is its zeroth-order approximation, $E[4,4]$ shows the effect of the $P_4^4(1/\bar{l})$ Padé approximant, equation (22). E_{VAM} from VAM, and E_{DNI} from DNI ([1], first reference).

D	$\bar{l}^2E^{(-2)}$	E_{P}	$E[4,4]$	E_{VAM}	E_{DNI}
2	7.581 139	8.485 461	8.485 369	8.485 384	8.485 378
3	7.919 880	8.564 352	8.564 355	8.564 358	8.564 356
4	8.339 920	8.795 436	8.795 440	8.795 440	8.795 440
5	8.840 678	9.163 092	9.163 093	9.163 093	9.163 093
6	9.416 352	9.646 701	9.646 701	9.646 701	9.646 701
7	10.058 042	10.225 045	10.225 045	10.225 045	10.225 045
8	10.755 870	10.879 077	10.879 077	10.879 077	10.879 077
9	11.500 402	11.592 982	11.592 982	11.592 982	11.592 982
10	12.283 349	12.354 183	12.354 183	12.354 183	12.354 183

Table 3. 2D and 3D nodeless states energies, with $l = 0, \ldots, 4$ (in $\hbar = m = 1$ units), for the potential $V(q) = (q^2 + 1000/q^b)/2$, where $E_{0,l}$ represents PSLET results with the $P_4^4(1/\bar{l})$ Padé approximant, equation (22).

D	b	$E_{0,0}$	$E_{0,1}$	$E_{0,2}$	$E_{0,3}$	$E_{0,4}$
2	0.5	415.886 751	415.898 889	415.935 293	415.995 938	416.080 780
	1	190.719 321	190.735 267	190.783 089	190.862 739	190.974 135
	1.5	104.404 517	104.427 341	104.495 769	104.609 681	104.768 874
	2	65.245 553	65.277 168	65.371 918	65.529 521	65.749 510
	2.5	44.945 030	44.986 838	45.112 071	45.320 150	45.610 129
	3	33.303 511	33.356 491	33.515 080	33.778 229	34.144 222
3	0.5	415.889 786	415.914 059	415.962 588	416.035 338	416.132 258
	1	190.723 31	190.755 196	190.818 940	190.914 475	191.041 704
	1.5	104.410 22	104.455 860	104.547 051	104.683 633	104.865 367
	2	65.253 459	65.316 665	65.442 888	65.631 753	65.882 705
	2.5	44.955 49	45.039 054	45.205 805	45.454 976	45.785 438
	3	33.316 76	33.422 634	33.633 677	33.948 503	34.365 078

Table 4. 2D and 3D k-state energies, in $\hbar = m = 1$ units, for the potential $V(q) = (q^2 + 1000/q^{3/2})/2$, where E_{P} represents PSLET results, equation (21), and $\bar{l}^2 E^{(-2)}$ is its zeroth-order approximation, $E[4, 4]$ shows the effect of the $P_4^4(1/\bar{l})$ Padé approximant, equation (22).

D	k	l	$\bar{l}^2 E^{(-2)}$	E_{P}	$E[4, 4]$
2	1	0	105.404 19	108.150 83	108.150 83
		1	105.674 66	108.173 79	108.173 79
		2	105.969 40	108.242 63	108.242 63
		3	106.289 70	108.357 21	108.357 21
3		0	105.536 48	108.156 57	108.156 57
		1	105.818 92	108.202 48	108.202 48
		2	106.126 28	108.294 21	108.294 21
		3	106.459 83	108.431 60	108.431 60
2	2	0	107.387 6	111.901 7	111.901 7
		1	107.738 2	111.924 8	111.924 8
		2	108.112 7	111.994 0	111.994 0
3		0	107.560 0	111.907 5	111.907 4
		1	107.922 4	111.953 6	111.953 6
		2	108.309 2	112.045 9	112.045 9

interdimensional degeneracies (equations (3) and (4)) or directly, the dimensionality D in l_D, we display the energies for $V(q) = (q^2 + 10/q^{1.9})/2$ in table 2. Clearly, our results compare excellently with those from direct numerical integrations. However, it should be noted that in [5] we have calculated the energy series up to $E_{0,l}^{(4)}/\bar{l}^4$ correction. Therefore, slight discrepancies obtain between the present results in table 1 and those reported in table 2 of [5].

Adhering to the implicated wisdom in equations (3) and (4), that the two- and three-dimensional cases are the basic ingredients of the energy ladder at larger dimensions, we report (in table 3) the 2D and 3D nodal bound-state energies when the coupling $c_2 = 1000$ and $b = 0.5, 1, \ldots, 2.5, 3$. The stability of the last three approximants of the Padé sequence indicates that the results are exact. For more details on this issue the reader may refer to [20, 24]. Nevertheless, our results $E_{0,0}$ for the 3D spiked harmonic oscillator are in exact accord with those from direct numerical integrations [2]. Following the same strategy, we display in table 4 the $k = 1$ and 2 nodal bound-state energies for $V(q) = (q^2 + 1000/q^{3/2})/2$.

Eventually, the leading term of PSLET, $\bar{l}^{\,2}E_{k,l}^{(-2)}$, turns out to be a good starting approximation. Tables 1, 2 and 4 bear this out.

Moreover, for the spiked harmonic oscillator, with $b = 2$, one would rewrite the effective potential term $(l(l+1)+c_2)/2q^2+q^2/2$ as $l'(l'+1)/2q^2+q^2/2$ with $l' = -\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2+c_2}$. For this particular case, the PSLET procedure yields, respectively, $w = 2$, $\beta = -\left(2k+\frac{3}{2}\right)$, $\bar{l} = 2k+l'+\frac{3}{2}$, $q_0^2 = \bar{l}$, $\bar{l}^{\,2}E_{k,l'}^{(-2)} = 2k+l'+\frac{3}{2}$ (the exact well known energies)

$$E_{k,l'}^{(0)} = E_{k,l'}^{(1)} = \cdots = E_{k,l'}^{(8)} = \cdots = E_{k,l'}^{(n)} = 0 \tag{25}$$

and when $k = 0$, for example,

$$\begin{aligned} U_{0,l'}(x) = &-\tfrac{1}{2}\left(y-\tfrac{1}{2}y^2+\tfrac{1}{3}y^3-\tfrac{1}{4}y^4+\tfrac{1}{5}y^5-\tfrac{1}{6}y^6+\tfrac{1}{7}y^7-\tfrac{1}{8}y^8+\cdots\right) \\ &+\bar{l}\left(y-\tfrac{1}{2}y^2+\tfrac{1}{3}y^3-\tfrac{1}{4}y^4+\tfrac{1}{5}y^5-\tfrac{1}{6}y^6+\tfrac{1}{7}y^7-\tfrac{1}{8}y^8+\cdots\right)-\tfrac{1}{2}\bar{l}y^2-\bar{l}y \end{aligned} \tag{26}$$

where $y = x\bar{l}^{\,-1/2}$. Obviously, the terms in parentheses in equation (26) are the infinite geometric series expansions for $\ln(1+y)$. Equation (26) thus becomes

$$U_{0,l'}(x) = \ln(1+y)^{-1/2}+\ln(1+y)^{\bar{l}}-\bar{l}y-\tfrac{1}{2}\bar{l}y^2. \tag{27}$$

Hence equation (8) (with $F_{0,l'}(x) = 1$ from (11)) reads

$$\Psi_{0,l'}(q) = N_{0,l'}\,q^{l'+1}\,\mathrm{e}^{-q^2/2} \tag{28}$$

the exact well known solutions [31], where $N_{0,l'}$ are the normalization constants. Proceeding exactly as above, one could obtain the well known solutions with $k \geqslant 1$. However, this already lies far beyond the scope of our present proposal.

Hall and Saad ([1], first reference) have therefore used, indirectly, the transformation of the angular momentum quantum number and cast the Hamiltonian of the spiked harmonic oscillator (1) as

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}q^2}+\frac{l_{\mathrm{H}}(l_{\mathrm{H}}+1)}{2q^2}+\frac{q^2}{2}+\frac{c_2}{2q^b}-\frac{A}{2q^2} \tag{29}$$

where $l_{\mathrm{H}} = -\frac{1}{2}+\sqrt{\left(l+\frac{1}{2}\right)^2+A}$, and A is used as a *further variational refinement* in their generalized variational analysis method. They found that $A = c_2$ is a *good* general estimate for the value of A. Indeed, this optimum value of A, which substantially reduced the number of the basis functions needed for a given accuracy in [1], first reference, enhances the convergence and accuracy of approximation method recipes. Practically, it minimizes the effect of the perturbation term c_2q^{-b} over the harmonic oscillator one (with the irrational quantum number l'), especially for values of $b \longrightarrow 2$. In table 5, the results of PSLET are obtained using such prescription. They compare excellently with direct numerical integrations and do not contradict the upper bounds from the generalized variational estimates.

4. Concluding remarks

We have generalized our pseudoperturbative shifted-l expansion technique PSLET [5, 20–22] for states with an arbitrary number of nodal zeros, $k \geqslant 0$. Starting with the central force problem, represented by the radial Schrödinger equation, and augmenting the orbital angular momentum by $l \longrightarrow l_D = l+(D-3)/2$, we have incorporated interdimensional degeneracies. To test the performance of PSLET, we have treated the spiked harmonic oscillator problem in

Table 5. $k = 2$ and $l = 1, 2$ energies, in units where $\hbar = m = 1$, for the potential $V(q) = (q^2 + 10/q^{2.1})/2$, where $E_{2,l,P}$ represents PSLET results, equation (21), $E_{2,1,\mathrm{V}}$ from VAM, and $E_{2,1,\mathrm{ex}}$ from DNI [1], first reference. $E_{2,l}[4,4]$ shows the effect of the $P_4^4(1/\bar{l})$ Padé approximant, equation (22).

D	$E_{2,1,\mathrm{ex}}$	$E_{2,1,\mathrm{V}}$	$E_{2,1,P}$	$E_{2,1}[4,4]$	$E_{2,2,P}$	$E_{2,2}[4,4]$
2	16.543 629	16.543 648	16.541 951	16.543 627	17.380 817	17.381 708
3	16.904 445	16.904 446	16.903 172	16.904 444	17.954 856	17.955 444
4	17.381 708	17.381 709	17.380 817	17.381 708	18.606 695	18.607 067
5	17.955 444	17.955 446	17.954 856	17.955 444	19.320 461	19.320 691
6	18.607 067	18.607 070	18.606 695	18.607 067	20.083 266	20.083 406
7	19.320 691	19.320 693	19.320 461	19.320 691	20.884 936	20.885 021
8	20.083 406	20.083 407	20.083 266	20.083 406	21.717 556	21.717 608
9	20.885 021	20.885 022	20.884 936	20.885 021	22.574 996	22.575 027
10	21.717 608	21.717 608	21.717 556	21.717 608	23.452 505	23.452 524

D dimensions and used results from direct numerical integrations and generalized variational analysis methods [1, 2] as a comparison. The comparison is satisfactory.

The salient features of the attendant proposal PSLET are in order.

It avoids troublesome questions such as those pertaining to the nature of small parameter expansions, the trend of convergence to the exact numerical values (marked in tables 1–3 and 5), the utility in calculating the eigenvalues and eigenfunctions in one batch to sufficiently higher orders (documented through the solution (28) of (1), with $b = 2$) and the applicability to a wide range of potentials. Provided that the potential $V(q)$ gives rise to one minimum of $E_{k,l}^{(-2)}$ and an infinite number of bound states. Moreover, beyond its promise of being quite handy (on the computational and practical methodical sides), it offers a useful perturbation prescription where the zeroth-order approximation $\bar{l}^{\,2} E_{k,l}^{(-2)}$ inherits a substantial amount of the total energy.

The above has been a very limited review and a number of other useful and novel approaches such as those presented by Papp [9, 32] and Bender and Wu [33], have not been touched on.

Finally, the scope of applicability of PSLET extends beyond the present D-dimensional spiked harmonic oscillator model. It could be applied to angular momentum states of multi-electron atoms [34–36], relativistic and non-relativistic quark–antiquark models [37], etc.

Appendix

Although some of the following expressions have appeared in previous articles [5, 20–22], we would like to repeat them to make this paper self-contained.

Expansions about $x = 0$ (i.e. $q = q_0$), yield

$$\frac{1}{q^2} = \sum_{n=0}^{\infty} (-1)^n \, \frac{(n+1)}{q_0^2} \, x^n \, \bar{l}^{\,-n/2} \tag{A1}$$

$$V(x(q)) = \sum_{n=0}^{\infty} \left(\frac{\mathrm{d}^n V(q_0)}{\mathrm{d}q_0^n} \right) \frac{(q_0 x)^n}{n!} \, \bar{l}^{\,-n/2}. \tag{A2}$$

Equation (5) thus becomes

$$\left[-\frac{1}{2} \frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{q_0^2}{\bar{l}} \tilde{V}(x(q)) \right] \Psi_{k,l}(x) = \frac{q_0^2}{\bar{l}} E_{k,l} \Psi_{k,l}(x) \tag{A3}$$

with

$$\frac{q_0^2}{\bar{l}}\tilde{V}(x(q)) = q_0^2\bar{l}\left[\frac{1}{2q_0^2}+\frac{V(q_0)}{Q}\right]+\bar{l}^{\,1/2}B_1x+B_2x^2+\tfrac{1}{2}(2\beta+1)$$
$$+(2\beta+1)\sum_{n=1}^{\infty}(-1)^n\tfrac{1}{2}(n+1)x^n\bar{l}^{\,-n/2}+\sum_{n=3}^{\infty}B_nx^n\bar{l}^{\,-(n-2)/2}$$
$$+\beta(\beta+1)\sum_{n=0}^{\infty}(-1)^n\tfrac{1}{2}(n+1)x^n\bar{l}^{\,-(n+2)/2} \tag{A4}$$

$$B_n=(-1)^n\tfrac{1}{2}(n+1)+\left(\frac{\mathrm{d}^nV(q_0)}{\mathrm{d}q_0^n}\right)\frac{q_0^{n+2}}{n!Q}. \tag{A5}$$

Equation (A3), along with (A4) and (A5), is evidently the one-dimensional Schrödinger equation for a perturbed harmonic oscillator

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{1}{2}w^2x^2+\varepsilon_0+P(x)\right]X_k(x)=\lambda_kX_k(x) \tag{A6}$$

where $w^2=2B_2$,

$$\varepsilon_0=\bar{l}\left[\frac{1}{2}+\frac{q_0^2V(q_0)}{Q}\right]+\frac{2\beta+1}{2}+\frac{\beta(\beta+1)}{2\bar{l}} \tag{A7}$$

and $P(x)$ represents the remaining terms in equation (A4) as infinite power series perturbations to the harmonic oscillator. One would then imply that

$$\lambda_k=\bar{l}\left[\frac{1}{2}+\frac{q_0^2V(q_0)}{Q}\right]+\left[\tfrac{1}{2}(2\beta+1)+(k+\tfrac{1}{2})w\right]+\frac{1}{\bar{l}}\left[\tfrac{1}{2}\beta(\beta+1)+\lambda_k^{(0)}\right]+\sum_{n=2}^{\infty}\lambda_k^{(n-1)}\bar{l}^{\,-n} \tag{A8}$$

and

$$\lambda_k=q_0^2\sum_{n=-2}^{\infty}E_{k,l}^{(n)}\bar{l}^{\,-(n+1)}. \tag{A9}$$

Hence, equations (A8) and (A9) yield

$$E_{k,l}^{(-2)}=\frac{1}{2q_0^2}+\frac{V(q_0)}{Q} \tag{A10}$$

$$E_{k,l}^{(-1)}=\frac{1}{q_0^2}\left[\tfrac{1}{2}(2\beta+1)+(k+\tfrac{1}{2})w\right] \tag{A11}$$

$$E_{k,l}^{(0)}=\frac{1}{q_0^2}\left[\tfrac{1}{2}\beta(\beta+1)+\lambda_k^{(0)}\right] \tag{A12}$$

$$E_{k,l}^{(n)}=\lambda_k^{(n)}/q_0^2 \qquad n\geqslant 1 \tag{A13}$$

where q_0 is chosen to minimize $E_{k,l}^{(-2)}$, i.e.

$$\frac{\mathrm{d}E_{k,l}^{(-2)}}{\mathrm{d}q_0}=0 \qquad \text{and} \qquad \frac{\mathrm{d}^2E_{k,l}^{(-2)}}{\mathrm{d}q_0^2}>0. \tag{A14}$$

Thereby, $V(q)$ is assumed to be well behaved so that $E_{k,l}^{(-2)}$ has a minimum q_0 and there are well defined bound states. Equation (A14) in turn gives, with $\bar{l} = \sqrt{Q}$

$$l_D - \beta = \sqrt{q_0^3 V'(q_0)}. \tag{A15}$$

Consequently, the second term in equation (A4) vanishes and the first term adds a constant to the energy eigenvalues. It should be noted that the energy term $\bar{l}^{\,2} E_{k,l}^{(-2)}$ corresponds roughly to the energy of a classical particle with angular momentum $L_z = \bar{l}$ executing circular motion of radius q_0 in the potential $V(q_0)$. It thus identifies the zeroth-order approximation, to all eigenvalues, as a classical approximation and the higher-order corrections as quantum fluctuations around the minimum q_0, organized in inverse powers of $\bar{l}$. The next correction to the energy series, $\bar{l} E_{k,l}^{(-1)}$, consists of a constant term and the exact eigenvalues of the harmonic oscillator $w^2x^2/2$.The shifting parameter β is determined by choosing $\bar{l} E_{k,l}^{(-1)} = 0$. This choice is physically motivated. In addition to its vital role in removing the singularity at $l = 0$, it also requires agreement between PSLET eigenvalues and eigenfunctions with the exact well known ones for the harmonic oscillator and Coulomb potentials. Hence

$$\beta = -\left[\tfrac{1}{2} + \left(k + \tfrac{1}{2}\right) w\right] \tag{A16}$$

where $w = \sqrt{3 + q_0 V''(q_0)/V'(q_0)}$, and the primes of $V(q_0)$ denote derivatives with respect to q_0. Then equation (A4) reduces to

$$\frac{q_0^2}{\bar{l}} \tilde{V}(x(q)) = q_0^2 \bar{l} \left[\frac{1}{2q_0^2} + \frac{V(q_0)}{Q}\right] + \sum_{n=0}^{\infty} v^{(n)}(x)\, \bar{l}^{\,-n/2} \tag{A17}$$

where

$$v^{(0)}(x) = B_2 x^2 + \tfrac{1}{2}(2\beta + 1) \tag{A18}$$

$$v^{(1)}(x) = -(2\beta + 1)x + B_3 x^3 \tag{A19}$$

and for $n \geqslant 2$

$$v^{(n)}(x) = B_{n+2}\, x^{n+2} + (-1)^n\, (2\beta + 1)\, \tfrac{1}{2}(n+1)\, x^n + (-1)^n\, \tfrac{1}{2}\beta(\beta + 1)\, (n-1)\, x^{(n-2)}. \tag{A20}$$

References

[1] Hall R L and Saad N 2000 *J. Phys. A: Math. Gen.* **33** 569
Hall R L and Saad N 1999 *J. Phys. A: Math. Gen.* **32** 133
[2] Hall R L and Saad N 1998 *J. Phys. A: Math. Gen.* **31** 963
[3] Hall R L, Saad N and Keviczky A 1998 *J. Math. Phys.* **39** 6345
[4] Hall R L and Saad N 1997 *J. Math. Phys.* **38** 4909
[5] Mustafa O and Odeh M 1999 *J. Phys. B: At. Mol. Opt. Phys.* **32** 3055
[6] Znojil M 1999 *Phys. Lett.* A **255** 1
[7] Znojil M 1999 *Phys. Lett.* A **259** 220
[8] Znojil M 1992 *Phys. Lett.* A **169** 415
[9] Papp E 1989 *Europhys. Lett.* **9** 309
[10] Klauder J R 1973 *Acta Phys. Austriaca Suppl.* **11** 341
[11] Detwiler L C and Klauder J R 1975 *Phys. Rev.* D **11** 1436
[12] Simon B 1973 *J. Funct. Anal.* **14** 295
[13] Harrell E M 1977 *Ann. Phys.* **105** 379
[14] Aguilera V C and Guardiola R 1991 *J. Math. Phys.* **32** 2135
[15] Znojil M 1993 *J. Math. Phys.* **34** 4914
[16] Flynn M F, Guardiola R and Znojil M 1993 *Czech. J. Phys.* **41** 1019
[17] Herschbach D R *et al* 1993 *Dimensional Scaling in Chemical Physics* (Dordrecht: Kluwer)

[18] Herschbach D R 1986 *J. Chem. Phys.* **84** 838
[19] Levai G, Konya B and Papp Z 1998 *J. Math. Phys.* **39** 5811
Znojil M 1997 *J. Math. Phys.* **38** 5087
[20] Mustafa O and Odeh M 1999 *J. Phys. A: Math. Gen.* **32** 6653
[21] Mustafa O and Odeh M 2000 *Eur. Phys. J.* B **15** 143
[22] Mustafa O and Odeh M 2000 *Commun. Theor. Phys.* **33** 469
[23] Maluendes S A, Fernandez F M and Castro E A 1987 *Phys. Lett.* A **124** 215
[24] Bender C M and Orszag S A 1978 *Advanced Mathematical Methods for Scientists and Engineers* (New York: McGraw-Hill)
[25] Imbo T, Pagnamenta A and Sukhatme U 1984 *Phys. Rev.* D **29** 1669
[26] Mustafa O and Chhajlany S C 1994 *Phys. Rev.* A **50** 2926
[27] Taseli H 1996 *J. Math. Chem.* **20** 235
[28] Mustafa O 1996 *J. Phys.: Condens. Matter* **8** 8073
[29] Barakat T, Odeh M and Mustafa O 1998 *J. Phys. A: Math. Gen.* **31** 3469
[30] Mustafa O and Sever R 1991 *Phys. Rev.* A **44** 4142
[31] Davydov A S 1976 *Quantum Mechanics* 2nd edn (Oxford: Pergamon)
[32] Papp E 1988 *Phys. Rev.* A **38** 5910
Papp E 1988 *Phys. Rep.* **161** 171
[33] Bender C M and Wu T T 1969 *Phys. Rev.* **184** 123
Bender C M and Wu T T 1973 *Phys. Rev.* D **7** 1620
[34] Dunn M and Watson D 1996 *Few-Body Syst.* **21** 187
[35] Dunn M and Watson D 1996 *Ann. Phys.* **251** 266
[36] Dunn M and Watson D 1999 *Phys. Rev.* A **59** 1109
[37] Lichtenberg D *et al* 1990 *Z. Phys.* C **46** 75