Studies on some singular potentials in quantum mechanics

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Abstract

A simple methodology is suggested for the efficient calculation of certain central potentials having singularities. The generalized pseudospectral method used in this work facilitates nonuniform and optimal spatial discretization. Applications have been made to calculate the energies, densities and expectation values for two singular potentials of physical interest, viz., (i) the harmonic potential plus inverse quartic and sextic perturbation and (ii) the Coulomb potential with a linear and quadratic term for a broad range of parameters. The first 10 states belonging to a maximum of \( \ell = 8 \) and 5 for (i) and (ii) have been computed with good accuracy and compared with the most accurate available literature data. The calculated results are in excellent agreement, especially in the light of the difficulties encountered in these potentials. Some new states are reported here for the first time. This offers a general and efficient scheme for calculating these and other similar potentials of physical and mathematical interest in quantum mechanics accurately.

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I. INTRODUCTION

Application of quantum mechanics to many branches of physics and chemistry, e.g., the atomic and molecular physics, nuclear physics, particle physics, solid-state physics, astrophysics, etc., often involves a potential term having *singularity* and usually some extra perturbation terms characterizing the physical system under study. Almost for all practical purposes, the radial Schrödinger equation to be solved requires approximations as the exact solutions can be obtained only for a few idealized cases such as the harmonic oscillator or the Coulomb potential. Consequently, a large number of analytical and numerical methodologies have been developed by many workers over the decades to obtain accurate solutions for such systems employing a variety of techniques. Although many attractive and elegant approaches exist in the literature for both the non-singular and singular potentials, the latter remains relatively less explored as one encounters considerable difficulties and challenges because of the singularity. Therefore, the search for a *general* scheme capable of producing accurate and reliable results, has continued to remain an active area of research.

The purpose of this article is to assess the performance of a simple numerical methodology for the singular potentials. Although the method would hold good for other singularities, we will restrict ourselves to two different classes of such potentials which have found applications in various branches of physics, viz.,

(a) the harmonic potential including an inverse quartic and sextic anharmonicity,

\[ V(r) = a_1 r^2 + \sum_{i=2}^{3} a_i r^{-2i}, \quad (a_1, a_3 > 0) \]  

and

(b) the Coulomb potential with a linear and quadratic coupling,

\[ V(r) = -b_1/r + \sum_{j=1}^{2} b_j r^j \]

In what follows we will adopt \( a_1 = a, a_2 = b, a_3 = c \); and \( b_1 = Z, b_2 = g, b_3 = \lambda \) for the sake of consistency with the literature.

The potential in Eq. (1) is defined in \( r \in [0, \infty] \) with Dirichlet boundary conditions. Such a potential may lead to many interesting and appealing features; both physically and mathematically. For example, there may be the so-called *Klauder phenomenon*\(^{[1-2]}\) signifying that once the singular perturbation is turned on, it cannot be completely turned off. It is
noticed that the effects of perturbation is never small enough to ignore. For example, the complete three-dimensional Schrödinger equation is exactly solvable without the inverse sextic perturbation in Eq. (1) for both the extreme cases $a = 0$ and $b = 0$. However subjecting the system to an infinitesimal perturbation $a \neq 0, b \neq 0$ induces such dramatic effects in the wave function near the origin that the perturbation theory fails to give any estimate at all [3]. On the other hand, when either $b$ or $c$ is large, the anharmonic terms compete with the harmonic term and none of the interacting terms can be considered negligible. Several methods are available for the calculation of the eigenvalues and eigenfunctions of this potential. Some of them, for example, include the singular perturbation theory [4-6] specially designed for this potential, variational methods [7,8], step-by-step analytic continuation method [9], numerical solution using finite-difference scheme [10,11] or the B spline techniques [12], etc. This potential also has the importance in the context of conditional exact solvability; in other words, exact analytic solutions can be obtained for some severely restricted set of parameters (related to each other through some special relations) for ground states [13] or excited states [14,15].

The potential in Eq. (2) also has many relevance to physics. Thus, the Coulomb plus the linear potential has been studied extensively for the spherical Stark effects in hydrogenic atoms [16], or in connection with the various non-relativistic quark confinement and other similar problems in particle physics [16-18], etc. On the other hand, the Coulomb plus the quadratic potential has been studied in the context of quadratic Zeeman effects in hydrogenic atoms [19], or in plasma physics [20], etc. Again various methodologies have been devised for the calculation of eigenvalues of this potential by many workers. For some special values of the parameters $Z, g$ and $\lambda$, this leads to a quasi exactly solvable potential and analytic solutions can be obtained [21,22]. Other works include Rayleigh-Schrödinger perturbation model [23], the Stieltjes moments method [21], the analytic continued fraction theory [24,25], the Hill-determinant method [26], the supersymmetric quantum mechanics coupled with the shifted $1/N$ method [22,27], the two-point quasifractional approximant method [28], etc. More references on this potential can be found in [28].

However, for both these potentials, good accuracy results can be achieved only by a few of the above mentioned methods. Thus leaving aside a few methods, (like [9] or [11], for example) it is usually quite difficult to reach beyond a six- or seven-decimal place accuracy for the potential in Eq. (1) for an arbitrary set of parameters. As another author [8] points
out, to obtain even this much accuracy by standard numerical methods for the potential like that in Eq. [1] sometimes requires one to use a mesh of at least 80,000 points for some cases. Also, some of these methods, although can provide good quality results for certain type of parameters, perform rather poorly or even can not provide any result at all in other occasions (see [22], for example). Finally while majority of the works have remained largely focused to the ground states, relatively less attention has been paid to the excited states (especially those associated with the higher angular momentum). Given these facts, a general method which can offer accurate as well as reliable results for a general set of parameters for both ground and excited states (low as well as high) with equal ease, would be highly desirable and demanding. This work attempts to make a small step in such a direction. The seed of the motivation grew from a study of singly- and doubly- and triply excited Rydberg states of many-electron atomic systems [29,30] within the density functional framework [31] using the generalized pseudospectral (GPS) [32,33] scheme which produced good quality results within the bounds of the theory.

The purpose of this article is to use this simple numerical scheme for the calculation of the above mentioned singular potentials. First we will present in brief the essentials of the GPS method for the solution of the single-particle radial Schrödinger equation in section II. This has witnessed many successful applications in electronic structure and dynamics calculations in the recent years involving mainly Coulomb singularities (see, for example, [29-30, 32-35]). Thereafter this has been extended to some other physical systems including the spiked harmonic oscillators, the logarithmic and power potentials as well as the Hulthen and Yukawa potentials [36-38] with considerable promise. Section III presents the computed eigenvalues, wave functions, radial densities and the expectation values for the tow cases. Both ground as well as higher excited states are calculated and a thorough comparison with literature data has been made, wherever possible. Finally few conclusions are drawn in section IV.

II. METHODOLOGY

In this section, we present an overview of the generalized pseudospectral method (GPS) employed to solve the radial eigenvalue problem with the singular potentials. A more detailed account can be found in the refs. [29-30, 32-38].
Without loss of generality, the desired radial Schrödinger equation can be written as (atomic units employed unless otherwise mentioned),

\[ \hat{H}(r) \phi(r) = \varepsilon \phi(r), \]  

where the Hamiltonian includes the usual kinetic and potential energy operators,

\[ \hat{H}(r) = -\frac{1}{2} \frac{d^2}{dr^2} + v(r), \]  

with

\[ v(r) = V(r) + \frac{\ell(\ell + 1)}{2r^2}, \]  

and \( V(r) \) is given by Eq. (1) or (2). The symbols have their usual significances. The usual finite-difference spatial discretization schemes often require a large number of grid points to achieve good accuracy since majority of these methods employ a uniform mesh (nonuniform schemes are used in a few occasions as well, e.g., in [11]). The GPS method, however, can give nonuniform and optimal spatial discretization accurately. This allows one to work with a denser mesh at shorter \( r \) regions and a coarser mesh at larger \( r \). Additionally the GPS method is computationally orders of magnitude faster than the finite-difference schemes.

One of the principal features of this scheme lies in the fact that a function \( f(x) \) defined in the interval \( x \in [-1, 1] \) can be approximated by the polynomial \( f_N(x) \) of order \( N \) so that,

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

and the approximation is exact at the collocation points \( x_j \), i.e.,

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

In this work, we have employed the Legendre pseudospectral method using \( x_0 = -1, x_N = 1 \), where \( x_j (j = 1, \ldots, N-1) \) are obtainable 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 cardinal functions, \( g_j(x) \) in Eq. (6) are given by the following expression,

\[ g_j(x) = -\frac{1}{N(N + 1)P_N(x_j)} \frac{(1 - x^2) P'_N(x)}{x - x_j}, \]
obeying the unique property \( g_j(x_{j'}) = \delta_{j'j} \). Now the semi-infinite domain \( r \in [0, \infty] \) is mapped into the finite domain \( x \in [-1, 1] \) by the transformation \( r = r(x) \). One can make use of the following algebraic nonlinear mapping,

\[
r = r(x) = L \frac{1 + x}{1 - x + \alpha},
\]

where \( L \) and \( \alpha = 2L/r_{\text{max}} \) may be termed as the mapping parameters. Now, introducing the following relation,

\[
\psi(r(x)) = \sqrt{r'(x)} f(x)
\]

coupled with the symmetrization procedure [32,33] leads to the transformed Hamiltonian as below,

\[
\hat{H}(x) = -\frac{1}{2} \frac{1}{r'(x)} \frac{d^2}{dx^2} \frac{1}{r'(x)} + v(r(x)) + v_m(x),
\]

where \( v_m(x) \) is given by,

\[
v_m(x) = \frac{3(r'')^2 - 2r''r'}{8(r')^4}.
\]

Note the advantage that this leads to a symmetric matrix eigenvalue problem which can be readily solved to give accurate eigenvalues and eigenfunctions. For the particular transformation used in Eq. (10), \( v_m(x) = 0 \). This discretization then leads to the following set of coupled equations,

\[
\sum_{j=0}^{N} \left[ -\frac{1}{2} D^{(2)}_j + \delta_{j'j} v(r(x_j)) + \delta_{j'j} v_m(r(x_j)) \right] A_j = E A_{j'}, \quad j = 1, \ldots, N - 1,
\]

where

\[
A_j = [r'(x_j)]^{1/2} \psi(r(x_j)) \left[ P_N(x_j) \right]^{-1}.
\]

and the symmetrized second derivative of the cardinal function, \( D^{(2)}_{jj} \) is given by,

\[
D^{(2)}_{jj} = [r'(x_j)]^{-1} d^{(2)}_{jj} [r'(x_j)]^{-1},
\]

with

\[
d^{(2)}_{jj} = \frac{1}{r'(x_j)} \left( \frac{N + 1)(N + 2)}{6(1 - x_j)^2} \frac{1}{r'(x)} \right), \quad j = j',
\]

\[
= \frac{1}{r'(x_{jj})} \frac{1}{(x_j - x_{jj})^2} \frac{1}{r'(x_j)}, \quad j \neq j'.
\]
The performance of the method has been tested for a large number of potentials with many other works in the literature with respect to the variation of the mapping parameters. The results have been reported only up to the precision that maintained stability with respect to these variations. Thus for all the calculations done in this work, a consistent set for the numerical parameters \((r_{\text{max}} = 200, \alpha = 25\) and \(N = 300)\) has been used which seemed to be appropriate for the current problem.

III. RESULTS AND DISCUSSION

In order to show the efficacy of the method, we first present some specimen results for a few odd- and even-parity high excited states of the pure three-dimensional quartic oscillator corresponding to the large vibrational quantum numbers \(v = 48, 49\) and the angular momentum quantum numbers \(\ell = 0, 1, \ldots, 9\) (these two quantum numbers must have the same parity). This was chosen because it has been quite extensively investigated by many authors over a long period and fairly accurate results are available making it amenable to easy comparison. At this point, it may be noted that all the results reported in this and all other subsequent tables throughout this article, have been truncated and not rounded-off. Therefore all the entries in the tables are to be taken as correct up to the place they are reported. The results used for comparison in Table II are chronologically: (a) the linear variation method involving diagonalization of matrices of large order \((800 \times 800)\) \([39]\), (b) the analytical formula based on the scaled oscillator approach \([40]\), (c) the finite-difference calculation \([10]\) and (d) the asymptotic shooting method \([41]\). As seen, the present result for all these states match exactly up to the 9th decimal place with the accurate results of \([41]\), demonstrating that higher excited states can be obtained fairly accurately and reliably.

Now we turn our focus on to the singular potentials. Table III shows the first 5 eigenvalues belonging to \(\ell = 0\) and 1 as obtained by the GPS method for a selected set of parameters for the even-power inverse anharmonic potentials. Besides the ground states, some of the excited states corresponding to \(\ell = 0\) have been reported in the literature and we quote them appropriately wherever possible. Exact analytical results are obtainable for parameters following certain relations among them for (i) ground \([7,15]\) and (ii) excited states \([15]\) (the exactly solvable conditionality, e.g., \(a = 0.5, b = -5.625, c = 1.7578125)\) and our results match very well with these. Both positive and negative values of the parameter \(b\) have been
considered, while the parameter $a$ has been fixed at 0.5 in all the cases. No results could be found for non-zero angular momentum states. For the first set, the numerical integration results are available for the first three states of $\ell = 0$ [42], while exact analytical result [15] exist for the first two states of $\ell = 0$. For the third set, there were some controversy in the literature regarding the position of the second state corresponding to $\ell = 0$. It was estimated to be at 6.048105 in [14]; later a numerical B-spline basis set calculation [12] re-estimated it at 4.24927125 a.u. The current scheme computes this with a higher accuracy (at 4.24927125613) than before and is more in keeping with the latter result. For the last two sets, no results are available except the exact analytical values for the ground states. A wide range of parameters has been used in this table, and these results may be useful to check the performances of other methods.

After comparing the GPS results for the harmonic potential with inverse even-power anharmonicities for ground and higher excited states, we now in Table III present the first 10 eigenvalues for the same belonging to $\ell = 0, 1, 2, 3, 4, 5$ with the parameter set $a = 0.5$, $b = 0.5$ and $c = 0.4$. The reason for the choice of this particular set lies in the fact that this is the only set for which we could find some nonzero angular momentum states with good accuracy [9]. Reference [9] employed the analytic continuation method and those are quoted. It is evident that for the available states, our results are in excellent agreement with those of [9]. However, these results are available only for the first four states of $\ell = 0, 1, 2, 3$. These results illustrate an advantage of the present method to treat the ground and excited states at the same footing without any special consideration for excited states as often required by

| $v$ | $\ell$ | This work | Ref. [39] | Ref. [40] | Ref. [10] | Ref. [41] |
|-----|--------|-----------|-----------|-----------|-----------|-----------|
| 48  | 0      | 250.18358697 | 250.183351 | 250.183369 | 250.183359 | 250.183358697 |
| 49  | 1      | 256.916238928 | 256.916220 | 256.916238 | 256.916239 | 256.9162389286 |
| 48  | 2      | 250.096690608 | 250.096679 | 250.096671 | 250.096691 | 250.096690608 |
| 49  | 3      | 256.773728914 | 256.773732 | 256.77369 | 256.7737289146 |
| 48  | 4      | 249.894552064 | 249.894545 | 249.894505 | 249.8945520647 |
| 49  | 5      | 256.517359165 | 256.517338 | 256.517316 | 256.5173591656 |
| 48  | 6      | 249.577151099 | 249.577138 | 249.577179 | 249.5771510991 |
| 49  | 7      | 256.147382583 | 256.147373 | 256.14750 | 256.1473825836 |
| 48  | 8      | 249.144812457 | 249.144801 | 249.1452 | 249.1448124575 |
| 49  | 9      | 255.664161642 | 255.664146 | 255.66480 | 255.6641616427 |
TABLE II: Comparison of the energies (in a.u.) with literature data for the singular potential in Eq. (1) with $a = 0.5$. First five eigenvalues are presented for $\ell = 0$ and 1.

| $b$  | $c$   | $\ell = 0$ | $\ell = 1$ |
|------|-------|------------|------------|
| −5.625 | 1.7578125 | $−0.999999999999(−1.0^a,−1.0^b)$ | 0.09972656243 |
|       |        | 2.999999999999(3.0^a,3.0^b) | 3.4535246920 |
|       |        | 5.48535332842(5.485353^b) | 5.8434077651 |
|       |        | 7.79200908589 | 8.1037987036 |
|       |        | 10.0249058750 | 10.3072928767 |
| −3.5  | 24.5  | 3.50000000000(3.5^c) | 3.7515331514 |
|       |       | 5.99788108291 | 6.2024854892 |
|       |       | 8.35808537819 | 8.5377961851 |
|       |       | 10.6486411431 | 10.8121723015 |
|       |       | 12.8960139536 | 13.0478732292 |
| 0.02041 | 0.09  | 2.04810689953(2.0481069^d,2.0481069^e) | 2.6368068656 |
|       |       | 4.24927125613(4.24927125^d,6.048105^e) | 4.7398165004 |
|       |       | 6.3922753858(6.3922759^d) | 6.8284134800 |
|       |       | 8.50708702884(8.507087^d) | 8.9068619165 |
|       |       | 10.6046536820 | 10.9776953418 |
| 0.5   | 0.5   | 2.50000000000(2.5^c) | 2.9358346225 |
|       |       | 4.7664152281 | 5.1271377958 |
|       |       | 6.95840432469 | 7.2782932569 |
|       |       | 9.11294921787 | 9.4059292925 |
|       |       | 11.2443693329 | 11.5177212332 |
| 22.5  | 112.5 | 5.49999999999(5.5^c) | 5.65277606191 |
|       |       | 7.97997008055 | 8.1141805562 |
|       |       | 10.3661382958 | 10.4882632705 |
|       |       | 12.6938328534 | 12.8072549804 |
|       |       | 14.9811074983 | 15.0878538581 |

$^a$Exact value, ref. [15].
$^b$Ref. [42].
$^c$Exact value, ref. [7].
$^d$Ref. [12].
$^e$Ref. [14].

some of the methods in the literature.

Now results are presented for the perturbed Coulomb potential. The basic strategy of presentation remains the same as earlier. First, a few low-lying states along with the literature results for a fairly large range of parameter sets and then higher states for a particular case. Table [LV] shows the first four computed eigenvalues for $\ell = 0$ and 1, of the five such sets along with other results. In this case the literature data seems relatively scarce and scanty. Both large and small $Z$ as well as $\lambda$ regions have been investigated. The
TABLE III: The first 10 eigenvalues (in a.u.) for $\ell = 0, 2, 4, 6, 8$ for the singular potential in Eq. (1).

The parameters are: $a = 0.5$, $b = 0.5$ and $c = 0.4$. Numbers in the parentheses denote the values taken from Ref. [9].

| $\ell = 0$ | $\ell = 2$ | $\ell = 4$ | $\ell = 6$ | $\ell = 8$ |
|------------|------------|------------|------------|------------|
| 2.46735982710 | 3.66898315916 | 5.54021470933 | 7.5163408012 | 9.50878342955 |
| (2.46735982710) | (3.66898315916) | | | |
| 4.72473466150 | 5.76433139697 | 7.55977095004 | 9.5218664743 | 11.5110218564 |
| (4.72473466150) | (5.76433139697) | | | |
| 6.91000701257 | 7.85154984749 | 9.58076033037 | 11.527837493 | 13.513680513 |
| (6.91000701257) | (7.85154984749) | | | |
| 9.05914846383 | 11.6028526028 | 13.5341458494 | 15.5158206760 | |
| (9.05914846383) | (11.6028526028) | | | |
| 11.1859453067 | 13.6257807401 | 15.5408308979 | 17.5183783293 | |
| 13.2973083828 | 15.6493304068 | 17.5477932761 | 19.5210395512 | |
| 15.3972525569 | 17.673301630 | 19.550974910 | 21.523802825 | |
| 17.4883415197 | 19.6976430683 | 21.5626976193 | 23.526665991 | |
| 19.572321622 | 21.722157681 | 23.570568873 | 25.5296292578 | |
| 21.650433563 | 23.7467929198 | 25.578185402 | 27.532689160 | |

The first three sets keep the $Z$ and $g$ fixed at $1$ and $0$ respectively varying $\lambda$ from $0.1$ to $1000$. There are no direct results for these to compare; however the lower and upper bounds for the ground-state energies are available [21] from the Stieltje’s moments method and these are mentioned appropriately. It is gratifying that our results fit very nicely within the small range of the bounds. For $Z = 8, g = 1, \lambda = 1/32$, the exact supersymmetric result for the lowest state of $\ell = 1$ is $-7.375$ (as quoted in [26]). The first four states of $\ell = 1$ are compared with the Hill-determinant results [26]. Table [IV] now gives the results for first 10 eigenvalues corresponding to $\ell = 0, 2, 5$ for the parameter set, $Z = 12, g = 1, \lambda = 1/32$ A few results are available for $\ell = 2$ including the exact supersymmetric result [26] as well as the Hill-determinant result [26]. The agreement in our results is seen to be excellent.

Additionally we now give the expectation values $\langle r^{-1} \rangle$ and $\langle r \rangle$ for both the potentials under consideration in Table [VI]. Three states belonging to $\ell = 0$ and $1$ are reported for both the potentials (one set for each of them). While no results could be found for the former case, a few results are available [43] for the perturbed Coulomb potential with $Z = g = \lambda = 0.5$ and good accuracy is observed for these. Finally, Fig. (1) depicts the radial probability distribution functions $|r R_{n\ell}|^2$ for the singular potentials in Eqs. (1) and (2) (in the left and right panel) for the first four states belonging to $\ell = 0, 1, 2$ respectively. The existence of
TABLE IV: Comparison of the calculated energies (in a.u.) with literature data for the singular potential in Eq. (2). First four eigenvalues are presented for $\ell = 0$ and 1.

| $Z$ | $g$ | $\lambda$ | $\ell = 0$ | $\ell = 1$ |
|-----|-----|------------|------------|------------|
| 1   | 0   | 0.1        | $-0.29608776768, -0.296087677$ | 0.57456732342 |
|     |     |            | 0.8791360777 | 1.5383941205 |
|     |     |            | 1.8709768364 | 2.4746029046 |
|     |     |            | 2.8225931925 | 3.3984488837 |
| 1   | 0   | 10         | $4.1501236516, 4.150123^b$ | 9.5524662112 |
|     |     |            | 13.602643792 | 18.672142320 |
|     |     |            | 22.793852381 | 27.731460369 |
|     |     |            | 31.8906276164| 36.76042590  |
| 1   | 0   | 1000       | $59.375469050, 59.3754646^c$ | 106.73670748 |
|     |     |            | 150.1747151  | 196.95803480 |
|     |     |            | 240.33685382 | 286.48090994 |
|     |     |            | 330.2541784  | 376.1905554  |
| 8   | 1   | 1/32       | $-31.841419073$, $-7.375000000, -7.375000^c$ | $-7.245571746$, $-2.048308777, -2.048308^c$ |
|     |     |            | $-7.245571746$, $-2.048308777, -2.048308^c$ | $-1.9150955585$, $0.5675978768, 0.567560^c$ |
|     |     |            | 0.7050052129 | 2.4020644372,2.402064^c |
| 10  | 5   | 1          | $-49.224345286$, $-9.8803468590$ | $-9.8803468590$ |
|     |     |            | $-9.289879040$, $0.7590170486$ | $-9.8803468590$ |
|     |     |            | 1.4166373230 | 7.418810789 |
|     |     |            | 8.1281375830 | 12.855211501 |

^a Lower and upper bounds to the eigenvalue are $-0.296088$ and $-0.296087$, from ref. [21].

^b Lower and upper bounds to the eigenvalue are $4.1501236$ and $4.1501239$, from ref. [21].

^c Lower and upper bounds to the eigenvalue are $59.3754689$ and $59.3754694$, from ref. [21].

^d Exact supersymmetric result, as quoted in ref. [26].

^e Hill-determinant method, ref. [26].

the required number of nodes is clearly manifest.

Before passing, a few remarks should be made. In the present method, no unphysical states are obtained. It is worthwhile to note that some of the methods employed for these kind of potentials in the literature often have the unwanted feature of producing unphysical roots, e.g., the Ricatti-Padé scheme for a class of singular potentials, commonly termed as spiked oscillators. On the other hand, existence of false (unphysical) eigenvalues in the Hill-determinant method for a perturbed oscillator or perturbed Coulomb potential has been suggested by some authors on mathematical grounds. Later it was pointed out [43] that these unphysical or false states manifest themselves by having the negative values for $\langle r \rangle$ or $\langle r^{-1} \rangle$. Some of the well-known methods have another undesirable feature that they give
FIG. 1: The radial probability distribution functions, $|r_{R_n\ell}|^2$ for the potentials in Eqs. (1) and (2) in left and right panel respectively. The first four states corresponding to $\ell = 0, 1, 2$ are shown: (a) the potential, (b) the ground, (c) first excited, and (d) the second excited state. The parameters are $a = 0.5, b = -5.625, c = 1.7578125$. and $Z = 10, g = 5, \lambda = 1$. 
TABLE V: The first 10 eigenvalues (in a.u.) for $\ell = 0, 2$ and 5 of the singular potential in Eq. (2) for the three sets of parameters $Z = 12, g = 1, \lambda = 1/32$.

| $\ell = 0$ | $\ell = 2$ | $\ell = 5$ |
|-----------|-----------|-----------|
| $-71.874422806$ | $-7.125000000$, $-7.125^a$, $-7.125000^b$ | $0.78955622011$ |
| $-17.494216229$ | $-2.7950831896$, $-2.795083^b$ | $2.3644580048$ |
| $-6.8642582202$ | $-0.2158824422$, $-0.215883^b$ | $3.744423185$ |
| $-2.5279008987$ | $1.6823565181$, $1.682357^b$ | $4.9984881647$ |
| $0.05747113632$ | $3.2467031143$ | $6.1643195425$ |
| $1.9612173543$ | $4.6183716246$ | $7.2648275518$ |
| $3.5304071400$ | $5.8655676414$ | $8.3148289025$ |
| $4.9063624018$ | $7.025708497$ | $9.3244751785$ |
| $6.1573955416$ | $8.1213708656$ | $10.301031550$ |
| $7.3210117750$ | $9.1671716851$ | $11.249883522$ |

$^a$Exact supersymmetric result, as quoted in ref. [26].

$^b$Hill-determinant result, ref. [26].

TABLE VI: Calculated expectation values (in a.u.) along with literature data for comparison for the two singular potentials in Eqs. (1) and (2) for the first three states corresponding to $\ell = 0$ and 1. The numbers in the parentheses denote the reference values from [43].

| $a$ | $b$ | $c$ | $\ell$ | $\langle r^{-1} \rangle$ | $\langle r \rangle$ |
|-----|-----|-----|--------|----------------|----------------|
| 0.5 | $-5.625$ | 1.7578125 | 0 | 1.037245259 | 1.04949541 |
| | | | | 0.6106362329 | 1.883380179 |
| | | | | 0.5127801051 | 2.390745126 |
| 1 | | | 0.9798264559 | 1.109065417 |
| | | | 0.5975951150 | 1.946934875 |
| | | | 0.5093809276 | 2.427714809 |

| $Z$ | $g$ | $\lambda$ | $\ell$ | $\langle r^{-1} \rangle$ | $\langle r \rangle$ |
|-----|-----|-----|--------|----------------|----------------|
| 0.5 | 0.5 | 0.5 | 0 | 1.426727774(1.4267278) | 0.9267277745(0.92672779) |
| | | | | 1.054078325(1.0540783) | 1.549650851(1.5496509) |
| | | | | 0.9037976872 | 1.990327571 |
| 1 | | | 0.8497088122(0.84970883) | 1.345281337(1.3452814) |
| | | | 0.7355708974(0.73557090) | 1.822100782(1.8221008) |
| | | | 0.6671751957 | 2.204434707 |

poor or erroneous results for potentials having multiple wells, for certain parameter sets or sometimes even for certain states within a particular parameter set. As an example, the shifted 1/N method for the perturbed Coulomb potential [22] fails to give any result when any four of the five quantities $Z$, $\lambda$, $g$, $\ell$, $n_r$ are kept fixed and only the fifth one is varied. The present method is general in the sense that it is applicable to a wide spectrum of
parameters without requiring any special relation among them, irrespective of the strength of the coupling involved and therefore lifts any such restrictions. In view of the simplicity and accuracy offered by this method for the polynomial as well as the singular potentials considered in this work for both ground and higher excited states, it may be hoped that this prescription may be useful for a wide range of other similar potentials of interest. Thus other singular potentials having higher order terms in Eqs. (1) or (2) or the nonsingular polynomial potentials with higher order anharmonicities like quartic, sextic, octic, etc., may as well be treated by this method very well. Finally, we mention that while practically all of the common methodologies in quantum mechanics for such systems involve the solution of the time-independent Schrödinger equation, recently a time-dependent (TD) formalism [44-47] has been proposed as well for the accurate calculation of static properties, which is, in principle, exact. Applications have been made for the ground and excited states of double well and anharmonic oscillators having higher order terms, multiple-well and self-interacting oscillators in one dimension [44-46], as well as the ground-state electronic properties of noble gas atoms [47] through an amalgamation of the density functional and quantum fluid dynamical treatment. It may be worthwhile to study the performance of such TD methods for the singular potentials dealt in this work.

IV. CONCLUSION

An accurate and simple methodology has been proposed for certain singular potentials employing the generalized pseudospectral method. The prescription is general and reliable. The energies, densities and expectation values presented for ground and excited states of the (i) harmonic potential with inverse quartic and sextic perturbation and (ii) the perturbed Coulomb potential with linear and quadratic terms are reported for a broad spectrum of potential parameters. This scheme is capable of producing very good quality results for both ground and higher excited states. The \( v = 48, 49, \cdots, 48, 49 \) states corresponding to the angular momentum quantum numbers \( \ell = 0, 1, \cdots, 8, 9 \) for the pure three dimensional quartic oscillator illustrates this fact. Many states have been reported here for the first time which might constitute a useful set for future referencing. A large number of states are shown to be in excellent agreement with those from other sophisticated methods available in the literature and augurs well for its practical applicability to other similar potentials of
physical and mathematical interest in quantum mechanics.

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