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Large-order perturbation expansions for the charged harmonic oscillator

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Abstract. The charged oscillator, defined by the Hamiltonian $H = -d^2/dr^2 + r^2 + \lambda/r$ in the domain $[0, \infty]$, is a particular case of the family of spiked oscillators, which does not behave as a supersingular Hamiltonian. This problem is analysed around the three regions $\lambda \to \infty$, $\lambda \to 0$ and $\lambda \to -\infty$ by using Rayleigh–Ritz large-order perturbative expansions. A path is found to connect the large λ regions with the small λ region by means of the renormalization of the series expansions in λ. Finally, the Riccati–Padé method is used to construct an implicit expansion around $\lambda \to 0$ which extends to very large values of $|\lambda|$.

1. Introduction

The family of quantum Hamiltonians known with the name of *spiked harmonic oscillators* is represented by the general Hamiltonian

$$H = -\frac{d^2}{dr^2} + r^2 + \frac{\lambda}{r^\alpha} \tag{1}$$

defined in the one-dimensional half space $[0, \infty]$, the eigenfunctions obeying Dirichlet boundary conditions. The Hamiltonian is characterized by means of two parameters, λ which plays the role of a coupling constant and $\alpha \geqslant 0$ which controls the type of the singularity of the potential at the origin.

The study for small λ reveals the presence of two different behaviours depending on the value of α. When α is smaller than 5/2, the ground-state energy has a power series expansion in terms of λ. Not very much is known about these expansions for $\alpha < 5/2$, with the exception of the exactly solvable case $\alpha = 2$, which generates a series expansion in powers of λ, its radius of convergence being 1/4. Nevertheless, plain application of the Rayleigh–Schrödinger perturbation theory does not generate the correct perturbative corrections to the wavefunction [1].

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The region $\alpha \geqslant 5/2$ is known by the name of *supersingular*. Klauder [2] and Detwiler and Klauder [3] realized that problems of this kind, or with similar behaviour, had very special properties in the small-coupling regime. Later, Harrell [4] was able to construct a special form of singular perturbation theory to determine the leading term of the ground-state energy for small λ, which turned out to depend on non-integral powers of the coupling parameter or even on logarithms of the coupling constant. Only very few terms of the expansion may be determined by using the method of Harrell [4]. Nevertheless, it is a simple task to generate many terms of the expansion in terms on an *effective* coupling constant in the strong-coupling regime [5, 6], i.e. for very large values of λ.

Our interest in the family of spiked oscillators was motivated by the analogy between the $\alpha = 5/2$ small-coupling expansion [4]

$$E(\alpha = 5/2) = 3 + \frac{2\lambda\Gamma(1/4)}{\Gamma(1/2)} + \frac{16\lambda^2 \ln \lambda}{\Gamma(1/2)} + O(\lambda^2) \tag{2}$$

and the low-density expansion of the energy per particle of a many-body boson system at zero temperature [7]

$$E/N = (2\pi\hbar^2/m)\rho a \left[1 + C_1(\rho a^3)^{1/2} + C_2\rho a^3 \ln(\rho a^3) + C_3\rho a^3 + \cdots\right] \tag{3}$$

where ρ is the particle density and a is the scattering length of the two-body problem with the bare interaction. Similar expansions have also been obtained for fermion systems [7].

The low-density expansions are not immediately useful for studying real many-body systems, in particular because in most cases the scattering length corresponding to the two-body system may be negative, so that equation (3) is meaningless. However, the use of constructive extrapolants, mainly based on Padé approximants of non-integral powers of the series equation (3), has proven to be a very precise method to determine the equation of state of several quantum systems near the equilibrium density [8–10]. For this reason, our interest will be focused on the study of connections between the expansions determined around finite (actually null) and infinite values of λ, for a given value of the exponent α.

In this work we are going to concentrate on a very *simple* case, namely $\alpha = 1$. The Hamiltonian equation (1) looks extremely simple, being a confined Coulomb potential,

$$H = -\frac{d^2}{dr^2} + r^2 + \frac{\lambda}{r}. \tag{4}$$

The amount of information which may be obtained for this simple spiked oscillator is quite impressive. First of all, it is possible to obtain perturbative expansions for the ground-state energy (and also for excited states) around $\lambda \to \infty$ as well as around $\lambda \to -\infty$. The former case will be referred to as the *strong-coupling regime*, and the latter will be called the *Coulomb regime*. These expansions may be obtained very efficiently by means of a combination of the hypervirial relations and the Hellmann–Feynman theorem. This method does not work in the $\lambda \to 0$ region, but it is still possible to obtain several terms of the small-coupling expansion by means of the standard Rayleigh–Schrödinger perturbation theory. These expansions are presented in section 2.

Next, the Hamiltonian, equation (4), has an infinite set of *elementary solutions* [11], i.e. solutions of the form of a polynomial times a Gaussian, for selected values of the coupling parameter λ. These solutions correspond to the ground state as well as to excited states, and they are found only for positive values of λ. The elementary solutions are discussed in section 3.

Section 4 deals with the *renormalized series* method (see for example [12]). This method is used to extend up to infinity the radius of convergence of series defined around the origin. Conversely, it also applies to series defined around infinity, extending them up to the origin. The only information required in one of the extremes is the leading non-integral power of the dominant term, whereas in the other extreme it is necessary to know many terms of the expansion. The renormalization of the large-order expansions determined in section 2 turns out to be a very accurate method to determine the ground-state energy in very wide domains and provides an *implicit* path of constructive extrapolation of the perturbative results. These extrapolations cover *half of the way*, so that the region $\lambda \to \infty$ is connected with the region $\lambda \to 0$, and the region $\lambda \to -\infty$ is also connected with the origin, but we have not found a (single) direct connection between the $\lambda \to -\infty$ and $\lambda \to \infty$ regions.

Finally, section 5 introduces a new method of dealing with the small-coupling perturbation expansion, i.e. in the region $\lambda \to 0$, by using the so called *Riccati–Padé* method [13–15], which consists in transforming the Schrödinger equation into a Riccati equation. The method produces very accurate results in a large domain around $\lambda = 0$, both for positive and negative values of λ and, moreover, is able to generate approximately several orders of the small-coupling expansion, as well as to reproduce the asymptotic expansion in the Coulomb regime.

A summary of the results and conclusions is presented in section 6.

2. Large-order expansions

We start by distinguishing the three regions where perturbative expansion in terms of an *effective* coupling constant may be determined. The regions are:

(i) *the Coulomb region*, corresponding to large and negative values of λ;

(ii) *the strong-coupling region*, (SC), corresponding to large and positive values of λ; and

(iii) *The weak-coupling region*, related to small (positive or negative) values of λ.

2.1. The Coulomb region

After a scaling transformation of the coordinate r the Hamiltonian equation (4) is converted into

$$H \to \lambda^2 \left[-\frac{d^2}{dr^2} - \frac{1}{r} + \beta r^2 \right] \tag{5}$$

where $\beta = \lambda^{-4}$ is the effective coupling constant for the forthcoming perturbation expansion. By using the hypervirial relations, [16–18], one may relate the eigenvalues $e(\beta)$ of the Hamiltonian H/λ^2 with the expectation value of powers of r,

$$2Ne(\beta)\langle r^{N-1}\rangle = (1-2N)\langle r^{N-2}\rangle + 2\beta(N+1)\langle r^{N+1}\rangle - N(N-1)(N-2)\langle r^{N-3}\rangle/2 \tag{6}$$

where the expectation values are taken with respect to any *exact* eigenstate of the Hamiltonian in square brackets of equation (5) and depend obviously on β. By combining equation (6) with the Hellmann–Feynman theorem, the expansion for the ground-state energy is given by

$$E(\lambda) = \lambda^2\left[-\frac{1}{4} + \frac{12}{\lambda^4} - \frac{1032}{\lambda^8} + \frac{348\,864}{\lambda^{12}} - \frac{211\,519\,200}{\lambda^{16}} + \frac{188\,054\,861\,568}{\lambda^{20}} - \frac{225\,337\,358\,179\,584}{\lambda^{24}} + \cdots\right] \tag{7}$$

valid for large and negative λ. We have included only few terms of this expansion but it is simple to obtain many more terms with the help of a computer algebra code.

2.2. *The strong-coupling region*

In the case of large and positive λ, the potential looks like a wide valley centred at some large value of r and rising to infinity both near the origin and at large distances. It is then convenient to expand the potential around its minimum,

$$r_{\min} = (\lambda/2)^{1/3} \tag{8}$$

so that

$$V(r_{\min} + x) = \frac{3}{\mu^2} + 3x^2 + 2\sum_{k=3}^{\infty}(-1)^k \mu^{k-2} x^k \tag{9}$$

where the effective coupling constant is now $\mu = (2/\lambda)^{1/3}$. The resulting potential has, apart from the constant term, a term depending on x^2 and infinite terms depending on higher powers of x multiplied by powers of the effective coupling constant. It is now possible to use a special form of the Rayleigh–Schrödinger perturbation expansion [1, 5] or, even better, the hypervirial relations [6], to get the expansion of the ground-state energy in powers of the effective constant μ. We show just a few terms of this expansion, namely

$$E = 3\mu^{-2} + \sqrt{3} + \frac{7\mu^2}{36} + \frac{37\mu^4}{432\sqrt{3}} + \frac{2573\mu^6}{139\,968} + \frac{168\,233\mu^8}{2\,239\,488\sqrt{27}} + \frac{11\,834\,297\mu^{10}}{725\,594\,112} + \frac{1\,982\,015\,237\sqrt{3}\mu^{12}}{156\,728\,328\,192} + \cdots. \tag{10}$$

Again, with the help of computer algebraic codes, one may obtain many more terms of this expansion.

2.3. *The weak-coupling expansion*

We have not found a way to use adequately the hypervirial relations in order to determine a large-order weak-coupling expansion, around $\lambda = 0$. However, by using standard perturbation theory the known coefficients of the expansion are [1]

$$E = 3 + \frac{2\lambda}{\sqrt{\pi}} - \frac{(2 + 2\ln 2 - \pi)\lambda^2}{\pi} + \cdots. \tag{11}$$

3. Elementary solutions

The words 'elementary solutions' refer to particular eigenstates of the Hamiltonian equation (4), which appear only for specific values of the coupling constant, and whose wavefunction may be expressed as the product of a polynomial times a Gaussian factor. To obtain these elementary solutions let us consider the wavefunction written as

$$\Psi(r) = \exp(-r^2/2)p(r) \tag{12}$$

and expand $p(r)$ in powers of r,

$$p(r) = \sum_{n=0}^{\infty} p_n r^n . \tag{13}$$

The resulting recurrence relation is

$$(n+1)(n+2)p_{n+2} = \lambda p_{n+1} + (2n+1-E)p_n \tag{14}$$

with the condition $p_0 = 0$, in order to satisfy the Dirichlet boundary condition at the origin, and p_1 arbitrarily chosen equal to 1. In order to have a finite number of terms in the expansion of $p(r)$ the two following equations must be satisfied

$$p_{n+1}(E, \lambda) = 0 \tag{15}$$

and

$$E = 2n + 1 \qquad n = 2, 3, \ldots \tag{16}$$

so that for all odd and positive values of the energy $E > 3$, there exist several values of λ, solutions of the polynomial equation (15), for which the function $p(r)$ is a polynomial. There is also a trivial solution for $E = 3$ which corresponds to $\lambda = 0$, i.e. the unperturbed Hamiltonian. Among all these values of λ corresponding to a given value of the energy, the largest is the one corresponding to the ground state, the corresponding wavefunction having no zeros, apart from the zeros at the origin and at infinity.

Table 1. Some elementary solutions of the Hamiltonian equation (4), for several energies E. The second column contains the polynomial equation to be solved and the third displays the largest solution, corresponding to the ground state.

E	Equation	λ
5	$\lambda^2 - 4 = 0$	2
7	$\lambda(\lambda^2 - 20) = 0$	$\sqrt{20}$
9	$\lambda^4 - 60\lambda^2 + 288 = 0$	$(30 + 6\sqrt{17})^{1/2}$
11	$\lambda(\lambda^4 - 140\lambda^2 + 2848) = 0$	$(70 + 6\sqrt{57})^{1/2}$
13	$\lambda^6 - 280\lambda^4 + 15\,280\lambda^2 - 86\,400 = 0$	14.450 001 026 966
15	$\lambda(\lambda^6 - 504\lambda^4 + 59\,184\lambda^2 - 1\,316\,736) = 0$	18.503 131 410 003

Table 1 lists some of the parameters characterizing the elementary solutions, and the equation for λ to be solved. It is also possible to obtain the resulting wavefunction. The simplest cases are

$$p(r, E = 5) = r(1 + r) \tag{17}$$

and

$$p(r, E = 7) = r(1 + \sqrt{5}r + r^2). \tag{18}$$

These elementary solutions will be of great help to analyse the constructive methods for extending the previous perturbation expansions.

4. The renormalization series approach

The method of renormalization of series is a mechanism which permits us to match two asymptotic expansions of a given function $f(x)$, one expansion defined around $x = 0$ and the other around $1/x = 0$. In this manner there results a representation for $f(x)$ which may be valid for all values of x. We assume these expansions to be of the form

$$f(x) = \sum_{j=0}^{\infty} f_j x^j \tag{19}$$

and

$$f(x) = x^a \sum_{j=0}^{\infty} F_j x^{-bj} \tag{20}$$

where $b > 0$. Moreover we will consider that sufficient coefficients f_j may be calculated. Following [12] let us define a new variable y by means of the implicit equation

$$x = \frac{y}{K(1 - y)^{1/b}} \tag{21}$$

which maps the x interval $[0, \infty]$ into the y interval $[0, 1]$. In the above equation K is a positive and, for the moment, arbitrary parameter. By considering that y may be expanded both in powers of x and in powers of $1/x$, the family of approximants

$$g_N(x) = \left[K(1 - y)^{1/b}\right]^{-a} \sum_{m=0}^{N} c_n y^n \tag{22}$$

defined in terms of the integer $N = 0, 1, \ldots$, satisfy expansions similar to (19) and (20). It is also possible to relate the set of coefficients c_n of the approximants with the coefficients f_n which define the original expansion [16, 19],

$$c_n = \sum_{j=0}^{n} K^{a-j}(-1)^{n-j} \binom{(a-j)/b}{n-j} f_j \tag{23}$$

where $\binom{d}{i} = d(d-1)\cdots(d-i+1)/i!$ and $\binom{d}{0} = 1$.

The choice of K depends on the problem in hand. In the case in which F_0 is known, one may fix K by requiring that for a given value of N, the approximant g_N reproduces exactly the value of F_0. The latter may be obtained by the condition

$$F_0 = \lim_{x\to\infty} x^{-a} g_N(x) = \sum_{m=0}^{N} c_m \tag{24}$$

which results in a polynomial equation for K. With this prescription no free parameters remain for the renormalization of the series.

We have applied this method to two of the cases presented in the previous section, namely the strong-coupling region and the Coulomb region. In both cases, a small modification of the described algorithm is necessary, because the known expansion is of the type of equation (20), involving non-integral powers of the variable, instead of the power series expansion of the type of equation (19). The modification is quite simple and consists in considering the function $x^{-a}f(x)$ instead of $f(x)$, and also in using as a free variable $z = x^{-b}$. Moreover, in both cases the reference value to determine the constant K is that the ground-state energy for the null coupling constant is 3. In the case of the strong-coupling expansion, two possible values for K result, which are shown in table 2 (this table corresponds to a renormalization based on 34 terms of the strong coupling series). In the case of the Coulomb regime, shown in table 3, one finds only one value of K from the constraint (this table corresponds to a renormalization based on 11 terms of the Coulomb regime series). These two tables include, for reference, the numerically determined eigenvalues.

Table 2. The ground-state energy of the spiked oscillator for several values of λ computed by means of the strong-coupling series (second column) and the renormalized series corresponding to two values of K (third and fourth column). The last column displays the numerically determined eigenvalue. The calculations based on the series correspond to a total of 34 terms.

λ	SC series	Renormalized $K = 3.483\,647\,994$	Renormalized $K = 5.961\,005\,319$	Numerical
0.001		3.001 094 21	3.001 142 52	3.001 128 301 2
0.01		3.010 939 02	3.011 417 20	3.011 276 010 5
0.1		3.109 062 04	3.113 386 01	3.112 066 906 5
1	5×10^6	4.047 745 49	4.064 649 65	4.057 877 008 0
5	7.478 888 02	7.383 056 76	7.386 453 45	7.384 031 725 9
10	10.577 549 39	10.577 439 51	10.577 824 87	10.577 483 394

A look at the relevant columns of these two tables shows the high efficiency of the renormalization mechanism, the original series being extended up to very small values of the coupling constant.

5. The Riccati–Padé method

The analysis of the previous section has enabled eigenvalues of a very high accuracy for all values of the coupling constant to be obtained, but was unable to provide a

Table 3. The ground-state energy of the spiked oscillator, for several values of λ, computed by means of the series of the Coulomb region (second column) and the renormalized series (third column). The last column displays the numerically determined eigenvalue. The calculations based on the series correspond to a total of 11 terms.

λ	Coulomb series	Renormalized $K = 488.680\,625\,5$	Numerical
−0.001		2.998 909 267	2.998 871 542 9
−0.01		2.989 074 410	2.988 708 411 3
−0.1		2.889 368 799	2.886 375 159 2
−1	-5×10^{27}	1.788 439 401	1.785 205 479 3
−5	−16.279 109 60	−5.816 158 040	−5.816 157 900 7
−10	−24.880 999 06	−24.880 999 070	−24.880 990 603

small-coupling series expansion for the ground-state energy. In this section we apply a recently developed method [13–15] based on a transformation of the Schrödinger equation into a Riccati differential equation, and using afterwards a Padé analysis of the resulting power series.

The Riccati method was applied many years ago [20], and quite recently [21] was also found to be adequate for studying the strong-coupling expansion of quartic and higher anharmonic oscillators. The method presented here introduces two important improvements. First, it explicitly includes the Dirichlet boundary condition. Second, the Padé transformation of the power series may improve the convergence and, as will be commented afterwards, is able to generate the lowest elementary solutions.

Consider the auxiliary function

$$\phi(r) = 1/r - \Psi'/\Psi \tag{25}$$

where Ψ is the ground-state wavefunction, and the equivalent equation

$$\Psi(r) = r \exp\left(-\int^r \phi(t)\,\mathrm{d}t\right). \tag{26}$$

The term r which appears in the right-hand side of equation (26) comes from the term $1/r$ of equation (25) and must be present in order to satisfy the Dirichlet boundary condition at $r = 0$.

Correspondingly to the Hamiltonian given in equation (4), the new function ϕ must satisfy the Riccati equation

$$\frac{\mathrm{d}\phi}{\mathrm{d}r} = -\frac{2}{r}\phi + \phi^2 - r^2 - \frac{\lambda}{r} + E. \tag{27}$$

Since $\phi(r)$ is regular at $r = 0$ we may expand it in a Taylor series around that point,

$$\phi(r) = \sum_{j=0}^{\infty} \phi_j r^j \tag{28}$$

and the coefficients ϕ_j have to fulfil the recurrence relation

$$\phi_n = \frac{1}{n+2} \sum_{j=0}^{n-1} \left[\phi_j \phi_{n-j-1} - \delta_{n3} + E\delta_{n1} - \lambda\delta_{n0}\right] \qquad n = 0, 1, \ldots. \tag{29}$$

Certainly, plain substitution of this expansion (which is fully determined) in equation (26) would give rise to a nonsensical wavefunction. In fact, the indefinite integral appearing in the exponential term of equation (26) will give rise to terms of the form $\exp(a_1 r + a_2 r^2 + a_3 r^3 + a_4 r^4 + \cdots)$. Consequently, either the wavefunction is non-normalizable, when the coefficient of the highest retained power of r is positive, or has an inadequate long-range behaviour, decaying faster than a Gaussian. A way to bypass these two abnormal behaviours is to use an appropriate Padé approximant constructed from series equation (28).

Surely an example will clarify this statement. Consider the values for $E = 5$ and $\lambda = 2$, which correspond to the first non-trivial elementary solution of section 3. The series corresponding to the function ϕ is in this case

$$\phi(r) = -1 + 2r - r^2 + r^3 - r^4 + r^5 - r^6 + r^7 + \cdots \tag{30}$$

and one recognizes quite easily that this series is the expansion of

$$\phi(r) = r - \frac{1}{1+r}. \tag{31}$$

In other words, any Padé approximant to the series above will degenerate into this simple form. Substituting in equation (26) results in the exact wavefunction corresponding to the elementary solution under consideration. Finally, a direct substitution of the full series equation (30) in equation (26) would have generated a nonsensical wavefunction.

By using a Padé approximant instead of the Riccati series expansion we have not yet solved the problem of the determination of the eigenvalues. In fact, the set of coefficients ϕ_n is defined in terms of the two quantities E and λ. A way to obtain a quantization condition is to assume that the corresponding Padé approximant $[N/D]$, which is defined in terms of $N + D + 1$ coefficients, produces exactly the next term of the expansion, ϕ_{N+D+2}. This will result in an implicit equation relating E and λ. It has been rigorously proved that for certain non-trivial problems this approach yields accurate upper and lower bounds to the ground-state energy [13–15]. Furthermore, for solvable and quasi-solvable problems, one obtains the exact answer both for the eigenvalues and eigenfunctions, provided the latter can be written as a finite polynomial times an exponential function.

The quantization condition is quite simple in the case of diagonal Padé approximants $[N/N]$, and corresponds to the Hankel determinantal equation $H_N = \det(a) = 0$, where $a_{ij} = \phi_{i+j-1}$ for $i, j = 1, 2, \ldots, N$ (see [13–15]). The determinant H_N is a polynomial of degree $N(N+1)/2$ in E and of the same degree in λ^2. The explicit equation for $N = 2$ is

$$(4E + \lambda^2)(64E^2 + 20E\lambda^2 + \lambda^4 - 576) = 0 \tag{32}$$

and for $N = 3$

$$E^6 + E^5\left(\frac{65\lambda^2}{72}\right) + E^4\left(\frac{713\lambda^4}{2304} + 3\right) + E^3\left(\frac{115\lambda^6}{2304} - \frac{385\lambda^2}{16}\right) + E^2\left(\frac{71\lambda^8}{18\,432} - \frac{909\lambda^4}{64} - 297\right) + E\left(\frac{5\lambda^{10}}{36\,864} - \frac{615\lambda^6}{256} - \frac{1395\lambda^2}{4}\right) + \left(\frac{\lambda^{12}}{589\,824} - \frac{103\lambda^8}{1024} - \frac{549\lambda^4}{8} + 1701\right) = 0. \tag{33}$$

There are two characteristics of the Hankel polynomial equations which should be mentioned. First of all, λ always appears in even powers, so that these equations do not distinguish between positive and negative λ. The space (λ, E) has been folded around the $\lambda = 0$ axis, and the roots of the polynomial equations are mixed. The second interesting property is the large λ limit, which is always of the form $E \to a\lambda^2$ for $\lambda \to \infty$, i.e. only the Coulomb solutions emerge in this asymptotic limit.

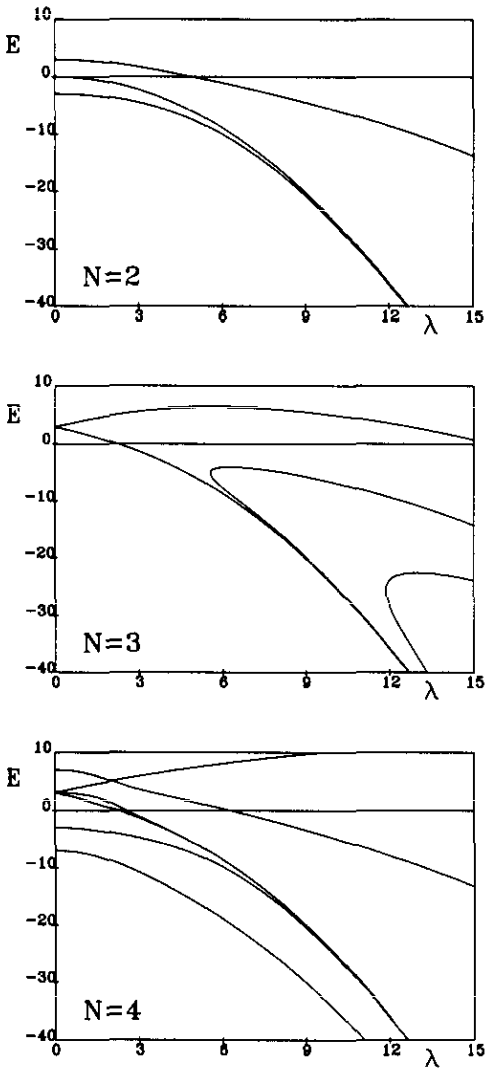

Figure 1. The solution of the Hankel determinantal equations related to the Riccati–Padé method for several values of the dimension of the determinant. The various roots of the polynomial equation in E are plotted against λ.

A detailed study of the solutions of several equations, corresponding to the lowest values of N, reveals other properties which appear systematically. This behaviour is exemplified in the three maps shown in figure 1, which correspond to the roots of the Hankel equation for $N = 2$, 3, and 4. At $\lambda = 0$ the solutions include some of the unperturbed harmonic oscillator, namely 3, 7, 11, ... as well as other spurious solutions corresponding to negative energies. The multiplicity of these solutions at the origin increases with the order of the Padé approximant. When λ increases,

these degenerate solutions split into several branches, and sometimes they jump to the complex plane. Some of these branches may be recognized as physical solutions for the ground-state energy for $\lambda > 0$, as well as for $\lambda < 0$. Other branches are related to excited states. Finally, there are also spurious branches with no connections with physical solutions. The way of identifying the nature of a given solution is to follow its trajectory from $\lambda = 0$ up to $\lambda \to \infty$. Due to the Hellmann–Feynman theorem, the derivative of the energy with respect to λ is given by the expectation value of $1/r$ in the exact eigenstate, namely $dE(\lambda)/d\lambda = \langle 1/r \rangle$, this derivative being always positive. So, monotonically decreasing functions correspond to negative values of λ. The solutions corresponding to positive λ increase for small values of the coupling constant, but ultimately they start to decrease and become negative. One may reasonably expect these solutions to be acceptable as far as they increase with λ. In any case, as mentioned above, all branches go to Coulomb-like solutions in the limit of very large and negative λ.

In conclusion, it is necessary to extract the appropriate root and also to interpret it by looking at its evolution. Table 4 presents a selected set of energies obtained by solving the determinantal equation for $N = 7$. By comparison with the numerically determined solutions for the same values of the coupling constant presented in tables 2 and 3 one may realize the high quality of the present method. Another very appealing characteristic of this method is that the lowest elementary solutions are obtained exactly, so that the Riccati–Padé method is, in a certain way, equivalent to an interpolation of the energy which goes through the eigenvalues of many elementary solutions. As a consequence, the quality of the approximation is particularly good for values of λ near the influence region of a given elementary solution.

Table 4. Ground-state energy for several values of λ obtained with the Riccati–Padé method, corresponding to $N = 7$. The second and fourth columns display the energies corresponding to positive and negative values of the coupling constant, respectively.

λ	E	λ	E
0	3		
0.001	3.001 128 301 31	−0.001	2.998 871 494
0.01	3.011 276 010 73	−0.01	2.988 708 411 06
0.1	3.1109	−0.1	2.886 370 2
1	4.057 906	−1	1.785 205 456
5	7.384 031 741	−5	−5.816 163
10	10.577 483 43	−10	−24.880 999 079

The best way to verify the accuracy of this method for small values of λ is to calculate the coefficients of the small coupling series $E(\lambda) = \sum_{n=0} E_n \lambda^n$. Certainly, and with the exception of the trivial case $E_0 = 3$, these coefficients are not exactly obtained with this method, but the accuracy of the coefficients increases very rapidly with the degree N of the determinant. To obtain the approximate small-coupling expansion we susbtitute the above expansion of the energy into the determinant and set the coefficients of every power of λ in the resulting polynomial equal to zero. The coefficient of λ^m exactly vanishes for all $m = 0, 1, \ldots, N-2$. The coefficient of λ^{N-1} is a polynomial equation for E_1, and one of the roots of this polynomial is the desired approximation for E_1 (see the above discussion on the roots). Once E_1 has been correctly identified, the rest of the expansion is simple: if $m \geqslant N$, the

coefficient of λ^m is linear in E_{m-N+2} and depends on the remaining lower order coefficients, so that the expansion coefficients are obtained sequentially.

The resulting coefficients are shown in Table 5, from E_1 up to E_4, for several values of N. From this table it turns out that the method converges very rapidly, as it is able to yield the first coefficients very accurately with determinants of moderate order. All the digits shown in the last row of this table coincide with the exact expansion coefficients given in equation (11).

Table 5. Coefficients of the weak-coupling expansion obtained from the roots of several Riccati–Padé determinants of different dimension N.

N	E_1	E_2	E_3	E_4
3	1.17	−0.072	−0.002	0
4	1.127	−0.077 77	0.008 17	−0.000 562
5	1.128 41	−0.077 897	0.000 795 1	−0.000 574 05
6	1.128 378 4	−0.077 890 8	0.007 957 1	−0.000 574 487
7	1.128 379 19	−0.077 890 98	0.007 956 951	−0.000 574 462 7
8	1.128 379 166	−0.077 890 972	0.007 956 955 0	−0.000 574 463 7

In an analogous way one may study the $\lambda \to \infty$ limit. As we have already commented, the leading term in the solution of the Hankel determinantal equation for large λ is proportional to λ^2, the proportionality constants being $-1/4$, $-1/16$, $-1/36$, and so on, for the different solutions. In other words, pure Coulomb solutions are obtained. It is possible to obtain the corrections to these asymptotic forms by expanding the solutions of the determinantal equations in a form similar to equation (7), which corresponds to the Coulomb regime. By selecting the appropriate root there results the following expansions, corresponding to several values of the dimension of the determinant

$$E(N=2) = \lambda^2\left(-\tfrac{1}{4}\right) \tag{34}$$

$$E(N=3) = \lambda^2\left(-\frac{1}{4} + \frac{12}{\lambda^4} - \frac{1032}{\lambda^8} + \frac{278\,304}{\lambda^{12}} + \cdots\right) \tag{35}$$

$$E(N=4) = \lambda^2\left(-\frac{1}{4} + \frac{12}{\lambda^4} - \frac{1032}{\lambda^8} + \frac{369\,024}{\lambda^{12}} + \cdots\right) \tag{36}$$

$$E(N=5) = \lambda^2\left(-\frac{1}{4} + \frac{12}{\lambda^4} - \frac{1032}{\lambda^8} + \frac{348\,864}{\lambda^{12}} - \frac{211\,519\,200}{\lambda^{14}} + \frac{186\,697\,690\,368}{\lambda^{18}} + \cdots\right). \tag{37}$$

In these equations we have only included up to the first non-exact term of the expansion.

One may thus temptatively conclude that the Riccati–Padé method provides a scheme extending from $\lambda = -\infty$ up to values of λ larger than zero (but not up to $+\infty$). There is, however, a question which we have not been able to answer in general, namely whether the solution with the proper small-coupling behaviour will smoothly evolve for increasing values of the coupling constant λ to the solution with

the proper strong-coupling behaviour. A glance at figure 1 reveals that this is not the case for the $N = 2$ case, where the branch which starts at $E = 3$ at $\lambda = 0$ moves to the first excited state at $\lambda = -\infty$, i.e. $-\lambda^2/16$. On the contrary, for the case $N = 3$, the lowest root has the correct behaviour at both extremes of the interval $[0, \infty]$. The situation is more complex in the case $N = 4$, as can be seen in figure 1. In fact there are four roots behaving as $-\lambda^2/4$ in the Coulomb regime limit. Only two of them reproduce the strong-coupling behaviour of equation (7) up to the term λ^{-6}, and these two roots go finally to $E = 3$ at $\lambda = 0$. In fact, these two roots can only be distinguished in the region of λ between 0 and 3, and it is not possible to decide which of these roots has the correct slope at $\lambda = 0$. Nevertheless, it seems that when N increases, apart from the contamination by unphysical branches, the physical branches are better reproduced. Note also in the plot labelled $N = 4$ of figure 1, the presence of a branch which evolves from $E = 7$ at $\lambda = 0$ to $E \to -\lambda^2/16$ at $\lambda \to -\infty$, and which corresponds to the first excited level.

6. Conclusions

This paper has been devoted to a simple spiked oscillator, characterized by a perturbative term of the Coulomb form λ/r, which results in a non-supersingular problem. The nature of the perturbation is such that large-order expansions may be obtained in the two strong-coupling regimes, i.e. very large positive and negative values of λ, as well as the first terms of the ordinary small-coupling expansion. Moreover, there is an infinite class of elementary solutions for specific, in general irrational, values of the coupling constant.

The aim of the paper was to find constructive methods to extend the convergence radius of these expansions. The use of the renormalization series method has provided an implicit, and somewhat involved, path to connect the strong-coupling regime ($\lambda \to \infty$) with the small-coupling regime, as well as to connect the Coulomb regime ($\lambda \to -\infty$) with the small-coupling regime. Unfortunately, no way seems to exist to connect the ∞ and the $-\infty$ regions directly.

Whereas the precision of the renormalized series expansion is acceptable for small values of λ, it worsens near the origin. This region, however, was studied with the Riccati–Padé method. We must recognize several uncomfortable aspects of this latter approach, such as the presence of unphysical roots as well as the folding of the λ domain $[-\infty, \infty]$ into the domain $[0, \infty]$. Because of these two facts, the identification of the appropriate root for a given value of λ is not immediate, requiring the study of the evolution of the root with the variation of λ to identify it correctly. Nevertheless, it is very satisfying that, for some elementary solutions, depending on the degree of the determinantal equation used, both the energy and the wavefunction are obtained exactly. This method seems to be very promising, but it still requires deeper study.

The next step would be the study of stronger spikes λ/r^α. The case λ/r^2 is trivial, because the Hamiltonian may be solved exactly. However the fact that the renormalization series approach is able to exactly reproduce the small-coupling series from the strong-coupling expansion for this spike is not so trivial. One is tempted to say that the domain of $\alpha \in [0, 2]$ may be accurately studied with the help of the renormalization method and the Riccati–Padé method. The real challenge is the supersingular region, which starts at $\alpha = 5/2$. For this and higher values of the exponent the small-coupling series contains fractional powers or logarithmic terms of

the coupling constant. A new renormalization mechanism must be invented to cover these cases.

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