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Convergent perturbation theory for multi-dimensional anharmonic oscillators

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Abstract. In this paper we analyze the Rayleigh-Schrödinger perturbation theory (RSPT) for anharmonic oscillators. Reasons of the divergence of the standard RSPT expansion are described. Possible analysis of the multidimensional cases is suggested.

Introduction

It is known that many physical problems can be approximately modeled as (systems of) linear harmonic oscillators (LHO), E.g. in vibrational spectra analysis. However LHO approximation has often limited usability, because the system far from ground state has behavior significantly different from LHO. It is better to model such situations using some type of anharmonical oscillator(s) i.e. oscillators which potential is different from x^2. Instead of the functions describing known potentials, it is possible to substitute (sometimes conveniently truncated) Taylor series into the potential part of Hamiltonian. From this point of view, we wold like to solve the eigenproblem of the form

$$\left[-\frac{d^2}{dx^2}+x^2+\beta_1 x^3+\beta_2 x^4+\beta_3 x^5\ldots\right]\psi=E\psi. \tag{1}$$

Only few terms of the infinite series are often used to describe concrete physical potential. Because the behavior of this finite sum strongly depends on the term with the highest power, it is interesting to study the simplified problem

$$\left[-\frac{d^2}{dx^2}+x^2+\beta x^{2m}\right]\psi=E(\beta)\psi,\quad \beta\geq 0,\ m\geq 0 \tag{2}$$

If there is no coupling between parts describing single independent variables, this equation can be extended to multi-dimensional problems.

Usually, perturbation methods are based on introducing a small parameter β into this problem. The problem must be solvable for $\beta=0$. Solution of the original equation is then assumed in form of the power series in β. We will attempt to extend known methods to more dimensional problems, which are needed for the solution of more general physical problems.

In this paper, we will discuss the eigenproblem

$$\left[-\frac{d^2}{dx^2}+x^2+\beta x^4\right]\psi=E(\beta)\psi. \tag{3}$$

Studying this problem we can explain the most important general features of the perturbation series. It can also be extended to more dimensions and applied to E.g. molecular vibration analysis. We are going to describe here shortly some features of the perturbation expansions and an elegant method called renormalization.

Renormalization

It was shown in [*W. J. Weniger*, 1996], [*L. Skála, J. Čížek, E. J. Weniger*, 1997], [*L. Skála, J. Čížek, J. Zamastil*, 1999] that it is convenient to study the so-called renormalized model. Renormalization is in fact suitable scaling transformation, which changes behavior of the perturbation expansion to a more convenient case. We will use the transformation

$$x \to (1-\kappa)^{1/4} x \tag{4}$$

in the explored eigenproblem (3). After applying this substitution, Eq. (3) becames

$$\left[-\frac{d^2}{dx^2} + x^2 + \kappa\left(\frac{x^4}{3} - x^2\right)\right]\psi = (1-\kappa)^{1/2} E(\beta)\psi. \tag{5}$$

and the renormalized energy $E_R(\kappa)$ and the renormalized coupling constant κ can be introduced by relations

$$E_R(\kappa) = (1-\kappa)^{1/2} E(\beta)\,, \qquad \beta = \frac{\kappa}{3(1-\kappa)^{3/2}}\,. \tag{6}$$

Number "3" in the denominator is a result of physically based optimization of β vs. κ relation, and need not be discussed here.

The reformulated eigenvalue problem (5) has the following advantages in comparison with the original problem (3). First, the original unbounded interval of the coupling constant $\beta \in (0,\infty)$ is transformed onto the bounded interval $\kappa \in (0,1)$. Second, the original energy $E(\beta)$ goes to infinity for β going to infinity. In contrast to it, the renormalized energy $E_R(\kappa)$ remains finite at the point $\kappa = 1$ corresponding to the point $\beta = \infty$

$$E_R(\kappa \to 1) = (1-\kappa)^{1/2} E(\beta \to \infty) = (1-\kappa)^{1/2} K_0 \beta^{1/3} = K_0/3^{1/3}, \tag{7}$$

where K_0 is finite number.

Perturbation expansions

Usually two types of the perturbation series, called "*the strong coupling expansion*" and "*the weak coupling expansion*" are used.

Weak coupling

Expanding the energy $E_R(\kappa)$ into the power series in the coupling constant κ we get the so-called weak coupling expansion

$$E_R(\kappa) = \sum_{n=0}^{\infty} a_n \kappa^n \tag{8}$$

A bad feature of this expansion is that it diverges for an arbitrary value of the coupling constant $\kappa \in (0,1)$ and, consequently, $\beta \in (0,\infty)$. However, the expansion coefficients are relatively easy evaluable. In the table one can see some of the expansion coefficients.

n	a_n
1	-0.25000000000000
2	-0.02083333333333
3	0.01562500000000
5	0.06576425057870
10	-46.68774596378166
20	$-0.22202683909984\times10^{11}$
50	$-0.16582982439360\times10^{48}$

Table the of expansion coefficients a_n. We can see that this series diverges.

Strong coupling

Reordering Eq. (5) we can expand the energy $E_R(\kappa)$ into the power series in $1-\kappa$, and obtain the so-called strong coupling expansion

$$E_R(\kappa) = \sum_{n=0}^{\infty} \Gamma_n (1-\kappa)^n \qquad (9)$$

which converges for $|1-\kappa| < 1$. The expansion coefficients Γ_n cannot be calculated as easily as the a_n coeffitients. Some of them are displayed in the following table.

n	Γ_n
1	0.2770556728799470
2	-0.0111788972096450
3	-0.0004661493115821
5	-0.0001480652568073
10	$-0.8820357960483973\times10^{-5}$
20	$-0.1711400738708880\times10^{-6}$
50	$-0.7635552518836174\times10^{-10}$

Table of the expansion coefficients Γ_n. This series converges.

We will try to explain some reasons of the convergence of Eq. (9) and divergence of Eq. (8) in the following paragraph. There is a theory that clarifies why some expansions converge and others diverge. We will mention only a little part of them. Details can be found in [*C. M. Bender* -a, 1969], [*C. M. Bender* -b, 1973], [*T. Banks* -a,b, 1973], [*E. Vrscay*, 1989], [*B. Simon*, 1970] .

Reasons of convergence and divergence

Regular perturbation problem is a problem, whose perturbation series is a power series in perturbation parameter β having a non-vanishing radius of convergence. Singular perturbation problem is a problem, whose perturbation series does not have the form of a power series or, if it does, the power series has a zero radius of convergence. Unperturbed part in the singular perturbation theory may not have a solution, or when it exist, its qualitative features are distinctly different from those of the exact solution for arbitrary small, but nonzero β.

Large number of practically used perturbation series has characteristic behavior — truncated series tends first to the exact solution, but there exists a turning point from which the series begins to diverge.

Reason of divergence of the perturbation series of (2) was found by Bender, Wu and Simon [*C. M. Bender* -a, 1969], [*B. Simon*, 1970], [*C. M. Bender* -b, 1973]. They found that $E_R(\kappa)$ assumed as a function of complex parameter κ has a cut on the negative real axis. There are also other singularities in the complex κ plane, having effect on the non-vanishing radius of convergence.

We can see that Eq. (9) is a regular perturbation problem and Eq. (8) is a singular perturbation problem (see Fig. 1). Short look at this two expansions shows (see Fig. 1) that expansion (8) is expanded in the point 0, in contrast to it, expansion (9) is expanded at the point 1. We can see that the expansion at 0 has vanishing radius of convergence due to presence of the cut on the negative real axis. Hamiltonian $H_R = p^2 + x^2 + \kappa(x^4/3 - x^2)$ does not have bound states for $\kappa < 0$ and the energy $E_R(\kappa)$ is not analytic at the point $\kappa = 0$. Therefore, this expansions is not convergent Taylor series and diverges for arbitrary $\kappa \in (0, 1)$.

Expansion at the point 1 has radius of convergence 1. It follows from the analytic structure of $E_R(\kappa)$ that $E_R(\kappa)$ is analytic in the circle $|1-\kappa| < 1$ in the complex κ-plane. Therefore, the series $E_R(\kappa) = \sum_n \Gamma_n(1-\kappa)^n$ is a convergent Taylor series for all $|1-\kappa| < 1$. The hamiltonian $H_R = p^2 + x^4/3 + (1-\kappa)(x^2 - x^4/3)$ becomes for $1-\kappa < 0$ the hamiltonian of the double-well problem that has bound states and the energy $E_R(\kappa)$ is at the point $\kappa = 1$ analytic.

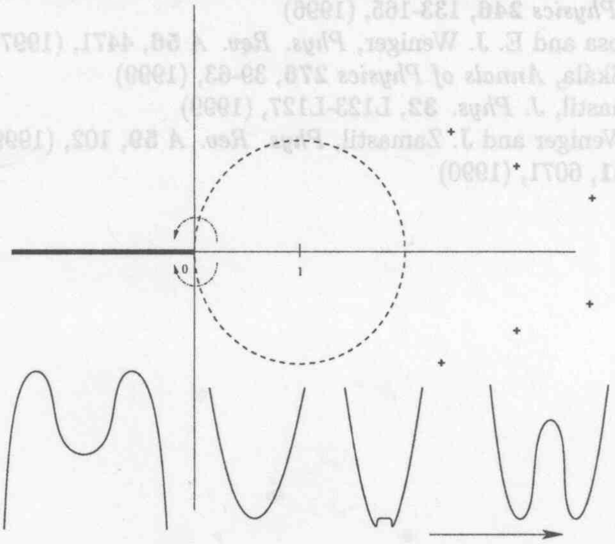

Figure 1. *Analytic structure of the energy plane E(κ). The dashed circle is the circle of convergence of perturbation series constructed at the point 1. The "+" marks are some poles. There is a cut on the negative real axis (thick line). The discontinuity of the energy on the negative real axis is twice the imaginary part of the energy. The imaginary part of the energy is related to the half-lifetime of the state. The curves at the bottom of the picture are qualitative plots of the potentials, depending on the value of the real part of the perturbation parameter. The right-arrow shows the character of the double-well with increasing the real part of the parameter κ.*

Conclusion

Multi-dimensional problems may be divided into three groups. The potentials of the first group doesn't contain any mixed terms i.e. terms containing more than one variable. In this case, the task may be easily separated into many one-dimensional problems the solution of which can be calculated separately.

The potentials of the second group contain mixed terms. They seems not to be convertible to previously mentioned group, general method of solution such eigenproblems is not known yet.

In the third case, these terms can be partially separated to a number of low-dimensional systems, whose dimension may exceed one. These systems can be partially separated and solved as above.

We hope that there is a perspective to extend the one-dimensional model to multidimensional ones. It was shown in [*W. Janke*, 1990] that the problem of the hydrogen atom in external magnetic field can be converted to the problem of the coupled harmonics oscillators. For this reason we started study the two-dimensional eigenproblem of the form

$$\left[p_x^2 + p_y^2 + x^2 + y^2 + \lambda(x^4 + y^4 + 2cx^2y^2)\right]\psi = E\psi \qquad (10)$$

which is usefull in the analysis of the Zeeman effect.

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