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Convergence radii of the Rayleigh–Schrödinger perturbation series for the bounded oscillators

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Abstract. The convergence radii of the Rayleigh-Schrödinger perturbation series for some bounded oscillators are calculated. The eigenvalues with quantum numbers $n = 0$ and $n = 2$, as well as those with $n = 1$ and $n = 3$, are found to cross at a pair of conjugate branch points of order two in the complex plane. Higher excited states are briefly discussed.

1. Introduction

The Rayleigh-Schrödinger perturbation theory is frequently applied to quantum mechanical problems to obtain an expansion of the energy E in powers of the perturbation parameter λ:

$$E = \sum_{j=0}^{\infty} E_j \lambda^j.$$

Quite often such a series has a finite convergence radius determined by the closest singularity to the origin (in the complex λ plane).

The calculation of the singular points of $E(\lambda)$ is very difficult for most physically interesting problems. However, the study of some simple examples may lead to a better insight into the subject. Among them we mention the delta-potential models (Certain and Byers Brown 1972, Fernández *et al* 1987 and references therein), the perturbed harmonic oscillator (Bender *et al* 1974), the Stark effect in rigid rotators (Fernández and Castro 1985, Maluendes *et al* 1985, Fernández *et al* 1987) and the Mathieu equation (McLachlan 1947, Fernández *et al* 1987). Except for some very simple problems, the direct calculation of the branch points of $E(\lambda)$ (Certain and Byers Brown 1972, Fernández and Castro 1985, Maluendes *et al* 1985, Fernández *et al* 1987) is quite cumbersome and it is sometimes preferable to obtain them from the behaviour of E_j for large j (Fernández *et al* 1987), though this method is less accurate.

The purpose of the present paper is to obtain the singular points of the eigenvalues $W(b)$ of the bounded oscillators

$$\Psi''(x) + (W - x^{2k})\Psi(x) = 0 \tag{1}$$

where $k = 1, 2, \ldots$, and $\Psi(-b) = \Psi(b) = 0$. The change of variables $x \to bx$ enables one to rewrite (1) as

$$\Phi''(x) + (E - \lambda x^{2k})\Phi(x) = 0 \tag{2}$$

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where $\lambda = b^{2(k+1)}$, $E = b^2 W$ and $\Phi(-1) = \Phi(1) = 0$. According to the Kato-Rellich theorem (Kato 1976) the λ perturbation series for $E(\lambda)$ has a finite convergence radius. Upper bounds to it have already been calculated in the case of two- and three-dimensional bounded harmonic oscillators (Aguilera-Navarro *et al* 1983).

The perturbation coefficients E_j for the one-dimensional oscillators (2) are obtained in § 2. A method for calculating the branch points of $E(\lambda)$ from the asymptotic form of E_j is shown in § 3. Numerical results are discussed in § 4.

2. Perturbation series

The perturbation series for the eigenvalues of (2) can be easily and accurately calculated by means of the hypervirial perturbative method (Fernández and Castro 1981a, 1982). The perturbation corrections are given by the following recurrence relations (Fernández and Castro 1981a, 1982):

$$A_0^N = 1/(N+1) - N(N-1)A_0^{N-2}/(4e_n) \tag{3a}$$

$$A_M^N = \frac{1-(k+1)M}{M(N+1)e_n} A_{M-1}^{2k} - \frac{N(N-1)}{4e_n} A_M^{N-2} + \frac{N+k+1}{(N+1)e_n} A_{M-1}^{N+2k} - \sum_{s=1}^{M} \frac{A_{s-1}^{2k} A_{M-s}^N}{se_n} \tag{3b}$$

$$E_j = \frac{1}{j} A_{j-1}^{2k} \qquad j > 0 \tag{3c}$$

where $N = 0, 2, \ldots$, $M = 1, 2, \ldots$, $e_n = (n+1)^2\pi^2/4$ and $n = 0, 1, \ldots$, is the quantum number. The starting point is $A_M^0 = \delta_{M0}$.

Equations (3) are not useful for large-order numerical calculations because the errors increase quickly with N and M. It is advisable to use the backward recurrence relations

$$A_0^{N-2} = \frac{4e_n}{N(N-1)} \left(\frac{1}{N+1} - A_0^N \right) \tag{4a}$$

$$A_M^{N-2} = \frac{4}{N(N-1)} \left(\frac{1-(k+1)M}{M(N+1)e_n} A_{M-1}^{2k} - e_n A_M^N + \frac{N+k+1}{N+1} A_{M-1}^{N+2k} - \sum_{s=1}^{M} \frac{A_{s-1}^{2k} A_{M-s}^N}{s} \right). \tag{4b}$$

Since A_M^N tends to zero as N increases we can choose $A_M^N = 0$ for a large enough N value and then proceed backwards calculating all the perturbation corrections for $M = 0, 1, \ldots$. The accuracy of the results is easily checked because the first perturbation corrections can be obtained analytically (Fernández and Castro 1981a, 1982). $N = 500$ is found to be an acceptable starting point for the procedure that ends when the calculated A_M^{2k} and A_M^0 ($M > 0$) are of the same order of magnitude (notice that A_M^0 will not be exactly equal to δ_{M0} when using the backward recurrence relation because the starting point is approximate).

3. Branch points

Let $f(z)$ be a function of the complex variable $z = x + iy$ so that $f(x)$ is real. Therefore, each singular point of $f(z)$ is either real or complex conjugate of another one.

The convergence radius of the Taylor series

$$f(z) = \sum_{j=0}^{\infty} f_j z^j \tag{5}$$

is determined by the closest singular point to the origin. We suppose that $f(z)$ has a pair of branch points at z_0 and z_0^*, where $z_0 = x_0 + iy_0$. In the neighbourhood of any of them $f(z)$ behaves approximately as

$$f(z) \simeq A(z^2 - 2x_0 z + x_0^2 + y_0^2)^a \tag{6}$$

where a is a real number and A can be real or complex.

Our main assumption is that the behaviour of f_j for large j can be obtained from the Taylor coefficients of (6) provided that the moduli of the other singularities are larger than $|z_0|$.

In order to obtain a and z_0 we proceed as follows. The coefficients Y_j of the Taylor expansion about the origin for the ansatz

$$Y(z) = B(z^2 - 2uz + r^2)^e \tag{7}$$

where B, u, r^2 ($\simeq x_0^2 + y_0^2$) and e are adjustable parameters, obey

$$(j-2e-1)Y_{j-1} + 2u(e-j)Y_j + r^2(j+1)Y_{j+1} = 0 \tag{8}$$

where $j = 0, 1, \ldots$, and $Y_j = 0$ if $j < 0$. If f_s is substituted for Y_s in (8) with $j = m$, $m+1$ and $m+2$, we obtain three equations that can be solved for the unknowns e, u and r^2. Since the results depend on m the procedure gives rise to three sequences e_m, u_m and r_m^2 that are expected to converge towards a, x_0 and $x_0^2 + y_0^2$, respectively, as m tends to infinity. Extensive numerical investigation covering a large number of examples shows that the method is convergent provided that the conditions stated above are fulfilled (Fernández *et al* 1987).

The results are largely improved when the actual a value is known beforehand. In such a case we substitute a for b in (8) and proceed as before (using only pairs of equations) to obtain the sequences u_m and r_m^2.

The eigenvalues of most linear operators exhibit branch points of order two characterised by the condition (Certain and Byers Brown 1972, Fernández and Castro 1985, Bender *et al* 1974, Simon 1970)

$$\partial\lambda/\partial E = 0. \tag{9}$$

In such cases $a = \frac{1}{2}$. Examples of this are the bounded oscillators (2) as shown below.

4. Results and discussion

We have investigated the cases $k = 1$, 2 and 3 drawing general conclusions that seem to apply to all the oscillators. For example, the large-order energy perturbation corrections for the first two even states have almost the same magnitude but different signs. This fact reveals that they are branches of the same branch point and thereby have the same convergence radius. This is also the case for the first two odd states.

The sequences e_m, u_m and r_m^2 for the bounded harmonic oscillator are partly displayed in table 1. The second column suggests that that $a = \frac{1}{2}$ and when introducing this value into the calculation the sequences u_m and r_m become smoother (compare columns 3 and 4 with 5 and 6, respectively). Since similar results have been obtained for all the states and oscillators investigated, we assume $a = \frac{1}{2}$ and consider only the u_m and r_m sequences obtained when $e = \frac{1}{2}$ from now on.

The estimated branch points for the harmonic oscillator are shown in table 2. The sequences e_m for the states with quantum number $n > 3$ are strongly oscillatory,

Table 1. Sequences e_m, u_m and r_m (cf (7)) for the ground state of the bounded harmonic oscillator ($k = 1$). a: using $e = a = \frac{1}{2}$.

m	e_m	u_m	r_m	u_m^a	r_m^a
36	0.5054	−17.7240	28.4518	−17.7271	28.4568
37	0.5089	−17.7220	28.4487	−17.7267	28.4563
38	0.5200	−17.7159	28.4395	−17.7268	28.4559
39	0.5017	−17.7261	28.4547	−17.7270	28.4561
40	0.5065	−17.7235	28.4508	−17.7267	28.4559

Table 2. Closest branch points to the origin for the first eigenvalues of the bounded harmonic oscillator. b_0 and λ_0 are related by the scaling transformation in (2).

n	Re λ_0	$\lvert$Im $\lambda_0\rvert$	$\lvert\lambda_0\rvert$	$b_0 = \lvert\lambda_0\rvert^{1/4}$
0	−17.727	22.260	28.456	2.310
1	−10.19	46.073	47.187	2.621
2	−17.727	22.260	28.456	2.310
3	−10.19	46.073	47.187	2.621
4	3.8	71	71	2.9
5	23.4	96	99	3.2
6	48	122	131	3.4

suggesting the interference of other singularities. However, when setting $e = \frac{1}{2}$ the sequences u_m and r_m are smooth enough to obtain approximate z_0 values. Their accuracy will be checked by diagonalising the matrix of the complex Hamiltonian operator and results will be published elsewhere in a forthcoming paper.

The s-state eigenvalues of a three-dimensional isotropic oscillator are equal to the odd-state ones of the one-dimensional model. However, the present convergence radius for the first excited state of the bounded harmonic oscillator is found to be larger than the upper bound obtained by Aguilera-Navarro *et al* (1983).

The conclusions about the branch points of the harmonic oscillator also apply to the other oscillators. Tables 3 and 4 show some numerical results for the quartic ($k = 2$) and sextic ($k = 3$) oscillators, respectively. It is clear that the convergence radius of the perturbation series in powers of b (Fernández and Castro 1981a, 1982) for a given state decreases as k increases. This is due to the fact that the larger the k values the stronger the perturbation.

Table 3. Closest branch points to the origin (λ_0) for the first eigenvalues of the bounded quartic oscillator ($k = 2$).

n	Re λ_0	$\lvert$Im $\lambda_0\rvert$	$\lvert\lambda_0\rvert$	$b_0 = \lvert\lambda_0\rvert^{1/6}$
0	−36.228	28.454	46.066	1.893
1	−30.744	54.870	62.896	1.994
2	−36.228	28.454	46.066	1.893
3	−30.744	54.870	62.896	1.994

Table 4. Closest branch points to the origin (λ_0) for the first eigenvalues of the bounded sextic oscillator ($k = 3$).

n	Re λ_0	$\lvert\text{Im } \lambda_0\rvert$	$\lvert\lambda_0\rvert$	$b_0 = \lvert\lambda_0\rvert^{1/8}$
0	−60.74	35.61	70.41	1.702
1	−56.40	67.04	87.61	1.749
2	−60.74	35.61	70.41	1.702
3	−56.40	67.04	87.61	1.749

The bounded oscillators in more than one dimension can also be treated as shown above because the peturbation series can be easily obtained by means of the hypervirial perturbative method (Fernández and Castro 1981b).

We hope that present conclusions will motivate a rigorous mathematical investigation of the singular points of the bounded-oscillator eigenvalues. It may be very helpful in understanding more complex problems.

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