The strong coupling expansion for anharmonic oscillators

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Abstract. We accurately calculate the strong coupling expansion for anharmonic oscillators by means of a robust and stable numerical algorithm. The method applies to any state and to any anharmonicity degree. By means of the perturbation coefficients, we estimate the location of the branch points that determine the convergence radius of the strong coupling expansion.

Anharmonic oscillators with Hamiltonian operators

$$H = p^2 + x^2 + \lambda x^K \qquad K = 4, 6, \ldots \tag{1}$$

are among the most widely studied models in quantum mechanics. Bender and Wu [1] and Simon [2] proved that the perturbation series in powers of λ for the eigenvalues $\mathcal{E}(\lambda)$ (i.e. the so-called weak coupling expansion) is divergent for all values of λ. The calculation of the coefficients of the weak coupling expansion is relatively simple and can be carried out analytically to large perturbation orders. This series gives reasonable results just for sufficiently small values of λ, and even then, only after appropriate truncation. For moderate and large values of the perturbation parameter one has to resort to summation methods, such as, for example, Padé and Borel–Padé approximants, and renormalization [3].

On the other hand, the strong coupling expansion of $E(g) = \mathcal{E}(\lambda)/\lambda^{2/(K+2)}$ in powers of $g = (1/\lambda)^{4/(K+2)}$ has a finite radius of convergence determined by a pair of branch points at which two eigenvalues coalesce [1, 2, 4]. Formally, one obtains this series by application of perturbation theory with $H_0 = p^2 + x^K$ as the unperturbed Hamiltonian operator and $H_1 = x^2$ as the perturbation. Clearly, one cannot obtain this expansion exactly because the eigenvalue equation for H_0 is not exactly solvable.

As far as we know, the first attempt to obtain the strong coupling expansion was due to Turbiner and Ushverizde [5], if one does not take into account earlier numerical fits [6, 7]. Later, Guardiola *et al* [8] obtained an accurate strong coupling expansion from a renormalized weak coupling series. Further developments are due to Fernández and Guardiola [9], Janke and Kleinert [10] and Weniger [11]. The last two papers exhibit the most accurate determination of the strong coupling expansion for the quartic anharmonic oscillator ($K = 4$), but the accuracy of their methods deteriorates considerably for the sextic ($K = 6$) and octic ($K = 8$) anharmonic oscillators. The accuracy decreases still further

for greater values of K because the renormalization procedure is unable to overcome the increasingly stronger divergence of the weak coupling series. For this reason no accurate strong coupling expansion for large values of the anharmonicity degree K have been yet reported, in spite of the renewed interest in the subject. None of the approaches used to obtain the strong coupling series is wholly algebraic and they may therefore be termed *seminumerical* emphasizing the fact that they resort to numerical calculations in some way or another.

It is our purpose to show that a straightforward numerical integration of the equations of Rayleigh–Schrödinger perturbation theory is a remarkably simple and accurate method for the calculation of the strong coupling coefficients of sufficiently large order, even for anharmonicity degrees as large as $K = 1000$. Additionally, we also consider the limit $K \to \infty$.

A numerical calculation of the strong coupling expansion was recently described by Skála and Čížek [12]. Although the mathematical foundation of their novel application of the Rayleigh–Schrödinger perturbation theory was criticized [13, 14] and later reformulated in a more rigorous way [15], the original idea of using a numerical approach appears to be sound [12]. The algorithm presented here is based on the standard Rayleigh–Schrödinger perturbation theory, and differs from the one proposed in [12, 15].

Assuming that the eigenfunctions ψ and eigenvalues E of a Hamiltonian operator of the form $H = H_0 + gH_1$ can be formally expanded in the g-power series, $\psi = \sum_n g^n \psi_n$ and $E = \sum_n g^n E_n$, respectively, one obtains the corresponding coefficients ψ_n and E_n from the hierarchical equations

$$H_0 \psi_n + H_1 \psi_{n-1} = \sum_{p=0}^{n} E_p \psi_{n-p}. \tag{2}$$

The solution of this set of equations is facilitated by the arbitrary choice of the *normalization* $\langle \psi_0 | \psi \rangle = 1$, which leads to the *intermediate orthogonality condition* $\langle \psi_0 | \psi_n \rangle = \delta_{n0}$. As a result, the correction of order n to the energy is given by the projection of equation (2) on $\langle \psi_0 |$:

$$E_n = \langle \psi_0 | H_1 | \psi_{n-1} \rangle \tag{3}$$

and the corresponding correction to the eigenfunction follows from the linear inhomogeneous equation

$$(H_0 - E_0)\psi_n = -H_1 \psi_{n-1} + \sum_{p=1}^{n} E_p \psi_{n-p}. \tag{4}$$

Only the first step ($n = 0$) requires the solution of an eigenvalue equation: $(H_0 - E_0)\psi_0 = 0$.

In our specific problem the unperturbed Hamiltonian operator and the perturbation are respectively $H_0 = -D^2 + x^K$ and $H_1 = x^2$, where D is the derivative operator. Equations (3) and (4) become

$$E_n = \int_{-\infty}^{\infty} \psi_0(x) x^2 \psi_{n-1}(x) \mathrm{d}x \tag{5}$$

and

$$(-D^2 + x^{2N} - E_0)\psi_n(x) = -x^2 \psi_{n-1}(x) + \sum_{p=1}^{n} E_p \psi_{n-p}(x) \tag{6}$$

respectively, with the boundary conditions

$$\lim_{x \to \pm\infty} \psi_n(x) = 0. \tag{7}$$

A straightforward numerical calculation of the perturbation coefficients E_n and ψ_n rests upon the substitution of the approximate boundary conditions $\psi_n(\pm X) = 0$, with a sufficiently large value of X, for the exact ones equation (7). In addition, the second derivative operator D^2 is approximated by the centred second difference operator δ^2/h^2, where h is the constant integration step of a uniform mesh in $[-X, X]$. The differential equation is thus converted into a three-point recurrence relation, equivalent to a tridiagonal linear system of equations. The special case $n = 0$ reduces to the determination of the chosen eigenvalue and corresponding eigenvector of a tridiagonal symmetric matrix. Finally, we calculate the integral in equation (5) by means of the repeated trapezoidal rule. All these tasks are commonly described in detail in any textbook of numerical analysis†.

It should be mentioned that there are alternate numerical methods to determine the perturbation expansion. However, one should have in mind that three procedures are required: one to solve the eigenvalue equation for ϕ_0, another to compute the nth-order perturbative energy, equation (5) and finally another to integrate the chain of inhomogeneous differential equations (6) for a two-point boundary value problem. To be efficient and consistent one should use algorithms of the same quality, i.e. with equivalent leading-error terms. Moreover, since a given nth-order requires the use of the previous $0, 1, \ldots n - 1$ functions, all of them should be determined in the same mesh. Our choice has been to use the simpler $O(h^2)$ algorithm for all the three tasks, and afterwards to improve the quality of the results by a deferred limit to null step. Alternatively, one could have used high-order single-step integration methods both for the eigenvalue equation (Numerov and extended Numerov methods [16–18], exponential fitted methods [19, 20], etc) and for the inhomogeneous equation (mid-point and Runge–Kutta methods [21, 22]), as well as high-order quadrature rules, like the familiar Simpsom, Simpsom-3/8, Bode etc rules.

In what follows we enumerate some advantages of our apparently naive scheme.

• The tridiagonal matrix to be diagonalized gives rise to a Sturm sequence, so that one selects a specific unperturbed level by just counting the number of sign changes in the Sturm sequence.

• The contributions to the error in the approximate perturbation corrections to the energy and eigenfunction are proportional to *even* powers of the mesh size h.

• It is possible to carry out a *deferred limit* to $h = 0$, called also *Richardson extrapolation*, by appropriate combination of the results of calculations with different values of h.

• One may *estimate* the error of the results by comparing the last two extrapolations.

In the case of the anharmonic oscillators, the algorithm has proved to be economical and robust, applying successfully to anharmonicities as strong as x^{1000} without special care. The error in the perturbation corrections to the energy through order 80 is uniformly estimated to be less than one part in 10^8 at worst. Quite tractable integration grids with 500–8000 points were enough for such an accuracy.

The method satisfactorily passed two tests, one at each end of the anharmonicity interval $2 \leqslant K < \infty$, within machine precision. For $K = 2$ one obtains the exact perturbation corrections to the ground-state energy from the Taylor expansion of $\sqrt{1 + g}$. On the other hand, when $K \to \infty$ the model becomes a harmonic oscillator in a box with impenetrable walls at $x = \pm 1$. In the latter case we obtained the perturbation corrections to the energy analytically by means of the hypervirial perturbative method [24].

Just to give a flavour of the values of the perturbation corrections to the energy E_n we

† The actual FORTRAN code was based in a custom library, from [23]. The authors will supply a copy of the full FORTRAN code upon e-mail request.

Table 1. Selected coefficients of the strong coupling expansion for small values of K. The quantities within brackets denote powers of 10. The last digit of each entry is uncertain.

E_n	$K = 4$		$K = 6$		$K = 8$	
E_0	1.060 362 09046		1.144 802 45383		1.225 820 1136	
E_8	−1.887 720 1490	[−7]	6.322 514 3404	[−9]	7.529 426 3506	[−10]
E_{16}	−1.522 121 7804	[−13]	−4.503 200 921	[−18]	1.066 954 515	[−18]
E_{24}	1.041 782 2073	[−18]	−2.915 646 411	[−24]	2.248 546 450	[−27]
E_{32}	−3.404 029 0538	[−24]	−9.923 668 018	[−32]	5.124 372 181	[−36]
E_{40}	7.539 834 269	[−30]	−4.594 454 27	[−40]	1.082 376 476	[−44]

Table 2. Selected coefficients of the strong coupling expansion for large values of K. The quantities within brackets denote powers of 10. The last digit of each entry is uncertain.

E_n	$K = 500$		$K = 1000$		$K = \infty$	
E_0	2.400 235 383		2.433 556 881		2.467 401 100 26	
E_8	1.847 326 44	[−15]	1.502 201 54	[−15]	1.221 108 985	[−15]
E_{16}	−1.196 070 51	[−29]	−7.800 800 35	[−30]	−5.083 858 08	[−30]
E_{24}	−1.795 339 84	[−43]	−9.391 303 57	[−44]	−4.906 910 136	[−44]
E_{32}	−1.212 733 58	[−57]	−5.087 932 24	[−58]	−2.131 333 963	[−58]
E_{40}	1.280 738 7	[−72]	4.309 642	[−73]	1.447 370 88	[−73]

show some of them for the ground state of anharmonic oscillators with small values of K in table 1 and for large values of K in table 2. The last column of table 2 corresponds to the harmonic oscillator in a box described above.

The algorithm applies also to excited states. However, the accuracy of the perturbation corrections to the energy decreases with the quantum number, exactly in the same way as in the numerical calculation of energy eigenvalues.

There are many reasons for the recent interest in the strong coupling expansion for anharmonic oscillators [10, 11]. However, it appears that the fact that one can obtain the radius of convergence of the series from accurate enough coefficients of sufficiently large order has been overlooked. In fact, pairs of eigenvalues of the anharmonic oscillators cross at branch points in the complex g plane [1, 2], and the branch point closest to the origin determines the asymptotic behaviour of the perturbation coefficients with the perturbation order. It is therefore possible to estimate the location of the branch point closest to the origin by means of the perturbation corrections calculated in the way described above.

Shanley has given a detailed map with the branch points for the quartic anharmonic oscillator [4]. The same kind of calculation for the anharmonic oscillators with increasing values of K must be a formidable numerical task. However, if one is interested only in the branch-point closest to the origin, then the generating function method is a thoroughly practical approach [25].

The branch points appear in complex conjugate pairs because $E^*(g) = E(g^*)$. It is possible to estimate the location of the branch point closest to the origin by means of a generating function with the appropriate branch-point structure. For the present purposes it is enough to consider the simple ansatz

$$W(g) = C\sqrt{(g - g_R)^2 + g_I^2}. \tag{8}$$

The coefficients of the Taylor expansion of this function around $g = 0$ satisfy the recurrence

relation

$$(n-1)W_{n-1} + (1-2n)g_R W_n + (g_R^2 + g_I^2)(n+1)W_{n+1} = W_{n-1}. \qquad (9)$$

We derive a second independent equation by simply substituting $n+1$ for n in equation (9). A system of two equations with two unknowns, g_R and $g_R^2 + g_I^2$, results from later substitution of the actual coefficients E_n for W_n in the equations thus generated. Solving for the unknowns we obtain corresponding sequences that converge towards the real part and modulus of the pair of branch points closest to the origin.

We have tested the generating function method by means of independent results for three cases. For $K = 2$ we know that $g_R = -1$ and $g_I = 0$ exactly. For $K = 4$ we compared our results with those obtained by Shanley [4]. For $K = \infty$ we derived the secular equation for the anharmonic oscillator in the basis set of eigenfunctions of the particle in the box which implicitly determines either $E(g)$ or $g(E)$. The condition $\partial g / \partial E = 0$ yields the location of the branch points with increasing accuracy for increasing values of the dimension of the secular determinant. In all three cases the agreement was satisfactory.

The position of the pair of branch points closest to the origin as a function of K is shown in figure 1 for the ground state. The branch points move left in the complex g plane as K increases. Some selected values of K are indicated in the figure for clarity. The left-most point corresponds to $K = \infty$ and the right-most point (exactly on the real axis) to $K = 2$. The figure also includes *non-integer* anharmonicities, corresponding to terms $|x|^\nu$ in the unperturbed Hamiltonian, with $\nu = 2.5$, 3 and 3.5.

In conclusion, a straightforward numerical treatment proves to be suitable for the study of the strong coupling regime of anharmonic oscillators.
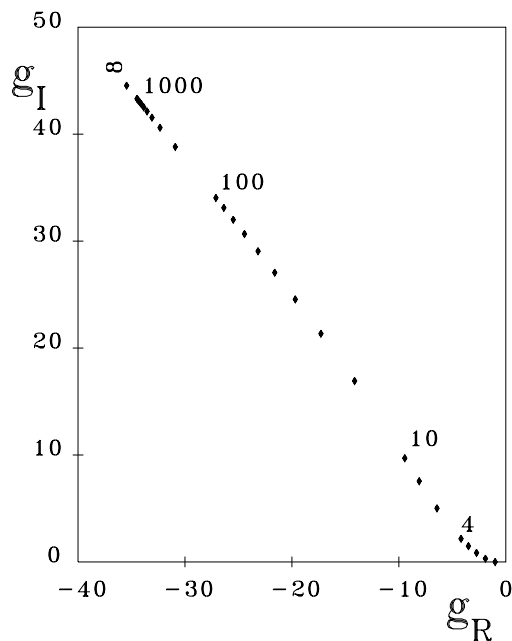

Figure 1. Position of the pair of branch points closest to the origin as a function of the oscillator anharmonicity K. Selected values of K are indicated above the corresponding points. The left-most point corresponds to $K = \infty$.

Acknowledgments

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