Calculation of the spiked harmonic oscillators through a generalized pseudospectral method

Amlan K. Roy

Department of Chemistry, University of New Brunswick, Fredericton, NB, E3B 6E2, Canada

Abstract

The generalized pseudospectral method is employed for the accurate calculation of eigenvalues, densities and expectation values for the spiked harmonic oscillators. This allows nonuniform and optimal spatial discretization of the corresponding single-particle radial Schrödinger equation satisfying the Dirichlet boundary conditions leading to the standard diagonalization of the symmetric matrices. The present results for a large range of potential parameters are in excellent agreement with those from the other accurate methods available in the literature. The ground and excited states (both low as well as high angular momentum states) are obtained with equal ease and accuracy. Some new states including the higher excited states are reported here for the first time. This offers a simple, accurate and efficient method for the treatment of these and a wide variety of other singular potentials of physical and chemical interest in quantum mechanics.

*Electronic address: akroy@unb.ca
I. INTRODUCTION

A class of interaction potentials in quantum mechanics characterized by the Hamiltonian,

\[ H = p^2 + r^2 + \lambda |r|^{-\alpha} \equiv H_0 + \lambda |r|^{-\alpha}, \quad r \in [0, \infty] \]  \tag{1}

where \( p = -i \partial / \partial r \), have found widespread applications in many areas of atomic, molecular, nuclear physics and are often referred as the spiked harmonic oscillators (SHO). Here \( H_0 \) formally denotes the simple harmonic oscillator Hamiltonian; the coupling parameter \( \lambda \) determines the strength of the perturbative potential and the positive constant \( \alpha \) represents the type of singularity at the origin. The higher the value of \( \lambda \), the higher the singularity.

There has been an upsurge of interest [1-20] to calculate the SHO eigenvalues over the past three decades and it continues to grow. An interesting feature of this potential is that once the perturbation \( \lambda |r|^{-\alpha} \) is switched on, complete turn-off is impossible; vestigial effects of the interaction persists leading to the so called “Klauder phenomenon” [1,2]. From a purely mathematical viewpoint, on the other hand, this poses considerable challenges to some of the well-established and widely used mathematical theories. For example, the commonly used Rayleigh-Schrödinger perturbation series diverges [3] according to the relation \( n \geq \frac{1}{\alpha - 2} \), where \( n \) is the order of the perturbation term. Consequently, a singular perturbation theory was to be specially devised to treat these potentials. These potentials also exhibit the phenomenon of supersingularity [1] in the region of \( \alpha \geq 5/2 \), i.e., every matrix element of the potential is infinite. The numerical solutions of the pertinent Schrödinger equations are notoriously difficult as well; especially those involving the finite-difference (FD) schemes and often require special care.

Several analytical (both variational and perturbative) methodologies [3-20] are available for the exact and approximate calculation of these systems. For example, the modified (nonpower) perturbation series [3] to finite order for the ground-state eigenenergies valid for small values of \( \lambda \) and arbitrary values of \( \alpha \), a large coupling perturbative expansion [5] for the approximate estimates of the same for large positive values of \( \lambda \), the weak coupling expansion expressions of the nonsingular (\( \alpha < 5/2 \)) SHO through the resummation technique for \( \alpha = 1/2, 1, 3/2 \) [6] and for \( \alpha = 2 \) [10], the exact and approximate (variational) solutions [8] for some particular values of the parameters in the interaction potential, a modified WKB treatment [11], etc. Besides, the upper and lower bounds of ground and excited states [12-16] of the SHO as well as the generalized SHO, the analytical pseudoperturbation
shifted-$\ell$ expansion technique (PSLET) [19,20] have also been developed. The extensions to N-dimensions are reported lately [14,20]. On the numerical side, the FD methods [21,22] through Richardson extrapolation, integration of the Schrödinger equation [23] using a Lanczos grid method for the cases of $\alpha = 4, 6$ for small values of the ($\lambda \leq 0.01$), the analytic continuation method [24] for ground and excited states have been reported.

Despite all these attempts, a general prescription which can accurately and reliably calculate the bound states of these potentials in a uniform and simple way for a general set of potential parameters with the promise of furnishing ground and excited states with equal ease, would be highly desirable. This is because physically meaningful and good accuracy results are obtainable only by some of these methods. Additionally some of these methods can give satisfactory results for a certain type of parameters while perform rather poorly in other cases. Much attention has been paid to the ground states; excited states are reported less frequently and definitively, presumably because of the greater challenges compared to the ground states. Moreover, much work has been devoted to the eigenvalues; only few results are available for the eigenfunctions [15]. Also some of these methodologies are often fraught with rather tedious and cumbersome mathematical complexities. This work proposes a simple methodology to study these systems by using the GPS scheme which has shown considerable promise for a variety of atomic and molecular processes including both static and dynamic situations in recent years (see, for example [25-29] and the references therein). This formalism helps alleviate some of the well-known discomfitures of the FD schemes widely used and discussed in the literature [5,21,22,30], e.g., the necessity of significantly larger spatial grid points to deal with the singularity at the origin. The GPS method essentially works in a nonuniform and optimal spatial grid; thus a much smaller number of points suffices to achieve good accuracy. However its applicability has been so far restricted to the cases of Coulomb singularities; no attempts have been made to deal with the other singularities characterizing many physical systems. The objective of this Letter is two-fold: (a) to extend the regions of applicability and judge the performance of it on the SHOs, (b) to calculate accurately the bound-state spectra of these systems. Comparison with the literature data has been made wherever possible.

The organization of the article is as follows. Section II presents an overview of the basic formalism. Section III makes a discussion of the results while a few concluding remarks are made in section IV.
II. THE GPS FORMALISM FOR THE SHO

In this section, we present the GPS formalism used to solve the radial eigenvalue problem with the SHO potentials. A detailed account of the GPS method can be found in the references [25-29].

The time-independent radial Schrödinger equation to be solved can be written in the usual way (atomic units employed unless otherwise mentioned),

\[
-\frac{1}{2} \frac{d^2}{dr^2} + \frac{\ell(\ell + 1)}{2r^2} + v(r) \psi_{n,\ell}(r) = E_{n,\ell} \psi_{n,\ell}(r)
\]  

where \( v(r) \) is the SHO potential given by,

\[
v(r) = \left[ r^2 + \frac{\lambda}{r^\alpha} \right] / 2.
\]

The \( 1/2 \) factor is introduced here only for easy comparison with the literature and \( \ell \) signifies the usual angular momentum quantum number. The GPS formalism facilitates the use of a denser mesh at small \( r \) regions and a relatively coarser mesh at the large \( r \) regions while preserving the similar accuracy at both the regions.

The key step in this formalism is to approximate a function \( f(x) \) defined in the interval \( x \in [-1, 1] \) by an \( N \)-th order polynomial \( f_N(x) \) exactly at the discrete collocation points \( x_j \) as in the following,

\[
f(x) \cong f_N(x) = \sum_{j=0}^{N} f(x_j) \ g_j(x),
\]

\[
f_N(x_j) = f(x_j).
\]

Within the Legendre pseudospectral method that the current work uses, \( x_0 = -1, \ x_N = 1, \) and \( x_j (j = 1, \ldots, N - 1) \) can be determined from the roots of the first derivative of the Legendre polynomial \( P_N(x) \) with respect to \( x \), i.e.,

\[
P'_N(x_j) = 0.
\]

The \( g_j(x) \)s in Eq. (4) are the cardinal functions expressed as,

\[
g_j(x) = -\frac{1}{N(N+1)P_N(x_j)} \frac{(1-x^2)P'_N(x)}{x-x_j},
\]

satisfying the relation \( g_j(x_{j'}) = \delta_{jj'} \). At this stage, we use a transformation \( r = r(x) \) to map the semi-infinite domain \( r \in [0, \infty] \) onto the finite domain \( x \in [-1, 1] \). One can make use of
the following algebraic nonlinear mapping,
\[ r = r(x) = L \frac{1 + x}{1 - x + \alpha}, \]
where \( L \) and \( \alpha = 2L/r_{\text{max}} \) are the mapping parameters. Finally, introduction of the following relation,
\[ \psi(r(x)) = \sqrt{r'(x)f(x)} \]
in conjunction with a symmetrization procedure gives the following transformed Hamiltonian
\[ \hat{H}(x) = -\frac{1}{2} \frac{1}{r'(x)} \frac{d^2}{dx^2} \frac{1}{r'(x)} + v(r(x)) + v_m(x), \]
The advantage of this is that one ends up with a symmetric matrix eigenvalue problem which can be solved readily and efficiently to give accurate eigenvalues and eigenfunctions by using standard routines. It may be noted that \( v_m(x) = 0 \) for the above transformation leading to the following set of discretized coupled equations,
\[ \sum_{j=0}^{N} \left[ -\frac{1}{2} D^{(2)}_{jj'} v(r(x_j)) + \delta_{jj'} v_m(r(x_j)) \right] A_j = E A_{j'}, \quad j = 1, \ldots, N - 1, \]
where
\[ A_j = [r'(x_j)]^{1/2} \psi(r(x_j)) \left[ P_N(x_j) \right]^{-1}. \]

III. RESULTS AND DISCUSSION

A. The charged harmonic oscillator, \( \alpha = 1 \)

Before considering the general case of relatively stronger spikes, \( \text{viz.}, \alpha \neq 1 \), it is worthwhile to study the simpler special case of \( \alpha = 1 \). This does not exhibit supersingularity and the Hamiltonian takes the simplified confined Coulomb potential type form. It has been
TABLE I: Some elementary solutions (in a.u.) of the SHO with $\alpha = 1$ for several values of $\lambda$ corresponding to the ground state.

| $\lambda$ | This work | Exact$^a$ |
|-----------|-----------|-----------|
| 0         | 1.499999999999 | 1.5 |
| 2         | 2.499999999999 | 2.5 |
| $\sqrt{20}$ | 3.500000000000 | 3.5 |
| $(30 + 6\sqrt{17})^{1/2}$ | 4.499999999999 | 4.5 |
| $(70 + 6\sqrt{57})^{1/2}$ | 5.499999999999 | 5.5 |
| 14.450001026966 | 6.499999999999 | 6.5 |
| 18.5031314100003 | 7.499999999999 | 7.5 |

$^a$Ref. [31]. These results have been halved to take care of a 2 factor.

TABLE II: Calculated ground-state energies $E$ (in a.u.) of the SHO with $\alpha = 1$ for several values of $\lambda$.

| $\lambda$ | This work | Literature$^a$ |
|-----------|-----------|----------------|
| -0.001    | 1.49943577146 | 1.49943577146 |
| -0.005    | 1.49717807794 | 1.49717807794 |
| -0.01     | 1.49435420563 | 1.49435420563 |
| -0.05     | 1.47169265799 | 1.47169265799 |
| -0.1      | 1.44318757957 | 1.44318757957 |
| -0.5      | 1.20765362342 | 1.20765362342 |
| -1        | 0.892602739638 | 0.892602739638 |
| -5        | -2.90807895034 | -2.90807895034 |
| -10       | -12.44049953015 | -12.44049953015 |
| -50       | -312.497600033 | -312.497600033 |
| -100      | -1249.999400000 | -1249.999400000 |

| $\lambda$ | This work | Literature$^a$ |
|-----------|-----------|----------------|
| 0.001     | 1.50056415064 | 1.50056415064 |
| 0.005     | 1.50281997477 | 1.50281997477 |
| 0.01      | 1.50563800525 | 1.50563800525 |
| 0.05      | 1.52811261097 | 1.52811261097 |
| 0.1       | 1.55603453244 | 1.55603453244 |
| 0.5       | 1.77283783394 | 1.77283783394 |
| 1         | 2.02893850398 | 2.02893850398 |
| 5         | 3.69201586294 | 3.69201586294 |
| 10        | 5.28874176968 | 5.28874176968 |
| 50        | 13.72005706824 | 13.72005706824 |
| 100       | 21.2314590573 | 21.2314590573 |

$^a$Ref. [31]. The quoted results are halved to take care of a 2 factor.

pointed out [31] that this possesses an infinite set of elementary solutions. Table I displays such elementary solutions calculated by the present method along with the exact analytical results. Note that $E = 3/2$ is a trivial solution corresponding to $\lambda = 0$, i.e., the unperturbed Hamiltonian. The other $\lambda$s in this table are taken from the solutions of the polynomial equation [31]. It may be noted that all the calculated results in this table and throughout the article are truncated and therefore all the digits in the reported numbers should be considered as correct. It is seen that for all values of $\lambda$, our results match excellently up to a 12 digit accuracy with the exact values.
Next we report in Table II the ground-state energies for a large range of (+)ve and (-)ve λs (left and right sides of the table respectively) along with the available literature data. One can envisage three distinct regions in this case depending on the values of λ, viz., (a) the Coulomb region, corresponding to large (-)ve λ, (b) the strong-coupling region having large (+)ve λ, and (c) the weak-coupling region having small (both (+)ve and (-)ve) λ. The perturbation expressions corresponding to regions (a) and (c) are obtained through an amalgamation of the hypervirial and Hellmann-Feynman theorem [31]. For some of the (-)ve and (+)ve λs ground states are examined by the Renormalization as well as the direct numerical integration methods [31]. Also for λ ≤ −1 and λ ≥ 1, the Coulomb series and strong coupling series solutions are available [31]. Good agreement is observed for λ = −10 and λ = 10 involving these methods; for other λs, they vary significantly from each other. Here, the numerical results are quoted for comparison. No results were available for λ = ±0.005, ±0.05, ±0.5, ±50, ±100). It is seen that the current results are in excellent agreement with theirs. At this point mention may be made of one of the uncomfortable features in some of the available methodologies, viz., the presence of the unphysical roots, e.g., in the Riccati-Padé method for the small λs of these potentials [31]. However, no such solutions have been found in the present calculations. In some instances, very slight differences are observed in our results from the literature data. Furthermore, in table III we present the calculated first three states corresponding to ℓ = 0, 1, 2, 3 for these systems. The ground states are repeated for the sake of completeness. Again a wide range of both positive and negative λ values are chosen. No results are available for these states to our knowledge and we hope that they could be useful in future calculations.

B. α ≠ 1

Now results are presented for α ≠ 1. Here we focus on the α values 4 and 6; however, the present scheme has been thoroughly checked to reproduce the results of similar accuracy and reliability for other values of α available in the literature. In table IV ground state energies are tabulated for these two cases (α = 4 in the left and α = 6 in the right), for small and large λs. Two new λ values are introduced here (500 and 1000) in addition to those employed in table II. Both of these α values can lead to supersingularity and have been investigated by many workers. The present results are seen to be in good agreement with the accurate
TABLE III: Excited state energies (in a.u.) of the charged harmonic oscillator for several positive and negative values of \( \lambda \). First three states are presented corresponding to \( \ell = 0, 1, 2, 3 \).

| \( \lambda \) | \( \ell = 0 \) | \( \ell = 1 \) | \( \ell = 2 \) | \( \ell = 3 \) |
|---|---|---|---|---|
| -0.001 | 1.49943577146 | 2.49962386468 | 3.49969095050 | 4.49974208263 |
| | 3.49952892655 | 4.49961481110 | 5.49970589211 | 6.49975411774 |
| | 5.49958155072 | 6.49967805046 | 7.49973670957 | 8.49976788986 |
| -0.1 | 1.44318757957 | 2.46229789284 | 3.46987169094 | 4.47418745607 |
| | 3.45282982176 | 4.46097466780 | 5.47033527134 | 6.47562904582 |
| | 5.45807015200 | 6.46866925358 | 7.47365242360 | 8.47676916627 |
| -10 | -12.4409953901 | -2.62119805046 | 3.49952982655 | 4.49966148110 |
| | -2.4172388317 | 5.51233459914 | 6.46976868780 | 7.47562904582 |
| | 0.86969218970 | 3.039429778956 | 4.46609746678 | 5.47203352713 |
| | -100 | -124.999400000 | -312.494000168 | -138.863694966 | -78.0530829912 |
| | -312.491600236 | -138.852989182 | -78.024335034 | -49.7760242855 |
| | -138.847499606 | -78.0051588012 | -49.7312779249 | -34.2071328286 |
| 0.001 | 1.50056415063 | 2.50037611746 | 3.50030089728 | 4.50025791310 |
| | 3.50047014252 | 4.50038505800 | 5.50029405566 | 6.50024358500 |
| | 5.50041843194 | 6.50032987472 | 7.50025326851 | 8.5002328755 |
| 0.1 | 1.55603345324 | 2.53752389333 | 3.53005208746 | 4.52577056704 |
| | 3.5468642702 | 4.53803079099 | 5.5279125734 | 6.5243425783 |
| | 5.54175768729 | 6.53126513099 | 7.52631014389 | 8.52320695048 |
| 10 | 5.2874176968 | 5.63241238009 | 6.1996201502 | 6.89697261559 |
| | 7.0753947857 | 7.46149523127 | 8.06916090729 | 8.79599713087 |
| | 8.89811648443 | 9.32030795656 | 9.96020685568 | 10.7102538225 |
| 100 | 21.2314590573 | 21.3064355531 | 21.454955286 | 21.6736073270 |
| | 22.9756496882 | 23.0536647120 | 23.2077138583 | 23.4341264159 |
| | 24.7309414007 | 24.8119454465 | 24.9716696244 | 25.2059214990 |

analytic continuation results [24]. These results are available for \( \lambda = 0.001, 0.01, 1, 10 \) for both \( \alpha = 4, 6, while \( \lambda = 0.1, 100, 1000 \) for \( \alpha = 4 \) only. Various other results are also available for the smaller \( \lambda \)s (0.005, 0.01) [23,21,1,33] and our results show good agreement with these. Direct integration results [8] for \( \lambda = 0.01, 0.1, 1, 5, 10 \) are also presented for comparison. It may be noted that the current results surpass in accuracy to all others except [24].

Now table V gives the results for low- and high-\( \ell \) states for a wide range of \( \lambda \)s (0.001, 0.01, 0.1,1,10) for both \( \alpha = 4, 6 \). Upper and lower bounds as well as the numerical eigenenergies for \( \ell = 3, 4, 5 \) have been studied recently by [16] for \( \alpha = 4 \) for first four \( \lambda \)s. Our results match almost completely with theirs except very slight discrepancies in three instances at the last digit (our results are lower by \( 10^{-11} \)). Also, the eigenvalues of \( \ell = 5, 10, 20 \cdots, 50 \) for all the mentioned values of \( \alpha \) and \( \lambda \) are given as a test of this method for the very high
TABLE IV: Calculated ground-state energies $E$ (in a.u.) of the SHO with $\alpha = 4$ and 6 for several values of $\lambda$. The literature results are divided by a 2 factor.

| $\lambda$ | Energy ($\alpha = 4$) | Energy ($\alpha = 6$) |
|-----------|------------------------|------------------------|
|           | This work | Literature | This work | Literature |
| 0.001     | 1.53438158545, 1.534385  | 1.63992791296          |
|           | 1.5417615416            | 0.574195               |
| 0.01      | 1.60253374753, 1.60254  | 1.75272613799          |
|           | 1.602533745, 1.6025354  | 1.752726195            |
| 0.05      | 1.71258069752           | 1.88277010302          |
| 0.1       | 1.78775995560, 1.787785  | 1.95783261264          |
|           | 1.7877750889168         | 2.24708899478          |
| 1         | 2.32996698478           | 2.32996698478, 2.329970 |
| 5         | 3.00160451444, 3.00160451 | 3.00160451444, 3.00160451 |
| 50        | 3.7677607255            | 4.20667914031          |
| 100       | 4.73277781767           | 5.57607711626          |
| 500       | 8.7393385806            | 10.6847312660, 10.68473  |
| 1000      | 10.6847312660, 10.68473  | 10.6847312659          |

$^a$Ref. [24].
$^b$Ref. [31].
$^c$Ref. [23].
$^d$Ref. [21].
$^e$Ref. [1].
$^f$Ref. [8].
$^g$Ref. [33].

excited states. The present result is in complete agreement with the lone available result of $\ell = 50$ (for $\alpha = 4, \lambda = 1$). Next table VII gives results for the first 10 eigenvalues of the SHO with the parameters $\alpha = 6, \lambda = 10$. We have considered $\ell = 0, 1, 2, 3, 4$ and no results could be found for these states.

As a test on the quality of the eigenfunctions, In table VII we present some of the calculated expectation values $\langle r^{-1} \rangle$ and $\langle r \rangle$ for $\alpha = 1, 4$ and 6. The parameter $\lambda$ is kept fixed at 10 in all these cases and the first three states are reported for $\ell = 0, 1, 2$. No results could be found for any of these values in the literature. Finally, figure 1 depicts the
TABLE V: Calculated $\ell \neq 0$ state energies (in a.u.) of the SHO with $\alpha = 4$ (top) and 6 (bottom) for several values of $\lambda$s. The literature results have been divided by a 2 factor.

| $\ell$ | $\lambda = 0.001$ | $\lambda = 0.01$ | $\lambda = 0.1$ | $\lambda = 1$ | $\lambda = 10$ |
|--------|-----------------|-----------------|-----------------|--------------|----------------|
| 3      | 4.50005713956   | 4.50057109970   | 4.50568201308   | 4.55432930375| 4.91961566042|
|        | 4.50005713956$^a$ | 4.50568201309$^a$ | 4.55432930376$^a$ |              |                |
| 4      | 5.50003174537   | 5.50031739444   | 5.50316804961   | 5.53112085969| 5.77200022575|
|        | 5.5003174537$^a$ | 5.50316804961$^a$ | 5.53112085969$^a$ |              |                |
| 5      | 6.50002020182   | 6.50020200030   | 6.50201821626   | 6.52000759152| 6.68566506197|
|        | 6.50002020182$^a$ | 6.50201821626$^a$ | 6.52000759153$^a$ |              |                |
| 10     | 11.5000050125   | 11.5000501247   | 11.5005011983   | 11.5050070693| 11.5495902896|
| 20     | 21.5000012507   | 21.500125077    | 21.501250765    | 21.5012506189| 21.5124915772|
| 30     | 31.500005556    | 31.500055570    | 31.5005556887   | 31.5055549875| 31.5055549875|
| 40     | 41.500003125    | 41.500031254    | 41.500312543    | 41.5031249904| 41.5031249904|
| 50     | 51.500001999    | 51.500020019    | 51.500020019    | 51.500020019 | 51.500020019 |
|        |                  |                | 51.500020018$^a$ |              |                |

$^a$Ref. [16].

TABLE VI: The first 10 eigenvalues (in a.u.) for $\ell = 0, 1, 2, 3, 4$, of the SHO. The parameters are: $\alpha = 6$ and $\lambda = 10$.

| $\ell$ | $\ell = 0$ | $\ell = 1$ | $\ell = 2$ | $\ell = 3$ | $\ell = 4$ |
|--------|------------|------------|------------|------------|------------|
| 3.0010451444 | 3.32389487858 | 3.91806927392 | 4.70345973112 | 5.60034573904 |
| 5.38666914834 | 5.6485918212 | 6.1491053052 | 6.84505383654 | 7.67818492569 |
| 7.66493489996 | 7.89510635043 | 8.34183646535 | 8.97697716408 | 9.7587666401 |
| 9.88940298242 | 10.0989808012 | 10.5089815278 | 11.096720737 | 11.839502067 |
| 12.0805100442 | 12.2752417097 | 12.6580500545 | 13.2142245371 | 13.919114855 |
| 14.2485304976 | 14.4318512146 | 14.7933959369 | 15.3217108425 | 15.996992830 |
| 16.3994450470 | 16.5736092280 | 16.9178854110 | 17.4230621225 | 18.0728546082 |
| 18.5370785045 | 18.7036642068 | 19.0352182032 | 19.5190555671 | 20.1466196426 |
| 20.6640433547 | 20.82402086533 | 21.147690049 | 21.6103351695 | 22.2182898578 |
| 22.7822131369 | 22.9368391875 | 23.2437342203 | 23.6974306875 | 24.2879213038 |

radial probability distribution functions for the first three states of $\ell = 0, 1, 2$ along with the potential ($\alpha = 6, \lambda = 10$). As expected they show the requisite number of nodes in these plots.
FIG. 1: The radial probability distribution function, $|r R_{nl}|^2$ (in a. u.) for the first three states corresponding to $\ell = 0, 1, 2$ of the spiked oscillator potential having the parameters, $\alpha = 6, \lambda = 10$.

(a) The potential, (b) the ground state, (c) the first excited state and (d) the second excited state.
TABLE VII: Calculated expectation values (in a.u.) for the SHO for some selected values of $\alpha$ and $\lambda$. The first three states corresponding to $\ell = 0, 1, 2$ are presented.

| $\alpha$ | $\lambda$ | $\ell$ | $\langle r^{-1} \rangle$ | $\langle r \rangle$ |
|---------|-----------|--------|----------------|------------------|
| 1       | 10        | 0      | 0.579335567     | 1.88860444       |
|         |           |        | 0.572186022     | 2.20351385       |
|         |           |        | 0.562374825     | 2.49562513       |
| 4       | 10        | 0      | 0.546623313     | 1.93946889       |
|         |           |        | 0.483512472     | 2.3864959        |
|         |           |        | 0.443751364     | 2.7404976        |
| 6       | 10        | 0      | 0.558986259     | 1.89176957       |
|         |           |        | 0.477245223     | 2.38688068       |
|         |           |        | 0.431013450     | 2.77224304       |

IV. CONCLUSION

The GPS formalism is shown to deliver accurate and reliable results for the eigenvalues, expectation values and the radial densities of the SHOs. The simplicity and viability of the method is demonstrated by calculating the low and high excited states of these potentials for weak and strong values of the interaction parameter in the potential. Excellent agreement with the literature data is observed in all cases. Some states are reported here for the first time. Finally the approach may be as well equally successful and useful for other singularities (e. g., the Hulthén, Yukawa, Hellman potentials etc.) in quantum mechanics. Work in this direction is under progress.

Acknowledgments

I gratefully acknowledge the hospitality provided by the Department of Chemistry, University of New Brunswick, Fredericton, Canada.

[1] L. C. Detwiler and J. R. Klauder, Phys. Rev. D 11 1436 (1975).
[2] J. R. Klauder, Science 199 735 (1978).
[3] E. M. Harrell, Ann. Phys., NY 105 379 (1977).
[4] E. Papp, Europhys. Lett. 9 309 (1989).
[5] V. C. Aguilera-Navarro, G. A. Estévez and R. Guardiola, J. Math. Phys. 31 99 (1990).
[6] V. C. Aguilera-Navarro and R. Guardiola, J. Math. Phys. 32 2135 (1991).
[7] M. Znojil, J. Math. Phys. 31 108 (1990); ibid. 34 4914 (1993).
[8] F. M. Fernández, Phys. Lett. A 160 511 (1991).
[9] M. Znojil, Phys. Lett. A 169 415 (1992); ibid. 255 1 (1999); ibid. 259 220 (1999).
[10] E. S. Estévez-Bretón and G. A. Estévez-Bretón, J. Math. Phys. 34 437 (1993).
[11] J. Trost and H. Friedrich, Phys. Lett. A 228 127 (1997).
[12] R. L. Hall and N. Saad, J. Phys. A 31 963 (1998).
[13] R. L. Hall, N. Saad and A. von Keviczky J. Math. Phys. 39 6345 (1998).
[14] R. L. Hall and N. Saad, J. Phys. A 33 569 (2000).
[15] R. L. Hall, N. Saad and A. von Keviczky J. Phys. A 34 1169 (2001).
[16] R. L. Hall, N. Saad and A. von Keviczky J. Phys. A 36 487 (2003).
[17] O. Mustafa and M. Odeh, Preprint quant-ph/006004 (2000).
[18] J. Skibiński, Preprint quant-ph/0007059 (2000).
[19] O. Mustafa and M. Odeh, J. Phys. B 32 3055 (1999).
[20] O. Mustafa and M. Odeh, J. Phys. A 33 5207 (2000).
[21] J. Killingbeck, J. Phys. B 15 829 (1982).
[22] J. P. Killingbeck, G. Jolicard, and A. Grosjean, J. Phys. A 34 L367 (2001).
[23] W. Solano-Torres, G. A. Estévez, F. M. Fernández and G. C. Groenenboom, J. Phys. A 25 3427 (1992).
[24] E. Buendiá, F. J. Gálvez and A. Puertas, J. Phys. A 28 6731 (1995).
[25] X. M. Tong and S. I. Chu, Phys. Rev. A 55 3406 (1997), ibid. 64 013417 (2001).
[26] A. K. Roy and S. I. Chu, Phys. Rev. A 65 043402 (2002), ibid. 65 052508 (2002).
[27] D. Telnov and S. I. Chu, Phys. Rev. A 59 2864 (1999).
[28] A. K. Roy and S. I. Chu, J. Phys. B 35 2075 (2002).
[29] A. K. Roy, J. Phys. G (in press).
[30] M. J. Jamieson, J. Phys. B 16 L391 (1983).
[31] V. C. Aguilera-Navarro, F. M. Fernández, R. Guardiola and J. Ros, J. Math. Phys. 25 6379 (1992).
[32] V. C. Aguilera-Navarro, A. C. Coelho and N. Ullah, Phys. Rev. A 49 1477 (1994).
[33] C. R. Handy, Phys. Lett. A 216 15 (1996).