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Eigenvalues of the Schrödinger equation with Coulomb potentials plus linear and harmonic radial terms

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Abstract. Analytic approximations for the eigenvalues have been obtained using the two-point quasifractional approximants method. Here we extend and generalize previous work where the method was applied to determine eigenenergies of two-dimensional Coulomb potentials in the presence of a magnetic field of arbitrary strength. We have also shown the advantage of our results with respect to other calculations using the shifted $1/N$ method or Padé approximants.

1. Introduction

Radial potentials represent simplified versions of important physical situations encountered in atomic and molecular physics as well as astrophysics, particle physics, plasma physics and solid-state physics. Here we study the eigenenergies of a hydrogenic atom with a Coulomb potential in the presence of an external linear term and an isotropic harmonic oscillator,

$$V(r) = -Z/r + gr + \lambda r^2. \quad (1)$$

Potentials of the form $V(r) = -Z/r + gr$ (linear plus Coulomb potential) have attracted great interest in atomic and molecular physics and quantum chromodynamics. It corresponds to a spherical Stark effect in hydrogen (Austin 1980, Vrscay 1985, Killingbeck 1977, 1978a), where g is essentially the electric field and is expressed in atomic units of the electric field $E_h e^{-1} a_0^{-1}$. For $g < 0$, $V(r)$ corresponds to an unstable potential, where $E(\lambda)$ is complex and $-\text{Im } E$ is inversely proportional to the mean lifetime of the exponentially decaying tunnelling states or resonances. The spectra of families of elementary particles may be well described by bound states of charmed-quark–charmed-antiquark pairs interacting through various non-relativistic confinement potentials. For this reason this potential has been studied in the context of non-relativistic quark confinement potentials and similar bound-state problems in particle physics (Vrscay 1985, Banerjee 1979, Eichten *et al* 1978, Müller-Kirsten *et al* 1979, Gupta and Khare 1979, Killingbeck 1977, Rein 1977, Eichten *et al* 1978, Quigg and Rosner 1979). The potential $V(r) = -Z/r + \lambda r^2$ has been studied in the context of:

- (a) the Zeeman quadratic effect in hydrogenic atoms (Avron 1991);
- (b) lineshapes of x-rays emitted by ions, used as a density diagnostic in laser-fusion experiments (Skupsky 1980); and

(c) several problems confronted in ion-sphere models in plasma physics (Stewart and Pyatt 1966, Cauble *et al* 1984).

In particular, for high plasma densities the shift frequency in the x-ray spectral lines emitted by laser-imploded plasmas can be explained using the ion-sphere model. In this case the potential considered is (Skupsky 1980)

$$V(r) = -\frac{Ze^2}{r} + \frac{(Z-1)e^2}{2R_0} \left[3 - \left(\frac{r}{R_0} \right)^2 \right] \quad r \leq R_0 \quad (2)$$

where R_0 is the radius of a sphere containing enough free electrons (plus the bound electron) to neutralize the ion, and it is given by $R_0 = ((Z-1)/(4\pi n_e/3))^{1/3}$. Here n_e is the number density for free electrons. The first term in (2) is the nuclear potential which gives rise to the normal hydrogen spectra. The remaining term is the potential generated by the surrounding free electrons. This is the source of the line shift.

Killingbeck (1978b) used a potential $V(r) = -Z/r + 2\lambda r + \lambda^2 r^2$ to show that the energy $E(\lambda)$ for $\lambda < 0$ contains a component not given by the Rayleigh–Schrödinger perturbation theory. In this analysis the $-1/r$ term represents the gluon exchange potential and the $2\lambda r + \lambda^2 r^2$ terms are responsible for confinement. Analytical solutions for the s-wave states for some particular values of λ were obtained by Saxena and Varma (1982b). A generalized version of the Killingbeck potential provides a convenient example to study quantum discontinuity phenomena (Saxena *et al* 1988), since there exists a discontinuity in the eigenvalue spectrum at $\lambda = 0$, as λ changes from positive to negative. The potential in (1) was suggested by Gupta and Khare (1979) as a quark-confining potential on the basis of 3P_J splittings of charmonium levels. Coincidences in the binding energy spectra of these potentials were analysed by Chhajlany (1993) based on the invariance of the kinetic energy operator under a discrete coordinate transformation.

For some special relations between Z , g and λ , the preceding potential (1) is a quasi-exactly solvable potential (Bessis *et al* 1987, Roychoudhury and Varshni 1988, Dutra 1988), and analytic solutions of the eigenfunctions and the eigenvalues can be found. However, we consider here the calculation of the eigenenergy for the general case, that is, for any value of g and λ . This potential and its particular cases have been studied in the context of the Rayleigh–Schrödinger perturbation method (Saxena and Varma 1982a, Killingbeck 1977, 1978a, 1980, 1986), the moment method (Bessis *et al* 1987), analytic continued fraction theory (Datta and Mukherjee 1980, Flessas 1982, Znojil 1983), the Hill determinant (Chaudhuri 1983, 1988, Chaudhuri and Mondal 1995), the Bender–Wu method (Avron 1991), the Padé method (Austin 1980), the Bender–Wu WKB method (Mehta and Patil 1978), supersymmetric quantum mechanics SUSYQM and the shifted $1/N$ method (Adhikari *et al* 1989, Roychoudhury and Varshni 1988), and other methods (Dutra 1988, Vrscay 1987, Ivanov 1996).

The shifted $1/N$ expansion, for example, has been proven to provide good results for potentials having a single minimum (Chatterjee 1990, Roychoudhury and Varshni 1990). However, the numerical errors increase with increasing values of the coupling constant, and the method becomes unreliable for large values of g and λ . Furthermore, the expressions obtained by the $1/N$ method are very cumbersome if one needs to determine the derivative of the eigenvalues in order to calculate, for instance, electric or magnetic susceptibilities, or other electromagnetic functions. Also derivatives of the eigenvalues appear in some calculations, as in the spectroscopy of heavy quarks (Müller-Kirsten *et al* 1979), where the value of the s-wave wavefunction at the origin (needed to derive the leptonic widths) depends on the eigenvalues and their derivatives. In these cases it is very convenient to have analytic solutions for the eigenvalues instead of numerical integrations.

In this paper we follow a methodology unlike the others. Using the perturbative quantum mechanics analysis one can obtain expansions in power series valid only for small values of the coupling parameter. It usually happens that the first term of these expansions does not give enough accuracy for the applications, so if we want to expand the region of validity of our series we should calculate more terms. However, the perturbation expansion fails quickly, due to the small radius of convergence of this series. For large values of the coupling parameter, we can obtain an asymptotic expansion exchanging the perturbed Hamiltonian with the non-perturbed Hamiltonian. This procedure can be used only when the new non-perturbed Hamiltonian has (old perturbed Hamiltonian) exact solutions for the eigenvalues and eigenvectors. The quality of the results obtained in both expansions depends on the radius of convergence of each expansion (Kleinert 1995).

The Padé, two-point Padé and Lauren–Padé methods have been used extensively in physics (Baker and Graves-Morris 1981a, b, Bultherl 1987). However, the improvement introduced by the two-point quasifractional approximant (TQA) method proposed by Martín and co-workers (Chaldbaud and Martín 1986, Martín and Baker 1991, Martín *et al* 1992) has proved to be a powerful procedure for obtaining the eigenvalues of a hydrogenic atom in a uniform magnetic field of arbitrary strength in two dimensions (Martín *et al* 1992). In this paper we show that this is also the case for three-dimensional (3D) radial potentials. The strategy of these quasifractional approximants is to build an analytic bridge between the power series and the asymptotic expansion, to obtain a unique analytic expression for the eigenenergies, using a few terms of both expansions. The accuracy of the analytic approximations obtained with this procedure is high for the whole range of values of the coupling parameters, even in the region where both expansions are not convergent. The results are usually good for all values of the coupling parameter independent of the radius of convergence of each expansion. In some cases approximations with seven exact digits are obtained with expansions of zero radius of convergence (Chaldbaud and Martín 1986).

The purpose of this work is to extend and improve the previous procedure using series other than those obtained by the usual perturbation quantum theory. We will derive a single analytic expression for the ground state and the first excited states energy 2S and 2P, with good accuracy for the eigenvalues independent of the value of the parameters.

One of the differences between the TQA and the two-point Padé method is that, a power-series and an asymptotic expansion are used, instead of two power series. Consequently, instead of using only fractional functions we are forced to introduce non-fractional functions, which we have denoted as auxiliary functions, in order to reproduce the singularities of the exact function. The golden rule is that the function and the approximant should have the same singularities in the region of interest. Undesirable singularities, that might appear in the approximant, must be located outside of that region. In this way highly accurate results are usually obtained with polynomials of low degree. In our case we look for the eigenvalues when λ is positive, therefore our region of interest is the positive axis ($\lambda > 0$). Thus the auxiliary functions must be chosen in such a way that the undesirable singularities have to be located in the negative axis or in the left-hand complex plane. Another important advantage of the TQA with respect to the Padé method is better accuracy for an equal number of parameters, and therefore the system of equations to obtain those parameters is simpler.

In this paper, we have not used the Rayleigh–Schrödinger perturbation method (RS) to obtain the power series for small values of the parameters. Instead of that, we have fixed Z and g , and obtained the power series for the parameter $\lambda > 0$, using the hypervirial theorem (HVT) and the Hellman–Feynman theorem (HFT). The HVT and HFT have been applied previously to the problems of anharmonic oscillators (Hirschfelder 1972, Swenson and Danforth 1972, Duncan and Jones 1993), the hydrogen atom with perturbation λr (Killingbeck 1978a), and

the treatment of the Coulombic-like potentials in the presence of screening effects (Grant and Lai 1979, Lai 1981). The energy and expectation values of the position coordinates can be calculated as power series of the perturbation coupling parameters. In the perturbation expansion method here used, there is no need to calculate the perturbed wavefunction, as happens with the RS perturbation method. To obtain the perturbed energy neither do we need the sum of matrix elements characteristic of the RS method. The preceding theorems mentioned above (HVT and HFT) are useful to obtain the expansion for small values of g and λ .

In contrast to our preceding paragraph, to obtain an asymptotic expansion, valid for the intermediate and high values of λ , the classical RS perturbation method has been used. For our calculations we have chosen a fixed value of g , obtaining approximants as a function of only one parameter, the parameter λ . We have preferred to choose small values of g in order to work with larger ranges of λ -values for bound states.

The form of our approximants for the ground state is just the same for all the excited states. However, we have calculated only the eigenenergies for the ground state and the first excited states 2S and 2P, because these are the important bound states. In these cases, the second and third excited bounded states exist only for very small values of g and λ . Thus the calculations of the approximants for those cases are not so important and can be omitted. Even for the cases considered here, we have to choose a very small value of g in order to obtain results of physical interest. Clearly the electron energy levels of the other states are so close to the free state that ionization is produced immediately.

In every case we have determined the accuracy of our results by numerical integration of the corresponding Schrödinger equation, using a fourth-order Runge–Kutta method. The approximants, found here, are valid for any value of the parameter λ . The shifted $1/N$ method fails for large values of λ . Furthermore, our method gives better accuracy than the shifted $1/N$ method even in the region where that method gives good results. In addition, our approximation involves only first-order polynomials, together with square roots of first-order polynomials, therefore the computation can be done easily with a pocket calculator or by hand. The accuracy of our approximants are very good, and as far as we know are well suited for all experimental and theoretical applications.

The paper is organized as follows. In section 2 we discuss the necessary theoretical background that is needed to yield the perturbation power series and the asymptotic expansions. We also discuss here the procedure to obtain the two-point quasifractional approximants. In section 3 we will compare, through a detailed numerical analysis, the accuracy of our results with those obtained by other methods, such as the Padé method and the shifted $1/N$ method. Finally, the last section is devoted to the conclusions.

2. Power series, asymptotic expansions and two-point quasifractional approximants

The Hamiltonian operator for a hydrogenic atom with a polynomial perturbation is

$$\hat{H} = -\frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} - \frac{Z}{r} + gr + \lambda r^2 + \frac{\hat{L}^2}{2r^2} \quad (3)$$

where g and λ are the coupling parameters, and \hat{L}^2 is the angular momentum operator. Here we use atomic units $\hbar = e = m_e = 1$. The number Z is like a scale factor, and is not important for the explanation of our method. Thus we will consider $Z = 1$. Let us consider first the calculation leading to the asymptotic expansion in λ . Here we take the unperturbed

Table 1. Values of the coefficients of the power series and the asymptotic expansions for the 1S, 2S and 2P states for different values of the coupling parameter g .

| State | g | a_0 | a_1 | a_2 | a_3 | b_0 | b_1 | b_2 | b_3 | b_4 |
|-------|--------|-----------|--------|-----------|---------|--------|---------|---------|---------|------------|
| 1S | 0 | -0.5 | 3 | -32.25 | 1801.13 | 2.1213 | -1.3418 | -0.1577 | 0.0297 | — |
| 2S | 0 | -0.125 | 42 | -2366.629 | — | 4.9497 | -1.0467 | 0.0307 | 0.0688 | 0.001 84 |
| 2P | 0 | -0.125 | 30 | -1674.339 | — | 3.535 | -0.8946 | -0.0354 | -0.0023 | -0.000 086 |
| 1S | 0.1 | -0.36 | 1.934 | 35.475 | 1362.75 | 2.1213 | -1.3418 | -0.1577 | 0.0652 | — |
| 2S | 0.0001 | -0.124 36 | 41.968 | -2349.956 | — | 4.9497 | -1.0466 | 0.0307 | 0.0689 | 0.001 8 |

Hamiltonian $\hat{H}_0(r)$ and the perturbed potential $V_1(r)$ as

$$\hat{H}_0(r) = -\frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} + \lambda r^2 + \frac{\hat{L}^2}{2r^2} \tag{4}$$

$$V_1(r) = -\frac{1}{r} + gr \quad \hat{H} = \hat{H}_0(r) + V_1(r). \tag{5}$$

The eigenvalues and eigenfunctions of the unperturbed states are

$$E_{nlm} = (2n + l + \frac{3}{2})\sqrt{2\lambda} \tag{6}$$

$$\Psi_{nlm}(r, \theta, \phi) = Nr^l e^{-(\lambda r^2/2)} {}_1F_1(-n, l + \frac{3}{2}; \lambda r^2) Y_{lm}(\theta, \phi). \tag{7}$$

Here N is the normalization constant, $Y_{lm}(\theta, \phi)$ are the spherical harmonics and the ${}_1F_1(-n, l + \frac{3}{2}; \lambda r^2)$ are the confluent hypergeometric functions (Greiner 1994). By using the perturbation method of RS to third order we obtain

$$E_{nl}^{(RS)}(\lambda) = b_0 \lambda^{1/2} + b_1 \lambda^{1/4} + b_2 + \frac{b_3}{\lambda^{1/4}} + \dots$$

$$= \sum_{j=0}^{\infty} (b_j^{(0)} \lambda^{(\frac{1}{2}+j)} + b_j^{(1)} \lambda^{(\frac{1}{4}+j)} + b_j^{(2)} \lambda^j + b_j^{(3)} \lambda^{-(\frac{1}{4}+j)}) \tag{8}$$

where the coefficients b_0, b_1, b_2 and b_3 are given in table 1 for the states 1S, 2S and 2P and for different values of g . The second right-hand side is a way to group the first one, which is convenient for the two-point quasifractional method. In the second part we change the notation slightly, that is $b_0^{(0)} = b_0, b_0^{(1)} = b_1, b_0^{(2)} = b_2$ and $b_0^{(3)} = b_3$. The asymptotic expansion (8) is decreasing in powers of $\lambda^{1/4}$ and in all cases the values of the coefficients are decreasing. This behaviour is different to that in the HF power series as is shown below.

Let us consider now how to calculate the power-series expansion valid for small values of λ . By applying the HVT and HFT to Hamiltonian in (3), we derive a power series as a function of both coupling parameters with a different split in perturbed and unperturbed terms. In the case where the potential is a polynomial, the HVT and HFT method is much easier to implement. It is the purpose of this paper to obtain the TQA as a function of only one parameter, so the parameter g is fixed and must be specified from the beginning. The power series is only convergent for small values of the coupling parameter of g . The dimensionless Hamiltonian (3) can be cast as

$$\hat{H} = -\frac{1}{2} \frac{d^2}{dr^2} - \frac{1}{r} \frac{d}{dr} + V_2(r) \tag{9}$$

where $V_2(r)$ is the sum of the centrifugal term and the confining potential defined in (1). The result after applying the HVT and HFT method (Grant and Lai 1979) are

$$E_{nl}^{(HF)}(\lambda) = a_0 + a_1 \lambda + a_2 \lambda^2 + a_3 \lambda^3 + \dots \tag{10}$$

where the coefficients a_0 , a_1 , a_2 and a_3 are given in table 1 for the states 1S, 2S and 2P, and for different values of g . These series are divergent for any λ different from zero, however, it will be used as the power series in our method.

Both expansions (8) and (10) together can be used to obtain quasifractional approximants of high accuracy for any value of the coupling parameter λ , still in the regions where the series are divergent.

Let us also point out another feature of our analysis, which we will call low or high effectiveness. In a previous work (Martín *et al* 1992) we have explained the motivation behind this terminology. However, it is also useful to stress the meaning of ‘effectiveness’ again in the present context. For us the term effectiveness is used in the sense that the series of the quasifractional approximant should have only powers of the variable appearing in the power series of the function. Thus we do not want to set to zero coefficients of the approximate series with no corresponding powers in the original series. Such a specification is necessary because there are sometimes power terms in the approximant that do not appear in the original series. In the Padé method this matter is usually ignored. Our effectiveness criterion is very relevant, because it reduces the number of parameters to be determined to just the needed ones. Considering the preceding expansions we note that the Hellman–Feynman expansion is expressed in powers of λ , while the asymptotic expansion, in contrast, is expressed in powers of $\lambda^{1/4}$. If we choose as our variable $\lambda^{1/4}$ instead of λ , then the approximant will have the right asymptotic expansion, but in this case we have to cope with many undesirable powers such as $\lambda^{1/4}$, $\lambda^{1/2}$, $\lambda^{3/4}$, etc, which do not appear in the HF power series. This means that many undesirable coefficients in the power series of the approximant have to be set to zero. This is what we denote by low efficiency, and what we want to avoid. In contrast, high efficiency will mean that the power series of the approximant have only terms with exponents equal to those appearing in the perturbative analysis.

Considering the form given to the asymptotic expansion in (8), there we see a combination of products of fractional powers with integer powers. The quasifractional approximant must have the same singularities in the region of interest, and we have to select points outside of the region of interest to put the undesirable singularities. If we choose λ or $\lambda^{1/4}$ as an auxiliary function we will have a branch point for $\lambda = 0$, which does not appear in the eigenvalue. The auxiliary functions must reproduce the asymptotic behaviour of the eigenvalues, but furthermore they should also be such that to reproduce the original power series, once combined with the fractional functions. We must keep in mind that the branch points come in pairs. So we should choose the form of auxiliary function as $(1 + \mu\lambda)^{1/4}$ with $\mu > 0$. In this way one of the branch points is at infinity as required, and the second one is on the negative axis, which is out of the region of interest for physics ($\lambda > 0$). Our simplest approximant will have the form

$$\hat{E}_{nl}^{(1)}(\lambda) = \frac{1}{1 + \mu\lambda} \left[(1 + \mu\lambda)^{1/2} (p_0 + p_1\lambda) + (1 + \mu\lambda)^{1/4} (P_0 + P_1\lambda) + (q_0 + q_1\lambda) + (1 + \mu\lambda)^{-1/4} (Q_0 + Q_1\lambda) \right] \quad (11)$$

where $(1 + \mu\lambda)^{1/2}$, $(1 + \mu\lambda)^{1/4}$ and $(1 + \mu\lambda)^{-1/4}$ are the non-fractional auxiliary functions.

The approximant in (11) is a combination of fractional powers with first-degree polynomials. Here we will denote this kind of approximant as first order, thus the order will be given by the degree of the polynomial with the highest degree.

The denominator for the fractional functions are the same. The reason is that we would like to obtain only linear algebraic equations to determine the parameters of the approximants. In the case of different denominators the equations for the parameters are not linear. It is useful to leave μ as a free parameter to be determined later using the eigenvalue at one point. Choosing the free parameter μ in this way we also avoid the occurrence of defects, so usual in

Table 2. Systems of equations obtained for the two-point quasifractional approximants in the cases of ground and first excited states.

| Powers of λ | Ground states | First excited states |
|---------------------|--|--|
| λ^0 | $a_0 = p_0 + P_0 + q_0 + Q_0$ | $a_0 = p_0 + P_0 + q_0 + Q_0$ |
| λ^1 | $a_1 + \mu a_0 = \frac{1}{2}\mu p_0 + \frac{1}{4}\mu P_0 - \frac{1}{4}\mu Q_0 + p_1 + P_1 + q_1 + Q_1$ | $a_1 + \mu a_0 = \frac{1}{2}\mu p_0 + \frac{1}{4}\mu P_0 - \frac{1}{4}\mu Q_0 + p_1 + P_1 + q_1 + Q_1$ |
| λ^2 | $a_2 + \mu a_1 = -\frac{1}{8}\mu^2 p_0 - \frac{3}{32}\mu^2 P_0 + \frac{5}{32}\mu^2 Q_0 + \frac{1}{2}\mu p_1 + \frac{1}{4}\mu P_1 - \frac{1}{4}\mu Q_1$ | $a_2 + \mu a_1 = -\frac{1}{8}\mu^2 p_0 - \frac{3}{32}\mu^2 P_0 + \frac{5}{32}\mu^2 Q_0 + \frac{1}{2}\mu p_1 + \frac{1}{4}\mu P_1 - \frac{1}{4}\mu Q_1$ |
| λ^3 | $a_3 + \mu a_2 = -\frac{3}{48}\mu^2 p_0 - \frac{7}{128}\mu^3 P_0 - \frac{15}{128}\mu^3 Q_0 - \frac{1}{8}\mu^2 p_1 + \frac{3}{32}\mu^2 P_1 - \frac{5}{32}\mu^2 Q_1$ | — |
| $\lambda^{1/2}$ | $p_1 = \sqrt{\mu}b_0$ | $p_1 = \sqrt{\mu}b_0$ |
| $\lambda^{1/4}$ | $P_1 = \mu^{3/4}b_1$ | $P_1 = \mu^{3/4}b_1$ |
| λ^0 | $q_1 = \mu b_2$ | $q_1 = \mu b_2$ |
| $\lambda^{-1/4}$ | $Q_1 = \mu^{5/4}b_3$ | $Q_1 = \mu^{5/4}b_3$ |
| $\lambda^{-1/2}$ | — | $p_0 = \frac{1}{\mu^{1/2}}(\mu b_4 + \frac{1}{2}b_0)$ |

the Padé method. Here the word ‘defect’ is applied in the same sense as in the Padé method, that is, an extraneous zero in the denominator and a nearby one in the numerator (Baker and Graves-Morris 1981a, b).

To determine the values of the parameters $p_0, p_1, P_0, P_1, q_0, q_1, Q_0$ and Q_1 in the quasifractional approximant (11), we have to consider that the power series and the asymptotic expansion of the quasifractional approximant should coincide with those power series and the asymptotic expansion, calculated previously in (8) and (10).

For the ground state we have used an equal number of terms coming from the power series and from the asymptotic expansion. In this way we find a system of eight equations with eight unknowns. Table 2 gives the system of equations used to calculate the parameters of the approximant of the eigenenergies for the 1S states with $g = 0$ and 0.1.

For the first excited state the coefficients of the power series increase strongly with the power of λ (see table 1), and the ranges of validity of these series are very small. Clearly, only the terms a_0, a_1 and a_2 can be used significantly. The coefficients of the other terms are too large. We have taken $g = 0.1$ and 0.0001 for the states 2S and 2P, respectively. The first excited state 2P for $g = 0.1$ is very close to the ionization level for any value of λ , which is the reason we have to choose a much smaller value of g in order to obtain significant values for the eigenvalues. This is also the reason for such large values of the coefficients of λ , for powers larger than λ^3 . The behaviour of the asymptotic expansion is much better, since the values of the coefficients do not change so much for any g . The preceding considerations lead us to use five terms of the asymptotic expansion (one term more than in the ground state) and three terms of the power series (one term less than in the ground state) for the first excited state 2S and 2P. In this way we are keeping the same number of equations as in the ground state, and all the parameters of the approximant can be determined as a function of the free parameter μ . Table 2 gives the system of equations used to calculate the parameters of the approximant for the eigenenergies of the 2S and 2P states in the cases $g = 0, 0.1$ and 0.0001.

To determine the free parameter μ , we calculate numerically the value of the eigenenergy $E_{nl}(\lambda)$ for one value of the coupling parameter λ . The value of μ is determined by the condition that the TQA $\hat{E}_{nl}^{(1)}(\lambda_b)$ is equal to $E_{nl}(\lambda_b)$. The value of λ to be considered, denoted by λ_b , should be for an intermediate value in the region where the potential series and the

Table 3. Values of the coefficients of the parameters $p's, q's, P's, Q's$ and $\mu_{optimal}$ for the TQA.

| State | g | p_0 | P_0 | p_1 | P_1 | q_0 | Q_0 | q_1 | Q_1 | $\mu_{optimal}$ |
|-------|--------|---------|---------|---------|----------|---------|---------|----------|----------|-----------------|
| 1S | 0 | 0.1363 | -0.4278 | 22.1761 | -45.3556 | -0.0806 | -0.1280 | -17.2376 | -10.4865 | 109.2843 |
| 2S | 0 | 0.3956 | -7.4679 | 31.9241 | -17.1439 | 14.9199 | -7.9725 | 1.2768 | 7.2683 | 41.5978 |
| 2P | 0 | 0.2646 | -2.3624 | 23.5694 | -15.3979 | 5.4361 | -3.4633 | -1.5750 | -0.2624 | 44.4412 |
| 1S | 0.1 | -0.0680 | -0.6620 | 27.9917 | -64.320 | -0.287 | -0.082 | -27.464 | 41.243 | 174.1192 |
| 2S | 0.0001 | 0.3969 | -7.5008 | 31.8052 | -17.048 | 15.0044 | -8.0248 | 1.2673 | 7.2062 | 41.2888 |

asymptotic expansion do not give good accuracy. This intermediate value acts as a bridge between both expansions.

To find the eigenenergy at this intermediate point, we can use exact solutions such as, for instance, a quasi-exactly solvable Hamiltonian or any other method, if there is any. In other cases we have to calculate it by numerical computation. It happens sometimes that the values of λ for which we can obtain an exact solution are very small or very large, and in that case we must also use a numerical computation at one point. We have determined this root for μ using the Newton–Raphson method (Nakamura 1992). In order to facilitate our analysis, we define the dimensionless parameter $\lambda' = \lambda/(1 + \lambda)$.

The procedure to determine μ by using the quasi-exactly solvable solutions fails, because the values of λ'_b are very small in the cases considered here, thus they are not in the intermediate region (see the appendix).

Our procedure is as follows: the eigenenergies $E_{nl}(\lambda)$ at the bridge point $\lambda'_b = 0.1$ are calculated from the Schrödinger equation, using the Runge–Kutta method (Neethiulagarajan and Balasubramanian 1989), with an accuracy of five digits and a step $\Delta h = 0.01$. Table 3 presents the optimal values of μ and the values of the parameters $p_0, p_1, P_0, P_1, q_0, q_1, Q_0$ and Q_1 calculated from the quasifractional approximant (11) for the states 1S, 2S and 2P for $g = 0, 0.1$ and 0.0001 .

3. Analysis and discussion

In figures 1(a) and (b) we present the values of the eigenenergies of all the states studied in this work, as a function of the normalized coupling parameter λ' , for some different values of the coupling parameter g . Our results are shown by several kinds of broken curves. On the other hand, we have determined the eigenvalues by using a numerical solution of the Schrödinger equation for several values of λ' , which are shown in the figures with crosses. The results obtained using TQA coincide to a high degree of accuracy with the numerical results. We can see that the first excited state has bound states only for small values of λ' . For other higher states ($n \geq 2$), the energy levels are just immediately the ionization level, and it is very difficult to put the atoms in those states. Thus we have not determined approximants in these cases. In order to find the accuracy of our results, we have calculated the absolute errors with respect to the numerical solution. They are shown in figures 2(a)–(c). The maximum errors of the approximants (i.e. ΔE_{max}) are 0.04 for both 2S ($g = 0$) and 1S ($g = 0.1$) states (see figures 2(b) and (c)). They are reached when λ' is about 1, which means they are out of the region of physical interest. These maximum errors are 0.002 for the 1S ($g = 0$) and 2S ($g = 0.1$) states (see figures 2(a) and (b)). For small values of λ' , in the region of bound states, for all the states the absolute errors are smaller than 0.005. However, if we consider only the bound state ($\lambda' < 0.2$) in the 1S ($g = 0$) state, the maximum error is smaller than 0.0003.

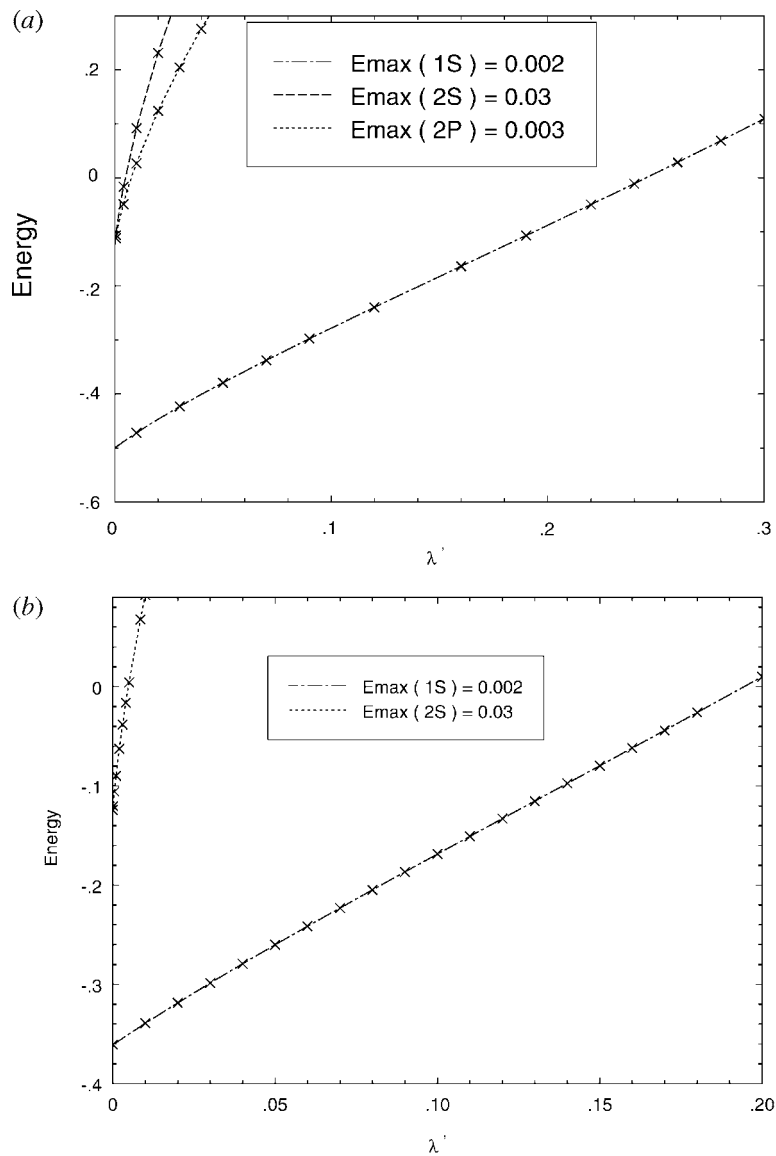


Figure 1. Eigenenergies of the two-point quasifractional approximant $\hat{E}_{nl}^{(1)}(\lambda')$ and its respective numerical values (crosses), as a function of the normalized coupling parameter λ' . (a) Eigenenergies spectra with $g = 0$. Chain curve, 1S state; broken curve, 2S state; dotted curve, 2P state. (b) Chain curve, 1S state ($g = 0.1$); dotted curve, 2S state ($g = 0.0001$).

To study the advantages of our method, we compare our results with those obtained using the shifted $1/N$ method for all the states calculated. In the ground state with $g = 0$ we have also calculated the one-point Padé approximant $P^{[2/1]}(\lambda)$ (Baker and Graves-Morris 1981a, b), using the power series $E_{10}^{HF}(\lambda)$ equation (8), giving

$$P^{[2/1]}(\lambda) = \frac{a_0 a_2 + (a_1 a_2 - a_0 a_3) \lambda + (a_2^2 - a_1 a_3) \lambda^2}{a_2 - a_3 \lambda}. \quad (12)$$

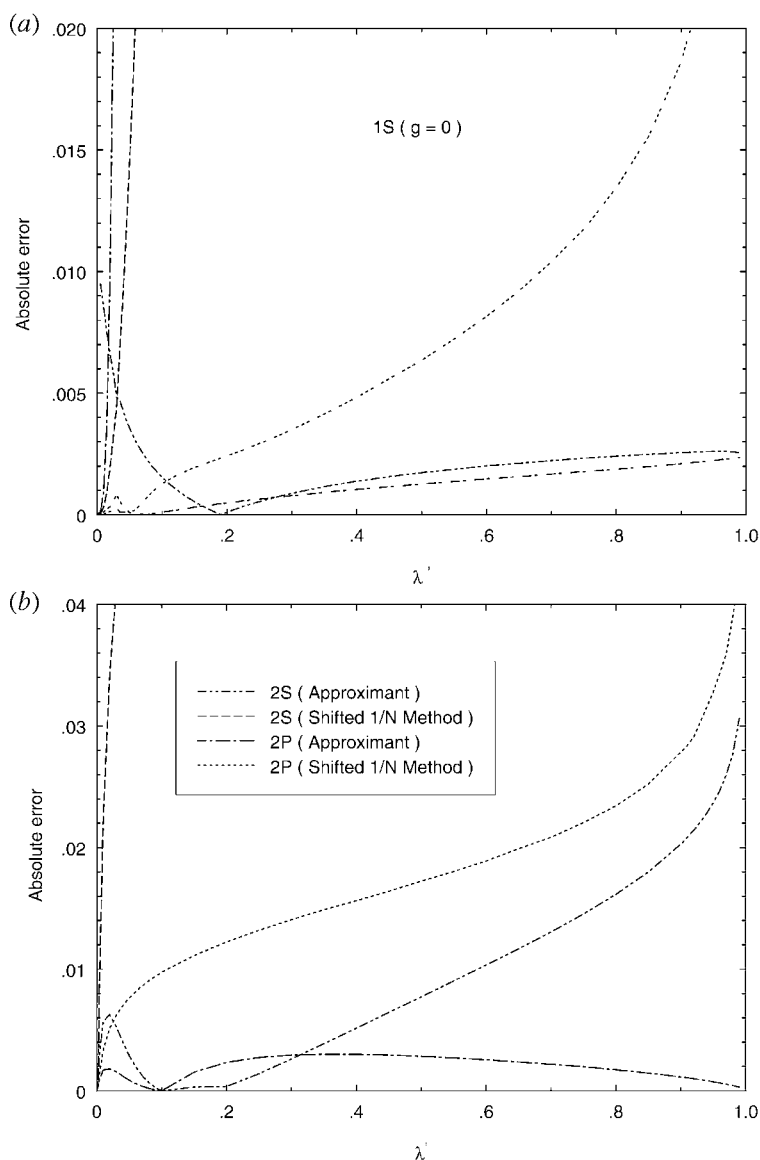


Figure 2. Absolute error as a function of the normalized coupling parameter λ' , corresponding to (a) the 1S state ($g = 0$): chain curve, two-point quasifractional approximant; triple-dotted curve, shifted $1/N$ method; double-dotted chain curve, asymptotic expansion (RS); broken curve, one-point Padé approximant $P^{[2/1]}(\lambda)$; long-chain curve, potential series (HF). (b) 2S state ($g = 0$): double-dotted chain curve, two-point quasifractional approximant; broken curve, shifted $1/N$ method. 2P state ($g = 0$): chain curve, two-point quasifractional approximant; dotted curve, shifted $1/N$ method. (c) 1S state ($g = 0.1$): double-dotted chain curve, two-point quasifractional approximant; broken curve, shifted $1/N$ method. 2S state ($g = 0.0001$): long-chain curve, two-point quasifractional approximant; dotted curve, shifted $1/N$ method.

Figure 2(a) illustrates the absolute errors of all the approximation methods determined here for the 1S state, with $g = 0$. In order to facilitate our analysis, our abscissa is the dimensionless parameter λ' . Looking at this figure we note that the potential series $E_{10}^{HF}(\lambda)$

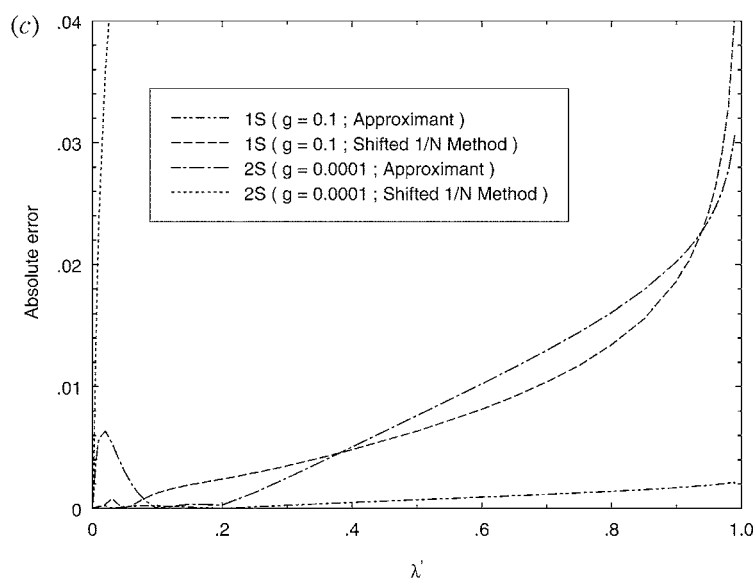


Figure 2. Continued.

and the Padé approximant $P^{[2/1]}(\lambda)$ are only suitable for small values of the coupling parameter. The asymptotic expansion, however, shows a wider range of applicability, with good accuracy not only for large values of λ , but also for intermediate values. The accuracy of our method is much better than that of any other methods for any λ' . Comparing our approximant with the shifted $1/N$ method, we see that the error of our approximant is always smaller, and the difference in accuracy for large values of λ' ($\lambda' \approx 1$) is even more remarkable.

Figure 2(b) shows the absolute errors for the first excited states 2S and 2P, with $g = 0$. Here if we compare with the shifted $1/N$ method we obtain much better accuracy for any λ' , and our results are even better than in the 1S case.

Figure 2(c) show the absolute errors of the two-point quasifractional approximant and the shifted $1/N$ method calculated as a function of the normalized coupling parameter λ' , for the ground state 1S and the first excited state 2S, with $g = 0.1$ and 0.0001 , respectively. Roychoudhury and Varshni (1988) have shown using SUSYQM that the accuracy of the shifted $1/N$ method varies considerably with the parameters Z , g and λ . However, the examination of figure 2 show that the accuracy of our first-order approximant is better than that of the shifted $1/N$ method for all values of the parameter λ' , and, furthermore, the difference in accuracy is very significant. Furthermore, our accuracy is better than four digits in the bound-state region, and also for large part of the region with positive eigenenergy. Approximants with higher accuracy can be obtained using higher approximants, which also means that more terms of the perturbation expansions have to be calculated.

Now consider the errors in detail. First, we have calculated numerically the eigenvalues for any value of λ . We have also performed the calculation using the shifted $1/N$ method. Here there is a difficulty, because the parameter r_0 has to be calculated to an accuracy of five digits. Thus the computation time is very large, and much larger than that used to determine all the parameters of our approximant. The computation of the energy using the approximant can be obtained easily, by hand or with a pocket calculator. Furthermore, we can derive and integrate the eigenenergy with respect to the parameter λ , and look for the behaviour of this

eigenvalues when λ is changed. The numerical computation of the eigenenergy using the Schrödinger equation is very cumbersome and it takes a lot of computer time. The advantage of the approximant is very clear. Furthermore, as we showed before, the accuracy of the approximant is so high that it will be sufficient for all the applications.

4. Conclusions

We have developed a new method to obtain an analytic approximation for the eigenenergies of a hydrogenic atom with linear and isotropic harmonic oscillator terms using two-point quasifractional approximants. Our approximant has been determined for the ground state 1S and for the first excited states 2S and 2P, which are the most important states for applications. The energy levels of the other excited states are very close to the ionization energy.

The approximants obtained here are for a fixed value of g and for any value of λ . There is only a unique approximant for any λ . Thus the study of the eigenenergies as a function of λ can be easily done. Differentiation or integration with respect to this parameter λ can also be performed. Thus, for instance, electric or magnetic susceptibilities can be obtained easily from our analytic results. Derivatives of eigenvalues also appear explicitly in some calculations in heavy quark spectroscopy and quantum chromodynamics. Though the numerical solution of the Schrödinger equation for given values of g and λ is not so difficult to obtain, the determination of the preceding electromagnetic functions by that method is very cumbersome. The structure of our approximant is a quotient of first-degree polynomials and also the square root of first-degree polynomials. Thus the calculation of the eigenvalues is very simple, and it can even be performed by hand.

Here we have used the Hellman–Feynman theorem, the hypervirial theorem and the Rayleigh–Schrödinger perturbation method to obtain the power series and asymptotic expansions, respectively.

In our procedure we find the TQA using the power series and the asymptotic expansion of the eigenvalues as a function of the coupling parameter λ . Our approximants depend on a given number of parameters p, q, P, Q and μ . The number of equations is equal to the number of unknowns p, q, P and Q , and μ is denoted as a free parameter. The optimum μ is obtained by calculating the eigenenergy for one value of λ denoted by λ_b , which is the bridge point between the power series and the asymptotic expansion.

The advantage of our method is that for a fixed value of g we obtain only one analytic expression with good accuracy for all values of the coupling parameter λ . Using a two-point quasifractional approximant to first order we can see that the maximum absolute error of our approximant is less than the maximum absolute error of the shifted $1/N$ method. The difference in accuracy of both methods is notable for intermediate and high values of the coupling parameter λ' . Our method gives an accuracy of at least four digits for most values of λ' , and the errors change very little with the parameter. Thus our accuracy will be enough for all the physical applications already known.

It is important to point out that, although the potential considered here is quasi-exactly solvable, the method presented here can be used, in principle, for any potential with spherical symmetry, because the quasi-exactly solvable conditions have not been used.

The energy values given by the shifted $1/N$ method can give poor or erroneous results (see the conclusions of Roychoudhury and Varshni (1990)) in the case where the potential has more than one well (it can also give incorrect radial quantum number for a level). However, our method does not have this limitation since for our calculations we do not depend on the minima of the potential. Therefore, the method presented here can be used, in principle, for a radial potential with several wells.

Appendix

By using the analytic methods proposed by Bessis *et al* (1987), or by Roychoudhury and Varshni (1990), we know that the potential given in (1) is quasi-exactly solvable, and for the ground state there is only one equation relating Z , g and λ (see equation (2.8) of Bessis *et al* (1987)) and for the first excited state there are two equations (see equation (24c) of Roychoudhury and Varshni (1990)). Fixing $Z = 1$ and $g = 0.1$, for the ground state, we obtain a unique value of λ'_b ($= 0.005$, i.e. $\lambda_b = 0.00497$), and the corresponding eigenenergy is $E_{10} = -0.35$ (see equation (21) of Roychoudhury and Varshni (1990)). Clearly, here λ is very small and if we find the root of μ such that $\hat{E}_{10}^{(1)}(\mu) = E_{10}(\lambda = 0.005)$, we find $\mu_{opt} = 5763.523$. This root has been determined using the Newton–Raphson method (Nakamura 1992). This value is not a good value and the accuracy of the approximant is not good. The reason for this is that the value of λ used as an intermediate point is very small, forcing the TQA to follow the behaviour of the potential series, which diverges very quickly.

In a similar way the λ'_b values for the first excited states 2S and 2P are 4.999×10^{-9} and 2.0016×10^{-8} . None of these points can be used as bridge point, between the power series and the asymptotic expansion. For the preceding reasons we decided in this paper to determine the values of the energy for all values of g with the bridge point $\lambda'_b = 0.1$. We could use any other intermediate point, for example, we could have chosen $\lambda'_b = 0.2$, and we have checked that the results are almost of the same accuracy.

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