

Chapter 1

Capabilities of Approximate Methods in Quantum Theory

The majority of physical phenomena in condensed matter, atomic and molecular systems is defined by electromagnetic interactions and governed by quantum mechanics laws. The systems possess an entirely defined Hamiltonian and the physical properties are described by the corresponding solutions of Schrödinger equation. The quantum description has an universal character, which assumes the wave functions of complex systems are the solutions of the linear equations, which have similar mathematical structure for the physical systems with essentially different physical properties. The mathematics plays a special role in a quantum mechanics [1], and any new method for the solution of Schrödinger equation results in essential progress in the description of numerous physical systems.

For the most of the problems in a quantum theory of many-body systems, the numerical solution of Schrödinger equation using a finite-element approximation for differential operators is ineffective, even by using modern powerful computers, because of the complexity of algorithms and large volume of processed information. The use of the functional integrals for quantum theory [2] faces a similar difficulty. Therefore, the development of new methods for approximate description of quantum systems plays a crucial role for both analytical investigations and design of the algorithms for numerical calculation of physical properties of the objects.

In the Chap. 1, we discuss the general criteria for the effectiveness of the approximate methods (AM), and make an assessment of most frequently used AMs in quantum theory. In this monograph, we apply exclusively the operator (Schrödinger's) formulation of quantum mechanics, and do not discuss the approximate methods for quantum theory in the form of Feynman's functional path integrals [2]. The analytical and approximate methods in the latter form have been widely presented in numerous monographs (for example, [3] and references therein). However, it is worth to mention that the non-perturbative investigations in both forms of quantum mechanics are pretty similar.

1.1 Effectiveness Criteria for Approximate Methods

The criteria for mathematical methods to be effective listed below have rather subjective nature, however, they are nevertheless important for the assessment of general effectiveness. To our opinion, they are:

- **universality**,

meaning the representation of the calculus scheme in a form, which is not related to the specific features of the physical problem. However, there is no universal method exists which delivers exact solution of Schrödinger equation for the system with an arbitrary Hamiltonian. Instead of, the method should include an iteration algorithm, which establishes the procedure for the successive approximations. Therefore, the following criteria have to be added:

- **high accuracy of the zeroth approximation**,

which has to describe correctly the most principal properties of the physical system, and

- **uniform convergence of successive approximations**, for calculation of the solution with any required accuracy. For practical applications, the following criterion is important:
- **simple enough algorithm for calculation of zeroth and successive approximations**, to be applicable for the systems with a large number of the degrees of freedom.

The detailed assessment of widely used AMs based on the above-mentioned criteria will be given in the following sections. The perturbation theory (PT) and its modifications (for example, [4, 5] and citations therein) seems to possess a highest universality in the sense of criteria listed above. The PT series can be constructed by the extraction of the operator \hat{H}_0 from the entire Hamiltonian \hat{H} , which has the known spectrum of eigenvalues (EV) and eigenfunctions (EF), and the operator of perturbation \hat{V} , both satisfying the condition $\hat{H} = \hat{H}_0 + \lambda \hat{V}$. The dimensionless parameter $\lambda \ll 1$ defines the characteristic value of the perturbation amplitude in relation with the distance between the energetic levels of the non-perturbed system with Hamiltonian \hat{H}_0 . Following a simple receipt, formally *applicable to arbitrary quantum system*, the series over the parameter λ for both EV and EF can be constructed. However, for the majority of physical systems, the series over λ , obtained on the basis of canonic form of PT, have an asymptotic nature. These series [5] are divergent and *do not permit to find a solution of Schrödinger equation* by a simple summation of the terms of series. Therefore, the quantitative description of the physical systems using PT is only possible in narrow diapason of small values of the parameter λ and for low energies of excitation.

All aforesaid is also true for the limit of strong coupling ($\lambda \gg 1$), where a small parameter is λ^{-1} [6], and for the quasi-classic approximation (with Planck constant \hbar as a small parameter), and for various modifications of adiabatic expansion,

where a small parameter is placed in a front of the operator of kinetic energy [7]. The asymptotic character of the expansions is manifested in the fact, that two-sided approximations being constructed for the same system, for instance, using parameters λ and λ^{-1} , result in a different functional dependence of EV on Hamiltonian parameters, which does not permit the continuous transition from one series to another. Thus, using the PT in real applications, the important property of *universality is lost*, because of the focus is switched from the mathematical procedure for construction of successive approximations to the deep understanding of the physics of processes, taking into account the qualitative characteristics of physical systems in operator \hat{H}_0 . This behavior is well described by the statement after L.Landau “There is no physical theory without a small parameter”.

The modern theoretical physics deals with the problems, the majority of which do not allow to select a small parameter having a certain physical sense. On the contrary, there are many problems exist where all parameters of Hamiltonian are varied in a wide range. Therefore, the development of the methods, which are able to build *a theory of quantum system without a small parameter*, or so called non-perturbative methods, is an actual trend of modern theoretical physics. For certainty, we mean here the avoidance of small parameters in the Hamiltonian of the system. At the same time, this does not exclude the use of supplementary or artificially introduced parameters in non-perturbative methods, which govern the accuracy of the numerical calculations.

There are also many methods exist, which investigate quantum systems without introduction of a physical small parameter (see, for example, [8–11] and citations therein). In a first turn, the direct numerical integration of Schrödinger equation using expansion over the artificially introduced parameter, for instance, the step of the finite-element approximation of derivatives, is an example of non-perturbative method. Another example is a lattice model of the quantum field theory, where the non-physical parameter is a lattice constant, which defines the accuracy of calculation of functional integrals for the transition from integration to summation [3]. The drawbacks of direct numerical methods are the exponential growth of the calculation volume and the loss of the algorithm stability when the dimension of the system s increases, for example, at $s \geq 3$ their effectiveness is already essentially low.

There are more examples of non-perturbative methods having a physical nature: variational principle, Hartree–Fock method for multi-electron atoms, approximating Hamiltonian method, etc. In the most cases, these methods deliver an approximate estimate for the energy of ground state and *are not capable to calculate the entire energy spectrum of the system with a required precision*.

In the majority of applications, the divergence of PT series is not related to the real properties of the physical system, but just points to necessary rearrangement of the received expansion over the Hamiltonian parameter to provide the analytical extension of EV and EF outside of the convergence region of the initial series. This task is partly solved by the summation methods for asymptotic series [12] and various modifications of Pade-approximation [13]. However, all these methods are

not really universal in the sense mentioned above, and cannot be generalized for the systems with the multiple degrees of freedom.

For quantitative characterization of the effectiveness and the accuracy of non-perturbative methods, the supplementary definitions have been introduced [14]. Let us assume that some characteristics of the quantum system is described by the function $F_n(\lambda)$, which depends on the quantum number n (quantum number set) of the state and on the parameter λ (parameter set), defining the perturbation amplitude in the system. We assume further that the non-perturbative method delivers both zeroth $F_n^{(0)}(\lambda)$ and successive $F_n^{(s)}(\lambda)$, $s = 0, 1, 2, \dots$ approximations for the function in question. Then these functions yield a *uniformly available approximation (UAA)* for the physical system, provided the following conditions are fulfilled for the entire range of parameter λ and for all quantum numbers n :

$$\left| \frac{F_n^{(s)}(\lambda) - F_n(\lambda)}{F_n(\lambda)} \right| \leq \xi^{(s)}, \quad (1.1)$$

where each parameter $\xi^{(s)} < 1$ is independent on n and λ and defines the accuracy of the approximation. The condition of the *convergence of non-perturbative method* corresponds to decreasing sequence of parameters $\xi^{(s)}$:

$$\lim_{s \rightarrow \infty} F_n^{(s)}(\lambda) = F_n(\lambda). \quad (1.2)$$

The asymptotic series obtained from PT are obviously not satisfying the conditions (1.1) and (1.2), because of they approximate the function in question in a narrow range of n, λ and are not convergent. At the same time, the two-side asymptotic expansions, corresponding to limits $\lambda \ll 1$ and $\lambda \gg 1$, allow to control the conditions of UAA for various non-perturbative methods [14]. In contrast to the asymptotic expansions, the UAA approximates the value with high relative accuracy $\xi^{(s)}$ in the entire range of the variation of physical parameters and quantum numbers of states. Thus, the effectiveness of the non-perturbative method can be quantitatively estimated from the infinitesimality of $\xi^{(s)}$ in primary approximations and the speed of their decay with the increase of s .

In this short introductory chapter dedicated to non-perturbative methods for quantum systems, we illuminate the techniques, which are to some extent related to the approach taking a central place in this monograph: operator method (OM). First of all, one of this techniques is a non-perturbative method utilizing the self-similar approximation for calculation of the dependence of system characteristics on the parameters of Hamiltonian. The basic ideas of this approach have been published for the first time in [15], and later it has been successfully applied to numerous problems of quantum mechanics and field theory (see, for instance, the review [16] and citations therein).

The non-perturbative method for calculation of functional integrals for the systems with a non-linear operation (see, for example, [17] and citations therein) has been used in the theory of strong interaction. The scheme of non-linear scaling of coupling constant in quantum chromodynamics makes possible the calculation of the processes in the range of energy variables, where the standard form of PT fails. The application area for this approach can be essentially extended, if the method is generalized for the theory of condensed matter and quantum mechanics of multiple-particle systems.

The method presented in this monograph is a kind of universal algorithm for rearrangement of PT series and it satisfies all the requirements for non-perturbative techniques listed above. This method is named an operator method in the sense that both for zeroth approximation and for high-order approximations there is no necessity to solve differential or integral equations: all calculations are reduced to the algebraic calculus with matrix elements of operators. In the book, we illustrate the application of OM to the description of various quantum systems, including the systems with infinite number of the degrees of freedom. The results demonstrate that already zeroth approximation gives a uniformly available approximation for EV and EF of Schrödinger equation at arbitrary values of Hamiltonian parameters, and the successive approximations converge to the exact solution for all values of quantum numbers of the system and for the entire range of parameters. The algebraic nature of calculations simplifies the development of the algorithms to obtain the higher approximations for the systems with a large number of the degrees of freedom, and to find the eigenvalues and eigenfunctions with a high accuracy.

A special attention is paid to the generalization of operator method for the quantum statistics. In this case, the physical system obtains one additional parameter: a temperature. In comparison with the description of pure quantum states, the calculation of the observed values in statistics involves a complex procedure of summation over all states of the system. Thus, the operator method for calculation of EV and EF is supplemented by the algorithm for the summation over the quantum states. This approach permits to calculate thermodynamical characteristics of physical systems in a wide range of temperature and is effective for the systems with the multiple degrees of freedom.

Prior the start of the detailed description of operator method in Chap. 2, we remind in current chapter the basic relationships from other recognized methods used for approximate evaluation of quantum systems. Their ability and limitations will be demonstrated by applying them to the model systems: the quantum anharmonic oscillator (QAO) and the coupled anharmonic oscillator (CAO), which both are widely used for approval of approximate methods in quantum [18, 19] as well as in classic [20] theories. The analysis of these problems shed the light on the difficulties of approximate methods, which are successfully overcome by the operator method.

1.2 Perturbation Theory for Solution of Stationary Schrödinger Equation

In 1939 Paul Dirac [21] introduced the notations and terminology, which are perfectly fitting the representation of perturbation theory in algebraic form. The state of the quantum system in arbitrary representation [22] is given by ket-vector $|\Psi_n\rangle$, where index n defines the set of quantum numbers corresponding to this state. In general case, these numbers may have both discrete (discrete spectrum) and continuous (continuous spectrum) values. The bra-vector $\langle\Psi_n|$ corresponds to Hermitian conjugate vector of the state. The wave function is determined by the projections of the state vector onto the axes of Hilbert space [22], which corresponds to this representation. For example, for wave functions in coordinate representation:

$$\Psi_n(x) \equiv \langle x|\Psi_n\rangle; \Psi_n^*(x) \equiv \langle\Psi_n|x\rangle; \int dx \Psi_m^*(x) \Psi_n(x) \equiv \langle\Psi_m|\Psi_n\rangle. \quad (1.3)$$

In these notations, the stationary Schrödinger equation for eigenvalues $E_n(\lambda)$, complete Hamiltonian and normalized eigenfunction $|\Psi_n\rangle$ take the following form:

$$\hat{H}|\Psi_n\rangle = E_n(\lambda)|\Psi_n\rangle, \quad \hat{H} = \hat{H}_0 + \lambda \hat{V}; \quad \langle\Psi_n|\Psi_n\rangle = 1. \quad (1.4)$$

For the unperturbed system:

$$\hat{H}_0|\psi_n\rangle = \epsilon_n|\psi_n\rangle, \quad \langle\psi_n|\psi_n\rangle = 1. \quad (1.5)$$

where \hat{H}_0 is a Hamiltonian of zeroth approximation, for which a complete set of eigenvalues ϵ_n and eigenfunctions $|\psi_n\rangle$ of the solutions of Eq. (1.5) is known. We assume that the ratio of the matrix elements of perturbation operator $\lambda \hat{V}$ to the difference between energy levels of non-perturbed system has an amplitude determined by the dimensionless physical parameter λ .

The state vector $|\Psi_n\rangle$ can be expanded into full set $|\psi_m\rangle$:

$$|\Psi_n\rangle = \sum_{m=0}^{\infty} C_{nm} |\psi_m\rangle, \quad (1.6)$$

and after substitution it into (1.5), we find an exact system of equations for the coefficients C_{nm} [4]:

$$(E_n - \epsilon_k) C_{nk} = \lambda \sum_m V_{km} C_{nm}; \quad V_{km} = \langle\psi_k|\hat{V}|\psi_m\rangle, \quad (1.7)$$

which include matrix elements V_{km} of the perturbation operator.

Formally the perturbation theory corresponds to the expansion of values in question into series over the λ :

$$\begin{aligned} C_{nk} &= C_{nk}^{(0)} + \lambda C_{nk}^{(1)} + \lambda^2 C_{nk}^{(2)} + \dots; \\ E_n(\lambda) &= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots \end{aligned} \quad (1.8)$$

There are two ways to obtain this expansion: the algorithm of Rayleigh-Schrödinger for perturbation theory (RSPT) [23, 24] and the method of Brillouin-Wigner for perturbation theory (BWPT) [25, 26]. They differ each from the other by the normalization of the state vector. In case of RSPT, the corrections for the coefficient $C_{nm}^{(l)}$ in each approximation order are selected from the condition for normalization $\langle \Psi_n | \Psi_n \rangle = 1$ to be satisfied with the accuracy up to the terms of the order λ^l . Assuming all the eigenvalues of Hamiltonian \hat{H}_0 are non-degenerate ($\epsilon_m \neq \epsilon_n$ for all $m \neq n$), we obtain [4]:

$$\begin{aligned} E_n(\lambda) &= \epsilon_n + \lambda V_{nn} - \lambda^2 \sum_{m \neq n} \frac{|V_{mn}|^2}{\epsilon_m - \epsilon_n} + \dots, \\ |\Psi_n\rangle &= |\psi_n\rangle - \lambda \sum_{m \neq n} \frac{V_{mn}}{\epsilon_m - \epsilon_n} |\psi_m\rangle + \lambda^2 \left[\sum_{m \neq n} \sum_{k \neq n} \frac{V_{mk}}{(\epsilon_m - \epsilon_n)} \frac{V_{kn}}{(\epsilon_k - \epsilon_n)} |\psi_m\rangle - \right. \\ &\quad \left. - \sum_{m \neq n} \frac{V_{nn} V_{mn}}{(\epsilon_m - \epsilon_n)^2} |\psi_m\rangle - \sum_{m \neq n} \frac{|V_{mn}|^2}{2(\epsilon_m - \epsilon_n)^2} |\psi_n\rangle \right] + \dots \end{aligned} \quad (1.9)$$

In the case of degeneration of the states of unperturbed Hamiltonian, each energy level ϵ_n has a corresponding set of the distinguished vectors:

$$|\psi_n 1\rangle; |\psi_n 2\rangle; \dots |\psi_n s_n\rangle, \quad (1.10)$$

where s_n is a multiplicity of degeneration. In this case, to obtain the RSPT series, a new set of states for zeroth approximation has to be constructed [4]:

$$|\psi_n^\sigma\rangle = \sum_{s=1}^{s_n} c_s^\sigma |\psi_n s\rangle; \quad \sigma = 1, 2, \dots s_n. \quad (1.11)$$

Here the coefficients c_s^σ and new eigenvalues ϵ_n^σ are calculated from the solution of the system of linear equations:

$$(\epsilon_n^\sigma - \epsilon_n) c_s^\sigma = \lambda \sum_{s'} V_{ss'}^{(n)} c_{s'}^\sigma; \quad V_{ss'}^{(n)} = \langle \psi_n s' | \hat{V} | \psi_n s \rangle; \quad \langle \psi_n^{\sigma'} | \psi_n^\sigma \rangle = \delta_{\sigma\sigma'}. \quad (1.12)$$

This additional operation does not influence the convergence and the general form of the series RSPT, if the set of indices n, σ is included in the definition of quantum number n .

If the BWPT form of the expansion over the parameter λ is used, the following fact is exploited: due to the linearity of Schrödinger equation (1.4) the solutions are defined with the accuracy of constant, and therefore the normalization vector can be found by applying the alternative normalization condition:

$$\begin{aligned}\hat{H}|\tilde{\Psi}_n\rangle &= E_n(\lambda)|\tilde{\Psi}_n\rangle, \\ \langle\psi_n|\tilde{\Psi}_n\rangle &= 1; |\Psi_n\rangle = A|\tilde{\Psi}_n\rangle; A^2 = [\langle\tilde{\Psi}_n|\tilde{\Psi}_n\rangle]^{-1}.\end{aligned}\quad (1.13)$$

As a result, the system of equations for coefficients of the expansion of state vector is found:

$$\begin{aligned}|\tilde{\Psi}_n\rangle &= |\psi_n\rangle + \sum_{k \neq n} \tilde{C}_{nk} |\psi_k\rangle, \\ E_n &= \epsilon_n + \lambda V_{nn} + \lambda \sum_{k \neq n} \tilde{C}_{nk} V_{nk}; \\ \tilde{C}_{nk} &= \frac{\lambda}{E_n - \epsilon_k} \left[V_{kn} + \sum_{m \neq n} \tilde{C}_{nm} V_{mk} \right]; \quad k \neq n.\end{aligned}\quad (1.14)$$

The successive approximations of the BWPT series are found by iterating the last equation in the expression (1.14):

$$\begin{aligned}\tilde{C}_{nk}^{(0)} &= 0; \quad \tilde{C}_{nk}^{(1)} = \frac{\lambda V_{kn}}{E_n - \epsilon_k}; \\ \tilde{C}_{nk}^{(2)} &= \frac{\lambda}{E_n - \epsilon_k} \left[V_{kn} + \lambda \sum_{m \neq n} \frac{V_{nm} V_{mk}}{E_n - \epsilon_m} \right]; \dots,\end{aligned}\quad (1.15)$$

and the energy levels for each approximation are found as the solutions of transcend equation. For example, in the second order BWPT this equation has a form:

$$E_n = \epsilon_n + \lambda V_{nn} + \lambda^2 \sum_{k \neq n} \frac{V_{nk} V_{kn}}{E_n - \epsilon_k}.\quad (1.16)$$

The expansion (1.14) is generalized for the case of degenerate states using the substitution of $|\psi_n\rangle, \epsilon_n$ by the states $|\psi_n^\sigma\rangle, \epsilon_n^\sigma$ in zeroth approximation. Thus, the formulas (1.9) and (1.14) define the *universal* method for calculation of eigenvalues

and eigenfunctions as a series over the ratio of matrix elements of perturbation operator to the distance between the energy levels of the zeroth approximation:

$$\xi_n = \sum_{k \neq n} \frac{\lambda V_{kn}}{\epsilon_n - \epsilon_k}. \quad (1.17)$$

However, these series allow to calculate eigenvalues and eigenfunctions within a limited range of the parameters of perturbation operator even for simple physical systems. As an example, we consider here one-dimensional QAO, which is often used for approbation of the solution of Schroödinger equation or as a basic model in the field theory with non-quadratic Hamiltonian [18]. The problem is reduced to the solution of the following equation (further we use the units system with Planck constant \hbar and particle mass m both equal unity) [19]:

$$\begin{aligned} \hat{H}|\Psi_n\rangle &= E_n(\lambda)|\Psi_n\rangle, \\ \hat{H} &= \frac{1}{2}(\hat{p}^2 + x^2) + \mu x^2 + \lambda x^4; \quad \hat{p} = -i \frac{d}{dx}. \end{aligned} \quad (1.18)$$

We start with the consideration of the case with $\lambda = 0$, which gives a good illustration of several obstacles in the canonic perturbation theory [27]. The perturbation operator is chosen as:

$$\hat{H}_0 = \frac{1}{2}(\hat{p}^2 + x^2); \quad \hat{V} = \mu x^2; \quad \mu > -\frac{1}{2}. \quad (1.19)$$

Here we use the algebraic calculations in the particle number representation [4], which is based on the canonic transformation to the creation and annihilation operators for unperturbed oscillator:

$$\begin{aligned} \hat{x} &= \frac{1}{\sqrt{2}} [\hat{a} + \hat{a}^+], \\ \hat{p} &= i \frac{1}{\sqrt{2}} [\hat{a}^+ - \hat{a}], \end{aligned} \quad (1.20)$$

The operators of annihilation \hat{a} and creation \hat{a}^+ satisfy to the permutation relation:

$$[\hat{a}, \hat{a}^+] = 1. \quad (1.21)$$

In this representation the operators \hat{H}_0 and \hat{V} have the following form:

$$\hat{H}_0 = \frac{1}{2} [1 + 2\hat{a}^+ \hat{a}], \quad (1.22)$$

$$\hat{V} = \frac{\mu}{2} [1 + 2\hat{a}^+ \hat{a} + (\hat{a}^+)^2 + (\hat{a})^2]. \quad (1.23)$$

The eigenfunctions for unperturbed oscillator in this representation coincide with the eigenvectors of the operator of the excitation numbers \hat{n} :

$$\begin{aligned} |n\rangle &= \frac{1}{\sqrt{n!}} [\hat{a}^+]^n |0\rangle, \quad n = 0, 1, 2, 3, \dots, \\ \hat{n} &= \hat{a}^+ \hat{a}, \quad \hat{n} |n\rangle = n |n\rangle, \\ \hat{a} |n\rangle &= \sqrt{n} |n-1\rangle, \quad \hat{a}^+ |n\rangle = \sqrt{n+1} |n+1\rangle, \end{aligned} \quad (1.24)$$

and the ground state of unperturbed system follows from the expression:

$$\hat{a} |0\rangle = 0. \quad (1.25)$$

Thus, the zeroth approximation for eigenvalues and eigenfunctions in the Eq. (1.19) is given by:

$$E_n^{(0)} = \frac{1}{2}(2n+1), \quad |\Psi_n^{(0)}\rangle = |n\rangle. \quad (1.26)$$

Using the algebra (1.21) for the creation and annihilation operators, the first terms of the series over the operator \hat{V} can be found from the formula (1.9):

$$E_n^{(1)} = \langle n | \hat{V} | n \rangle = \frac{\mu}{2}(2n+1), \quad (1.27)$$

$$E_n^{(2)} = -\frac{|\langle n+2 | \hat{V} | n \rangle|^2}{E_{n+2}^{(0)} - E_n^{(0)}} = -\frac{\mu^2}{8}(n+1)(n+2), \quad (1.28)$$

and in a similar way for further terms. As follows from the expression (1.27), even for the ground state with $n = 0$ the series of the perturbation theory converges only in the domain $|\mu| < \frac{1}{2}$. At the same time, the operator (1.19) is evidently a Hamiltonian of the harmonic oscillator with frequency:

$$\omega(\mu) = \sqrt{1+2\mu}, \quad (1.29)$$

with known set of eigenfunctions and exact spectrum of eigenvalues:

$$E_n = \omega(\mu) \left(n + \frac{1}{2} \right) = \left(n + \frac{1}{2} \right) \sqrt{1+2\mu}. \quad (1.30)$$

The eigenvalues (1.30), considered as the functions of parameter μ , have a singularity at $\mu = -\frac{1}{2}$, because of at $\mu < -\frac{1}{2}$ the Hamiltonian (1.19) does not possess a discrete spectrum. In general, the convergence radius of the power series

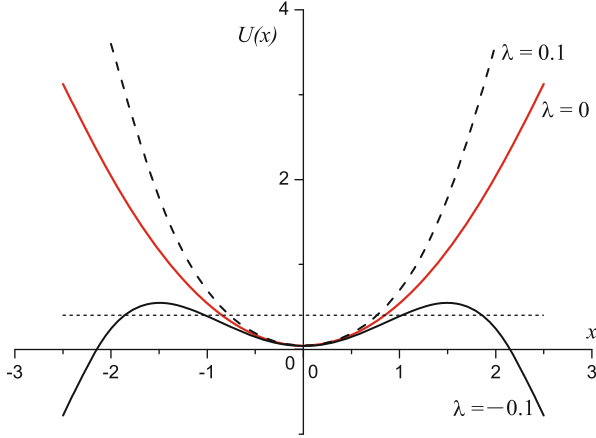


Fig. 1.1 The potential energy of anharmonic oscillator for different values of λ

is determined by the distance to the nearest singular point in complex plane μ [5], that limits the convergence of PT series to the values of perturbation parameter in interval $|\mu| < \frac{1}{2}$. However, from (1.29) follows that all the values of the parameter are permissible in the interval $(-\frac{1}{2}; \infty)$. Thus, even in this simple situation the calculation of EV spectrum for the entire range of Hamiltonian parameter requires an essential reconstruction of PT series. For the operator (1.18) with $\mu = 0$, $\lambda \neq 0$ the situation becomes even more complicated:

$$\hat{H}_0 = \frac{1}{2}(\hat{p}^2 + x^2); \quad \hat{V} = \lambda x^4. \quad (1.31)$$

The potential energy $U(x) = x^2/2 + \lambda x^4$ at various λ for the oscillator is shown in Fig. 1.1. At the values $\lambda < 0$, the motion of particle in this potential becomes infinite due to the subbarrier tunneling. That means the system has not discrete spectrum at infinitesimal negative λ and the functions $E_n(\lambda)$ have a singularity at $\lambda = 0$. In this case, the power series over this parameter have a zeroth convergence radius and are not converging at any values of λ . Such series are called asymptotic, and they can be used with a limited number of terms and only for estimate of eigenvalues at small λ [5]. The described above properties of PT series are confirmed when the formulas (1.9) are used for calculations in the particle number representation for operators (1.31):

$$\hat{H}_0 = \frac{1}{2} [1 + 2\hat{a}^+ \hat{a}], \quad \hat{V} = \frac{\lambda}{16} [\hat{a}^+ + a]^4. \quad (1.32)$$

Using the Eq. (1.24) for matrix elements of the creation and annihilation operators, the following expressions are found for the first terms of the RSPT series [4]:

$$\begin{aligned}
 E_n(\lambda) = & \left(n + \frac{1}{2}\right) + \frac{3}{4}\lambda[2n^2 + 2n + 1] - \\
 & - \frac{\lambda^2}{8}[34n^3 + 51n^2 + 59n + 21] + \\
 & + \frac{\lambda^3}{16}[375n^4 + 750n^3 + 1416n^2 + 1041n + 333] + \dots \quad (1.33)
 \end{aligned}$$

For the ground state of the system ($n = 0$), the calculations are easier, and we show here more terms of the series [19]:

$$E_0(\lambda) = \sum_{s=0}^{\infty} \lambda^s A_0^s = \frac{1}{2} + \frac{3}{4}\lambda - \frac{21}{8}\lambda^2 + \frac{333}{16}\lambda^3 - \frac{30885}{128}\lambda^4 + \frac{916731}{256}\lambda^5 - \dots \quad (1.34)$$

In the formula (1.33) the effective expansion parameter is λn , and for high excitation levels the RSPT series can only be used for very small λ . The graph on the Fig. 1.2, calculated on the basis of expression (1.34) for the function

$$E_0^{(l)}(\lambda) = \sum_{s=0}^l \lambda^s A_0^s,$$

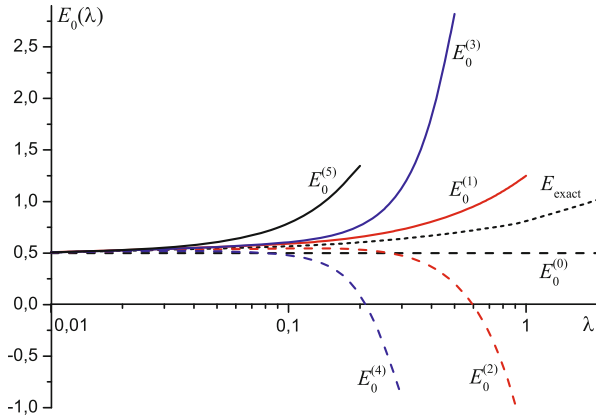


Fig. 1.2 The estimate for the energy of ground state of QAO for different numbers of terms $E_0^{(l)}$ in (1.34). The accurate values for $E_0(\lambda)$ are obtained in [28] from numerical solution of Schrödinger equation

illustrates the asymptotic character of the series with zeroth convergence radius: the larger the number of the involved terms in the expansion, the narrower is the applicability range of the series.

The divergence of RSPT series for the eigenvalues follows from its representation as power series, for example, for ground state:

$$E_0(\lambda) = \sum_{s=0}^{\infty} \lambda^s A_0^{(s)}. \quad (1.35)$$

The general behavior of the coefficients of the series at $s \gg 1$ was found in [18]:

$$A_0^{(s)} \approx (-1)^{s+1} \left(\frac{6}{\pi^3} \right)^{1/2} \Gamma\left(s + \frac{1}{2}\right) 3^s, \quad (1.36)$$

and using the general expression for the convergence radius R of the power series [5], we obtain:

$$R = \lim_{s \rightarrow \infty} \left| \frac{A_0^{(s)}}{A_0^{(s+1)}} \right| \approx \lim_{s \rightarrow \infty} \frac{1}{3(s + 1/2)} = 0. \quad (1.37)$$

Summarizing all written above, the demonstrated in this section examples show that even for relatively simple physical systems the canonic perturbation theory is not able to find an uniformly available approximation for the solution of Schrödinger equation.

1.3 Non-perturbative Methods for Stationary Schrödinger Equation

The other than canonic perturbation theory methods are usually formulated not universally and relate to the specific properties of quantum system. To illustrate the principle idea of these methods, we again use the quantum anharmonic oscillator problem. One of the effective non-perturbative method is the *strong coupling approximation* (SCA), which is conveniently formulated in the coordinate representation of Schrödinger equation:

$$-\frac{1}{2} \frac{d^2 \Psi_n(x)}{dx^2} + \frac{1}{2} x^2 \Psi_n(x) + \lambda x^4 \Psi_n(x) = E_n(\lambda) \Psi_n(x). \quad (1.38)$$

The basic idea of SCA in the range $\lambda \gg 1$ consists of the transformation of independent variable in such a way that new small parameter is introduced in the

equation, which depends on $\lambda^{-1} \ll 1$. By re-scaling the variable in the Eq. (1.35) as:

$$x = \xi y; \Psi_n(y\xi) = \Phi_n(y);$$

$$-\frac{1}{2\xi^2} \frac{d^2 \Phi_n(y)}{dy^2} + \frac{1}{2} \xi^2 y^2 \Phi_n(y) + \lambda \xi^4 y^4 \Phi_n(y) = E_n(\lambda) \Phi_n(y), \quad (1.39)$$

and choosing the parameter ξ under the condition that the coefficients at highest derivative in the equation and the largest term in the limit $\lambda \gg 1$ coincide:

$$\xi^{-2} = \lambda \xi^4; \xi = \lambda^{-1/6};$$

$$-\frac{1}{2} \frac{d^2 \Phi_n(y)}{dy^2} + \frac{1}{2\lambda^{2/3}} y^2 \Phi_n(y) + y^4 \Phi_n(y) = \epsilon_n(\lambda) \Phi_n(y);$$

$$E_n(\lambda) = \lambda^{1/3} \epsilon_n(\lambda), \quad (1.40)$$

we reduce the problem to the form, which can be treated by the perturbation theory with the effective parameter $\lambda^{-2/3} \ll 1$ and the equation for zeroth approximation, which is independent on λ :

$$-\frac{1}{2} \frac{d^2 \phi_n(y)}{dy^2} + y^4 \phi_n(y) = \epsilon_n^{(0)} \phi_n(y). \quad (1.41)$$

In strong coupling approximation, contrary to the case $\lambda \ll 1$, the equation for zeroth approximation does not have an analytical solution for eigenvalues and eigenfunctions, and therefore the dependence on λ is manifested as a series:

$$E_n(\lambda) = \lambda^{1/3} \sum_{s=0}^{\infty} B_n^s \lambda^{-2s/3}, \quad (1.42)$$

and for the coefficients B_n^s the numerical calculation of EV and EF is required from the differential equation (1.41) and matrix elements of the perturbation operator $\frac{1}{2\lambda^{2/3}} y^2$ (see, for example, [19]). In the next chapters we compare the analytical results after OM with the numerical calculations, and here we show some few results for the coefficients B_0^s to demonstrate the asymptotic character of SCA series, illustrated in Fig. 1.3, where the following functions are presented:

$$\tilde{E}_0^{(l)}(\lambda) = \lambda^{1/3} \sum_{s=0}^l B_0^s \lambda^{-2s/3};$$

$$B_0^0 \approx 0.6680; B_0^1 \approx 0.1437; B_0^2 \approx -0.0088. \quad (1.43)$$

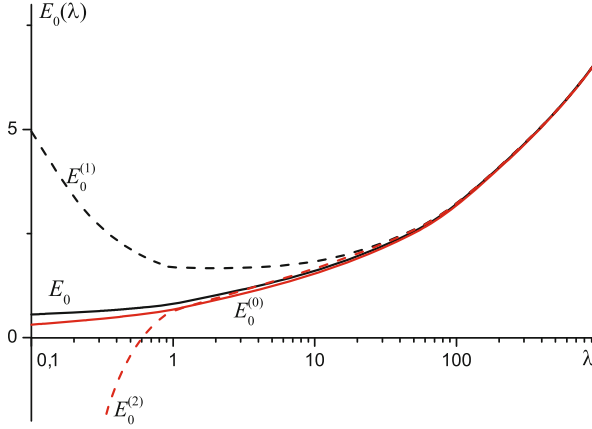


Fig. 1.3 The estimate for the energy of ground state of QAO for different numbers of terms $\tilde{E}_0^{(l)}$ in (1.43) for the case of SCA

As has been previously discussed in the Sect. 1.2, the applicability area of the perturbation theory is determined both by parameter λ and small values of a quantum number n . In the range $n \gg 1$, the *quasi-classic approximation* of Wentzel-Kramers-Brillouin (WKB) [4] can be used for calculation of eigenvalues. For the Eq. (1.38), this method is reduced to the Bohr-Sommerfeld quantization procedure:

$$\int_{x_n}^{x'_n} [2E_n - x^2 - 2\lambda x^4]^{1/2} dx = \pi \left(n + \frac{1}{2} \right) + O(1/n), \quad (1.44)$$

where stationary points x_n, x'_n are defined as real solutions of the equation:

$$2E_n - x^2 - 2\lambda x^4 = 0.$$

In general case of arbitrary λ , the use of WKB is ineffective because of requires the time-consuming calculation of the elliptic integrals [29]. However, in the limit $\lambda \gg 1$ these integrals can be approximated by using the expansion over the parameter $\lambda^{-1/3}$ and the series similar to (1.42) is obtained with approximate analytical expressions for coefficients [19]:

$$\begin{aligned} B_n^0 &\approx 3^{4/3} \pi^2 \left[\Gamma \left(\frac{1}{4} \right) \right]^{-8/3} \left(n + \frac{1}{2} \right)^{4/3}; \\ B_n^1 &\approx 3^{4/3} 4\pi^3 \left[\Gamma \left(\frac{1}{4} \right) \right]^{-16/3} \left(n + \frac{1}{2} \right)^{2/3}; \quad B_n^2 \approx -\frac{1}{32} + 6\pi^4 \left[\Gamma \left(\frac{1}{4} \right) \right]^{-8}. \end{aligned} \quad (1.45)$$

Another asymptotic expression used further for the analysis of the effectiveness of methods is obtained from the numerical solution of the Eq. (1.38) by using the power series [5]. To execute this procedure, the asymptotic behavior of wave function at $|x| \gg 1$ has to be studied, where the wave function is determined from the solution of the equation:

$$-\frac{1}{2} \frac{d^2 \Psi_n(x)}{dx^2} + \lambda x^4 \Psi_n(x) \approx 0;$$

$$\Psi_n(x) \sim e^{-|x|^3 \sqrt{2\lambda}} + O\left(\frac{1}{|x|}\right). \quad (1.46)$$

Using the design of the wave function in the form:

$$\Psi_n(x) = e^{-|x|^3 \sqrt{2\lambda}} \sum_{k=0}^{\infty} a_{nk} x^k,$$

the coefficients a_{nk} satisfy to the system of recurrent equations, which can be investigated analytically in the limiting case:

$$\lambda \rightarrow 0; n \rightarrow \infty; \lambda n = \beta < 1,$$

and for eigenvalues the following asymptotic expansion is obtained [19]:

$$E_n = (n + \frac{1}{2}) \left[1 + \frac{3}{2} \beta - \frac{17}{16} \frac{4 + 9\beta}{(1 + 3\beta)^2} \beta^2 + \dots \right]. \quad (1.47)$$

Summarizing the above presented approaches, all the approximate methods described in this chapter are able to estimate the functions $E_n(\lambda)$, each method in a particular domain of the parameters n, λ . However, neither algorithm provides the uniformly available approximation in the entire range of the parameters. Another essential drawbacks of all methods are the divergence of the successive approximations and cumbersome form of wave functions for zeroth approximations.

The *variational method* (VM) is used often for the evaluation of ground state energy for arbitrary amplitude of perturbation. This method is based on the fact that Schrödinger equation for the wave function $\Psi_0(\{\zeta\})$, which depends on the set of variables $\{\zeta\}$ parameterizing the physical system, corresponds to the extremum of the following functional [5]:

$$I_0[\Psi] = \int d\{\zeta\} \Psi_0^*(\{\zeta\}) [\hat{H} - E_0] \Psi_0(\{\zeta\});$$

$$\frac{\delta I}{\delta \Psi_0^*} = 0; \int d\{\zeta\} \Psi_0^*(\{\zeta\}) \Psi_0(\{\zeta\}) = 1. \quad (1.48)$$

The principle idea of VM consists of the replacement of the exact solution of Schrödinger equation by the function, which is modeled by analytical expression (trial function) containing the set of variational parameters $\omega_i, i = 1, 2, \dots, s$:

$$\Psi_0(\{\xi\}) \approx \psi_0(\{\xi\}, (\{\omega_i\})); \int d\{\xi\} \psi_0^*(\{\xi\}) \psi_0(\{\xi\}) = 1. \quad (1.49)$$

By substituting (1.49) into (1.48), we find the approximate value of the energy, which depends on these parameters:

$$E_0 \rightarrow \epsilon_0(\{\omega_i\}) = \int d\{\xi\} \psi_0^*(\{\xi\}) \hat{H} \psi_0(\{\xi\}),$$

and the best approximation for the energy on the selected class of functions is obtained on the basis of the choice of variational parameters from the minimum condition for $\epsilon_0(\{\omega_i\})$:

$$\begin{aligned} \frac{\partial \epsilon_0(\{\omega_i\})}{\partial \omega_i} &= 0; \quad i = 1, 2, \dots, s; \Rightarrow \{\omega_i^{(0)}\}; \\ E_0 &\approx \epsilon_0(\{\omega_i^{(0)}\}). \end{aligned} \quad (1.50)$$

In general case, the function $\epsilon_0(\{\omega_i\})$ is non-linear. Therefore, in this formulation of VM it is difficult to design the regular procedure for improvement of the accuracy of zeroth approximation as well as to evaluate the convergence of the resulted estimate for the large number of parameters. Moreover, the use of VM for excited states becomes complicated due to the accounting of additional orthogonality of wave function to the wave functions of all lower states, which have to be implemented in the variation of the functional.

$$\begin{aligned} I_n[\Psi] &= \int d\{\xi\} \Psi_n^*(\{\xi\}) [\hat{H} - E_n] \Psi_n(\{\xi\}); \quad \int d\{\xi\} \Psi_n^*(\{\xi\}) \Psi_n(\{\xi\}) = 1; \\ \int d\{\xi\} \Psi_m^*(\{\xi\}) \Psi_n(\{\xi\}) &= 0, \quad m = 0, 1, \dots, (n-1). \end{aligned} \quad (1.51)$$

To some extent, these problems are eliminated when using the variational principle based on the Ritz-Bubnov-Galerkin method [30]. In this method, the trial function consists of limited number of terms of the series (1.6) in the expansion of the state vector:

$$|\Psi^{(N)}\rangle = \sum_{m=0}^N C_m |\psi_m\rangle. \quad (1.52)$$

The set of the coefficients C_m represents the variational parameters in this case. By substituting expression (1.52) into functional (1.48), and calculating the variational

derivatives, the system of N linear uniform equations for these coefficients is found and the determinant Δ_N is written as:

$$(E - \epsilon_k)C_k = \lambda \sum_{m=0}^N V_{km}C_m; \\ \Delta_N(E, \lambda) = \| (E - \epsilon_k)\delta_{km} - \lambda V_{km} \| . \quad (1.53)$$

The solution of the equation $\Delta_N(E, \lambda) = 0$ delivers $(N + 1)$ eigenvalues $E_n^N(\lambda); n = 0, \dots, N$ and corresponding eigenvectors $|\Psi_n^{(N)}\rangle$. This method is one of the techniques to numerically solve the Schrödinger equation, which has been used in [28] for calculation of eigenvalues and eigenfunctions for QAO. However, this method is not able to investigate analytically the qualitative behavior of quantum system for various ranges of physical parameters, which is a key subject for the presented in this monograph operator method. There are also substantial difficulties of the application of Ritz-Bubnov-Galerkin method for the physical systems with a large number of the degrees of freedom because of the cumbersome matrix elements and the increase of the dimension of the determinant in (1.53). To illustrate the non-perturbative nature of VM, we consider here the functional (1.48), which corresponds to the Eq. (1.38) for the ground state of anharmonic oscillator:

$$I_0[\Psi] = \int_{-\infty}^{\infty} dx \left\{ \left| \frac{d\Psi_0(x)}{dx} \right|^2 + \Psi_0^*(x)[x^2 + 2\lambda x^4 - E_0]\Psi_0(x) \right\}; \\ \int_{-\infty}^{\infty} dx |\Psi_0(x)|^2 = 1. \quad (1.54)$$

The trial function is chosen in compliance with the wave function of harmonic oscillator, but with arbitrary frequency ω [4]:

$$\Psi_0(x) \approx \tilde{\Psi}_0(x) = C \exp \left[-\frac{\omega x^2}{2} \right], \quad (1.55)$$

and the normalizing constant C and the frequency ω are treated as variational parameters. The calculation of integrals in (1.54) with the function (1.55) results in:

$$I_0[\Psi] \approx \tilde{I}_0[\omega, C] = C^2 \sqrt{\frac{\pi}{\omega}} \left[\frac{1}{2} \left(\omega + \frac{1}{\omega} \right) + \frac{3\lambda}{\omega^2} - \tilde{E}_0 \right]; \quad C^2 \sqrt{\frac{\pi}{\omega}} = 1. \quad (1.56)$$

The calculation of the derivatives over C from the functional gives to the equation for energy, and the value C is found from the normalization condition:

$$\tilde{E}_0 = \frac{1}{2} \left(\omega + \frac{1}{\omega} \right) + \frac{3\lambda}{\omega^2}; \quad C = \left(\frac{\omega}{\pi} \right)^{1/4}, \quad (1.57)$$

and the derivative over ω determines the dependence of the variational parameter on the coupling constant λ :

$$\omega^3 - \omega - 6\lambda = 0. \quad (1.58)$$

Thus, the Eqs. (1.57) and (1.58) define the parametric form of the function $\tilde{E}_0(\lambda)$, which can be used for the estimate of the eigenvalue $E_0(\lambda)$ in the entire range of the parameter λ . The analytical solution of these equations at $\lambda \ll 1$ and $\lambda \gg 1$ results in the following expansions:

$$\begin{aligned} \tilde{E}_0(\lambda) &\approx \frac{1}{2} + \frac{3}{4}\lambda - \frac{9}{4}\lambda^2 + \dots, \quad \lambda \ll 1; \\ \tilde{E}_0(\lambda) &\approx \lambda^{1/3} \left[\left(\frac{3}{4}\right)^{4/3} + \frac{1}{4(36\lambda)^{2/3}} - \frac{1}{144\lambda^{4/3}} + \dots \right], \quad \lambda \gg 1. \end{aligned} \quad (1.59)$$

These expansions are in a good agreement with the asymptotic series RSPT (1.34) and SCA (1.43), respectively, but contrary to them are convergent for all λ . Thereby the variational method delivers an uniformly available approximation for the eigenvalues in a zeroth approximation. It is worth to notice that in VM the wave function of physical system is modeled and not the Hamiltonian, as in the case of perturbation theory. Being used in the systems with several degrees of freedom, VM faces some specific issues, which can be illustrated by a simple model of two coupled harmonic oscillators [31]. The dimensionless form of Hamiltonian for this system is written as [32]:

$$\hat{H} = \frac{1}{2}\hat{p}_x^2 + \frac{1}{2M}\hat{p}_y^2 + \frac{1}{2}x^2 + \frac{1}{2}y^2 + \lambda xy, \quad (1.60)$$

where M is the ratio of the oscillator masses and λ is the interaction parameter. In spite of its simplicity, this Hamiltonian is often used for the approbation of various approximate methods in many-particle quantum theory [31]. The classical trajectories of the system are described by rather complicated Lissajous figures which demonstrates the essential dependence of the quantum levels on the interaction and mass parameters. The exact eigenvalues of the Hamiltonian are found straightforward:

$$E_{nm} = \nu_1 \left(n + \frac{1}{2} \right) + \nu_2 \left(m + \frac{1}{2} \right), \quad (1.61)$$

where $\nu_{1,2}$ are defined by the expression:

$$\nu_{1,2}^2 = \frac{1}{2M} (1 + M \pm \sqrt{(1 - M)^2 + 4\lambda^2 M}). \quad (1.62)$$

The formula (1.62) shows that the system energy has singularities if it is considered as an analytical function in the complex plane of the parameters λ and M . Thus, the series in terms of powers of these parameters have the finite convergence radii. This is the mathematical reason of the restrictions for various approximate methods, as has been discussed earlier for one-dimensional system.

The analogous restrictions for the convergence of the series appear when the interactions between the oscillators are considered by some approximate method. Let us consider the results of VM in one-particle approximation used for the Hamiltonian (1.60). The wave functions of the system in the zeroth order are chosen as the product of one-particle functions, i.e. Hartree approximation is applied (the symmetrization of the function in the case of $M = 1$ is not essential for our discussion):

$$\Psi_{VM}(x, y) = \varphi(x)\chi(y); \quad \int_{-\infty}^{\infty} dx |\varphi(x)|^2 = \int_{-\infty}^{\infty} dy |\chi(y)|^2 = 1. \quad (1.63)$$

The system of the approximate equations for one-particle functions follows from the exact variational principle (1.48):

$$\begin{aligned} \left\{ \frac{1}{2} \hat{p}_x^2 + \frac{1}{2} x^2 + \lambda xy_{mm} - \epsilon_n \right\} \varphi_n &= 0; \\ \left\{ \frac{1}{2M} \hat{p}_y^2 + \frac{1}{2} y^2 + \lambda yx_{nn} - \epsilon_m \right\} \chi_m &= 0. \end{aligned} \quad (1.64)$$

Both equations correspond to the uncoupled harmonic oscillators with displaced equilibrium positions defined as:

$$\bar{x} = y_{mm} = \int_{-\infty}^{\infty} dy \chi_m(y)^* y \chi_m(y); \quad \bar{y} = x_{nn} = \int_{-\infty}^{\infty} dx \varphi_n(x)^* x \varphi_n(x). \quad (1.65)$$

The energy spectrum of the system in this approximation is:

$$E_{nm}^{VM} = \left(n + \frac{1}{2} \right) + \frac{1}{\sqrt{M}} \left(m + \frac{1}{2} \right) - \frac{1}{2} \lambda^2 (x_{nn}^2 + y_{mm}^2) - \lambda x_{nn} y_{mm}. \quad (1.66)$$

This expression is actually the power series of the parameter λ , and taking into account the conditions of self-consistency for the values \bar{x} , \bar{y} :

$$\bar{x} = -\lambda \bar{y}; \quad \bar{y} = -\lambda \bar{x},$$

one finds $\bar{x} = \bar{y} = 0$ for arbitrary value of λ .

Thus, the zeroth-order approximation of E_{nm}^{VM} differs essentially from the corresponding exact value. Certainly, the consequent corrections take into account

the particle correlations, but in any case VM fails to describe the energy levels over the entire range of parameters λ and M . The so-called adiabatic approximation ($M \gg 1$) being applied to the Schrödinger equation with the Hamiltonian (1.60) leads to analogous problem. A similar calculation has also been considered in [31] to illustrate the general method for calculation of high-order corrections for the adiabatic approximation. In the adiabatic zeroth-order approximation the operator \hat{p}_y^2 should be neglected and the “adiabatic” terms $\epsilon_n(y)$ are defined by the energy levels of that part of the Hamiltonian which depends on the “quick” variable x :

$$\epsilon_n(y) = n + \frac{1}{2} - \frac{1}{2}\lambda^2 y^2.$$

These values play the role of the potential energy in the Schrödinger equation for the “slow” oscillator y in the next order of the approximation. In the result, the energy spectrum of the system, taking into account two orders of the series in the parameter $1/\sqrt{M}$, has the form:

$$E_{nm}^{AA} = n + \frac{1}{2} + \sqrt{\frac{1-\lambda^2}{M}} \left(m + \frac{1}{2} \right). \quad (1.67)$$

Comparing this expression with formula (1.62), it becomes evident that the adiabatic (Born-Oppenheimer) [33] approximation also does not lead to the uniformly suitable estimation for the energy levels, even for such a simple system. Certainly, the same restrictions of the considered methods appear for more complicated model when the anharmonicity of the oscillators is included. In any case, the singularities of the energy, considered as an analytical function of the Hamiltonian parameters, define the finite radii of convergence for the power series in these parameters and do not allow to find an uniformly suitable approximation.

As we have shown above, while working with the real physical systems, the perturbation methods applied for the solution of the Schrödinger equation have led to the divergent asymptotic series for the energy corrections. However in some cases it is possible to develop the methods of regular summation of such series. We will mention here one of these methods—the Borel’s summation [34], which is very effective for calculation of the divergent or very slowly convergent series. This method was developed in the end of the nineteenth century by Emile Borel and then generalized by Gösta Mittag-Leffler [35].

First of all, we recall some main ideas of the method, starting with the investigation of power series:

$$f(z) = \sum_{k=0}^{+\infty} c_k z^k. \quad (1.68)$$

The series (1.68) could be divergent at a certain area of value z , or very slowly convergent. Therefore, instead of (1.68) we consider another series called the Borel transform of (1.68):

$$F(z) = \sum_{k=0}^{+\infty} \frac{1}{k!} c_k z^k. \quad (1.69)$$

The Borel transform (1.69) is obviously converging faster than (1.68), and assuming it converges to the analytical function near the point $z = 0$, the analytical continuation can be performed along the positive real axis. The following integral is defined:

$$f(z)(Borel) = \int_0^{+\infty} e^{-t} F(zt) dt, \quad (1.70)$$

which is called the Borel summation of (1.68). The function (1.70) can converge to a certain value even in the region where the series (1.68) is divergent.

This method is very effective for the calculation of divergent series, which depends on single variable. The method was generalized and adjusted to different problems, for example, in [36–40]. Here we generalize the Borel summation (1.69) by applying the Pade approximant [38, 39] of the order m/n to obtain the result with a better convergence:

$$P(z) = \frac{a_0 + a_1 z + \dots + a_m z^m}{1 + b_1 z + \dots + b_n z^n}, \quad (1.71)$$

where the coefficients are defined by the following equations:

$$\begin{aligned} P(0) &= F(0), \quad P'(0) = F'(0), \quad P''(0) = F''(0), \dots \\ \dots P^{(m+n)}(0) &= F^{(m+n)}(0). \end{aligned} \quad (1.72)$$

These equations reflect the fact that the Taylor expansion of $P(z)$ at zero point has the first $m+n$ terms coinciding with the first $m+n$ terms of $F(z)$. Using the notation for Pade approximant as $[m/n]_F(z)$, the Borel summation (1.70) is rewritten as:

$$f^{[m/n]}(z)(Borel - Pade) = \int_0^{+\infty} e^{-t} [m/n]_F(zt) dt. \quad (1.73)$$

The method of Borel summation with the Pade approximant can be applied to the problem of the anharmonic oscillator. In quantum mechanics, the use of

the perturbation theory delivers the energy in the form of a power series of the perturbation parameter:

$$E(\lambda) = E^{(0)} + \sum_{k=1}^{+\infty} C_k \lambda^k. \quad (1.74)$$

Here we consider a specific case of the anharmonic oscillator with the perturbation term λx^4 . Using the Rayleigh-Schrödinger scheme, the energy of the ground state is written in the form:

$$\begin{aligned} E_0(\lambda) = & 1 + 0.214286 \times \left(\frac{7\lambda}{2}\right) - 0.107143 \times \left(\frac{7\lambda}{2}\right)^2 \\ & + 0.121356 \times \left(\frac{7\lambda}{2}\right)^3 - 0.200990 \times \left(\frac{7\lambda}{2}\right)^4 \\ & + 0.426130 \times \left(\frac{7\lambda}{2}\right)^5 - 1.087689 \times \left(\frac{7\lambda}{2}\right)^6 + O[\lambda^7]. \end{aligned} \quad (1.75)$$

The series (1.75) has a zero radius of convergence [40], which means even for a very small parameter λ , the high-order corrections for the energy do not result in a right value. For large values of λ , the terms of high order in (1.75) grow very fast, and the series (1.75) quickly becomes divergent. However, applying the Borel-Pade technique described above in the formulae (1.68–1.73), the correct values of energy $E_0(\lambda)$ can be obtained from (1.75) in the wide range of the parameter λ .

For the illustration of this technique, we reproduce in the Table 1.1 the energy values with the different orders of Pade approximation [38]. The results show the convergence to the known values of the energy for anharmonic oscillator. In the work [39], the Borel-Pade method of regular summation has been applied to obtain the asymptotic energy values for large parameter $\lambda \gg 1$: $E_0(\lambda) \sim \lambda^{1/3}$.

Table 1.1 Energy of ground state $E_0^{[m/n]}(\lambda)$ for different orders of Pade approximant

$m/n = m$	$\lambda = 0.1$	$\lambda = 0.2$	$\lambda = 1.0$
1	1.063829787234	1.111111111111	1.272727272727
2	1.065217852490	1.117540578275	1.348289096707
3	1.065280680051	1.118183011861	1.373799864956
4	1.065285049128	1.118272722955	1.383756497228
5	1.065285455239	1.118288405206	1.388075603389
6	1.065285502030	1.118291631128	1.390103754651
7	1.065285508357	1.118292382860	1.391116612108
8	1.065285509335	1.118292576357	1.391648018148
9	1.065285509503	1.118292630404	1.391938365335
10	1.065285509535	1.118292646573	1.392102495074
11	1.065285509541	1.118292651703	1.392198009942
12	1.065285509543	1.118292653416	1.392255010021

The table demonstrates the fast convergence of the method, however, the generalization of this technique for calculation of the energies of high excited states, and especially for multi-dimensional case, encounters substantial difficulties. Moreover, the partial summation of the series (1.74) for energy does not define the wave function and other physical characteristics of the system.

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2015, XV, 362 p. 63 illus., 43 illus. in color., Softcover

ISBN: 978-3-319-13005-7