Quantum anharmonic oscillators: a new approach

2005 J. Phys. A: Math. Gen. 38 3193

(http://iopscience.iop.org/0305-4470/38/14/009)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS A: MATHEMATICAL AND GENERAL

J. Phys. A: Math. Gen. **38** (2005) 3193–3202 doi:10.1088/0305-4470/38/14/009

Quantum anharmonic oscillators: a new approach

F J Gómez and J Sesma

Departamento de Física Teórica, Facultad de Ciencias, 50009, Zaragoza, Spain

Received 19 October 2004, in final form 2 February 2005
Published 21 March 2005
Online at stacks.iop.org/JPhysA/38/3193

Abstract

The determination of the eigenenergies of a quantum anharmonic oscillator consists merely in finding the zeros of a function of the energy, namely the Wronskian of two solutions of the Schrödinger equation which are regular respectively at the origin and at infinity. We show in this paper how to evaluate that Wronskian exactly, except for numerical rounding errors. The procedure is illustrated by application to the $gx^2 + x^{2N}$ (N a positive integer) oscillator.

PACS number: 03.65.Ge

Quantum anharmonic oscillators have been frequently used in different branches of physics to simulate a great variety of situations and to explain a multitude of phenomena. Apart from this, since the publication of the seminal papers by Bender and Wu [1] and by Simon and Dicke [2] showing the failure of the Rayleigh–Schrödinger perturbation method, they have served to test plenty of approximate methods of solution of the Schrödinger equation. Papers dealing with the most recently proposed methods [3] contain references to older ones, which we omit for brevity. It seems, however, to have been passed unnoticed that an exact procedure exists to obtain a quantization condition that gives the eigenenergies as zeros of an easily calculable function. The idea is the same as that exploited in the solution of the Schrödinger equation for the harmonic oscillator or the Coulomb potential, although the procedure is slightly more tricky than in those two simple cases.

The starting point is the Schrödinger equation written as a second-order differential equation free of first-derivative terms. Such an equation is satisfied by the wavefunction, in the case of an even one-dimensional anharmonic oscillator, or by the reduced wavefunction, if one is considering an isotropic D-dimensional oscillator. A solution $u_{\rm reg}$ of the differential equation physically acceptable at the origin can be immediately obtained as a power series of the variable. Two other solutions $u^{(1)}$ and $u^{(2)}$, characterized by their behaviour at large distances, can also be considered. To be specific, let $u^{(1)}$ represent the solution going exponentially to zero as the variable increases, whereas $u^{(2)}$ corresponds to an exponentially diverging one. Since $u^{(1)}$ and $u^{(2)}$ are independent, $u_{\rm reg}$ can always be written as a linear combination of them with coefficients, called *connection factors*, which depend on the energy and on the parameters of the potential. For a generic value of the energy, both connection factors are different from

zero and $u_{\rm reg}$ is not a physical solution because of its behaviour at infinity. The eigenenergies are then determined by requiring the cancellation of the connection factor multiplying $u^{(2)}$.

The connection problem for a differential equation with two singular points (let us say, one at the origin and the other at infinity) was discussed by Naundorf [4]. He considered the case of one of the singular points (that at infinity, for instance) being irregular of integer rank $R > 0$ and the other one being either irregular of integer rank $r > 0$ or regular ($r = 0$). Here we are interested in this last case. Naundorf gave a procedure consisting of obtaining $2R$ independent formal power series, with an integer index running from $-\infty$ to $+\infty$, having well-defined asymptotic behaviours, and whose coefficients can serve as a basis in the $2R$-dimensional space of solutions of the recurrence obeyed by the coefficients of $u_{\rm reg}$. To obtain such basis, Naundorf replaces, in the known expressions of $u^{(1)}$ and $u^{(2)}$ [5], the exponential term determining their respective asymptotic behaviours by R independent formal expansions of the type of Heaviside's exponential series. Multiplication of those formal expansions by the Taylor series of the rest of the exponential terms and the descending power series in $u^{(1)}$ and $u^{(2)}$ produces $2R$ formal expansions whose coefficients obey the above-mentioned recurrence, i.e., the required basis. Comparison of $2R$ consecutive coefficients of the power series expression of $u_{\rm reg}$ with the analogous coefficients of the elements of the basis leads to a system of $2R$ linear equations whose solution allows one to obtain the connection factors. That procedure has been applied to the solution of several physical problems, such as the hydrogen atom with fine structure [6], the quarkonium [7], the spherical Stark effect in the hydrogen atom [8] or the quartic and sextic anharmonic oscillators [9].

The method suggested here is related to Naundorf's one insofar as it also rests on the vanishing of one of the connection factors and makes use of Heaviside's exponential series to obtain formal expansions, but differs from Naundorf's method in the procedure of computation: instead of following the steps detailed in the preceding paragraph, we benefit from the fact that the connection factor multiplying $u^{(2)}$ is given by the quotient of Wronskians $\mathcal{W}[u_{\rm reg}, u^{(1)}]/\mathcal{W}[u^{(2)}, u^{(1)}]$ and, since the denominator does not vanish, the quantization results from the fulfilment of the condition

$$\mathcal{W}[u_{\rm reg}, u^{(1)}] = 0. \tag{1}$$

To implement this condition, we need suitable expressions of $u_{\rm reg}$ and $u^{(1)}$. The series expansion mentioned above is adequate to represent the first of these solutions. For the second one a closed expression does not exist, in general, but a formal (asymptotic) expansion can be easily obtained by substitution in the differential equation. Then it is trivial to write a formal expression of the Wronskian and to require its cancellation.

To illustrate the method, let us apply it to the determination of the eigenenergies of the one-dimensional anharmonic oscillator represented by the potential

$$V(x) = gx^2 + x^{2N}, \quad N \text{ a positive integer.} \tag{2}$$

This problem has been tackled by several authors [10–12] by using different approximations. We discard the trivial case $N = 1$. The cases $N = 2$ (usually referred to as quartic oscillator) and $N = 3$ (sextic) can be easily solved following the steps we will detail, but the resulting equations do not fit in the general form given below. Therefore, we assume $N \geqslant 4$. The Schrödinger equation (in adequate units for the variable x and the energy E)

$$\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + gx^2 + x^{2N}\right) u(x) = Eu(x), \tag{3}$$

admits solutions, regular at the origin, of the form

$$u_{\rm reg}(x) = \sum_{n=0}^{\infty} a_n x^{n+\nu}, \qquad a_0 \neq 0, \tag{4}$$

with $\nu = 0$ (even states) or 1 (odd states). Alternatively, two independent solutions, $u^{(1)}$ and $u^{(2)}$, with asymptotic expansions (for $x \to +\infty$)

$$u^{(j)}(x) \sim \exp\left[\frac{\alpha^{(j)}}{N+1}x^{N+1}\right] x^{\mu^{(j)}} \sum_{m=0}^{\infty} h_m^{(j)} x^{-m}, \qquad h_0^{(j)} \neq 0, \quad j = 1, 2, \tag{5}$$

can also be considered. Substitution of this formal expansion in (3) gives for the exponents

$$\begin{aligned} &\alpha^{(1)} = -1, && \mu^{(1)} = \mu \equiv -N/2, \\ &\alpha^{(2)} = +1, && \mu^{(2)} = \mu \equiv -N/2, \end{aligned} \tag{6}$$

and for the coefficients

$$2\alpha^{(j)} m h_m^{(j)} = (m - N/2)(m - N/2 - 1)h_{m-N-1}^{(j)} + E h_{m-N+1}^{(j)} - g h_{m-N+3}^{(j)}. \tag{7}$$

Instead of computing directly the left-hand side of (1), let us introduce two auxiliary functions

$$v_{\text{reg}}(x) = \exp(x^{N+1}/(N+1))u_{\text{reg}}(x), \tag{8}$$

$$v^{(1)}(x) = \exp(x^{N+1}/(N+1))u^{(1)}(x), \tag{9}$$

which obey the differential equation

$$\frac{\mathrm{d}^2 v}{\mathrm{d}x^2} - 2x^N \frac{\mathrm{d}v}{\mathrm{d}x} + (E - gx^2 - Nx^{N-1})v = 0, \tag{10}$$

and whose Wronskian satisfies

$$\mathcal{W}[v_{\text{reg}}, v^{(1)}] = \exp(2x^{N+1}/(N+1))\mathcal{W}[u_{\text{reg}}, u^{(1)}]. \tag{11}$$

Now, by using the series expansion

$$v_{\text{reg}}(x) = \sum_{n=0}^{\infty} b_n x^{n+\nu}, \qquad b_0 \neq 0, \tag{12}$$

with coefficients given by the recurrence

$$(n+\nu)(n+\nu-1)b_n = -E b_{n-2} + g b_{n-4} + 2(n - N/2 - 1 + \nu)b_{n-N-1}, \tag{13}$$

and the asymptotic expansion

$$v^{(1)}(x) \sim \sum_{m=0}^{\infty} h_m^{(1)} x^{-m+\mu}, \tag{14}$$

one obtains for the left-hand side of (11) a formal expansion

$$\mathcal{W}[v_{\text{reg}}, v^{(1)}] \sim \sum_{k=-\infty}^{\infty} \gamma_k x^{k-1+\nu+\mu}, \tag{15}$$

with coefficients

$$\gamma_k = \sum_{m=0}^{\infty} (-2m - k - \nu + \mu) b_{m+k} h_m. \tag{16}$$

A similar expansion can be obtained for the right-hand side of (11) by recalling Heaviside's exponential series

$$\exp(t) \sim \sum_{n=-\infty}^{\infty} \frac{t^{n+\delta}}{\Gamma(n+1+\delta)}, \tag{17}$$

introduced by Heaviside in the second volume of his *Electromagnetic Theory* (London, 1899) and probed by Barnes [13] to be an asymptotic expansion for arbitrary δ and $|\arg(t)| < \pi$. Let us construct $N+1$ expansions

$$\exp(2x^{N+1}/(N+1)) \sim \mathcal{E}_L \equiv \sum_{n=-\infty}^{\infty} \frac{(2x^{N+1}/(N+1))^{n+\delta_L}}{\Gamma(n+1+\delta_L)} \tag{18}$$

of the type (17) with appropriate choices for δ,

$$\delta_L = (\nu+\mu+L)/(N+1), \qquad L = 0, 1, \ldots, N. \tag{19}$$

It is evident that, for any set of constants β_L $(L = 0, 1, \ldots, N)$ restricted by the condition

$$\mathcal{W}[u_{\mathrm{reg}}, u^{(1)}] = \sum_{L=0}^{N} \beta_L, \tag{20}$$

one has

$$\exp(2x^{N+1}/(N+1))\mathcal{W}[u_{\mathrm{reg}}, u^{(1)}] \sim \sum_{L=0}^{N} \beta_L \mathcal{E}_L. \tag{21}$$

If, according to equation (11), this formal expansion has to coincide with that in (15), the constants β_L must be

$$\beta_L = \frac{\Gamma(n+1+\delta_L)}{(2/(N+1))^{n+\delta_L}} \gamma_{k_L}, \qquad k_L = n(N+1)+1+L, \tag{22}$$

where the integer n can be chosen at will. Substitution of those values in (20) allows one to write the quantization condition (1) in the final form

$$\sum_{L=0}^{N} \Gamma(n+1+\delta_L)((N+1)/2)^{L/(N+1)} \gamma_{k_L} = 0. \tag{23}$$

We have used the last expression of the quantization condition to find the lowest eigenenergies of the anharmonic oscillator (2) for different values of the coupling parameter g and four different choices of N. In the computation, we have used a FORTRAN program with double precision. The results are shown in tables 1 to 4.

The procedure presented above assumes the capability to compute the $N+1$ coefficients γ_{k_L} $(L = 0, 1, \ldots, N)$ by summation of the series in (16). We have not yet proved rigorously the convergence of such series, albeit extensive numerical explorations guarantee its convergence for sufficiently large k, i.e., for n, in equation (22), above a certain threshold which depends on the values of the coupling parameter g and on the energy. Moreover, those explorations show that, the larger n is taken, the faster becomes the convergence. Investigations tending to elucidate that question are currently in progress.

Besides the eigenenergies, our method determines also, in principle, the eigenfunctions. In the example considered, they are given by equations (8) and (12). Nevertheless, although the series in (12) converges for all finite x, it cannot be used safely for large values of x, unless a considerable number of digits are maintained in the successive arithmetical operations. Certainly, the asymptotic expansion (5) can be used for sufficiently large values of x (above about 5 units). But the advantage of this procedure over the conventional numerical integration of the Schrödinger equation is not clear, especially if one needs the normalized wavefunction for a large number of points.

To facilitate understanding the method, we have chosen above a very simple example: a one-dimensional anharmonic oscillator with only two terms in the potential. The procedure is

Table 1. The four lowest eigenenergies of the oscillator (2), for $N = 4$ and several values of g. The energies E_0 and E_2 correspond to even states ($\nu = 0$ in (4)); E_1 and E_3 to odd ones ($\nu = 1$).

g	E_0	E_1	E_2	E_3
−20	−15.627 817 90	−15.603 428 43	−1.997 596 74	0.049 137 69
−10	−3.898 942 14	−3.325 413 35	3.264 150 45	8.822 126 29
−1	0.935 278 62	4.113 468 27	9.490 089 84	16.491 632 53
−0.1	1.197 981 14	4.692 996 58	10.169 682 29	17.258 079 61
0	1.225 820 11	4.755 874 41	10.244 946 98	17.343 087 97
0.1	1.253 406 43	4.818 457 27	10.320 150 25	17.428 061 87
1	1.491 019 90	5.368 778 06	10.993 737 34	18.191 100 02
10	3.212 964 74	9.868 891 92	17.200 021 66	25.523 114 99
20	4.487 415 20	13.545 432 09	22.894 307 80	32.782 471 04

Table 2. The four lowest eigenenergies of the Hamiltonian (2), for $N = 5$ and several values of g.

g	E_0	E_1	E_2	E_3
−20	−11.566 301 47	−11.458 546 77	0.564 947 00	4.907 290 85
−10	−2.837 826 75	−1.830 754 83	4.909 461 47	11.942 792 56
−1	1.032 058 34	4.515 333 89	10.486 979 85	18.454 644 82
−0.1	1.273 081 85	5.040 588 36	11.087 624 65	19.115 376 34
0	1.298 843 70	5.097 876 53	11.154 318 20	19.188 809 56
0.1	1.324 412 24	5.154 953 87	11.220 994 52	19.262 244 08
1	1.546 263 51	5.659 337 72	11.819 967 88	19.923 103 57
10	3.217 117 08	9.932 293 22	17.515 895 63	26.434 508 76
20	4.486 235 13	13.553 292 64	22.992 318 28	33.193 547 64

Table 3. The four lowest eigenenergies of the Hamiltonian (2), for $N = 6$ and several values of g.

g	E_0	E_1	E_2	E_3
−20	−9.366 071 77	−9.130 105 87	2.010 354 59	7.975 546 84
−10	−2.241 874 09	−0.870 044 33	6.121 596 77	14.165 128 36
−1	1.113 699 83	4.844 702 02	11.281 306 98	19.999 879 59
−0.1	1.339 499 07	5.333 472 17	11.831 812 76	20.595 393 82
0	1.363 779 71	5.386 942 02	11.893 009 08	20.661 637 60
0.1	1.387 865 79	5.440 245 56	11.954 205 20	20.727 894 95
1	1.597 990 50	5.912 646 17	12.504 708 42	21.324 741 09
10	3.224 418 73	10.006 304 19	17.831 647 30	27.278 764 98
20	4.486 801 92	13.570 820 13	23.113 716 63	33.632 812 10

equally applicable to isotropic D-dimensional oscillators with any number of integer powers of the radial variable in the potential and for any value of the D-dimensional 'angular momentum'. It is also applicable, of course, to easier problems. Let us consider, for instance, three anharmonic oscillators algebraically solvable, namely, the Pöschl–Teller, the modified Pöschl–Teller and the Morse potentials. Their exact solution can be found in [14], whose notation we adopt. In what follows, we concentrate on obtaining, by our procedure, the eigenenergies of the bound states. But, since the reflection and transmission coefficients are trivially related to the connection factors, our method is also useful for calculating phase shifts.

Table 4. The four lowest eigenenergies of the oscillator (2), for $N = 7$ and several values of g.

g	E_0	E_1	E_2	E_3
−20	−7.974 891 49	−7.590 267 06	3.059 161 12	10.192 691 95
−10	−1.847 462 4	−0.171 591 44	7.073 200 94	15.872 592 91
−1	1.183 937 65	5.123 291 91	11.939 119 91	21.262 040 13
−0.1	1.398 320 30	5.585 520 94	12.454 750 50	21.813 415 53
0	1.421 438 88	5.636 185 03	12.512 101 99	21.874 775 20
0.1	1.444 422 47	5.686 711 75	12.569 460 66	21.936 152 83
1	1.645 427 30	6.135 342 77	13.085 814 00	22.489 304 58
10	3.233 359 19	10.084 158 88	18.134 656 08	28.044 330 38
20	4.488 353 26	13.594 289 39	23.247 812 10	34.074 174 53

In the case of the Pöschl–Teller potential

$$V(x) = \frac{1}{2}V_0\left(\frac{\kappa(\kappa-1)}{\sin^2(\alpha x)} + \frac{\lambda(\lambda-1)}{\cos^2(\alpha x)}\right), \qquad V_0 = \frac{\hbar^2\alpha^2}{m}, \quad \kappa, \lambda > 1, \tag{24}$$

defined in the interval $x \in [0, \pi/2]$, the Schrödinger equation can be written in the form

$$y(y-1)u'' + \left(\frac{1}{2} - y\right)u' + \frac{1}{4}\left(\frac{k^2}{\alpha^2} - \frac{\kappa(\kappa-1)}{y} - \frac{\lambda(\lambda-1)}{1-y}\right)u = 0, \tag{25}$$

in terms of a new variable

$$y = \sin^2(\alpha x) \tag{26}$$

and using, instead of the energy E, the parameter

$$k^2 = \frac{2mE}{\hbar^2}. \tag{27}$$

Equation (25) can be written as a hypergeometric one by means of the change of function done in [14]. Then, it is immediate to write the connection factors and to obtain the quantization condition. Nevertheless, let us ignore this fact and try to apply our method directly to equation (25), to be solved between the two regular singular points $y = 0$ and $y = 1$. The solution regular at $y = 0$ can be written as a power series

$$u_{\mathrm{reg}}(y) = \sum_{n=0}^{\infty} a_n y^{n+\kappa/2}, \qquad a_0 \neq 0, \tag{28}$$

with coefficients given by the recurrence

$$n\left(n - \frac{1}{2} + \kappa\right)a_n = \left(\left(n - 1 + \frac{\kappa}{2}\right)\left(2n - \frac{5}{2} + \kappa\right) - \frac{1}{4}\left(\frac{k^2}{\alpha^2} + \kappa(\kappa-1) - \lambda(\lambda-1)\right)\right)a_{n-1}$$
$$-\left(\left(n - 2 + \frac{\kappa}{2}\right)^2 - \frac{k^2}{4\alpha^2}\right)a_{n-2}. \tag{29}$$

The solution regular at $y = 1$ can be immediately written if one realizes that the differential equation (25) is invariant under the interchange

$$\begin{Bmatrix} y \\ \kappa \end{Bmatrix} \longleftrightarrow \begin{Bmatrix} 1-y \\ \lambda \end{Bmatrix}$$

and, therefore,

$$u^{(1)}(y) = \sum_{n=0}^{\infty} b_n (1-y)^{n+\lambda/2}, \qquad b_0 \neq 0, \tag{30}$$

with coefficients given now by

$$n\left(n-\frac{1}{2}+\lambda\right)b_n=\left(\left(n-1+\frac{\lambda}{2}\right)\left(2n-\frac{5}{2}+\lambda\right)-\frac{1}{4}\left(\frac{k^2}{\alpha^2}+\lambda(\lambda-1)-\kappa(\kappa-1)\right)\right)b_{n-1}$$
$$-\left(\left(n-2+\frac{\lambda}{2}\right)^2-\frac{k^2}{4\alpha^2}\right)b_{n-2}. \tag{31}$$

Both series in equations (28) and (30) are convergent for $y\in(0,1)$. We can, therefore, write a convergent (not merely formal, as in the problem considered before) expansion of the Wronskian. At the point $y=1/2$, for instance, one has

$$\mathcal{W}[u_{\rm reg},u^{(1)}](y=1/2)=-\frac{1}{2^{(\kappa+\lambda)/2}}\left(\left(\sum_{n=0}^{\infty}\frac{a_n}{2^n}\right)\left(\sum_{m=0}^{\infty}\frac{(m+\lambda/2)b_m}{2^{m-1}}\right)\right.$$
$$\left.+\left(\sum_{n=0}^{\infty}\frac{(n+\kappa/2)a_n}{2^{n-1}}\right)\left(\sum_{m=0}^{\infty}\frac{b_m}{2^m}\right)\right). \tag{32}$$

Giving numerical values to κ and λ, one can check that the Wronskian vanishes whenever

$$\frac{k^2}{\alpha^2}=(\kappa+\lambda+2n)^2,\qquad n=0,1,2,\ldots, \tag{33}$$

as it should be.

The modified Pöschl–Teller potential, defined for $x\in(-\infty,+\infty)$, reads

$$V(x)=-\frac{\hbar^2}{2m}\alpha^2\frac{\lambda(\lambda-1)}{\cosh^2(\alpha x)},\qquad \lambda>1. \tag{34}$$

Instead of the (negative) energy E, we use the parameter

$$\kappa^2=\frac{2m(-E)}{\hbar^2}. \tag{35}$$

Once again, the Schrödinger equation can be written as a hypergeometric one with adequate changes of variable and function. The change of variable used in [14] maps the interval $(-\infty,+\infty)$ for the variable x onto $[1,+\infty)$ for the new variable. Here we prefer, however, to make a different change of variable, namely

$$y=\frac{1}{\cosh^2(\alpha x)}, \tag{36}$$

in order to get the mentioned interval, where the differential equation has to be solved, mapped onto $[0,1]$. The Schrödinger equation then turns into

$$y^2(1-y)u''+y\left(1-\frac{3}{2}y\right)u'+\frac{1}{4}\left(-\frac{\kappa^2}{\alpha^2}+\lambda(\lambda-1)y\right)u=0. \tag{37}$$

The regular solution at the regular singular point $y=0$ can be written as a series

$$u_{\rm reg}(y)=\sum_{n=0}^{\infty}a_n y^{n+\kappa/(2\alpha)},\qquad a_0\neq 0, \tag{38}$$

with coefficients obtainable by means of

$$n\left(n+\frac{\kappa}{\alpha}\right)a_n=\left(\left(n-1+\frac{\kappa}{2\alpha}\right)\left(n-\frac{1}{2}+\frac{\kappa}{2\alpha}\right)-\frac{\lambda(\lambda-1)}{4}\right)a_{n-1}. \tag{39}$$

Now we need to write the well-behaved solution at $y = 1$. Two independent expansions in power series of $1 - y$ of the form

$$u(y) = \sum_{n=0}^{\infty} b_n (1-y)^{n+\mu}, \qquad b_0 \neq 0, \tag{40}$$

with

$$\mu = 0 \qquad \text{or} \qquad \mu = 1/2$$

and coefficients obeying the recurrence

$$(n+\mu)\left(n+\mu-\frac{1}{2}\right) b_n = \left(2\,(n-1+\mu)^2 + \frac{\kappa^2}{4\alpha^2} - \frac{\lambda(\lambda-1)}{4}\right) b_{n-1} - \left((n-2+\mu)\left(n-\frac{3}{2}+\mu\right) - \frac{\lambda(\lambda-1)}{4}\right) b_{n-2}, \tag{41}$$

are physically acceptable. Those solutions with $\mu = 0$ and $\mu = 1/2$ correspond, respectively, to even and odd wavefunctions in the variable x. Choosing the point $y = 1/2$ to evaluate the Wronskian of $u_{\rm reg}$ and each one of those functions, one has

$$\mathcal{W}[u_{\rm reg}, u](y = 1/2) = -\frac{1}{2^{\kappa/(2\alpha)+\mu}}\left(\left(\sum_{n=0}^{\infty}\frac{a_n}{2^n}\right)\left(\sum_{m=0}^{\infty}\frac{(m+\mu)b_m}{2^{m-1}}\right) + \left(\sum_{n=0}^{\infty}\frac{(n+\kappa/(2\alpha))a_n}{2^{n-1}}\right)\left(\sum_{m=0}^{\infty}\frac{b_m}{2^m}\right)\right). \tag{42}$$

It can be checked numerically that the right-hand side of (42) becomes zero if,

$$\text{for } n = 0, 1, 2, \ldots, \quad 0 < \frac{\kappa}{\alpha} = \begin{cases} \lambda - 1 - 2n & \text{for even states,} \\ \lambda - 2 - 2n & \text{for odd states.} \end{cases}$$

We arrive finally to the case of the Morse potential

$$V(r) = D(\exp(-2\alpha x) - 2\exp(-\alpha x)), \qquad x = (r - r_0)/r_0, \quad \alpha > 0, \tag{43}$$

exactly solvable for angular momentum $l = 0$. By introducing, as in [14], a new variable

$$y = \frac{2\gamma}{\alpha}\exp(-\alpha x), \tag{44}$$

and denoting

$$\beta^2 = -\frac{2mEr_0^2}{\hbar^2}, \qquad \gamma^2 = \frac{2mDr_0^2}{\hbar^2}, \qquad \beta, \gamma > 0, \tag{45}$$

the Schrödinger equation becomes

$$y^2 u'' + y u' + \left(-\frac{\beta^2}{\alpha^2} + \frac{\gamma}{\alpha}y - \frac{1}{4}y^2\right) u = 0. \tag{46}$$

This equation presents a regular singular point at the origin and an irregular one at infinity. The physical solution, however, needs to be defined only between $y = 0$, corresponding to $x \to \infty$ ($r \to \infty$), and $y = y_0 \equiv (2\gamma/\alpha)\exp(\alpha)$, corresponding to $x = -1$ ($r = 0$). Such physical solution must be regular at $y = 0$ and become zero at $y = y_0$. The solution regular at $y = 0$ can be given as a series

$$u_{\rm reg}(y) = \sum_{n=0}^{\infty} a_n y^{n+\beta/\alpha}, \qquad a_0 \neq 0, \tag{47}$$

with coefficients obeying

$$n(n+2\beta/\alpha)a_n = -(\gamma/\alpha)a_{n-1} + (1/4)a_{n-2}. \tag{48}$$

The other extreme of the interval of definition of the wavefunction, $y = y_0$, is an ordinary point. There are two independent solutions of the differential equation, both finite at $y = y_0$. But only the linear combination of them becoming zero at that point is physically acceptable. Let us call it $u^{(1)}$. Now, following our procedure, we should impose the cancellation of the Wronskian of $u_{\rm reg}$ and $u^{(1)}$ at any point of $[0, y_0]$. If we choose $y = y_0$, it becomes

$$\mathcal{W}[u_{\rm reg}, u^{(1)}](y = y_0) = u_{\rm reg}(y_0)u^{(1)\prime}(y_0), \tag{49}$$

and, since $u^{(1)\prime}$ cannot vanish at $y = y_0$, the quantization condition reads

$$u_{\rm reg}(y_0) = 0, \tag{50}$$

an expression that could have been obtained trivially, without having recourse to our method. It is not difficult to see that, if one takes $a_0 = 1$ in (47), one has

$$u_{\rm reg}(y) = y^{\beta/\alpha}\exp(-y/2)\,{}_1F_1\left(\frac{1}{2}+\frac{\beta}{\alpha}-\frac{\gamma}{\alpha}, 1+2\frac{\beta}{\alpha}; y\right), \tag{51}$$

and the quantization condition (50) coincides with that given in [14].

Unlike what happened in the case of potential (2), the numerical convergence of the power series giving the solutions of the Schrödinger equation in the three last examples is rapid enough to guarantee an accurate computation of the eigenfunctions. For instance, in the case of the Pöschl–Teller potential, the series in (28) can be used for $y \leqslant 1/2$ and that in (30) for $y \geqslant 1/2$, the coefficients a_0 and b_0 being determined by continuity at $y = 1/2$ and normalization in the interval $y \in [0, 1]$.

Acknowledgments

It is a great pleasure to dedicate this work to Professor Rafael Guardiola on the occasion of his 60th birthday. The suggestions of two anonymous referees have contributed to improve considerably a first version of the paper. Financial support from Comisión Interministerial de Ciencia y Tecnología is acknowledged.

References

[1] Bender C M and Wu T T 1969 *Phys. Rev.* **184** 1231
Bender C M and Wu T T 1971 *Phys. Rev. Lett.* **27** 461
Bender C M and Wu T T 1973 *Phys. Rev.* D **7** 1620
[2] Simon B and Dicke A 1970 *Ann. Phys., NY* **58** 76
[3] Zamastil J, Čížek J and Skála L 2000 *Phys. Rev. Lett.* **84** 5683
de Castro A S and de Souza Dutra A 2000 *Phys. Lett.* A **269** 281
Müller M and Heiss W D 2000 *J. Phys. A: Math. Gen.* **33** 93
Álvarez G and Casares C 2000 *J. Phys. A: Math. Gen.* **33** 2499
Álvarez G and Casares C 2000 *J. Phys. A: Math. Gen.* **33** 5171
Pathak A 2000 *J. Phys. A: Math. Gen.* **33** 5607
Child M S, Dong S H and Wang X G 2000 *J. Phys. A: Math. Gen.* **33** 5653
Chen G F 2001 *J. Phys. A: Math. Gen.* **34** 757
Zappalá D 2001 *Phys. Lett.* A **290** 35
Giller S and Milczarski P 2001 *J. Math. Phys.* **42** 608
Jafarpour M and Afshar D 2002 *J. Phys. A: Math. Gen.* **35** 87
Álvarez G, Howls C J and Silverstone H J 2002 *J. Phys. A: Math. Gen.* **35** 4003
Álvarez G, Howls C J and Silverstone H J 2002 *J. Phys. A: Math. Gen.* **35** 4017

Meurice Y 2002 *J. Phys. A: Math. Gen.* **35** 8831
de Souza Dutra A, de Castro A S, da Silva E A and Castilho L C O 2003 *J. Phys. A: Math. Gen.* **36** 1711
Amore P, Aranda A and De Pace A 2004 *J. Phys. A: Math. Gen.* **37** 3515
Dusuel S and Uhrig G S 2004 *J. Phys. A: Math. Gen.* **37** 9275
[4] Naundorf F 1976 *SIAM J. Math. Anal.* **7** 157
[5] Olver F W J and Stenger J 1965 *SIAM J. Numer. Anal.* **2** 244
[6] Naundorf F F 1978 *J. Math. Phys.* **19** 1426
[7] Gómez F J and Sesma J 1994 *J. Comput. Phys.* **115** 296
[8] Gómez F J and Sesma J 1996 *Phys. Lett.* A **219** 187
[9] Gómez F J and Sesma J 2000 *Phys. Lett.* A **270** 20
[10] Guardiola R, Solís M A and Ros J 1992 *Nuovo Cimento* B **107** 713
[11] Nanayakkara A and Bandara V 2002 *Can. J. Phys.* **80** 959
[12] Amore P, Aranda A, De Pace A and López J A 2004 *Phys. Lett.* A **329** 451
[13] Barnes E W 1906 *Trans. Camb. Phil. Soc.* **20** 253
[14] Flügge S 1974 *Practical Quantum Mechanics* (New York: Springer)