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ANALYTIC SOLUTION OF THE ONE-DIMENSIONAL SCHRÖDINGER EQUATION. SOME NEW RESULTS AND APPROACHES

Summary

A few different approaches suitable for obtaining analytic or at least partly analytic solutions of the Schrödinger equation are summarized and discussed.

Contents

1. Introduction

In this paper, we are interested in the analytic or at least partly analytic solutions of the one-dimensional Schrödinger equation

$$\left(-\frac{d^2}{dx^2}+V\right)\psi = E\psi \tag{1}$$

where $V(x)$ is a potential. We investigate bound states only.

We consider four different levels of solutions.

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•• Paper dedicated to Prof. Hans Müller on the occasion of his 65-th birthday.

- Both energies and wave functions are known analytically. It is the most favourable case.
- The Schrödinger equation is solvable analytically in the initial steps. In the last steps, however, a numerical solution of a finite order eigenvalue problem or a similar problem is necessary. Such solutions are called usually next to solvable or quasi exact solutions.
- Most of the steps of the solution are numerical. At the end, however, we may be able to perform, for example, asymptotical analysis of the perturbation coefficients which can yield further useful information.
- Only the numerical solution is possible.

In the rest of this paper, we discuss the first three cases only.

2. Analytical solutions

There are numerous approaches for obtaining analytic solutions of the Schrödinger equation (1) (see e.g. [1], [2]). In this paper, we use the approach described in [2]. Its advantage is considerable generality and possibility to introduce two generalizations discussed below.

In this approach, we write the wave function in the form

$$\psi = \sum_m c_m \psi_m , \tag{2}$$

where c_m are coefficients of the linear combination and the function ψ_m is assumed in the form

$$\psi_m = \left[f(x)\right]^m g(x) . \tag{3}$$

Here, $f(x)$ and $g(x)$ are functions examples of which are given below. An important step in our method is the assumption that we can express $H\psi_m$ as a finite linear combination

$$H\psi_m = \sum_n h_{mn} \psi_n , \tag{4}$$

where h_{mn} are numerical coefficients. Substituting Eqs. (2), (3) and (4) into the Schrödinger equation (1) we get a non-hermitian matrix eigenvalue problem

$$\sum_m c_m h_{mn} = E c_n . \tag{5}$$

If this eigenvalue problem is of the infinite order, its solution is difficult. However, for a finite eigenvalue problem, its analytical solution is in many cases possible. If necessary, we can solve this problem numerically and get quasi-exact solutions.

It can be shown [2] that this eigenvalue problem has especially simple structure if the potential V and the functions f and g obey the following equations

$$V(x) = \sum_i V_i \left[f(x)\right]^i , \tag{6}$$

$$df(x) \big/ dx = \sum f_i \left[f(x)\right]^i \tag{7}$$

and

$$dg(x) \big/ dx = -g(x) \sum g_i \left[f(x)\right]^i . \tag{8}$$

For this case, the explicit expression for the matrix h in terms of V_i, f_i and g_i is given in [2].

2.1. Standard approach

In this approach, we assume that the potential is 'quadratic'

$$V(x) = V_1 f(x) + V_2 \left[f(x)\right]^2 , \tag{9}$$

and the functions f and g obey the equations

$$df(x) \big/ dx = f_0 + f_1 f(x) + f_2 \left[f(x)\right]^2 \tag{10}$$

and

$$dg(x) \big/ dx = -g(x) \left\{ g_0 + g_1 f(x) + g_2 \left[f(x)\right]^2 \right\} . \tag{11}$$

It can be shown [2] that the potential coefficients can be arbitrary, i.e. to get analytic solutions no constraints on the potential coefficients need not be introduced.

To present some examples, we consider the equation

$$df / dx = 1 \tag{12}$$

which gives, except for a constant,

$$f(x) = x\,. \tag{13}$$

The corresponding potential

$$V(x) = V_0 + V_1 x + V_2 x^2 \tag{14}$$

leads to the harmonic oscillator as a special case.

Further examples include the Morse potential [3, 4] which can be obtained from the equations

$$df/dx = a - f\,, \tag{15}$$

$$f(x) = 1 - \exp(-x) \tag{16}$$

and

$$V(x) = V_0 + V_1[1 - \exp(-x)] + V_2[1 - \exp(-x)]^2\,, \tag{17}$$

the Kratzer potential [5, 4, 6] and the one-dimensional Coulomb potential which follow from

$$df/dx = (a - f)^2\,, \tag{18}$$

$$f(x) = a - 1/x \tag{19}$$

and

$$V(x) = V_0 + V_1[1 - 1/x] + V_2[1 - 1/x]^2\,. \tag{20}$$

The symmetric Pöschl-Teller potential [7], the Rosen-Morse potential [8], the Eckart potential [9], the Hulthen potential[10] and the Manning-Rosen potential [11] can be obtained from

$$df/dx = k(a \pm f)(b - f)\,, \tag{21}$$

$$f = \left[b \pm a\exp(\pm k(a-b)x)\right]/\left[1 \pm \exp(\pm k(a-b)x)\right] \tag{22}$$

and

$$V(x) = V_0 + V_1 f(x) + V_2 f(x)^2 \tag{23}$$

These examples of the well-known analytically solvable problems which are a special case of our approach indicate that our method can be generalized to further cases which may be of physical interest.

2.2. First generalization

In this approach we assume the same equation for the function $f(x)$ as in the standard approach

$$df(x)/dx = f_0 + f_1 f(x) + f_2[f(x)]^2\,, \tag{24}$$

however, we consider a higher order potential

$$V(x) = V_0 + V_1 f(x) + \ldots + V_{2M}[f(x)]^{2M}\,. \tag{25}$$

As examples, we consider the anharmonic oscillators

$$V(x) = V_0 + V_1 x + \ldots + V_{2M} x^{2M}\,. \tag{26}$$

To be more concrete, we assume the potential

$$V(x) = V_2 x^2 + V_4 x^4 + V_6 x^6 \tag{27}$$

leading to the analytical solution if

$$V_2 = V_4^2/(4V_6) - 3\sqrt{V_6}\,. \tag{28}$$

The ground state energy and wave function for this potential equal [2]

$$E = V_4/\left(2\sqrt{V_6}\right) \tag{29}$$

and

$$\psi(x) = \exp\left(-V_4 x^2/\left(4\sqrt{V_6}\right) - \sqrt{V_6}\,x^4/4\right). \tag{30}$$

The second example is the ground state of the generalized Morse potential

$$V(x) = V_1[1 - \exp(-x)] + \ldots + V_4[1 - \exp(-x)]^4\,. \tag{31}$$

Introducing

$$g_2 = -\sqrt{V_4}\,,\ g_1 = V_3/(2g_2)\,,\ g_0 = \left(V_2 - g_1^2\right)/(2g_2) - 1\,, \tag{32}$$

the potential constraint can be written as

$$V_1 = 2g_1g_0 - 2g_2 + g_1 . \tag{33}$$

The ground state energy and wave function equal [2]

$$E = g_1 - g_0^2 \tag{34}$$

and

$$\psi(x) = \exp\{-g_0x - g_1[x + \exp(-x)] - g_2[x + 2\exp(-x) - \exp(-2x)/2]\} . \tag{35}$$

2.3. Second generalization

We can consider also a higher order equation for the function $f(x)$

$$df(x)/dx = f_0 + f_1f(x) + ... + f_N[f(x)]^N . \tag{36}$$

For example, the equation

$$df/dx = (-1)^{k+1}(a-f)^k \tag{37}$$

with the solution

$$f(x) = a + [(k-1)x]^{1/(k-1)} \tag{38}$$

leads to the potentials with fractional powers. A similar case is obtained from

$$df/dx = 1/f^k \tag{39}$$

with the solution

$$f(x) = (-1)^k[(k+1)x]^{1/(k+1)} \tag{40}$$

Another example of the equation for $f(x)$ which can be solved in the implicit form is

$$df/dx = 1 \pm f^N \tag{41}$$

The corresponding function $f(x)$ is more complex than in the preceding cases.

These examples show that also the second generalization can lead to problems which are of physical interest.

2.4. General case

In this case, we consider a general equation for $f(x)$

$$df(x)/dx = f_0 + f_1f(x) + ... + f_N[f(x)]^N \tag{42}$$

and a general form of the potential

$$V(x) = V_0 + V_1f(x) + ... + V_{2M}[f(x)]^{2M} . \tag{43}$$

It is obvious that there are many cases in which also the general case may be solved analytically or at least partly analytically. It appears, however, that the number of the potential constraints equals $M-1$ and that, in general, the potential constraints are different for different states. Thus, different analytic states correspond usually to different potentials. The only exception is $M = 1$ case when there are no potential constraints and all analytic solutions correspond to the same potential [2, 12].

The eigenvalue problem (5) depends parametrically on f_i, g_i and V_i and its solution is in general difficult. For this reason, it is usually easy to find the ground state or low excited states analytically. Higher order states, however, can be often found only via a numerical solution of Eq. (5). In such a case, only quasi exact solutions can be found.

3. Perturbation theory for anharmonic oscillators

In this Section, we investigate the anharmonic oscillator with the quartic term in the hamiltonian

$$H = -d^2/dx^2 + x^2 + \beta x^4 , \tag{44}$$

where $\beta > 0$. It is well-known that the analytical solutions of the Schrödinger equation for this hamiltonian do not exist [13].

The weak coupling perturbation series in β

$$E(\beta) = \sum_{n=0}^{\infty} b_n\beta^n \tag{45}$$

diverges for any β. The strong coupling series

$$E(\beta) = \beta^{1/3}\sum_{n=0}^{\infty} K_n\beta^{-2n/3} \tag{46}$$

is convergent for large β only.

After the renormalization

$$\beta = \frac{1-\tau^2}{3\tau^3} \tag{47}$$

the weak coupling series

$$E(\beta) = \frac{1}{r}\sum_{n=0}^{\infty} c_n (1-\tau)^n \tag{48}$$

diverges similarly to Eq. (45). In contrast to it, the renormalized strong coupling series

$$E(\beta) = \frac{1}{\tau}\sum_{n=0}^{\infty} \Gamma_n \tau^{2n} \tag{49}$$

converges for all τ or β [13]. In [13], we calculated 200 perturbation coefficients Γ_n numerically. From this information, we suggested the large order formula for Γ_n

$$\Gamma_n = -\frac{12^K 4\sqrt{6}}{K!\pi e^2}(2n)^{(K-1)/2}\exp\left(-2\sqrt{2n}\right), \tag{50}$$

where $K = 0, 1, 2, \ldots$ denotes the ground and excited states.

This formula is an example of the problem when the exact solution of the problem is not known, however, the knowledge of numerical values of the first perturbation coefficients together with their analytical large order behavior makes possible to calculate the energy $E(\beta)$ for any value of the coupling parameter β with very high accuracy.

References

[1] A.G. Ushveridze, *Quasi-Exactly Solvable Models in Quantum Mechanics*, Institute of Physics Publishing, Bristol 1994

[2] L. Skála, J. Dvořák, J. Čížek, V. Špirko, Phys. Rev. **A53** (1996) 2009

[3] P. M. Morse, Phys. Rev. **34** (1929) 57

[4] S. Flügge, *Rechenmethoden der Quantentheorie dargestelt in Aufgaben und Lösungen*, Springer, Berlin 1947

[5] A. Kratzer, Zs. Phys. **3** (1920) 289

[6] J. Dvořák, L. Skála, Bulletin de la Société des Sciences et des Lettres de Łódź **46** (1996) 11

[7] G. Pöschl, E. Teller, Z. Phys. **83** (1933) 1439

[8] N. Rosen, P.M. Morse, Phys. Rev. **42** (1932) 210

[9] C. Eckart, Phys. Rev. **35** (1930) 1303

[10] L. Hulthen, Arkiv math. Astron. Fys. **28A** (1942) 5; **29B** (1942) 1

[11] M.F. Manning, N. Rosen, Phys. Rev. **44** (1933) 953

[12] L. Skála, J. Dvořák, V. Kapsa, Int. J. Theor. Phys. **36** (1997) 2953

[13] L. Skála, J. Čížek, V. Kapsa, E.J. Weniger, Phys. Rev. **A 56** (1997) 4471

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ANALITYCZNE ROZWIĄZANIA JEDNOWYMIAROWEGO RÓWNANIA SCHRÖDINGERA. NIEKTÓRE NOWE PODEJŚCIA I WYNIKI

Streszczenie

W pracy dyskutuje się kilka różnych wygodnych metod otrzymywania analitycznych lub prawie analitycznych rozwiązań równania Schrödigera.