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Operator Method in the Problem of Quantum Anharmonic Oscillator

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The problem of quantum anharmonic oscillator is considered as a test for a new non-perturbative method of the Schrödinger equation solution—the operator method (OM). It is shown that the OM zeroth-order approximation permits us to find such analytical interpolation for eigenfunctions and eigenvalues of the Hamiltonian which ensures high accuracy within the entire range of the anharmonicity constant changing and for any quantum numbers. The OM subsequent approximations converge quickly to the exact solutions of the Schrödinger equation. These results are justified for different types of anharmonicity (double-well potential, quasistationary states, etc.) and can be generalized for more complicated quantum-mechanical problems. © 1995 Academic Press, Inc.

CONTENTS

INTRODUCTION

There is no doubt at present that the whole variety of atomic and molecular physics phenomena are defined by electromagnetic interaction and quantum mechanics laws. Therefore any atomic and molecular system states can be described by corresponding solutions of the Schrödinger equation (SE) with completely definite Hamiltonian. Besides, the quantum description is universal and simple enough, because the wave function of any complex system is a solution of linear equation with a mathematical structure which is often similar for systems with different physical

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properties. That is why we may say, as Wigner once said [1], there is a special role for mathematics in quantum mechanics. In particular, the development of a new effective method of the SE approximate solution provides essential progress in describing a number of real physical systems.

It is necessary to point out that a lot of modern methods for obtaining solutions for many quantum mechanical and field theory problem solutions have arisen, not from the development of well-known branches of mathematical physics, but from the generalization of some unconventional approaches proposed in describing real physical systems. Such "physical" methods of quantum system theoretical description have obtained a strict foundation only after a successful explanation of complex physical phenomena has been given. Some of these methods are still unsubstantiated.

For example, one can cite the theory of distributions [2] which arose after the introduction of the Dirac delta-function in quantum mechanics; the Bogoliubov method of approximate second quantization [3], which was the first to give the microscopic explanation of superfluidity; the method model or of approximating Hamiltonians [4] allowed one to describe the most essential superconductor [5] and ferromagnetic [6] properties; the method of a coherent wave and the effective refraction index for considering the interaction of radiation and particles with condensed matter [7]—this method established close analogy between many optics and nuclear physics phenomena [8]; the method of the Hartree–Fock self-consistent field for atomic and nuclear systems, which has no general mathematical proof of its convergence for the present [9].

New methods of the SE solution are of great interest not only for analytical description of quantum systems but for the construction of an effective algorithm for numerical computation of their characteristic as well. The thing is that despite considerable increase in modern computer power it is still unsufficient, for instance, in solving the SE for the system of three interacting particles if one uses canonical methods for the numerical solution of differential equations on the basis of the finite difference approximation of derivatives. The above-mentioned difficulty has its principal meaning in considering the systems with an infinite number of degrees of freedom. At present the only method of such a numerical investigation problem is based on applying the physical ideas proposed by Feynman in the path integral formulation of quantum mechanics [10]. However, the volume of calculation with such an approach remains so great that sufficient accuracy can be obtained only for the simple models of the quantum field theory in the so-called numerical experiments [11].

What requirements should the mathematical method satisfy to be widely adopted in describing the real quantum systems? In our opinion, the first one is universality, that is, the possibility of representation of the main computer procedure in such form which is not bound up with special properties of a concrete system. We mean, of course, that any universal method cannot provide a ready-made formula for solution of the SE with an arbitrary Hamiltonian, but which gives only a prescription for the calculation of successive approximation to it. First, it requires that the

zeroth approximation of the method should describe qualitatively the most essential properties of the considered physical system, and, second, the consequent approximations should uniformly converge to the exact solution in order to calculate it with any necessary accuracy. Finally, the important condition is that the calculation algorithm for the successive approximations should be sufficiently simple so as to be carried out on a computer.

Among the approximate methods that are well known at present, the perturbation theory (PT) and its various modifications seem to have the largest universality (see, for example, [12]). In order to construct a PT series it is sufficient to select the zeroth-order operator $\hat{H}_0$ with known eigenvalue spectrum and eigenfunction set and the perturbation operator $\hat{V}$ from the total Hamiltonian $\hat{H}$ to that $\hat{H} = \hat{H}_0 + \lambda \hat{V}$. The nondimensional parameter λ determines the characteristic amplitude of the perturbation with respect to a distance between energy levels of unperturbed system with Hamiltonian $\hat{H}_0$. Then, one can construct the expansion in powers of the parameter λ both for the eigenvalues and for the eigenfunctions by a simple scheme which is formally applicable to any system. It proves, however, that the series in powers of λ obtained on the basis of the PT canonical form are asymptotic in the majority of non-trivial problems of current interest. It means that these series [12] do not allow us to find the SE solution by simple summation of a sufficiently great number of terms. That is why the use of PT is suitable only for sufficiently small λ. All the above equally correct for the so-called limit of strong coupling ($\lambda \gg 1$), when the value λ^{-1} is used as a small parameter [13] and for quasiclassical approximation with a small parameter, proportional to the Plank constant h and defined by the coefficient in front of the kinetic energy operator [14]. The asymptotic character of these expansions is clearly displayed in the fact that if one can construct two-way approximation in the parameters λ and λ^{-1} for the same system, these series provide essentially different functional dependences of the eigenvalues on the Hamiltonian parameter without analytical continuation from one series to another. Thus, in order to describe the most essential system features on the basis of the PT one should have deep understanding of the physics of processes taking place in the considered system and there is no universal procedure for choosing $\hat{H}_0$. In this connection it is useful to recall the Landau remark: "physical theory without a small parameter is impossible."

However, the nontrivial physical problems with some small parameter are almost exhausted at present. On the contrary, the practical value of problems with arbitrary Hamiltonain parameters in increasing. Thus, the necessity arises to develop the mathematical methods for physical theories without small parameters. At present there are many nonperturbative methods for describing of quantum systems. First, it is the direct numerical solution of the Schrödinger equation, when one uses actually the expansion in a small non-physical parameter, being a step of the derivative finite-difference approximation. The use of lattice model in field quantum theory on the basis of the path-integral method has the analogous character [15]. We can list examples of more "physical" nonperturbative methods such as the variational principle, the method of approximating Hamiltonains, the

Hartree–Fock method, and others. The known analytical and numerical methods, however, do not satisfy all the above-mentioned requirements. We belive that the operator method (OM) of the Schrödinger equation solution, described in the present paper, to a certain extent fills up this gap.

It is natural to suppose that in the majority of physical problems the divergence of perturbation theory series for a quantum system is not determined by the properties of the system, but only points out the necessity of reconstruction of the perturbation expansion to realize the eigenvalue and eigenfunction analytical continuations out of the convergence region of the initial series. In some cases this problem can be solved by the method of asymptotic series summation [16] and different modifications of the Padé-approximant method [17]. However, these methods are not sufficiently universal and theirs applications in the case of a system with many degrees of freedom [18] are bound up with serious difficulties.

The proposed method is actually a universal procedure of transformation of the perturbation series. We call it an operator method in the sense that all calculations are reduced to algebraic manipulations with operator matrix elements without solving any differential or integral equations both in the zeroth-order approximation and in calculating the successive ones. It proves that the OM zeroth-order approximation provides uniformly fitted estimation of the Schrödinger equation eigenvalues and eigenfunctions in the entire range of the Hamiltonian parameters. As a result the OM sequential approximations converge to the exact solution in the entire range of the system parameters and quantum numbers. The algebraic nature of the method also allows one to construct the effective procedure of the highest approximation calculation and to determine the system eigenvalues and eigenfunctions with high accuracy.

The fact, that the OM series convergence does not depend on Hamiltonian parameters and quantum numbers of the considered state, give rise to the natural question: "What is the difference between two successive approximations to eigenvalues and eigenfunctions defined by the OM?" Unfortunately we do not know the correct answer to this question because it requires special mathematical investigation. But we can give the "experimental" answer obtained on the basis of many specific results described in the paper: "The OM successive approximations converge as the geometric progression with the denominator defined by the ratio of nondiagonal to diagonal matrix elements of the Hamiltonian." This value depends on the choice of the initial basis set of quantum states but is less than unity under all conditions.

The operator method had been introduced in the papers [19, 20] and then some of its applications for specific systems were considered [21–30]. This method was developed by Fernandes, Meson, and Castro [31–36], Gerry and Silverman [37], Witchel [38], and others [39, 40]. Several ideas, which we used in our concept of the OM, were introduced earlier in the papers [41–47].

Analogous results were obtained later by other authors [48–51]. We hope that the application of the method is not confined to specific examples listed in this

paper. We believe that it can be an effective way of analysis of real physical systems despite the absence of strict mathematical grounding.

Any new method for the solution of the SE, describing real quantum systems, has to be investigated in detail by an example of well-known, but non-trivial model problem. In the case of non-relativistic quantum mechanics the role of such a test is played by the problem of the one-dimensional system, described by the Hamilton operator,

$$\hat{H} = \tfrac{1}{2}\hat{p}^2 + \mu\hat{x}^2 + \lambda\hat{x}^4, \tag{i}$$

where $\hat{x}$ and $\hat{p}$ are the operators of coordinate and momentum, satisfying the following permutable relation

$$[\hat{x}, \hat{p}] \equiv \hat{x}\hat{p} - \hat{p}\hat{x} = i.$$

Here Plank's constant $\hbar$ and a particle mass are equal to unity.

Hamiltonian (i) corresponds to the symmetrical quantum anharmonic oscillator in the case of $\mu > 0$ and $\lambda > 0$ and to the particle moving in the double-well potential field in the case of $\mu < 0$ and $\lambda > 0$. The Hamiltonian spectrum consists of quasistationary state set for $\mu > 0$ and $\lambda < 0$. These peculiarities of the quantum system with Hamiltonian (i) allow one to simulate different properties of the real physical systems successfully and to determine the permanent interest in its investigation. Apart from that this problem has important applications in atomic, molecular, and solid state physics. It can be considered as one-dimensional field quantum theory containing many problems that are typical for four-dimensional quantum field models. Under these reasons practically all known methods (see, e.g., [52]) are approved in the operator (i) eigenvalue and eigenfunction calculations.

In the present paper we also use the QAO problem in order to introduce main ideas of the operator method (OM) of the SE solution, to discuss its possibilities in comparison with other methods, to consider the calculation procedure of successive approximations to the exact eigenvalues and eigenfunctions and the convergence of this procedure.

1. Symmetrical Anharmonic Oscillator

1.1. *The Zeroth Approximation Choice*

Let us start with a simple example [31]. We need to find eigenvalues and eigenfunctions of the operator

$$\hat{H} = \tfrac{1}{2}(\hat{p}^2 + \hat{x}^2) + \mu\hat{x}^2, \tag{1.1}$$

where $\mu > -\frac{1}{2}$.

As is generally known, this problem with a quadratic Hamiltonian can be solved algebraically by means of the second quantization representation with the help of operators of the excitation annihilation and creation

$$\hat{x} = \frac{1}{\sqrt{2\omega}} [a(\omega) + a^+(\omega)], \qquad \hat{p} = i\sqrt{(\omega/2)}\,[a^+(\omega) - a(\omega)], \tag{1.2}$$

where ω is an arbitrary positive real value. The operators of annihilation $a(\omega)$ and creation $a^+(\omega)$ satisfy the permutable relations

$$[a(\omega), a^+(\omega)] = 1. \tag{1.3}$$

By substiting (1.2) to (1.1) and reducing the operator $\hat{H}$ to the normal form (all operators of creation are to the left of the annihilation operators) by the permutable relations (1.3) we obtain

$$\hat{H} = \frac{\omega}{4} [1 + 2a^+(\omega)\, a(\omega) - (a^+(\omega))^2 - (a(\omega))^2] + \frac{1 + 2\mu}{4\omega} [1 + a^+(\omega)\, a(\omega) + (a^+(\omega))^2 + (a(\omega))^2]. \tag{1.4}$$

If we choose

$$\omega = \omega_0 = \sqrt{1 + 2\mu}, \tag{1.5}$$

the operator $\hat{H}$ is reduced to the "diagonal" form

$$\hat{H} = \tfrac{1}{2}\omega_0 [1 + 2a^+(\omega_0)\, a(\omega_0)], \tag{1.6}$$

and its eigenvectors are the following normalized state vectors:

$$|n(\omega_0)\rangle = \frac{1}{\sqrt{n!}} [a^+(\omega_0)]^n\, |0(\omega_0)\rangle, \qquad n = 0, 1, 2, 3, \ldots,$$
$$a^+(\omega_0)\, a(\omega_0)\, |n(\omega_0)\rangle = n\, |n(\omega_0)\rangle. \tag{1.7}$$

The state of "vacuum" of the excitations is defined by equation

$$a(\omega_0)\, |0(\omega_0)\rangle = 0. \tag{1.8}$$

Equations (1.6) and (1.7) define the operator (1.1) eigenvalues

$$E_n = \tfrac{1}{2}\omega_0(2n + 1) = \tfrac{1}{2}(2n + 1)\sqrt{1 + 2\mu}. \tag{1.9}$$

Let us note that the eigenvalues (1.9) considered as a function of μ have singular point at $\mu = -\frac{1}{2}$ (in the range of $\mu < -\frac{1}{2}$ the Hamiltonian (1.1) does not have a discrete spectrum).

In order to construct the operator (1.3) eigenfunctions and eigenvalues on the basis of the perturbation theory (PT) let us suppose that $\mu\hat{x}^2$ is a small correction

to the unperturbed Hamiltonian $\hat{H}_0$ which can be reduced to the diagonal form at $\omega = 1$,

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \tag{1.10}$$

$$\begin{aligned} \hat{H}_0 &= \tfrac{1}{2}[1 + 2a^+(1)\,a(1)], \\ \hat{H}_1 &= \frac{\mu}{2}[1 + 2a^+(1)\,a(1) + (a^+(1))^2 + (a(1))^2]. \end{aligned} \tag{1.11}$$

The operator $\hat{H}_0$ eigenvalues and eigenfunctions are equal to

$$E_n^{(0)} = \tfrac{1}{2}(1 + 2n), \qquad |\psi_n^{(0)}\rangle = |n(1)\rangle,$$

in the chosen representation. One can easily find the first item of PT series in terms of the operator $\hat{H}_1$,

$$\begin{aligned} E_n^{(1)} &= \langle n(1)|\,\hat{H}_1\,|n(1)\rangle = \frac{\mu}{2}(1 + 2n), \\ E_n^{(2)} &= -\frac{|\langle n+2|\,\hat{H}_1\,|n\rangle|^2}{E_{n+2}^{(0)} - E_n^{(0)}} = -\frac{\mu}{8}(n+1)(n+2). \end{aligned} \tag{1.12}$$

It turns our that the series (1.12) converges only in the range of $|\mu| < \frac{1}{2}$ which is determined by the exact eigenvalue (1.9) singular point at $\mu = -\frac{1}{2}$ in the complex plane of the parameter μ [12]. At the same time all the values of this parameter in the range of $(-\frac{1}{2}, \infty)$ are possible. In connection with this it is necessary to carry out analytical continuation of the PT series by changing the zeroth approximation Hamiltonian choice so that we could find its spectrum in closed form and to make the PT series converging at all possible parameter μ values. The main idea of the OM [19] satisfying both the mentioned requirements is to include the part of the operator $\hat{H}$ (1.4) which commutes with the excitation number operator $\hat{n}(\omega) = a^+(\omega)\,a(\omega)$ at arbitrary ω into $\hat{H}_0$, that is,

$$\hat{H} = \hat{H}_0 + \hat{H}_1$$

with new division of the operator $\hat{H}$:

$$\hat{H}_0 = \frac{1}{4\omega}(\omega^2 + 1 + 2\mu)[1 + 2a^+(\omega)\,a(\omega)]; \tag{1.13}$$

$$\hat{H}_1 = -\frac{1}{4\omega}(\omega^2 - 1 - 2\mu)[(a^+(\omega))^2 + a^2(\omega)]. \tag{1.14}$$

Thus the zeroth approximation of the operator (1.1) eigenvalues should have the form

$$E_n^{(0)}(\omega) = -\frac{1}{4\omega}(\omega^2 + 1 + 2\mu)(1 + 2n), \qquad n = 0, 1, 2, \ldots. \tag{1.15}$$

In order to find the parameter on powers of which the operator (1.1) eigenvalue expansion should be carried out in using PT with the perturbation Hamiltonian (1.14) one has to use (1.13) and (1.14) in the PT series or represent the exact formula (1.9) in the form

$$E_n = (1+2n)\frac{1}{4\omega}(\omega^2+1+2\mu)\left[1-\left(\frac{\omega^2-1-2\mu}{\omega^2+1+2\mu}\right)^2\right]^{1/2}. \tag{1.16}$$

In this case the perturbation parameter is

$$\varepsilon = \left(\frac{\omega^2-1-2\mu}{\omega^2+1+2\mu}\right)^2$$

and the PT series converges at $\varepsilon < 1$ or at any real positive ω and $\mu < -\frac{1}{2}$. Thus, the above-mentioned choice of the zeroth approximation Hamiltonian allows one to construct the analytical continuation of the converging PT series in order to calculate the Hamilton operator eigenvalues and eigenfunctions at all possible values of the parameter μ.

We would like to draw your attention to the fact that the parameter ω value in (1.13)–(1.15) has not yet been fixed. This fact gives us an additional degree of freedom, allowing acceleration of convergence of the rebuilt PT series. Since the exact eigenvalues of the total hermitian Hamiltonian do not depend on the choice of a concrete representation of the full wave function set that is on the parameter ω in our case, the following condition has to be satisfied for exact energies:

$$\frac{\partial E_n}{\partial \omega} = 0. \tag{1.17}$$

In carrying out the concrete calculation on the basis of PT, it is natural to choose the parameter ω value so that the zeroth approximation (1.15) satisfies the condition (1.17) or

$$\frac{\partial}{\partial \omega} E_n^{(0)}(\omega) = 0. \tag{1.18}$$

This equation leads to the choice of $\omega = \omega_0$, defined by (1.5) and, hence, the described procedure of the zeroth approximation Hamiltonian construction and condition (1.18) lead to the exact solution of the problem of obtaining operator (1.1) eigenvalues and eigenfunctions (perturbation Hamiltonian (1.14) becomes equal to zero at $\omega = \omega_0$).

The above-mentioned example first proposed in [31] permits us to illustrate the ideas of the zeroth approximation of the OM. However, it is necessary to test the suitability of this method in solving a non-trivial problem before making any generalization. Therefore, turn to consideration of the QAO with corresponding Hamiltonian

$$\hat{H} = \tfrac{1}{2}(\hat{p}^2 + \hat{x}^2) + \lambda \hat{x}^4, \qquad \lambda \geqslant 0. \tag{1.19}$$

Since operator (1.19) does not have a discrete spectrum at $\lambda < 0$, it results from [12] that the PT series with perturbation operator $\lambda\hat{x}^4$ has a zero radius of convergence in the complex plane of the parameter λ. Hence, it is asymptotic at all $\lambda > 0$ [53]. By this reason other methods [52], requiring sufficiently complex numerical calculations [53], were used to compute the QAO eigenvalues and eigenfunctions with any necessary accuracy. In this connection let us construct the Hamiltonian (1.19) zeroth approximation by the above-mentioned way. Let us substitute the canonical transformation (1.2) in (1.19) and reduce operator $\hat{H}$ to the normal form

$$\hat{H} = \hat{H}_0 + \hat{H}_1,$$

where

$$\hat{H}_0 = \frac{1}{4\omega}(\omega^2 + 1)(1 + 2a^+a) + \frac{3\lambda}{4\omega^2}[1 + 2a^+a + 2(a^+a)^2], \tag{1.20}$$

$$\hat{H}_1 = -\frac{1}{4\omega}(\omega^2 - 1)[(a^+)^2 + a^2] + \frac{\lambda}{4\omega^2}[2(a^+)^2(2a^+a + 3)) + 2(2a^+a + 3)a^2 + (a^+)^4 + a^4]. \tag{1.21}$$

We omit argument ω of the annihilation and creation operators and assume that it should be clear from the text to which values of ω the operators correspond.

The eigenvectors of the OM zeroth approximation of the Hamilton operator (1.20) are vectors (1.7) and the corresponding eigenvalues are

$$E_n^{(0)}(\omega, \lambda) = \frac{1}{4\omega}(\omega^2 + 1)(1 + 2n) + \frac{3\lambda}{4\omega^2}(1 + 2n + 2n^2), \qquad n = 0, 1, 2, \ldots. \tag{1.22}$$

According to condition (1.17), we choose parameters ω at every value of the operator (1.20) eigenvalue from the equation

$$\frac{\partial}{\partial\omega} E_n^{(0)}(\omega, \lambda) = 0, \tag{1.23}$$

which has the following form for the definite n:

$$\omega_n^3 - \omega_n - 6\lambda\frac{1 + 2n + 2n^2}{1 + 2n} = 0. \tag{1.24}$$

Contrary to the case of the harmonic oscillator and usual form of PT the parameter $\omega = \omega_n$ appears to be different for different states in the problem of QAO. Due to this fact the dependence of the energy levels on the quantum number n is sufficiently

complex even in the zeroth approximation. While combining (1.22) and (1.24), we find the zeroth approximation of the QAO energy levels

$$E_n^{(0)}(\lambda)=\frac{1}{4}\left(3\omega_n+\frac{1}{\omega_n}\right)\left(n+\frac{1}{2}\right), \tag{1.25}$$

where ω_n is the algebraic equation (1.24) solution.

It seems unusual that a parameter in the Hamiltonian depends on the energy level. But we emphasize that the parameter ω is not the real parameter of the system. It was introduced into the Hamiltonian artificially in order to rebuild the perturbation operator. Condition (1.23) reconstructs the independence of the eigenvalues on this artificial parameter in the zeroth approximation. Actually, Equations (1.23) and (1.25) define the energy of the nth level as a function of λ in parametric form.

Condition (1.23) has formal resemblance to the variational principle. But they coincide only for energies of the lowest ($n=0$) and the first excited ($n=1$) states. The difference between conditions (1.23) and variational evaluation at $n\geqslant 2$ is determined by the fact that in the given approach, the operator (1.20) eigenvectors are not orthogonal to the vectors with lower numbers. Indeed, the vectors $|n(\omega_n)\rangle$ and $|n(\omega_m)\rangle$ are not orthogonal because, according to Eq. (1.24) they correspond to wave functions of the harmonic oscillators with different frequencies. At the same time, according to (1.7), every vector $|n(\omega_n)\rangle$ provides accurate symmetry and a corresponding number of branch points of the wave function in coordinate representation. It proves that it is sufficient to obtain an appropriate approximation of $E_n^{(0)}(\lambda)$ to the exact values of $E_n(\lambda)$ (see below). However, we should use only the full orthonormal set of the state vectors in order to compute higher approximations for the energy level corresponding to the quantum number n. The diagrams of Fig. 1 illustrate the relation between states used in the canonical PT and in the

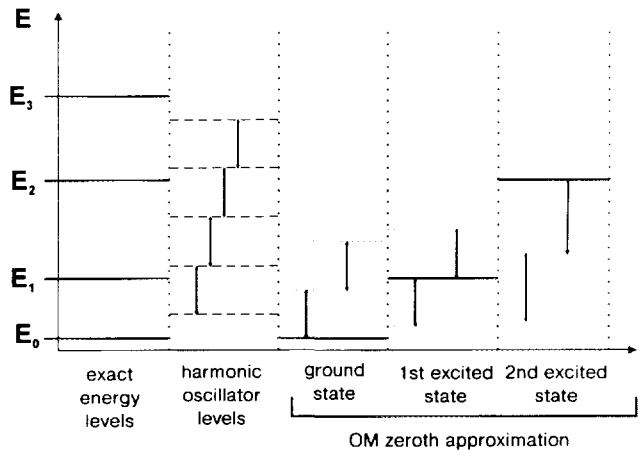

FIG. 1. The scheme of the full sets of states used in the canonic PT series and the OM zeroth approximation.

OM. Evidently, the main difference between these approaches is in the fact that the different full sets of wave functions are used to compute the various eigenvalues. The set of functions for the definite state does not coincide with those introduced to consider other states.

Let us point out that the method considered for the choice of the parameter ω, introduced in Hamiltonian by transformation (1.4), is closely connected with the transformations introduced by other authors in order to exceed the bounds of PT in computing QAO energy levels. First, it is the *principle of minimum sensitivity* considered by Caswell [42]. The coordinate scale transformation was introduced by Dmitrieva and Plindov [44] as a method for approximate calculation of the QAO levels. The results of these papers are similar to ours in the case of the lowest energy levels in the zeroth approximation. However, the approaches considered by these authors were not presented in the universal form because they were based on peculiarities of the QAO problem. Besides, the regular method of calculation of consequent approximations to exact eigenvalues was not considered in these papers.

Recently the delta-expansion method has been considered as a non-perturbation approach in quantum field theory (see, for example, the paper of Duncan and Jones [86]). This method is similar to the OM in many respects. An artificial parameter was also introduced in order to rebuild the perturbation operator and to optimize the convergence of the PT series. But in comparison with this method the OM contains the additional idea—to include all diagonal elements of the perturbation operator to the Hamiltonian of the zeroth approximation. This condition has a principal significance for convergence of the subsequent approximation (see below Section 1.4).

The canonical transformation, being more common then (1.2), was considered in [55]. This transformation corresponds to complex values of the parameter ω and defines the three-parametric group of transformation of the operators a and a^+. The conducted investigation has shown that the applied choice of real ω provided the best evaluation of energy of the QAO stationary states.

Now compare the eigenvalue zeroth approximation defined by Eqs. (1.24) and (1.25) with known exact results. In the weak coupling limit ($\lambda \to 0$) we find the expansion solving Eq. (1.24),

$$\omega_n = 1 + 3\lambda \frac{1+2n+2n^2}{1+2n} - \frac{3}{2}\left(3\lambda \frac{1+2n+2n^2}{1+2n}\right)^2 + 4\left(3\lambda \frac{1+2n+2n^2}{1+2n}\right)^3 + O(\lambda^4), \tag{1.26}$$

which substitution in formula (1.25) results in

$$E_n^{(0)}(\lambda) = n + \frac{1}{2} + \frac{3}{4}\lambda(1+2n+2n^2) - \frac{9}{4}\lambda^2 \frac{(1+2n+2n^2)^2}{1+2n} + \frac{27}{2}\lambda^3 \frac{(1+2n+2n^2)^3}{(1+2n)^2} + O(\lambda^4). \tag{1.27}$$

This should be compared with the Rayleigh–Schrödinger canonical PT application to this problem [52–53, 54],

$$E_n(\lambda) = n + \tfrac{1}{2} + \tfrac{3}{4}\lambda(1 + 2n + 2n^2) - \tfrac{1}{8}\lambda^2(21 + 59n + 51n^2 + 34n^3) + \tfrac{1}{16}\lambda^3(333 + 1041n + 1416n^2 + 750n^3 + 375n^4) + O(\lambda^4). \quad (1.28)$$

Table I compares the numerical values of some coefficients of both expansions presented in the following forms

$$E_n^{(0)}(\lambda) = \sum_{k=0}^{\infty} a_{nk}^{(\mathrm{OM})}\lambda^k, \qquad E_n(\lambda) = \sum_{k=0}^{\infty} a_{nk}^{(T)}\lambda^k.$$

Let us consider the opposite limit case when anharmonicity parameter $\lambda \to \infty$. Functional dependence on λ in the asymptotic expansion of the operator (1.19) exact eigenvalues can be determined by changing the variables in the SE coordinate representation [52]:

$$-\frac{1}{2}\frac{d^2\psi_n(x)}{dx^2} + \frac{1}{2}x^2\psi_n(x) + \lambda x^4\psi_n(x) = E_n(\lambda)\,\psi_n(x). \quad (1.29)$$

Suppose that

$$\xi = x\lambda^{1/6}, \qquad \psi_n(x) = \varphi_n(\xi). \quad (1.30)$$

TABLE I

Coefficients of the Weak Coupling Series for the QAO

	k			
$a_{nk}^{(\mathrm{OM})}$ $(a_{nk}^{(T)})$	0	1	2	3
$n=0$	0.5 (0.5)	0.75 (0.75)	−2.25 (−2.63)	13.5 (20.8)
$n=1$	1.5 (1.5)	3.75 (3.75)	−18.75 (−20.63)	187.5 (244.7)
$n=2$	2.5 (2.5)	9.75 (9.75)	−76.05 (−76.88)	1186.38 (1254.94)
$n=3$	3.5 (3.5)	18.75 (18.75)	−200.893 (−196.875)	4304.8469 (4176.5625)
$n=10$	10.5 (10.5)	165.75 (165.75)	−5232.964 (−4963.875)	330424.3 (290771.4)

Then instead of (1.29) we obtain

$$-\frac{1}{2}\frac{d^2\varphi}{d^2\xi}+\frac{1}{2\lambda^{2/3}}\xi^2\varphi_n(\xi)+\xi^4\varphi_n(\xi)=\frac{E_n(\lambda)}{\lambda^{1/3}}\varphi_n(\xi), \tag{1.31}$$

which results in

$$E_n(\lambda)=\lambda^{1/3}\sum_{k=0}^{\infty} b_{nk}^{(T)}(\lambda)^{(-2/3)k} \tag{1.32}$$

at $\lambda \gg 1$. Let us note that, by contrast with PT series, coefficients of an asymptotic expansion (1.32) are determined now by differential equation solutions [52]. On the other hand, the solution of algebraic equation (1.24) has the expansion at $\lambda \gg 1$

$$\omega_n=\lambda^{1/3}\left[6^{1/3}\left(\frac{1+2n+2n^2}{1+2n}\right)^{1/3}+\frac{1}{3\cdot 6^{1/3}}\left(\frac{1+2n}{1+2n+2n^2}\right)^{1/3}\times\frac{1}{\lambda^{2/3}}+O\left(\frac{1}{\lambda^2}\right)\right], \tag{1.33}$$

which results in

$$E_n(\lambda)=\lambda^{1/3}\left[\frac{3^{4/3}}{2^{8/3}}(1+2n+2n^2)^{1/3}(1+2n)^{2/3}+\frac{1}{4\cdot 6^{1/3}}\frac{(1+2n)^{4/3}}{(1+2n+2n^2)^{1/3}}\frac{1}{\lambda^{2/3}}-\frac{1}{144}\frac{(2n+1)^2}{(1+2n+2n^2)}\frac{1}{\lambda^{4/3}}+O\left(\frac{1}{\lambda^2}\right)\right] \tag{1.34}$$

TABLE II

Coefficients of Strong Coupling Series for QAO

	k		
$b_{nk}^{(\mathrm{OM})}$ $(b_{nk}^{(T)})$	0	1	2
$n=0$	0.68142 (0.66799)	0.13758 (0.14367)	−0.0069 (−0.0088)
$n=1$	2.42374 (2.39364)	0.34812 (0.35780)	−0.0125 (−0.0140)
$n=2$	4.68526 (4.69680)	0.50027 (0.49397)	−0.0133 (−0.0125)
$n=3$	7.29111 (7.33573)	0.63005 (0.61826)	−0.0136 (−0.0116)

TABLE III

Comparison of Some Numerical and OM Zeroth Approximation Results for QAO

$E_n^{(T)}$ ($E_n^{(OM)}$)	λ			
	0.1	1	10	100
$n=0$	0.560307 (0.559146)	0.812500 (0.803771)	1.53125 (1.50497)	3.19244 (3.13138)
$n=10$	17.26588 (17.35190)	32.66349 (32.93326)	68.17094 (68.03695)	145.8383 (147.2270)
$n=40$	94.84034 (95.56017)	192.7883 (194.6022)	409.8935 (413.9383)	880.546 (889.325)

after substitution in (1.25). As is evident from comparing (1.34) with (1.32), the OM zeroth approximation also results in the correct parameter λ functional dependence of eigenvalues in the range of strong anharmonicity. Numerical values of coefficients b_{nk} in formulas (1.32) and (1.34) are listed in Table II.

Thus, comparing formulas (1.27) and (1.34) with formulas (1.28) and (1.32) we can see that the function $E_n^{(0)}(\lambda)$ correctly reproduces the functional structure of an asymptotic series in the corresponding limits. In contrast to PT series or strong coupling limit, when it is necessary to take into account higher approximations to compute addends containing new powers of λ, the function $E_n^{(0)}(\lambda)$ initially contains all the necessary powers of a coupling constant in expanding into the corresponding series although coefficients of these converged series have to differ slightly from their values in the asymptotic series.

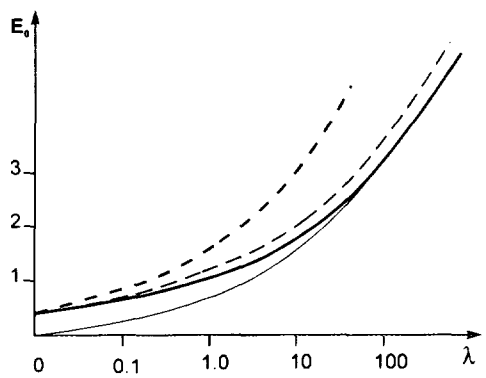

FIG. 2. Comparison of the function $E_0(\lambda)$ with its different approximations: ——— exact; ——— strong coupling; – – – PT; - - - OM zeroth approximation.

Therefore, it is natural to expect that $E_n^{(0)}(\lambda)$ should provide a suitable approximation to the exact eigenvalues $E_n(\lambda)$ in the range of intermediate λ. Indeed, comparing the energy values defined by formulas (1.24) and (1.25) with the numerical calculation results [52], we see that the function $E_n^{(0)}(\lambda)$ provides a valid approximation of the QAO energy levels at any n and λ (Table III), this evaluation precision being about 2–3%. This statement is illustrated by Fig. 2 which shows the functions $E_n^{(0)}(\lambda)$ and $E_n(\lambda)$ and analogous functions found by PT and strong coupling approximation.

1.2. *Iteration Scheme of the Successive Approximation Calculation*

The fact that the function $E_n^{(0)}(\lambda)$ is the best approximation for the exact eigenvalue $E_n(\lambda)$ means that the operator H_0 (1.20), separated from $\hat{H}$ according to the OM prescription, takes into account all the peculiarities of the initial Hamiltonian. Therefore we may expect that applying operator $\hat{H}_1$ (1.21) in solving SE for considered system will not result in qualitative changes in the energy spectrum and allows us to construct the algorithm for calculation of eigenvalues and eigenfunctions with any required accuracy at all n and λ.

Thus, let us consider SE for eigenvector $|\psi_n\rangle$, corresponding to the energy E_n,

$$(\hat{H}_0 + \hat{H}_1)\,|\psi_n\rangle = E_n\,|\psi_n\rangle, \tag{1.35}$$

where operators $\hat{H}_0$ and $\hat{H}_1$ are determined by formulas (1.20) and (1.21). Let us represent vector $|\psi_n\rangle$ in terms of the operator $\hat{H}_0$ eigenfunctions

$$|\psi_n\rangle = |n(\omega_n)\rangle + \sum_{k \neq n} C_{nk}\,|k(\omega_n)\rangle \tag{1.36}$$

with the coefficient C_{nk} to be defined by Eq. (1.35). Note that all state vectors $|k(\omega_n)\rangle$ correspond to the same parameter ω_n values at fixed n and, hence, satisfy the ordinary conditions of orthogonality and completeness. State vectors (1.36) should be normalized by the condition

$$\langle n(\omega_n)\,|\psi_n\rangle = 1, \tag{1.37}$$

which essentially simplifies the further relations. As a rule, a similar condition is used in solving Eq. (1.35) by means of the unstationary PT [56]. Substitute the expansion (1.36) in Eq. (1.35) and find its projection on bra-vector $\langle n|$ by taking into account (1.37):

$$E_n = H_{nn} + \sum_{k \neq n} C_{nk} H_{nk}. \tag{1.38}$$

In order to be brief we should not write index ω in the subsequent formulas and we should assume that by the definition

$$(\hat{H}_0)_{nn} \equiv H_{nn}, \qquad (\hat{H}_1)_{nk} \equiv H_{nk}, \qquad k \neq n.$$

Equations for coefficients C_{nm} are found by projecting Eq. (1.35) on different vectors $|m\rangle$ of the full set of states

$$C_{nm} = -[H_{mm} - E_n]^{-1} \left[H_{nm} + \sum_{k \neq n} H_{nk} C_{km} \right], \qquad m \neq n. \tag{1.39}$$

By using the well-known expressions for matrix elements of creation and annihilation operators ($\delta_{k,n}$—Kroneker symbol)

$$\langle k| a |n\rangle = \sqrt{n}\,\delta_{k,n-1}, \qquad \langle k| a^+ n\rangle\rangle = \sqrt{n+1}\,\delta_{k,n+1}, \tag{1.40}$$

one can find the expressions for diagonal matrix elements H_{nn} and nonzero transition matrix elements H_{nk} in the case of QAO:

$$H_{nn} = \frac{1}{4\omega}(\omega^2 + 1)(1 + 2n) + \frac{3\lambda}{4\omega^2}(1 + 2n + 2n^2); \tag{1.41}$$

$$\begin{aligned} H_{n,n+2} &= H_{n+2,n} = \frac{1}{4}\sqrt{(n+1)(n+2)}\left[\frac{1-\omega^2}{\omega} + \frac{2\lambda}{\omega^2}(2n+3)\right] \\ H_{n,n+4} &= H_{n+4,n} = \frac{\lambda}{4\omega^2}\sqrt{(n+4)!/n!}. \end{aligned} \tag{1.42}$$

The system of nonlinear algebraic equations (1.38), (1.39) is exact and completely equivalent to the initial SE (1.35). As has been mentioned above, the dependence of coefficients C_{nk} on the parameter ω is determined by the fact that the wave function form depends on the choice of specific representation, defined by ω in our case. In contrast to SE in coordinate representation, where numerical solving requires finite-difference derivative approximative approximation, in the present case the problem reduces only to algebraic calculations with the matrix elements of the Hamiltonian. On the basis of the results, described in Section 1.1 in the case of QAO, there is a suitable zeroth approximation,

$$\omega = \omega_n, \qquad E_n^{(0)} = H_{nn}(\omega_n), \qquad C_{nk}^{(0)} = 0, \qquad |\psi_n^{(0)}\rangle = |n(\omega_n)\rangle. \tag{1.43}$$

This circumstance makes it natural to suppose that the non-diagonal matrix elements H_{nk} provide a small contribution to the system energy in the range of $\omega \sim \omega_n$ and permits one to develop a scheme of successive approximation to E_n. It is expedient to consider several different variants of such a scheme. First, we should choose a calculation procedure [29, 32] based on the solution of equations (1.38), (1.39) by an ordinary form of Rayleigh–Schrödinger PT [12]. By adding to the operator $\hat{H}_1$ formal small-parameter β ($\hat{H}_1 \to \beta \hat{H}_1$), one can present unknown quantities E_n and C_{nk} in the form of the following series:

$$E_n = H_{nn} + \sum_{s=1}^{\infty} \beta^s \varepsilon_n^{(s)}, \qquad C_{nk} = \sum_{s=1}^{\infty} \beta^s C_{nk}^{(s)}; \qquad k \neq n. \tag{1.44}$$

Certainly the parameter β is equal to unity in formulas (1.44) while performing specific calculations. By substituting expansion (1.44) in Eq. (1.38), (1.39) and equating the coefficients at similar powers of β, we find recurrence formulas connecting the values of $\varepsilon_n^{(s)}$ and $C_{kn}^{(s)}$ with the corrections of lower order

$$\varepsilon_n^{(1)} = 0,$$

$$\varepsilon_n^{(s)} = \sum_{k \neq n} H_{nk} C_{kn}^{(s-1)}, \qquad s = 2, 3, \ldots, \tag{1.45}$$

$$C_{mn}^{(s)} = [H_{nn} - H_{mm}]^{-1} \left\{ \sum_{k \neq m,n} H_{mk} C_{kn}^{(s-1)} - \sum_{t=1}^{s-1} C_{mn}^{(t)} \varepsilon_n^{(s-t)} \right\}.$$

Generally speaking, parameter ω in Eq. (1.45) still remains arbitrary and it is not obvious that the choice of $\omega = \omega_n$ on the basis of condition (1.18), which is optimal in the zeroth approximation, remains the best in the consequent approximations. Moreover, it was shown in the paper [32] that in the case of QAO recurrence, the relations (1.45) diverge at $\omega = \omega_n$, starting from some $s \geqslant s_0$, that is, the value of $|\varepsilon_n^{(s)}|$ stops decreasing at $s \geqslant s_0$. As we shall see later on, the matter is that the choice of different values of ω results in the reconstruction of a series (1.45) coefficients, although it does not change the total structure of these series, similarly to partial summation of some sequences of ordinary PT terms. Therefore it is natural, that the sequence (1.45) convergence and that its rate depend on the ω value. Generally speaking, $\omega_{n0}^{(s)}$ depends on the number of iterations of s. In connection with this, let us consider the calculation procedure for the optimal value of $\omega_{n0}^{(s)}$ in Eq. (1.45) in the case of QAO, following [28].

Let us introduce the partial sums

$$S_n^{(t)}(\omega) = H_{nn}(\omega) + \sum_{s=2}^{t} \varepsilon_n^{(s)}(\omega), \tag{1.46}$$

which should become equal to the exact eigenvalues E_n at $t \to \infty$ and, hence, should not depend on parameter ω. It is interest to retrace how this dependence disappears for QAO. Figure 3 shows several functions $S_n^{(t)}(\omega)$ at different n and t, computed by Eqs. (1.45) and (1.46). It should be noted that the algebraic nature of this calculation requires a minor computing time input even for small PC. The computational time of functions $S_n^{(t)}(\omega)$ at $t \leqslant 10$ is practically defined by rate of the results readout and is much less than the time of a direct numerical solution with the same accuracy of the SE in a coordinate representation by using finite-difference approximation for the derivative [57], or by other known methods [52]. Analysis of the curves reproduced in Fig. 3 shows the character of function $S_n^{(t)}$ convergence to the value E_n: with t increasing, the difference $|S_n^{(t)} - E|$ become a more oscillating function of ω; this oscillation magnitude, however, quickly aims at zero.

Therefore, locations of the function $S_n^{(t)}$ extremum essentially change at different t and conditions like (1.18) of ω; choosing becomes variational in the highest approximations. At the same time one can note that there are such values of ω_{n0} at which $S_n^{(t)}$ coincides with its limit value E_n. This statement is valid at $t \geqslant 2$, if $n = 0, 1$.

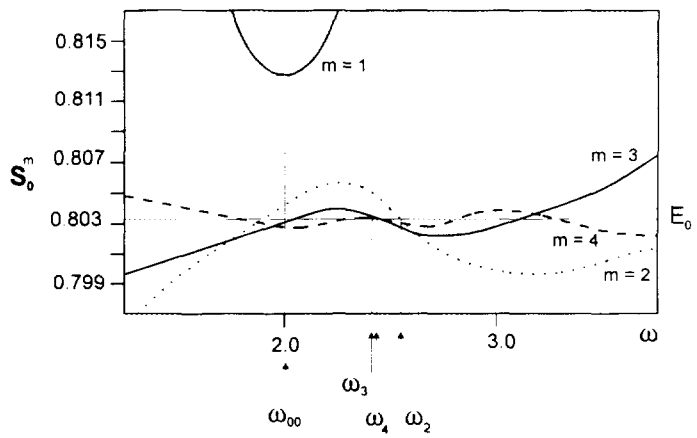

FIG. 3. The dependence of the OM subsequent approximations on the parameter ω.

We can consider the following numerical method for the regular calculation of the ω_{n0} optimal value. We shall choose it as the solution of the equation

$$\begin{aligned} &H_{nn}(\omega_{n0}) + \varepsilon^{(2)}(\omega_{n0}) = E_n, \qquad n = 0, 1, ..., \\ &H_{nn}(\omega_{n0}) = E_n, \qquad n \geqslant 2. \end{aligned} \tag{1.47}$$

Evidently, the exact value E_n is not known in advance and, in fact, ω_{n0} is calculated as a limit of

$$\omega_{n0} = \lim_{t \to \infty} \omega_{n0}^{(t)}, \qquad \omega_{n0} > \omega_n,$$

with parameter $\omega_{n0}^{(t)}$ being determined by one of the equations

$$\begin{aligned} &\sum_{s=3}^{t} \varepsilon_n^{(s)}(\omega_{n0}^{(t)}) = 0, \qquad n = 0, 1, \\ &\sum_{s=1}^{t} \varepsilon_n^{(s)}(\omega_{n0}^{(t)}) = 0, \qquad n \geqslant 2, \end{aligned} \tag{1.48}$$

for every eigenvalue after calculating tth correction. Moreover, it is necessary to choose such an equation solution, which is the closest to the value ω_n of (1.24) and optimal in its zeroth approximation. It is essential that condition (1.48) simplifies reccurent formulas (1.45) which take the form

$$C_{nk}^{(s)} = (H_{kk} - H_{nn})^{-1} \sum_{m \neq k} H_{nm} C_{mk}^{(s-1)}. \tag{1.49}$$

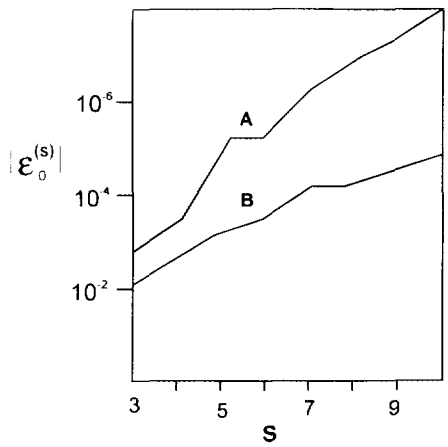

FIG. 4. The convergence of the OM series in cases of fixed (B) and optimized (A) parameter ω.

The results of the numerical calculation (Fig. 4) show that for an optimal choice of parameter ω the successive corrections $\varepsilon_n^{(s)}$ decrease with increasing s as the terms of a geometric progression with denominator $q \sim \frac{1}{8}$, when relations (1.45) are used, while fixed ω [32] convergence rate proves to be essentially less ($q \simeq \frac{1}{3}$). The comparison of exact values for QAO with results of computing based on the operator method with parameter optimization is in Table IV.

One can introduce other ways for the parameter ω adjustment in computing high order corrections which change convergence rate [32, 58]. It is important that such a change of ω is necessary in computing energy and coefficients C_{nk} in the form of series (1.44) because divergence of these series for fixed ω, although for the operator method the addend growth takes place in the approximations of essentially higher orders than for ordinary PT. In specific computations the ω optimization depending on approximation order s requires repeated computing by the recurrent

TABLE IV

Results of Optimal Choice of the Parameter ω

λ	E_0	$H_{00}+\varepsilon_0^{(2)}(\omega_{00}^{(8)})$	$H_{00}+\varepsilon_0^{(2)}(\omega_{00}^{(9)})$	$\omega_{00}^{(9)}$
1	0.80377065	0.80377079	0.80377071	2.5170107
50	2.49970877	2.49971045	2.49970957	8.7704769
	E_2	$H_{22}+\varepsilon_2^{(2)}(\omega_{20}^{(8)})$	$H_{22}+\varepsilon_2^{(2)}(\omega_{20}^{(9)})$	$\omega_{20}^{(9)}$
1	5.17929169	5.17929328	5.17929202	3.0118979
50	17.4369921	17.4370082	17.4369958	10.712937

Note. Figure 4 illustrates the successive approximation convergence in computing ω_{n0} and eigenvalues E_n by formulas (1.45)–(1.48) for QAO.

formulas (1.45) at different values of ω that leads to an essential increase of the calculation time. Besides, an optimization algorithm has an experimental character in a certain sense and its application in describing systems more complex than QAO may lead to some computation difficulties.

In connection with this we introduce another scheme of the initial equation (1.38) solution which is much more effective, to our mind, especially in describing physical systems with several degrees of freedom. The present approach is based on simple iterations in a nonlinear equation (1.38), (1.39), system and, practically, is a modification of PT in the form of Vigner–Brillouin over operator $\hat{H}_1$. In this case the higher approximation computing is reduced not to the calculation of corrections to zeroth order values, as it is in (1.44), but to computing sequences of $E_n^{(s)}$ and $C_{nk}^{(s)}$,

$$E_n = \lim_{s \to \infty} E_n^{(s)}, \qquad C_{nk} = \lim_{s \to \infty} C_{nk}^{(s)}. \tag{1.50}$$

The two neighbouring terms of sequences (1.50) satisfy the algebraic recurrences, which appear in the iteration of exact equations (1.38), (1.39),

$$E_n^{(s)} = H_{nn}(\omega) + \sum_{k \neq n} C_{nk}^{(s-1)} H_{kn}(\omega),$$

$$C_{nk}^{(s)} = [E_n^{(s-1)} - H_{kk}]^{-1} \left\{ H_{nk}(\omega) + \sum_{m \neq k,n} H_{nm}(\omega) C_{mn}^{(s-1)} \right\}, \tag{1.51}$$

$$E_n^{(0)} = H_{nn}, \qquad C_{nk}^{(0)} = 0. \tag{1.52}$$

The volume of calculations required to compute high order approximations by formulas (1.51) is essentially less than using PT in the form of Vigner–Brillouin, when we need to solve a sufficiently complex nonlinear equation relative to $E_n^{(s)}$ to calculate the energy in sth-approximation [59]:

$$E_n^{(s)} = H_{nn} + \sum_{k \neq n} H_{kn} [E_n^{(s)} - H_{kk}]^{-1} \left\{ H_{nk} + \sum_{m \neq k,n} H_{nm} C_{mn}^{(s-1)} \right\}.$$

At the same time, the calculation of both energy and wave functions of the given state with any precision by an iteration scheme (1.51) with the initial condition (1.52) requires a single calculation of a sufficient amount of terms for a recurrent sequence (1.51) which proves to converge evenly in the whole range of parameter ω values satisfying the condition

$$\omega > \omega_n, \tag{1.53}$$

where ω_n is the Eq. (1.26) solution. The results of such a calculation for QAO are listed in Table V, which shows that the rate of convergence hardly depends on the choice of a specific value of ω. A record precision was reached in [35] on the basis of these formulas for the QAO energy level calculation.

TABLE V

Convergence of the OM Iteration Scheme (1.51)

	$(n; \lambda)$	
$E_n^{(s)} - E_n^{(s-1)}$	(10; 10)	(0; 1)
$s = 4$	$-0.1212077 \cdot 10^{-5}$	$-0.911329466 \cdot 10^{-8}$
$s = 8$	$-0.10778 \cdot 10^{-9}$	$0.3108703 \cdot 10^{-10}$
$s = 12$	$0.737 \cdot 10^{-11}$	$0.4712 \cdot 10^{-11}$
$s = 16$	$0.57 \cdot 10^{-13}$	$0.172 \cdot 10^{-14}$
$E_n^{(\text{exact})}$ $(s \geqslant 25)$	68.80369551829225	0.8037706512344274

We hope that the reader, who had the patience to reach formula (1.53), has suspected already that the SE solution for QAO is not an aim in itself. Therefore, despite the simplicity of iteration scheme (1.51), we improve it in such a way that it is not connected with specific QAO properties. The fact is that we should make a summation over all state $|k\rangle$, for which the operator $\hat{H}$ provides nonzero transition probability to calculate every iteration in (1.51) at certain n. In the case of QAO $\hat{H}$ has only four nonzero matrix elements at a given n, which cuts down the volume of calculation for this specific problem. However, in the common case of non-polynomial Hamiltonian, the number of matrix elements H_{nk} will be infinite and the problem concerning the principle of limitation for the summation over k in (1.5) arises in real numerical calculations.

In connection with this we recall once again that the OM zeroth approximation $E_n^{(0)} = H_{nn}$, when transitions in states different from $|n\rangle$ are not considered at all, correctly describes the qualitative peculiarities of the system energy spectrum. Thus, it is natural to expect that the value of corrections to the zeroth approximation, determined by the influence of other states $|k\rangle$, $k \neq n$, decreases with the growth of the difference $l = |n - k\rangle$. This might be settled by using the representation

$$H_{n,k} = \sum_{l=1}^{\infty} \{ V_{nl}^{(+)} \delta_{k,n+l} + V_{nl}^{(-)} \delta_{k,n-l} \}, \qquad k \neq n, \tag{1.54}$$

where

$$V_{nl}^{(\pm)} = H_{n,n\pm l}.$$

Let us suppose that every term of series (1.54) is to be taken into account, starting only from such element of sequences (1.50) for which the iteration number s coin-

cides with the "transition length" $l=|n-k|$. Then the recurrent relations (1.51) result in the expressions

$$E_n^{(s)}=H_{nn}+\sum_{l=1}^{s-1}\{C_{n,n+l}^{(s-l)}V_{nl}^{(+)}+C_{n,n-l}^{(s-l)}V_{nl}^{(-)}\},$$
$$C_{nk}^{(s)}=\frac{H_{nk}}{E_n^{(s-1)}-H_{kk}}+\sum_{l=1}^{s-1}\left\{\frac{V_{nl}^{(+)}}{E_n^{(s-l)}-H_{kk}}C_{n+l,k}^{(s-l)}+\frac{V_{nl}^{(-)}}{E_n^{(s-l)}-H_{kk}}C_{n-l,k}^{(s-l)}\right\}, \tag{1.55}$$

with the initial conditions (1.54) remaining invariant.

To calculate any approximation, summation is to be carried out only in finite limits due to the use of formulas (1.55), which determine the iteration scheme with successive inclusion of Hamiltonian matrix elements. These relations are the basis of the calculating procedure of the OM for the SE solution with any precision for discrete spectrum states.

Matrix elements (1.42), where $l=2$ and $l=4$ for QAO, are divided into two classes, from the point of view of expansion (1.54). It is interesting to compare the results of calculations by formulas (1.55) with a similar one based on the full iteration scheme (1.51) for this problem. This comparison shows that successive inclusion of matrix elements does not lead to tangible changes in the convergence rate of OM but makes this convergence smoother. Convergence of the OM iteration scheme (1.51) is shown in Table V.

1.3. *About a Precision of the Wave Function Calculation*

The results of the previous sections show that the OM permits one to find the QAO eigenvalue spectrum with any precision. However, for any method of the SE solution, precision of the eigenfunction calculation is a much more serious test due to the importance of eigenfunctions for applications.

We use several criteria to determine the wave function qualities. First we consider matrix elements of different operators. For this it is interesting to discuss separately the results of the OM zeroth approximation and, also, to consider the possibility of exact calculation of matrix elements by the iteration scheme (1.55).

The case appears to be simple when we calculate the diagonal matrix elements since they are reduced to the well-known matrix elements of transition between harmonic oscillator states. For instance, the formulas of value x_{nn}^2 calculation in the zeroth approximation ($(x_{nn}^2)_0$) and after s iterations ($(x_{nn}^2)_s$) have the form

$$(x_{nn}^2)_0=\langle n(\omega_n)|\frac{1}{2\omega_n}(a^{+2}+a^2+2a^+a+1)\,|n(\omega_n)\rangle=\frac{2n+1}{2\omega_n};$$
$$(x_{nn}^2)_s=\langle\psi_n^{(s)}|\frac{1}{2\omega}(a^{+2}+a^2+2a^+a+1)\,|\psi_n^{(s)}\rangle\cdot\langle\psi_n^{(s)}|\psi_n^{(s)}\rangle^{-1}; \tag{1.56}$$
$$|\psi_n^{(s)}\rangle=|n(\omega)\rangle+\sum_{k\neq n}C_{nk}^{(s)}|k(\omega)\rangle;$$

$$\langle\psi_n^{(s)}|\psi_n^{(s)}\rangle\equiv A_n^{(s)}=1+\sum_{k\neq n}[C_{nk}^{(s)}]^2; \tag{1.57}$$

$$(x^2_{nn})_s = \frac{1}{2\omega A^{(s)}_n}\Big\{2n+1+\sum_{k\neq n}(2k+1)[C^{(s)}_{nk}]^2+\sqrt{n(n-1)}\,C^{(s)}_{n,n-2}$$
$$+\sqrt{(n+1)(n+2)}\,C^{(s)}_{n,n+2}+\sum_{k\neq n}\Big[\sqrt{k(k-1)}\,C^{(s)}_{nk}C^{(s)}_{n,k-2}$$
$$+\sqrt{(k+1)(k+2)}\,C^{(s)}_{nk}C^{(s)}_{n,k+2}\Big]\Big\}.$$

In formula (1.56) parameter ω_n is the Eq. (1.22) solution. In (1.57) ω takes any value for which iterations (1.55) converge. Results listed in Table VI show that in calculating diagonal matrix elements OM has the same characteristics as in calculating eigenvalues; zeroth order produces evenly valid approximation at every λ. Matrix element value $(x^2_{nn})_s$ rate of convergence to the exact value x^2_{nn} is of the same order, that is, for $E^{(s)}_n$.

Calculation of nondiagonal matrix elements requires additional consideration. In order to be fully confident we take into account values $x_{n,n+k}$ which are used to calculate the dipole transition possibility. The problem is that in zeroth approximation it is necessary to compute the values

$$(x_{n,n+k})_0 = \langle n, \omega_n\,|\hat{x}|\,n+k, \omega_{n+k}\rangle, \tag{1.58}$$

in which different frequencies ω_n and ω_{n+k} correspond to the initial and finite states. Operator $\hat{x}$ might be represented in terms of operators a_ω and a^+_ω, related to any of the frequencies. To remove this uncertainty and to preserve the algebraic

TABLE VI

Calculation Results for QAO Matrix Elements and the Inverse Problem ($\hat{H} = \frac{1}{2}(\hat{p}^2+\hat{x}^2)+\alpha\hat{x}^3+\lambda\hat{x}_4$ [24])

α	0.0	1.0	1.0
λ	1.0	1.0	0.6
$x^{(0)}_{01}$	0.501263	0.528346	0.594462
$x^{(s\geq 8)}_{01}$	0.506600	0.527097	0.595176
$x^{(0)}_{03}$	0.023587	0.029017	0.298617
$x^{(s\geq 8)}_{03}$	0.022483	0.027096	0.031825
$n_2 \to n_1$ ($\alpha = 0$)	$1 \to 0$	$3 \to 0$	$2 \to 1$
$\Omega^{[52]}_{n_2 n_1}$	1.934221	8.775756	5.025446
λ	1	2	10
$\lambda^{(0)}$	0.998562	1.999673	9.994531
$\lambda^{(10)}$	0.999998	1.999998	9.999985
$E^{(10)}_{n_1} = E^{[52]}_{n_1}$	0.803771	0.954568	5.321609

nature of the calculations we construct operator $R(\omega, \omega')$ which transforms the state $|n, \omega\rangle$ to the state $|n, \omega'\rangle$, corresponding to the other frequency ω' [23]. As a basis of construction of $\hat{R}(\omega, \omega')$ we use the invariance of coordinate $\hat{x}$ and momentum $\hat{p}$ operators under the transformations

$$\begin{aligned} \hat{x} &= \frac{1}{\sqrt{2\omega}}(a_\omega^+ + a_\omega) = \frac{1}{\sqrt{2\omega'}}(a_{\omega'}^+ + a_{\omega'}), \\ \hat{p} &= i\sqrt{\frac{\omega}{2}}(a_\omega^+ - a_\omega) = i\sqrt{\frac{\omega'}{2}}(a_{\omega'}^+ - a_{\omega'}); \end{aligned} \tag{1.59}$$

that is,

$$\begin{aligned} a_{\omega'}^+ &= \left(\sqrt{\frac{\omega'}{\omega}} + \sqrt{\frac{\omega}{\omega'}}\right) a_\omega^+ + \left(\sqrt{\frac{\omega'}{\omega}} - \sqrt{\frac{\omega}{\omega'}}\right) a_\omega \\ a_{\omega'} &= \left(\sqrt{\frac{\omega'}{\omega}} + \sqrt{\frac{\omega}{\omega'}}\right) a_\omega + \left(\sqrt{\frac{\omega'}{\omega}} - \sqrt{\frac{\omega}{\omega'}}\right) a_\omega^+. \end{aligned} \tag{1.59a}$$

One can find the explicit form of the operator $\hat{R}(\omega, \omega')$ realizing the transformation (1.3),

$$\begin{aligned} \hat{R}(\omega', \omega) &= \exp\left\{\frac{1}{4}(a_\omega^{+2} - a_\omega^2)\ln\frac{\omega'}{\omega}\right\}; \\ a_{\omega'} &= \hat{R}(\omega', \omega)\, a_\omega \hat{R}^{-1}(\omega', \omega), \qquad |n, \omega'\rangle = \hat{R}(\omega', \omega)\,|n, \omega\rangle, \end{aligned} \tag{1.60}$$

by using simple identities arising from the algebra of creation and annihilation operators. Since there are only quadratic combinations of the operators a_ω and a_ω^+ in the exponent index of $\hat{R}(\omega, \omega')$ the latter can be reduced to normal form exactly [60],

$$\hat{R}(\omega', \omega) = \exp(\varphi_1 a_\omega^{+2}) \exp[\varphi_2(a_\omega^+ a_\omega + \tfrac{1}{2})] \exp(-\varphi_1 a_\omega^2), \tag{1.61}$$

where

$$\varphi_1 = \frac{\omega - \omega'}{2(\omega + \omega')}, \qquad \varphi_2 = \ln\frac{2\sqrt{\omega\omega'}}{\omega + \omega'}.$$

By using (1.61) in formula (1.58), we find the following expression for the considered matrix element in the zeroth approximation:

$$\begin{aligned} (x_{n,n+k})_0 &= \left\langle n, \omega_n \left| \frac{a_{\omega_n}^+ + a_{\omega_n}}{\sqrt{2\omega_n}} \hat{R}(\omega_{n+k}, \omega_n) \right| n+k, \omega_n \right\rangle \\ &= \frac{1}{\sqrt{2\omega_n}} \{\sqrt{n}\langle n-1|\, \hat{R}(\omega_{n+k}, \omega)\,|n+k\rangle \\ &\quad + \sqrt{n+1}\langle n+1|\, \hat{R}(\omega_{n+k}, \omega)\,|n+k\rangle\}. \end{aligned} \tag{1.62}$$

For example,

$$(x_{01})_0 = \frac{1}{\sqrt{2\omega_0}} \left[\frac{2\sqrt{\omega_0 \omega_1}}{\omega_0 + \omega_1} \right]^{3/2}.$$

At the same time the $(x_{n,n+k})_s$ calculation formula is similar to (1.57) after s iterations, since the recurrent relations (1.55) converge in a wide range of frequencies ω, and coefficients C_{nk} of the initial and finite states can be computed at the same values of the parameter ω,

$$(x_{n,n+k})_s = \frac{1}{\sqrt{2\omega A_n^{(s)} A_{n+k}^{(s)}}} \left\{ \sqrt{n+1}\, \delta_{k,1} + \sqrt{n}\, \delta_{k,-1} + \sum_{j \neq n} C_{nj} [\sqrt{j}\, C_{n+k,j-1} + \sqrt{j+1}\, C_{n+k,j+1}] + \sqrt{n}\, C_{n+k,n-1} + \sqrt{n+1}\, C_{n+k,n+1} \right\}. \tag{1.63}$$

Here we have taken into account the normalizing condition $\langle n | \psi_n^{(0)} \rangle = 1$ for wave functions. The results of calculations by formulas (1.62) and (1.63) are also listed in Table VI.

The possibility of conversion of the OM under Hamiltonian parameters is a good test for the iteration scheme (1.55) as well. This task also arises in describing real physical systems, when it is required to determine potential parameters by given frequencies of transitions between energy levels (the inverse problem of spectroscopy [61]). Let us show that this problem can be also reduced to the recurrent formulas, analogous to (1.55), for calculation of the parameter λ in the QAO Hamiltonian represented in the form

$$\hat{H} = (\hat{H}_0 + \hat{H}_1) + \lambda(\hat{V}_0 + \hat{V}_1), \tag{1.64}$$

where $\hat{H}_0 + \hat{H}_1$ is the harmonic oscillator Hamiltonian and $\hat{V}_0 + \hat{V}_1$ is the anharmonic part of the potential, divided into diagonal and nondiagonal parts, according to the recipe of the OM:

$$\hat{H}_0 = \frac{1}{4}\left(\omega + \frac{1}{\omega}\right)(2\hat{n} + 1), \qquad \hat{H}_1 = \frac{1}{4}\left(\frac{1}{\omega} - \omega\right)(a^{+2} + a^2), \qquad \hat{n} = a^+ a,$$

$$\hat{V}_0 = \frac{3}{4\omega^2}(1 + 2\hat{n} + 2\hat{n}^2), \tag{1.65}$$

$$\hat{V}_1 = \frac{1}{4\omega^2}[6(a^2 + a^{+2}) + a^4 + a^{+4} + 4(\hat{n}a^2 + a^{+2}\hat{n})].$$

Let us suppose that we know the transition frequencies,

$$\Omega_{mn} = E_m - E_n.$$

Using expansions

$$|\psi_m\rangle = |m\rangle + \sum_{l \neq m} C_{ml} |l\rangle, \qquad |\psi_n\rangle = |n\rangle + \sum_{k \neq n} C_{nk} |k\rangle,$$

we obtain equations analogous to (1.38) for energy levels E_m and E_n,

$$E_m = H_{mm} + \lambda V_{mm} + \sum_{l \neq m} C_{ml}(H_{lm} + \lambda V_{lm}), \tag{1.66}$$

$$C_{ml} = -[H_{ll} + \lambda V_{ll} - E_m]^{-1} \left\{ H_{ml} + \lambda V_{ml} + \sum_{i \neq m,l} C_{mi}(H_{il} + \lambda V_{li}) \right\},$$

$$E_n = H_{nn} + \lambda V_{nn} + \sum_{k \neq n} C_{nk}(H_{kn} + \lambda V_{kn}), \tag{1.67}$$

$$C_{nk} = -[H_{kk} + \lambda V_{kk} - E_n]^{-1} \left\{ H_{nk} + \lambda V_{nk} + \sum_{j \neq n,k} C_{nj}(H_{jk} + \lambda V_{jk}) \right\}.$$

Solution of these equations in the zeroth approximation over operators $\hat{H}_1$ and $\hat{V}_1$ permits one to express the anharmonicity constant λ and the absolute value of energy E_n in terms of the transition frequency:

$$C_{nk}^{(0)} = C_{ml}^{(0)} = 0,$$

$$\lambda^{(0)} = \frac{\Omega_{mn} - (H_{mm} - H_{nn})}{V_m^{(0)} - V_l^{(0)}}, \qquad E_n^{(0)} = H_{nn} + \lambda^{(0)} V_{nn}, \tag{1.68}$$

$$\frac{\partial \lambda^{(0)}}{\partial \omega} = 0, \qquad \omega = \frac{2\Omega_{mn}}{m - n}. \tag{1.69}$$

In this case it is natural to determine these values as the initial conditions for recurrent formulas arising in the iteration of exact equations (1.66), (1.67):

$$\lambda^{(s)} = [V_{mm} - V_{nn}]^{-1} \left\{ \Omega_{mn} - \sum_{l \neq m} C_{ml}^{(s-1)}(H_{lm} + \lambda^{(s-1)} V_{lm}) \right.$$

$$\left. + \sum_{k \neq n} C_{nk}^{(s-1)}(H_{kn} + \lambda^{(s-1)} V_{kn}) - (H_{mm} - H_{nn}) \right\};$$

$$E_n^{(s)} = H_{nn} + \lambda^{(s-1)} V_{nn} + \sum_{k \neq n} C_{nk}^{(s-1)}(H_{kn} + \lambda^{(s-1)} V_{kn}); \tag{1.70}$$

$$C_{nk}^{(s)} = -[H_{kk} + \lambda^{(s-1)} V_{kk} - E_n^{(s-1)}]^{-1} \left\{ H_{nk} + \lambda^{(s-1)} V_{nk} \right.$$

$$\left. + \sum_{j \neq n,k} C_{nj}^{(s-1)}(H_{jk} + \lambda^{(s-1)} V_{jk}) \right\}.$$

So as it is in (1.51), the exact values of the desired quantities are defined as limits of the corresponding consequences:

$$\lambda = \lim_{s \to \infty} \lambda^{(s)}, \qquad E_n = \lim_{s \to \infty} E_n^{(s)}.$$

By analogy with (1.55), iteration scheme (1.70) can be generalized for non-polynomial interaction potentials used in modelling interatomic potentials [61]. Comparing the exact values of λ with one calculated by (1.70), carried out in Table VI, shows that OM is also efficient in solving the inverse problem, as it is in SE solving.

The above-considered examples relate to calculations with the wave functions corresponding to small quantum numbers when these functions have a small number of nodes. Thus it is interesting to put to one more test the quality of the wave functions found by OM, so that we may consider such system characteristics which are defined by quickly oscillating wave functions of highly excited states. We deal with such characteristics, for example, in studying the properties of the quantum mechanical systems in the classic limit which corresponds to the Plank constant $\hbar \to 0$. In considering this limit by OM we can act in the following way. First we find approximate analytical solutions to the SE for an arbitrary quantum number n,

$$(\hat{H} - E_n)\,\psi_n(x) = 0, \tag{1.71}$$

with the Hamiltonian

$$\hat{H} = \frac{1}{2}\,\hat{p}^2 + v(\hat{x}), \qquad \hat{p} = -i\hbar \frac{d}{dx}, \tag{1.72}$$

where $v(x)$ is any arbitrary potential. With these solutions one can determine time dependence of the average value of the coordinate $\hat{x}$ operator at an arbitrary initial state. Then we pass over to the limit $\hbar \to 0$ in the obtained expression (for this, $n \to \infty$ so that the system energy should remain a finite value) and we find the classic law of motion $x(t)$ which should be the approximate solution to Newton's equation

$$\frac{d^2x(t)}{dt^2} = -\frac{\partial v(x)}{\partial x}. \tag{1.73}$$

For systems with the Hamilton function (1.72), the mentioned scheme of the limit transition might be considered as a uniformly fitted method in the theory of non-linear oscillations of classic Hamilton systems [23] having a wider field of application in comparison with known asymptotic methods of averaging (see, e.g., [62]). It permits one to find oscillation characteristics at any values of the system of physical parameters, as will be shown below.

We consider specific calculations by an example of problem (1.71), having supposed that a part of Eq. (1.71) solutions relates to a discrete spectrum. This corresponds to the existance of periodic solutions in the equation (1.71) in the classic limit. In addition for simplicity we suppose function $v(x)$ to be an even function of its argument.

Carrying out canonic transformation

$$\hat{x} = \frac{\hbar}{2\omega}(a^+ + a), \qquad \hat{p} = i\frac{\hbar\omega}{2}(a^+ - a), \qquad aa^+ - a^+a = 1, \tag{1.74}$$

we reduce Hamiltonian (1.72) to the form

$$\hat{H} = \frac{1}{4}\hbar\omega(1 + 2a^+a - a^{+2} - a^2) + \frac{1}{2\pi}\int_{-\infty}^{\infty} dy\, v(y) \int_{-\infty}^{\infty} dk\, e^{-iky} e^{-\hbar k^2/4\omega} e^{ik\sqrt{\hbar/2\omega}\, a^+} e^{ik\sqrt{\hbar/2\omega}\, a}. \tag{1.75}$$

According to the recipe of the OM for Eq. (1.71) in the zeroth approximation we extract the part of Hamiltonian (1.75) which commutates with the excitation number operator $\hat{n} = a^+a$,

$$\hat{H} = \hat{H}_0 + \hat{H}_1, \tag{1.76}$$

where

$$\hat{H}_0 = \frac{\hbar\omega}{4}(1 + 2a^+a) + \frac{1}{2\pi}\int_{-\infty}^{\infty} dy\, v(y) \int_{-\infty}^{\infty} dk\, e^{-\hbar k^2/4\omega} \sum_{s=0}^{\infty} \frac{(-1)^s}{(s!)^2}\left(\frac{\hbar}{2\omega}\right) k^{2s}(a^+)^s a^s; \tag{1.77}$$

$$\hat{H}_1 = -\frac{\hbar\omega}{4}(a^{+2} + a^2) + \frac{1}{2\pi}\int_{-\infty}^{\infty} dy\, v(y) \int_{-\infty}^{\infty} dk\, e^{-iky} e^{-\hbar k^2/4\omega} \left(e^{ik\sqrt{\hbar/2\omega}\, a^+} e^{ik\sqrt{\hbar/2\omega}\, a} - \sum_{s=0}^{\infty} \frac{(-1)^s}{(s!)^2}\left(\frac{\hbar}{2\omega}\right)^s k^{2s}(a^+)^s a^s \right). \tag{1.78}$$

In accordance with the definition, operator $\hat{H}_0$ eigenvectors are the vectors

$$|n\rangle = \frac{1}{\sqrt{n!}}(a^+)^n |0\rangle, \qquad n = 0, 1, 2, \ldots, \qquad a|0\rangle = 0, \tag{1.79}$$

belonging to the eigenvalues

$$E_n^{(0)} = \frac{\hbar\omega}{4}(1+2n) + \frac{1}{2\pi}\int_{\infty}^{\infty} dy\, v(y) \int_{-\infty}^{\infty} dk\, e^{-iky} e^{-\hbar k^2/4} \times \sum_{s=0}^{n} \frac{(-1)^s}{(s!)^2} \frac{n!}{(n-s)!} \left(\frac{\hbar k^2}{2\omega}\right)^s. \tag{1.80}$$

We carry out the transition to the classic limit in expression (1.82) for eigenvalues in the following way. Supposing that in the given limit,

$$h \to 0, \quad n \to \infty, \qquad \hbar n \to \beta = \text{const}, \tag{1.81}$$

and taking into account that for $n \to \infty$

$$\frac{n!}{(n-s)!} \to n^s,$$

we find the energy of classic motion in the field of potential $v(x)$ using the following formula:

$$\lim_{\substack{h\to 0 \\ n\to\infty}} E_n^{(0)} = E = \frac{1}{2}\omega\beta + \frac{1}{2\pi}\int_{-\infty}^{\infty} dy\, v(y) \int_{-\infty}^{\infty} dk\, e^{-iky} \times \sum_{s=0}^{\infty} \frac{(-1)^s}{(s!)^2} \left(\frac{1}{2} k \sqrt{2\beta/\omega}\right)^{2s}, \tag{1.82}$$

which brings together energy E with parameter β. Let us note that the value β might be considered with respect to an arbitrary choice of the parameter ω. Taking note of that the sum in the right part of Eq. (1.82) is the Bessel function $J_0(k\sqrt{2\beta/\omega})$ and, using integral [63],

$$\int_0^{\infty} dk \cos ky J_0(k\sqrt{2\beta/\omega}) = \begin{cases} \sqrt{2\beta/\omega - y^2}, & \dfrac{2\beta}{\omega} - y^2 > 0; \\ 0, & \dfrac{2\beta}{\omega} - y^2 < 0, \end{cases} \tag{1.83}$$

we finally found the formula

$$E = \frac{1}{2}\omega\beta + \frac{2}{\pi}\int_0^{\sqrt{2\beta\omega^{-1}}} dy \frac{v(y)}{\sqrt{2\beta\omega^{-1} - y^2}}. \tag{1.84}$$

Expression (1.84) derives from Hamiltonian (1.72) eigenvalue formulas, obtained in the OM zeroth approximation. If in calculating the mentioned eigenvalues one takes into account the corrections caused by perturbation operator $\hat{H}_1$, this leads,

generally speaking, to the change in Eq. (1.84) form. However, Eq. (1.84) remains unchanged with respect to these corrections as well. This happens when the optimal value of the parameter ω is chosen from the condition that the second-order correction to the zeroth approximation eigenvalues over H_1 approaches to zero (the OM first-order correction equals zero by definition). Application of this condition after a transition to the classic limit results in the following equation which determines parameter ω (we omit calculation details since they are analogous to the transition from (1.80) to (1.84)):

$$-\frac{\omega^2\beta}{8v}-\frac{1}{8}\omega^2\beta^2 A+\frac{\omega}{8\pi v}\int_0^\zeta dy\,\frac{yv'(y)}{\sqrt{\zeta^2-y^2}}+\frac{2\omega\beta A}{\pi}\int_0^\zeta dy\,\frac{v(y)}{\sqrt{\zeta^2-y^2}}\left(2\frac{y^2}{\zeta^2}-1\right)$$
$$-\frac{1}{\pi\beta v}\int_0^\zeta dy\,\frac{yv'(y)\,v(y)}{\sqrt{\zeta^2-y^2}}+\frac{2}{\pi^2\beta v}\int_0^\zeta dy\,\frac{yv'(y)}{\sqrt{\zeta^2-y^2}}\int_0^\zeta dz\,\frac{v(z)}{\sqrt{\zeta^2-z^2}}$$
$$+\frac{4A}{\pi^2}\left(\int_0^\zeta dy\,\frac{v(y)}{\sqrt{\zeta^2-y^2}}\right)^2-\frac{2A}{\pi}\int_0^\zeta dy\,\frac{v^2(y)}{\sqrt{\zeta^2-y^2}}=0, \tag{1.85}$$

where to shorten the expression we introduced the signs

$$\zeta=\sqrt{2\beta/\omega};\qquad v=\frac{1}{2}\omega+\frac{1}{\pi\beta}\int_0^\zeta dy\,\frac{yv'(y)}{\sqrt{\zeta^2-y^2}},\qquad v'(y)=\frac{dv}{dy},$$
$$A=\frac{\zeta^2}{4\pi v^2\beta^2}\int_0^\zeta dy\,\frac{v''(y)}{\sqrt{\zeta^2-y^2}}\left(2\frac{y^2}{\zeta^2}-1\right).$$

Thus, the classic motion energy E dependence on the problem parameters ω and β is defined by algebraic equations (1.84) and (1.85), without defining the potential function $v(x)$ form. Let us also note, that, if we use the condition of the eigenvalue E independence on the parameter ω (see Section 1.1), but not the optimal choice of this parameter, we obtain a much more simple equation,

$$\frac{\partial E}{\partial\omega}=\frac{1}{2}\beta-\frac{4}{\pi\omega}\left\{1+\zeta^2\int_0^\zeta\frac{dy}{(\zeta^2+y)\sqrt{\zeta^2-y^2}}\left[v'(y)-\frac{3}{2}\frac{v(y)}{\zeta+y}\right]\right\}=0, \tag{1.86}$$

instead of (1.85).

As we see below Eq. (1.86) provides less accuracy than (1.85) does in calculating the parameters of classic motion law, but it allows presenting the results in an analytical form.

Let us turn now to defining the classic law of motion $x(t)$ based on the approximate solution of the SE found above. Let us suppose that we know the exact eigenfunctions $|\psi_m\rangle$ and corresponding eigenvalues E_m and construct the wave packet

$$|\psi(t)\rangle=\sum_m C_m e^{-(i/\hbar)E_m(t-t_0)}|\psi_m\rangle,\qquad \sum_m |C_m|^2=1. \tag{1.87}$$

Coefficients C_m determine the packet form at $t = t_0$. According to the general rules of quantum mechanics we find the average value of the coordinate $\hat{x}$ operator in the state (1.87)

$$x(t) = \sum_{mm'} C^*_{m'} C_m e^{(i/\hbar)(E_{m'} - E_m)(t - t_0)} \langle \psi_{m'} | \hat{x} | \psi_m \rangle, \tag{1.88}$$

or

$$x(t) = \sum_{mk} C^*_{m+k} C_m e^{(i/\hbar)(E_{m+k} - E_m)(t - t_0)} \langle \psi_{m+k} | \hat{x} | \psi_m \rangle. \tag{1.89}$$

Classic trajectory of a particle corresponds to such a wave packet in which the coefficients C_m, as a function of m, have a maximum near value $n \gg 1$, defined by (1.81) and (1.82):

$$E_n = E, \qquad \hbar n = \beta.$$

This definition shows that the classical law of motion does not depend on the wave packet form and is defined by the expression

$$x(t) = \sum_{k=-\infty}^{\infty} e^{ik\Omega(t - t_0)} \lim_{\substack{\hbar \to 0 \\ n \to \infty}} \langle \psi_{n+k} | \hat{x} | \psi_n \rangle, \tag{1.90}$$

where

$$\Omega = \partial E / \partial \beta \tag{1.91}$$

is the frequency of the classical periodic motion.

For the following calculations we use approximate expressions, obtained by OM for wave vectors of stationary states $|\psi_n\rangle$ in (1.90). In the zeroth approximation these wave functions are defined by formula (1.79), i.e.,

$$|\psi_n^{(0)}\rangle = |n, \omega_n\rangle, \tag{1.92}$$

where it is specially noted that in the OM zeroth approximation every state with n excitations corresponds its own value ω_n due to the choice of the parameter ω described above. Owing to this the states $|n, \omega_n\rangle$ and $|m, \omega_m\rangle$ are nonorthogonal at $m \neq n$ and that results in some change of definition (1.90) for the classical law of motion,

$$x^{(0)}(t) = \frac{1}{N(t)} \sum_{k=-\infty}^{\infty} e^{ik\Omega(t - t_0)} \lim_{\substack{\hbar \to 0 \\ n \to \infty}} \langle n + k, \omega_{n+k} | \hat{x} | n, \omega_n \rangle, \tag{1.93}$$

where

$$N(t) = \sum_{k=-\infty}^{\infty} e^{ik\Omega(t - t_0)} \lim_{\substack{\hbar \to 0 \\ n \to \infty}} \langle n + k, \omega_{n+k} | n, \omega_n \rangle. \tag{1.94}$$

Further calculations are based on use of the unitary transformation (1.62). Using the transformation operator normal form (1.63) we find, for example, that

$$\langle n+k, \omega_{n+k} | n, \omega_n \rangle = (\operatorname{ch} 2\zeta)^{-1/2} \langle n+k | e^{-(A^+/2)\, th 2\zeta} e^{-\hat{n} \ln \operatorname{ch} 2\zeta} e^{(A/2)\, th 2\zeta} | n \rangle, \quad (1.95)$$

where

$$\zeta = \frac{1}{4} \ln \frac{\omega_{n+k}}{\omega_n} \simeq \frac{1}{2} \gamma \frac{k}{n}, \qquad \gamma = \frac{\beta}{2\omega} \frac{\partial \omega}{\partial \beta}, \quad (1.96)$$

and now all the operators and wave vectors have been reduced already to the same value of the parameter ω_n. Carrying out the limit transition in formula (1.95), we find that

$$\lim_{\substack{\hbar \to 0 \\ n \to \infty}} \langle n+k, \omega_{n+k} | n, \omega_n \rangle = \begin{cases} J_{(1/2)k}(\gamma k), & k = 2l, \\ 0, & k = 2l+1, \end{cases} \quad (1.97)$$

where $J_\nu(x)$ is the νth-order Bessel function. Then, applying the integral representation of the Bessel function [63]

$$J_k(z) = \frac{1}{\pi} \int_0^\pi d\varphi \cos(k\varphi - z \sin \varphi), \quad (1.98)$$

one can reduce the expression for the normalizing factor $N(t)$ to the form ($t_0 = 0$)

$$N(t) = 1 + \frac{2}{\pi} \int_0^\pi \lim_{\varepsilon \to 0} \sum_{k=1}^{\infty} e^{-\varepsilon k} \cos(2\Omega t k) \cos(k\varphi - 2\gamma k \sin \varphi) \quad (1.99)$$

and takes its final form after carring out summation and integration,

$$N(t) = \frac{1}{1 - 2\gamma \cos \varphi}, \quad (1.100)$$

with phase φ being determined by the equation

$$\Omega t - \tfrac{1}{2}\varphi + \gamma \sin \varphi = 0. \quad (1.101)$$

When doing similar calculations in the numerator of formula (1.93), we find that the use of the OM zeroth approximation for eigenvalues and eigenfunctions of the Hamiltonian in the range of high quantum numbers leads to the following expression for the classical law of motion

$$x^{(0)}(t) = \sqrt{(2\beta/\omega)} \cos \frac{\varphi}{2}, \quad (1.102)$$

with phase φ being defined by Eqs. (1.101). The parameters β, γ, ω, and Ω are defined by classical motion energy E by formulas (1.84), (1.85) or (1.86), (1.91),

and (1.96). Let us note that the parameter ω value proves to coincide exactly with classical motion frequency in using the simple equation (1.86) to calculate this parameter, i.e.,

$$\omega(E) = \Omega(E). \tag{1.103}$$

Having finished with the bulky analytical computations in general case, we pass over to quantitative comparison of the results obtained above with exact solution of the specific problem concerning the classical law of motion of AO, which is the main feature of this section.

In this case function $x(t)$ is the solution of the differential equation in the form (1.73)

$$\frac{d^2x}{dt^2} + x + 4\lambda x^3 = 0 \tag{1.104}$$

and is known to be defined by the formula

$$x(t) = \left[\frac{\sqrt{1+16\lambda E}-1}{4\lambda}\right]^{1/2} cn(\tau, k), \tag{1.105}$$

where

$$\tau = t(1+16\lambda E)^{1/4}, \qquad k^2 = \frac{1}{2}\left[1 - \frac{1}{\sqrt{1+16\lambda E}}\right];$$

E is the energy of the classical motion, $cn(\tau, k)$ is the elliptical Jakobi function.

The classical motion frequency is defined by the following expression

$$\Omega = \frac{\pi}{2K(k)}(1+16\lambda E)^{1/4}, \tag{1.106}$$

where $K(k)$ is the full elliptical integral of the first kind [63].

Let us recall also that the application of well-known methods of averaging for this problem [62] allows one to find only asymptotic expansions for functions (1.105) and (1.106), which are valid at $\lambda E \ll 1$.

Within the limits of the OM zeroth approximation analytical formula for a classical AO oscillation frequency might be found by Eq. (1.86) and relation (1.103)

$$\Omega_0(E) = \left(\frac{1+2\sqrt{1+18\lambda E}}{3}\right)^{1/2}.$$

The results of the calculation of the oscillation period $T^{(0)}(E) = 2\pi/\Omega_0(E)$ by this formula are listed in the Table VII as a function of the dimensionless parameter λE. These results have been compared with the exact values of period $T(E)$ and function $T_2(E)$, obtained by Eq. (1.85) which corresponds to the second order of the

TABLE VII

Oscillation Period and Motion Law of a Classical AO

	λE				
T	0.1	0.5	1.0	10	$(\lambda E)^{1/4} T$, $\lambda E \gg 1$
$T(E)$	5.21198	4.00431	3.47306	2.04604	3.70815
$T^{(2)}(E)$	5.21195	4.00425	3.47302	2.04605	3.70820
$T^{(0)}(E)$	5.21992	4.02115	3.49105	2.06007	3.73600
	$\tau = 2(\lambda E)^{1/4} t$, $\lambda E \gg 1$				
x	0	0.4	1.0	1.4	1.6
$x(\tau)$	1	0.923	0.596	0.321	0.176
$x^{(0)}(\tau)$	1.017	0.905	0.551	0.293	0.164

OM. In the same table the laws of the AO motion obtained by the exact formula (1.105) and the approximate one (1.102) are compared in the case of $\lambda E \gg 1$ which is the most unfavourable from the point of view of result precision of the consideration described above. Formulas (1.101) and (1.102) obtained above have the universal form which does not depend on the form of the potential function. If anharmonicity parameter $\lambda \ll 1$ they lead to the same results that the asymptotical method of averaging does [62]. However, Table VII shows that these formulas provide motion laws similar to the exact one in the case of $\lambda E \gg 1$. Thus obtained results indicate that OM provides evenly valid interpolation of the SE solution for AO within the limits of asymptotically high quantum numbers.

Let us note one more result obtained here. It arises from formulas (1.106) and (1.103) that we have incidentally found analytical approximation of the full elliptical integral of the first kind: at $0 \leqslant k \leqslant 1/\sqrt{2}$ we obtain

$$K(k) \approx \frac{\pi}{2}\left(\frac{3}{1-2k^2+2\sqrt{1+\frac{1}{2}k^2(1-k^2)}}\right)^{1/2}. \tag{1.107}$$

Approximation precision has the same order that it has for estimation of the classical motion period. We shall be dealing further with analogous approximations of other special functions which are useful in qualitative analysis of different physical problems.

1.4. *Why Do the OM Successive Approximations Converge?*

The set of empirical results obtained above in using the OM prescriptions for a particular problem of QAO is not a fully sufficient basis to expand this method to other systems. It is necessary to find the reason why the special choice of a zeroth approximation Hamiltonian with some arbitrary parameter results in the radical reconstruction of the successive approximation series which converge evenly at any

quantum numbers within the entire range of the Hamiltonian parameters and are not asymptotic with the zeroth convergence radius, as it is in the PT canonical scheme.

For this purpose we compare once again the ways of division of the QAO Hamiltonian into the zeroth approximation Hamiltonian $\hat{H}'_0$ and the perturbation operator $\hat{H}'_1$ in the case of canonical PT,

$$\hat{H}'_0 = \frac{1}{2}(2\hat{n}+1), \qquad \hat{n} = a^+ a, \qquad \hat{H}'_1 = \frac{\lambda}{4}(a+a^+)^4, \tag{1.108}$$

and in using OM ($\hat{H}_0$ and $\hat{H}_1$),

$$\begin{aligned}
\hat{H}_0 &= \frac{1}{4\omega^2}[\omega(\omega^2+1)(2\hat{n}+1)+3\lambda(2\hat{n}^2+2\hat{n}+1)], \\
\hat{H}_1 &= \frac{1}{4\omega^2}a^{+2}[2\lambda(2\hat{n}^2+3)-\omega(\omega^2-1)] \\
&\quad + \frac{1}{4\omega^2}[2\lambda(2\hat{n}+3)-\omega(\omega^2-1)]\,a^2 + \frac{\lambda}{4\omega^2}(a^{+4}+a^4).
\end{aligned} \tag{1.109}$$

As we see, formula (1.109) differs from (1.108) in two essential features: (i) in including all addends commutating with the operator of excitation number $\hat{n}$ into $\hat{H}_0$; (ii) in free parameter (frequency ω) dependence of the zeroth approximation Hamiltonian $\hat{H}_0$. Parameter ω might be used either to choose the best zeroth approximation, or to increase the convergence rate of successive approximations. Let us note straight away that the possibility of Hamiltonian division similar to (1.109) is not the specificity of the given system and might be carried out on the basis of any full set of state vectors as it will be shown in describing other applications of the OM [27]–[30].

Now let us discuss the role of each of the mentioned factors in the PT series reconstruction separately. Point (i) results in that the coupling constant λ and the quantum numbers of intermediate states appear in denominators of series terms of the SE exact solution expansion in operator $\hat{H}_1$ powers due to propagator $(E_n^{(0)} - H_0)^{-1}$. Really, the exact eigenvalues and eigenfunctions of Hamilton operator $\hat{H}$ might be represented in the form of the following operator series (see, e.g., [64])

$$\begin{aligned}
|\psi_n\rangle &= \lim_{\alpha \to 0} \frac{\hat{U}_\alpha |n\rangle}{\langle n|\, \hat{U}_\alpha |n\rangle}, \\
E_n &= E_n^{(0)} + \lim_{\alpha \to 0} \frac{\langle n|\, \hat{H}_1 \hat{U}_\alpha |n\rangle}{\langle n|\, \hat{U}_\alpha |n\rangle},
\end{aligned} \tag{1.110}$$

where

$$\hat{U}_\alpha = 1 + \sum_{s=1}^{\infty} \frac{1}{E_n^{(0)} - \hat{H}_0 + is\alpha} \hat{H}_1 \frac{1}{E_n^{(0)} - \hat{H}_0 + i(s-1)\alpha} \hat{H}_1 \cdots \times \frac{1}{E_n^{(0)} - \hat{H}_0 + i\alpha} \hat{H}_1, \tag{1.111}$$

i.e., successive approximations are defined by the operator powers

$$\hat{B}_n = \frac{1}{E_n^{(0)} - \hat{H}_0} \hat{H}_1, \tag{1.112}$$

which provides the following results when it impacts the arbitrary intermediate k-quantum state

$$\begin{aligned}
\hat{B}_n^{\mathrm{PT}} |k\rangle = {} & \frac{\lambda}{4} \frac{1}{E_n^{(0)} - (k+4+1/2)} \sqrt{\frac{(k+4)!}{k!}} |k+4\rangle \\
& + \frac{\lambda}{2} \frac{2k+3}{E_n^{(0)} - (k+2+1/2)} \sqrt{\frac{(k+2)!}{k!}} |k+2\rangle + \frac{3}{4} \lambda \frac{1+2k+2k^2}{E_n^{(0)} - k} |k\rangle \\
& + \frac{\lambda}{2} \frac{2k-1}{E_n^{(0)} - (k-2+1/2)} \sqrt{\frac{k!}{(k-2)!}} |k-2\rangle \\
& + \frac{\lambda}{4} \frac{1}{E_n^{(0)} - (k-4+1/2)} \sqrt{\frac{k!}{(k-4)!}} |k-4\rangle
\end{aligned} \tag{1.113}$$

in the case of PT for H_0' and H_1', defined by formulas (1.108) and

$$\begin{aligned}
& \hat{B}_n^{\mathrm{OM}} |k\rangle \\
& = \frac{\lambda}{4\omega^2} \frac{1}{E_n^{(0)} - (1/4\omega^2)[\omega(\omega^2+1)(1+2k+8) + 3\lambda(1+2k+8+2k^2+16k+32)]} \\
& \quad \times \sqrt{\frac{(k+4)!}{k!}} |k+4\rangle \\
& \quad + \frac{1}{4\omega^2} \frac{2\lambda(2k+3) - \omega(\omega^2-1)}{E_n^{(0)} - (1/4\omega^2)[\omega(\omega^2+1)(1+2k+4) + 3\lambda(1+2k+4+2k^2+8k+8)]} \\
& \quad \times \sqrt{\frac{(k+2)!}{k!}} |k+2\rangle \\
& \quad + \frac{1}{4\omega^2} \frac{2\lambda(2k-1) - \omega(\omega^2-1)}{E_n^{(0)} - (1/4\omega^2)[\omega(\omega^2+1)(1+2k-4) + 3\lambda(1+2k-4+2k^2-8k+8)]}
\end{aligned}$$

$$\times \sqrt{\frac{k!}{(k-2)!}}\,|k-2\rangle$$

$$+\frac{\lambda}{4\omega^2}\left\{E_n^{(0)}-\frac{1}{4\omega^2}[\omega(\omega^2+1)(1+2k-8)\right.$$

$$\left.+3\lambda(1+2k-8+2k^2-16k+8)]\right\}\frac{1}{\sqrt{(k-4)!}}\,|k-4\rangle \tag{1.114}$$

for operators (1.109) corresponding to the OM.

Apparently for any finite n in the limit of $k \gg 1$ any matrix element of operator $\hat{B}_n^{\mathrm{PT}}$ behaves as

$$\|\hat{B}_n^{\mathrm{PT}}\| = c\lambda k \qquad (c = \mathrm{const}),$$

while for arbitrary finite values of n, λ, and ω any matrix element of $\hat{B}_n^{\mathrm{OM}}$ at $k \gg 1$ do not exceed

$$\|\hat{B}_n^{\mathrm{OM}}\| < \tfrac{2}{3},$$

that derives from including the operator

$$\frac{3\lambda}{4\omega^2}(2\hat{n}^2+2\hat{n}+1)$$

in $\hat{H}_0$ and results in power decrease of all coefficients in expansion (1.110) instead of their factorial increase when taking into account the whole unharmonicity by PT. To prove this, let us consider some particular sequences (1.110) determining the nth steady state energy. The sequence of addends of the form

$$I_k = n \to \boxed{n+4} \to \boxed{n+8} \to \cdots \to \boxed{n+4k\cdot 4} \to \boxed{n+4k} \to \boxed{n+4k+4} \to$$

$$\cdots \to \boxed{n+4} \to n \tag{1.115}$$

proves to be one of the most quickly increasing within the limits of ordinary PT. Here we use a symbolic graphic presentation of intermediate states which sense derives from the analytical formula for series (1.110) kth term corresponding to diagram (1.115)

$$I_k = H_{n,n+4}\frac{1}{E_n^{(0)}-H_{n+4,n+4}}H_{n+4,n+8}\frac{1}{E_n^{(0)}-H_{n+8,n+8}}$$

$$\cdots\frac{1}{E_n^{(0)}-H_{n+4,n+4}}H_{n+4,n}. \tag{1.116}$$

Substituting the form of operators $\hat{B}_n^{\mathrm{PT}}$ and $\hat{B}_n^{\mathrm{OM}}$ matrix elements defined by formulas (1.113) and (1.114) into (1.116), we find the following expressions for I_k in the limits of PT and OM

$$I_k^{\mathrm{PT}} = -\left(\frac{\lambda}{4}\right)^{2k} \frac{1}{[(k-1)!]^2} \frac{(n+4k)!}{n!}, \tag{1.117}$$

$$I_k^{\mathrm{OM}} = -\left(\frac{\lambda}{8}\right)^{2k} \frac{2k[\omega(\omega^2+1)+3\lambda(4k+2n+1)]}{\omega^2 n!\,(k!)^2}. \tag{1.118}$$

For fixed m, λ, and ω we find at $k \gg 1$,

$$I_k^{\mathrm{PT}} = -\left(\frac{4\lambda}{e}\right)^{2k} k^{2k+n+3/2} A_n^{\mathrm{PT}} \tag{1.119}$$

$$I_k^{\mathrm{OM}} = -\frac{1}{6^{2k}} \frac{1}{k^{\omega(\omega^2+1)/6\lambda}} A_n^{\mathrm{OM}}, \tag{1.120}$$

where A_n^{PT} and A_n^{OM} are certain constants not depending on k. As follows from (1.119) the series formed of addends (1.115) diverges at any $\lambda > 0$ in the case of PT. At the same time formula (1.120) shows that for OM the similar series converges even at $\lambda \gg 1$ not worse than the geometrical progression with denominator $q = \frac{1}{36}$. Such a radical change of convergence is caused by including the intermediate state quantum numbers in propagator $[E_n^{(0)} - \hat{H}_0]^{-1}$.

Similar considerations of the series formed of addends corresponding to the following diagrams

$$J_k = n - \boxed{n+2} - \cdots - \boxed{n+2k\cdot 2} - \boxed{n+2k} - \boxed{n+2k+2} -$$

$$\cdots - \boxed{n+2} - n. \tag{1.121}$$

results (at $k \gg 1$) in the estimation

$$J_k^{\mathrm{OM}} = -\left(\frac{4}{9}\right)^k \frac{1}{k^{\omega(\omega^2+1)/3\lambda + \omega(\omega^2-1)/4\lambda}} A_n^{(1)}. \tag{1.122}$$

Thus the sequence of addends corresponding to diagrams (1.121) converges not worse than the geometrical progression with denominator $\frac{4}{9}$.

The results obtained above allow us to conclude that the first peculiarity of the OM (including all the diagonal matrix elements in $\hat{H}_0$) results in the absolute convergence of different sequences appearing in the operator $\hat{H}_1$ power series in the whole range of Hamiltonian parameters. As was shown in [19]–[39] in considering various physical systems, this property of OM is universal and does not depend on the choice of the concrete representation form.

It should be noted that the above choice of the zeroth approximation Hamiltonian is very close to some methods widely used in describing systems of many particles. As a first example one can mention the Hartree–Fock method where the state vectors $|N_i\{\phi_i\}\rangle$ play the role of the basis set and correspond to N noninteracting particles, the role of arbitrary parameters is played by a one-particle wave function chosen from the variation analogue of condition (1.18) [9]. Another example is given by the method which is based on the separation of the so-called coherent wave [7] in describing particle interaction with a system possessing an infinite number of degrees of freedom. In this case the basis set corresponds to the plane waves with a refractive index different from 1 and is an analogue of the parameter ω in the QAO problem.

However, the adequate choice of the zeroth approximation Hamiltonian in the OM, resulting in the convergence of partial sequences of PT series over the operator $\hat{H}_1$ does not mean that this series converges with the arbitrary choice of the basic set of functions. The fact is that the number of possible diagrams rapidly increases with the increasing PT order. As an example we pointed out in Fig. 5 all the diagrams corresponding to the corrections of the 2–4th order of the QAO nth-level energy (the analytical expression of any diagram can be written by the same rules as those in formula (1.116)). Thus, series convergence in general depends not only on the convergence of partial sequences of diagrams, but on the rate of the number of such sequences S_k, increasing with the growth of the number k which determines PT order. Therefore to limit S_k growth and therefore to accelerate PT series convergence one can use additional degrees of freedom which are included in the given scheme of the OM: (1) the possibility of the choice of a full set of functions properly describing exact solution peculiarities; (2) using optimal values of the parameters such as ω; (3) carring out calculations on the basis of an iteration procedure providing the most rapid convergence. Undoubtedly, the way to use this possibility depends on specific peculiarities of real problems. It proves, however, that one can consider a wide range of real physical problems, for which it is possible to construct some general recipes [19]–[30].

Concluding the section we would like to discuss briefly how the additional degrees of freedom of the OM influence the value of S_k in the case of QAO. For example, all the uncoupled diagrams (diagrams 17–32 of the 4th-order correction in Fig. 5) disappear due to the wave function normalizing condition (1.37). Special choice of the parameter ω lessens the number of diagrams that are different from zero. In particular, if according to [23] we choose ω from the condition that the matrix element of transition (in the nearest state for given level) turns into zero, then all the odd order diagrams disappear and the diagram number in PT even order essentially decreases (for example, at Fig. 5 only diagrams 1, 4 in the second order and diagrams 1, 2 and 15, 16 in the fourth order are different from zero). Choosing ω_{opt} from the condition (1.48), we set such a parameter value, for which the sum of all the diagrams beyond some given order turns to zero. At last, the recurrent sequence defined by the iteration procedure (1.51) permits one to

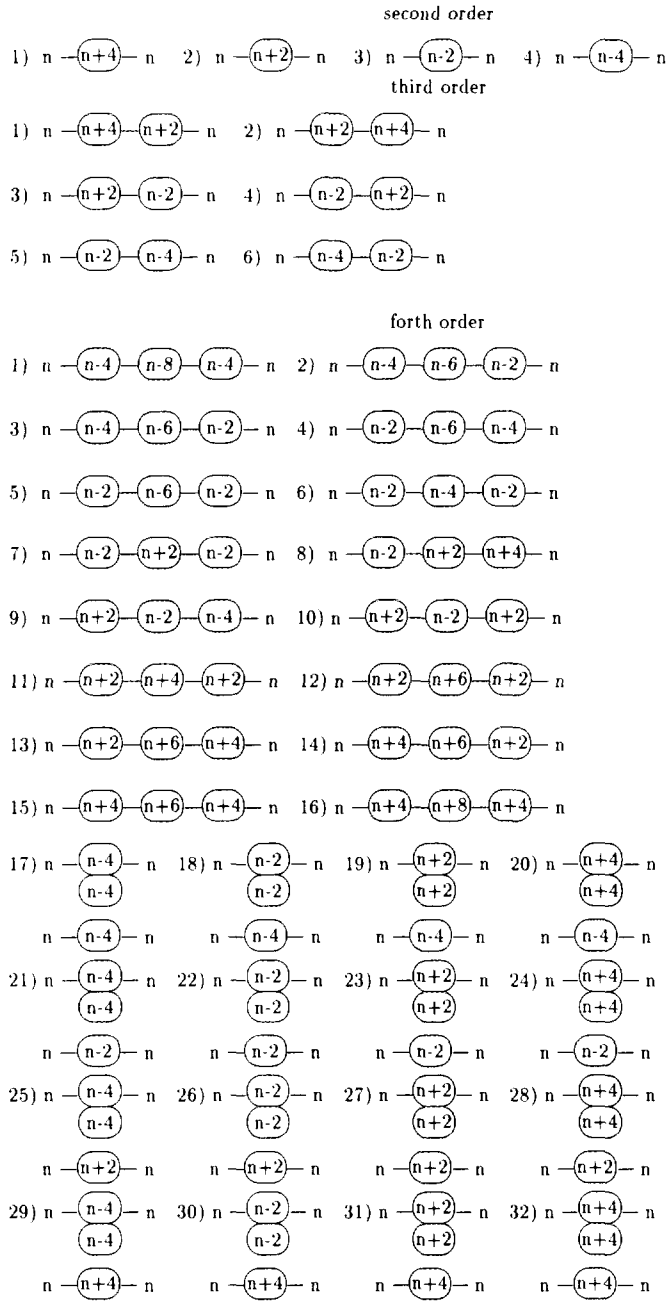

FIG. 5. The diagrams corresponding to the OM approximations of the second and fourth orders.

calculate not the successive corrections but still more precise values of energy, and it is a full analogue of the Dayson equations arising in summing the diagrams which describe any quantum mechanical system.

Qualitative arguments listed in this section are not a mathematical proof of the OM convergence, but to a certain extent they explain the high efficiency of the method in describing various physical systems which will be mentioned in the following sections.

2. Other Forms of Anharmonicity

2.1. *Calculation of Energy and the Level Width of Quasistationary States*

As it has been noted in the Introduction, the QAO model allows us to consider various versions of quantum system behaviour and, in particular, the case when its states have finite lifetime or become quasistationary. Let us consider an operator in the form

$$\hat{H} = \tfrac{1}{2}(\hat{p}^2 + \hat{x}^2) - \lambda \hat{x}^4 \equiv \tfrac{1}{2}\hat{p}^2 + V(x). \tag{2.1}$$

Quasistationary nature of such system states at any values of $\lambda > 0$ can be seen from Fig. 6 which shows the form of a potential pit in which the particle moves. A particle cannot stay infinitly long in the section I corresponding to the classical finite movement, due to the quantum mechanical tunnel effect. This effect results in particle tunnelling into the section III after some period of time and extending to infinity [64].

The probability of the particle penetrating P through the barrier is known to decrease exponentially with its height and width increasing. P happens to be $\sim \exp(-a/\lambda)$ at $\lambda \to 0$, where a is a certain constant [65]. Hence, Hamiltonian (2.1) eigenvalues E_n should be complex-valued,

$$E_n = E'_n - i\frac{\Gamma_n}{2},$$

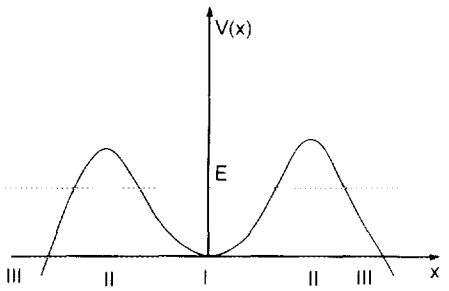

Fig. 6. Form of the potential pit for quasistationary states.

$\Gamma_n \sim P$ and the level width $\Gamma \sim P$, being inverse proportional to this state lifetime. Thus, SE solutions

$$\hat{H}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle, \tag{2.2}$$

considered as functions of parameter λ, have essential singularity at $\lambda = 0$. Therefore the use of the PT canonical form in this problem does not permit one to calculate level width at any small λ although such a problem often arises for real systems [66]. The most widespread method allowing us to exceed the limits of PT and to estimate a value Γ is based on the use of quasiclassical approximation to calculate a coefficient of the barrier permeability [67]. However, this approach can be applied only within the range of exponentially small values of Γ.

The method of coordinate rotation in the complex plane is used in the numerical integrating equation (2.2) for complex-valued E_n [68]. In this case the change of variables

$$x = \rho e^{i\varphi} \tag{2.3}$$

allows us to choose such an Eq. (2.2) integration in the complex plane ρ at $\varphi > \varphi_0$, along which the wave function $|\Psi_n\rangle$ becomes absolutely normalized. However, the Hamiltonian becomes nonhermitian and all the numerical method problems concerning the finite-difference approximation of derivatives over the infinite integration interval essentially grow.

As is known from the general theory of differential equations [69], the solutions in complex-valued variables and parameters of the system are the analytical continuation of the solutions on real axis. Therefore the considered OM is expected to permit calculating, not only the real energies of the discrete spectrum states, but also complex eigenvalues of the states with finite lifetime. To investigate these new possibilities of the OM we consider the problem defined by Eqs. (2.1), (2.2).

First of all we consider what the formal application of the simple canonical transformation (1.2) to this problem results in, limiting ourselves to the OM zeroth approximation. Since the Hamiltonian (1.19) differs from operator (2.1) only in the parameter λ sign, simple transformation of Eqs. (1.22) and (1.24) results in the following equation for calculating the zeroth approximation of energy $E_n^{(0)}(\omega, \lambda)$ of state with the quantum number n and the corresponding parameter ω value:

$$E_n^{(0)} = \frac{1}{4}\left(\omega + \frac{1}{\omega}\right) - \frac{3\lambda}{4\omega^2}(1 + 2n + 2n^2), \qquad n = 0, 1, 2, \ldots, \tag{2.4}$$

$$(\omega^3 - \omega)(2n + 1) + 6\lambda(1 + 2n + 2n^2) = 0. \tag{2.5}$$

To analyze the possible solutions of Eq. (2.5) we recall that in coordinate representation the wave function is

$$|0, \omega\rangle \to \Psi_0(x) = \left(\frac{\omega}{\pi}\right)^{1/4} e^{-(\omega/2)x^2},$$

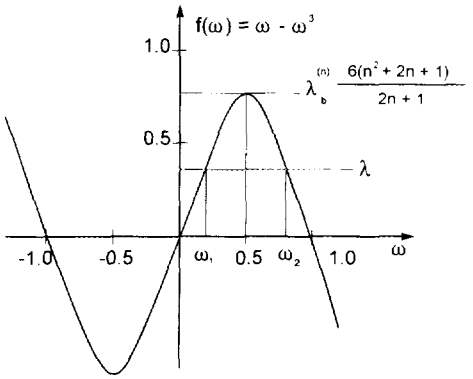

FIG. 7. Choice of the parameter ω for quasistationary states.

where it is absolutely normalized only in fulfilling the condition

$$\omega' \equiv \mathrm{Re}(\omega) > 0, \tag{2.6}$$

where $\mathrm{Re}(\omega)$ is the real part of the parameter ω, corresponding to the state vector $|0, \omega\rangle$ which is the basic state of the OM basic set.

In contrast to Eq. (1.24), with a single root satisfying condition (2.6) at any λ, the situation in Eq. (2.5) depends on the λ value (see Fig. 7). In particular, these are two real roots $\omega_{1,2}$ at $\lambda < \lambda_b^{(n)}$, where

$$\lambda_b^{(n)} = \frac{2n+1}{9\sqrt{3(2n^2+2n+1)}} \tag{2.7}$$

and there is a single complex root with $\omega' > 0$ at $\lambda > \lambda_b^{(n)}$. One should choose in the range $0 < \lambda < \lambda_b^{(n)}$ the root ω_2 satisfying the adiabaticity condition and in the limit $\lambda \to 0$ transforming to the solution $\omega = 1$ which corresponds to the harmonic oscillator (HO).

Thus, the OM zeroth approximation allows us to find complex-valued eigenvalues only at $\lambda > \lambda_b^{(n)}$, when the energy level width becomes sufficiently high, $\Gamma_n^{(0)} > 0.01\ \mathrm{Re}\, E_n^{(0)}$. It follows from the results listed in Section 1.1 that in calculating the real energy values the above-mentioned approximation can provide an accuracy of several percentages. Therefore at the parameter values satisfying condition (2.6), simple analytical formulas (2.4) and (2.5) permit us to estimate the energy and level width with sufficiently high precision as is shown in Table VIII, where the quantities $\Gamma_n^{(0)}$ and $\mathrm{Re}\, E_n^{(0)}$ calculated by Eqs. (2.4) and (2.5) are compared with the results of computing quantities Γ_n and E_n', obtained in [68] on the basis of a bulky numerical solution of the SE with Hamiltonian (2.1). The value $\lambda = 0, 1$ used in the calculation satisfies condition (2.6) even for the basic state. Let us note that when λ is increasing, the accuracy of estimation of energy and level width is almost unvariable and accounts for ~ 2–3% that is typical of the OM zeroth approximation.

TABLE VIII

Comparison of the Results of Numerical E_n [68] and Approximate $E_n^{(0)}$ Calculation of Energy and Level Width of QAO Quasistationary States

$\lambda = 0.1$	E'_n	Γ_n	Re $E_n^{(0)}$	$\Gamma_n^{(0)}$
$n=0$	0.397	0.045	0.384	0.042
$n=1$	1.096	0.340	1.074	0.353
$n=2$	1.753	0.969	1.769	0.971

Formal application of the OM zeroth approximation algorithm results in the necessity for using the complex-valued parameter ω. In connection with this it is necessary to define strictly the basic set of states $|n, \omega\rangle$ when the imaginary part ω'' ($\operatorname{Im}\omega = \omega''$) differs from zero. It is easier to construct this definition using the operator $\hat{R}(\omega, \omega_1)$, which transforms the operators of creation and annihilation from parameter ω_1 into the unit ω, corresponding to the secondary quantization representation for an ordinary HO,

$$\begin{aligned} a_\omega &= \hat{R}^{-1} a_1 \hat{R}, \qquad a_\omega^+ = \hat{R}^{-1} a_1^+ \hat{R}, \\ |n;\omega\rangle &= \hat{R}(\omega, 1)\,|n;1\rangle, \qquad a_1\,|0;1\rangle = 0. \end{aligned} \tag{2.8}$$

Since, according to formula (1.60), the operator $R(\omega, 1)$ is defined by the simple analytical expression

$$\hat{R}(\omega;1) = \exp[\tfrac{1}{4}(a^{+2} - a_1^2)\ln\omega]$$

and the full set of HO eigenfunctions is well known too, one can consider formula (2.8) as the analytical continuation of the basic sequence of the state vectors on complex-valued ω. We should note that operators a_ω and a_ω^+ and also state vectors $|n, \omega\rangle$ and $\langle\omega, n|$ are not Hermitian-conjugated at complex ω. Using the closed form of operator $\hat{R}(\omega)$ one can prove the following expression:

$$(|n;\omega\rangle)^+ = \langle\omega^*; n|, \qquad (a_\omega)^+ = a_{\omega^*}^+.$$

If one takes into account that ω is a canonical parameter of transformation (1.2)

$$\hat{x} = \frac{1}{\sqrt{2\omega}}(a_\omega^+ + a_\omega)$$

to the secondary quantization representation, it becomes clear that in using OM for quasistationary states introduction of the complex ω is equivalent to coordinate rotation in the complex plane when we numerically integrate SE for such states [68].

Now we are ready to apply the iteration procedure for the OM successive approximation calculation described in Section 1.2 so that to consider its con-

vergence at complex ω and possibility of E_n' and Γ_n calculation with any necessary accuracy. Calculating the algorithm is based on the use of the algebraic recurrent relations [29]

$$E_n = \lim_{s \to \infty} E_n^{(s)}, \qquad C_{nk} = \lim_{s \to \infty} C_{nk}^{(s)} \tag{2.9}$$

$$E_n^{(s)} = H_{nn} + \sum_{k \neq n} C_{nk}^{(s-1)} H_{nk}$$

$$C_{nk}^{(s)} = (E_n^{(s-1)} - H_{kk})^{-1} \left(H_{nk} + \sum_{l \neq n,k} C_{nl}^{(s-1)} H_{lk} \right), \tag{2.10}$$

where C_{nk} are the coefficients of the state vector expansion

$$|\Psi_n\rangle = |n, \omega\rangle + \sum_{k \neq n} C_{nk} |k, \omega\rangle$$

with the normalization condition

$$\langle \omega, n \mid \Psi_n \rangle = 1.$$

The initial elements of sequences (2.9) are defined by the OM zeroth approximation

$$E_n^{(0)} = H_{nn}(\omega), \qquad C_{nk}^{(0)} = 0. \tag{2.11}$$

To give a complete picture we list the formulas for nonzero Hamiltonian matrix elements included in (2.10):

$$H_{nn} = \frac{1}{4}\left(\omega + \frac{1}{\omega}\right)(2n+1) - \frac{3\lambda}{2\omega^2}\left(n^2 + n + \frac{1}{2}\right),$$

$$H_{n,n+2} = H_{n+2,n} = -\frac{\sqrt{(n+1)(n+2)}}{4\omega^2}\left[\lambda(4n+6) + \omega(\omega^2 - 1)\right],$$

$$H_{n,n+4} = H_{n+4,n} = -\frac{\lambda}{4\omega^2}\left[(n+1)(n+2)(n+3)(n+4)\right]^{1/2}.$$

Obviously one has to choose a definite parameter ω value in calculating by formulas (2.10). As has been shown in Section 1.4, the optimal value ω_{opt} at which sequence (2.10) converges to the exact solution most rapidly is usually different from Eq. (2.5) solutions ω_n that correspond to the best OM zeroth approximation. In particular, the value ω_n can not be used in (2.10) at $\lambda < \lambda_b^{(n)}$ because it cannot provide values for $\Gamma_n \neq 0$. The same situation arises in the method of coordinate complex rotation, when to calculate Γ_n one should rotate (2.3) through some finite angle $\varphi > \varphi_0 \neq 0$ which makes the state vector $|\Psi_n\rangle$ normalized. Numerical computing by formulas (2.9) shows that the OM successive approximations converge

sufficiently rapidly to the exact values of E'_n and Γ_n in a wide range of complex planes $\omega = \omega' + i\omega''$, where the inequalities

$$\omega' > \omega'_n, \qquad \omega'' > \omega''_n \tag{2.12}$$

are satisfied. When $\omega''_n = 0$ at $\lambda < \lambda_b^{(n)}$ one can choose $\omega'' \geqslant 0.1\,\omega'$ relatively arbitrary because in satisfying conditions (2.12) to be the convergence rate in (2.11) hardly depends on the specific values of ω' and ω''. In the limits of calculating the precision the eigenvalues E_n do not change with ω changing, and that is one of the iteration convergence criteria. At the same time the coefficients C_{nk} depend on the parameter ω choice which defines the basis set of states $|n, \omega\rangle$ in the exact vector $|\Psi_n\rangle$ expansion.

Some results of our calculations are listed in the Table IX. At some values of λ one manages to obtain essentially higher precision for a very small volume of numerical calculations by formulas (2.10), in comparison with results obtained by other authors by more complex numerical methods (see, e.g., [70]) in the given problem.

At the conclusion of the section we consider a problem of eigenvalue calculation for QAO Hamiltonian with cubic nonlinearity:

$$\hat{H} = \frac{\hat{p}^2}{2} + V_3(x) \equiv \frac{1}{2}p^2 + \frac{1}{2}x^2 + \lambda x^3. \tag{2.13}$$

Such system states are quasistationary at any λ sign. The system is rather peculiar in the sense that the operator $\hat{H}$ does not commutate with the parity operator in

TABLE IX

The Energy Levels of QAO with $\hat{H} = \frac{1}{2}(\hat{p}^2 + \hat{x}^2) - \lambda\hat{x}^4$

	$\lambda = 0.1$			
$E_0^{(s)}(E', \frac{\Gamma}{2})$	$\omega = 0.1 + i0.8$		$\omega = 1.0 + i1.0$	
$E_0^{(0)}$	0.392400	0.122665	0.375000	0.162500
$E_0^{(6)}$	0.397473	0.044629	0.397682	0.044932
$E_0^{(10)}$	0.397441	0.044705	0.397682	0.044715
$E_0^{(s \geqslant 13)}$	0.397441	0.044706	0.397441	0.044706
$E_0^{[70]}$	0.397	0.045	0.	0.
	$\lambda = 0.025$		$\lambda = 0.5$	
$E_n^{(s)}(E', \frac{\Gamma}{2})$	$\omega = 1.0 + i0.2$		$\omega = 2.0 + i1.5$	
$E_0^{(s \geqslant 10)}$	0.479117	0.000007	0.373874	0.304990
$E_0^{[70]}$	0.479117	0.000007	0.37	0.31
$E_1^{(s \geqslant \geqslant 20)}$	1.385667	0.000771	1.205286	1.257500
$E_1^{[70]}$	1.38564	0.00077	1.	1.3
$E_2^{(s \geqslant 20)}$	2.157234	0.021984	2.198786	2.68970
$E_2^{[70]}$	2.157	0.021	2.	2.5

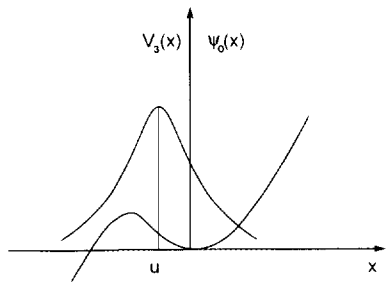

FIG. 8. Form of the potential $V_3(x)$ and localization of the of the ground state wave function.

comparison with the problem considered above. In this case the potential energy is not symmetric with respect to the origin of coordinate system. Therefore in the general case one should use functions, localized closely to some value $x = u \neq 0$, in the basic set to construct the OM. At the operator level one can take this circumstance into account by generalizing the canonical transformation (1.2) [23],

$$\hat{x} = u + \frac{1}{\sqrt{2\omega}}(a^+ + a), \qquad \hat{p} = i\sqrt{(\omega/2)}(a^+ - a), \tag{2.14}$$

introducing (together with ω) another arbitrary parameter u defining the equilibrium position of the considered system (Fig. 8).

The principal scheme of subsequent calculations remains unchangeable. It is based on using recurrent relations (2.10) with the following matrix elements which are simply calculated by means of substituting the operators (2.14) in the Hamiltonian (2.13):

$$H_{nn} = \frac{1}{4}\left(\omega + \frac{1}{\omega}\right)(2n+1) + \frac{1}{2}u^2 - \lambda\left[u^3 + \frac{3u}{2\omega}(2n+1)\right],$$

$$H_{n,n+1} = H_{n+1,n} = \frac{u}{\sqrt{2\omega}}\sqrt{n+1}\left[1 - 3\lambda\left(u^2 + \frac{n}{2\omega} + 1\right)\right],$$

$$H_{n,n+3} = H_{n+3,n} = -\frac{\lambda}{(2\omega)^{3/2}}[(n+1)(n+2)(n+3)]^{1/2}.$$

Parameter u values can be found by the equation

$$\frac{\partial E_n^{(0)}}{\partial u} = \frac{\partial H_{nn}}{\partial u} = u - 3\lambda\left(u^2 + \frac{2n+1}{2\omega}\right) = 0$$

and the ω value can be obtained by the same algorithm that is in the previous problem. Table X shows the OM effectiveness in describing states of the considered QAO.

TABLE X

The Energy Levels of QAO with $\hat{H} = \frac{1}{2}(\hat{p}^2 + \hat{x}^2) - \lambda\hat{x}^3$

$E_n^{(s)}(E', \Gamma/2)$	$\lambda = 0.1$ $\omega = 1.5 + i\,0.5$		$\lambda = 0.5$ $\omega = 2.7 + i\,1.9$	
$E_0^{(0)}$	0.494862	0.012833	0.385852	0.142919
$E_0^{(s \geq 20)}$	0.484316	0.000008	0.472129	0.252714
$E_0^{[70]}$	0.48432	0.000001	0.5	0.25
$E_1^{(s \geq 30)}$	1.378073	0.003141	1.631	1.051
$E_1^{[70]}$	1.3782	0.003	1.5	1.
$E_2^{(s \geq 30)}$	2.09437	0.09101	2.70	1.31
$E_2^{[70]}$	2.09	0.1	3.	2.

2.2. *The Problem of Double-Well Potential*

At present, when investigating some applied and fundamental problems of field quantum theory, a new trend has formed for description of the systems with spotaneously broken symmetry (see, e.g., [71]).

In the general case the solution of such problems is reduced to investigation of the system states which do not possess symmetry of the initial Hamiltonian. The general form of the QAO Hamiltonian (1.1) proves to be sufficiently flexible to model such a situation. Let us consider the solution of a SE with the Hamiltonian:

$$H = \tfrac{1}{2}\hat{p}^2 + V_D(x) = \tfrac{1}{2}\hat{p}^2 - \tfrac{1}{2}x^2 + \lambda x^4. \tag{2.15}$$

In this case the function $V_D(x)$ consists of two symmetrical potential pits. The depth and the distance between them increase with λ decreasing (Fig. 9).

The analysis of common properties of the one-dimensional quantum system [64] shows that the operator (2.15) eigenfunction at energy $E < 0$ has to be concentrated

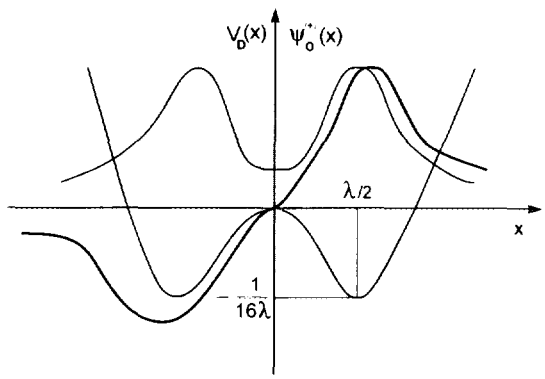

FIG. 9. The double-well potential and the function of the lowest symmetrical (———) and antisymmetrical (———) states.

near one of the potential energy minima. Like in the previous section one can take into account this condition in operator form that is required for using OM. For this we may apply the canonical transformation (2.14)

$$\hat{x} = \frac{1}{\sqrt{2\omega}}(a^+ + a), \qquad \hat{p} = i\sqrt{\frac{\omega}{2}}(a^+ - a), \qquad a = u + b, \qquad a^+ = u + b^+. \quad (2.16)$$

One can consider the state vector $|n\rangle$ which is the vacuum state with respect to the operators b,

$$b\,|u\rangle = (a-u)\,|u\rangle = 0, \quad (2.17)$$

as the zeroth approximation to the wave function of a system basic state. Let us note that in the coordinate representation state the vector $|n\rangle$ corresponds to the wave function

$$\langle x\,|u\rangle = \left(\frac{\omega}{\pi}\right)^{1/4} e^{-\omega(x-u)^2/2}$$

which describes the HO concentrated near the point $x = u$. On the other hand, $|n\rangle$ is the coherent state that is an eigenvector of the operator a [71],

$$\begin{aligned} a\,|u\rangle &= u\,|u\rangle \\ |u\rangle &= e^{ua^+}\,|0\rangle\, e^{-u^2/2}, \qquad a\,|0\rangle = 0. \end{aligned} \quad (2.18)$$

In contrast to operator (2.13) the Hamiltonian (2.14) commutates with the parity operator $\hat{P}$. Therefore, its eigenfunctions

$$\hat{H}\,|\Psi_\mu\rangle = E_\mu\,|\Psi_\mu\rangle \quad (2.19)$$

are to be eigenfunctions of $\hat{P}$ as well:

$$\hat{P}\,|\Psi_\mu\rangle = \mu\,|\Psi_\mu\rangle, \qquad \mu = \pm 1, \qquad [\hat{P}\hat{H}] = 0. \quad (2.20)$$

At the same time the canonical transformation (2.16) does not commutate with the parity operator which can be represented in terms of operators a and a^+ as [72]

$$\hat{P} = e^{i\pi a^+ a}.$$

Therefore one has to take into account the exact integral of motion defined by Eq. (2.20) in the function $|\Psi_\mu\rangle$, before using any approximation for this function. Within the limits of such approach it is natural to do this, not by means of choosing the wave function especially, but in the operator form. This problem can be solved in general by introducing an operator of arbitrary vector projection on the state with a definite value of the integral of motion. In the given case the

operator of projection on the state with a given value of parity $\mu = \pm 1$ has the form

$$T_\mu = \tfrac{1}{2}(1 + \mu e^{i\pi a^+ a}), \qquad T_\mu^2 = T_\mu. \tag{2.21}$$

If we find now the solution $|\mu\rangle$ of the equation

$$\hat{L}_\mu |\mu\rangle \equiv (\hat{H} - E_\mu)\, \hat{T}_\mu |\mu\rangle = 0, \tag{2.22}$$

the state vector $|\Psi_\mu\rangle = \hat{T}_\mu |\mu\rangle$ should satisfy both Eqs. (2.19) and (2.20) at the same time. As the state vector $|\mu\rangle$ is not bound with any additional conditions, we can apply a usual OM procedure to solve (2.22) on the basis of the canonical transformation (2.16) in the operator $\hat{L}_\mu$. In particular, to construct the OM zeroth approximation one has to reduce operator $\hat{L}_\mu$ to the normal form and then to retain only the operators which commutate with the operator of the excitation number $b^+ b$. For example, the parity operator is reduced to the normal form as

$$\hat{P} = e^{2u^2} e^{-2ub^+} e^{i\pi b^+ b} e^{-2ub}.$$

As a result, the expressions for energies of the two lowest states with different parity in the OM zeroth approximation are presented in the form

$$E_{0\mu}^{(0)}(\omega, u) = \frac{1}{4}\left(\omega - \frac{1}{\omega} + \frac{3\lambda}{4\omega^2}\right) + \frac{u^2}{\omega^2}(6\lambda - \omega + 4\lambda u^2)$$
$$- \mu u^2 Z(u^2)\left(\omega - \frac{1}{\omega} + \frac{6\lambda}{\omega^2} + \frac{4\lambda u}{\omega^2}\right), \qquad Z(u^2) = \frac{e^{-2u^2}}{1 + \mu e^{-2u^2}}.$$

As usual, the parameters ω and u are calculated, deriving the hermitian operator eigenvalue independence on the representation choice that in the given approximation results in the equations

$$\frac{\partial E_{0\mu}^{(0)}}{\partial u} = \frac{\partial E_{0\mu}^{(0)}}{\partial \omega} = 0,$$

$$\omega^3 + \omega + 4\omega u^2 + 5e^{-2u^2}(\omega^3 + \omega - 4\omega^3 u^2) - \lambda(6 + 48u + 32u^2 + 6\mu e^{-2u^2}) = 0,$$

$$2\lambda(3 + 4u^2) - \omega + 2u^2 Z^2(u^2)[\omega(\omega^2 - 1) + 2\lambda(3 + 2u^2)]$$
$$- \mu Z(u^2)[\omega(\omega^2 - 1) - 6\lambda - 2u^2\omega(\omega^2 - 1) - 4\lambda u^2(1 + 2u^2)] = 0.$$

Analytical solution to these equations can be found in the limit of big or small λ. In particular, in the most interesting case when $\lambda \to 0$ one can find

$$E_{0\mu}^{(0)} \simeq -\frac{1}{16\lambda} + \frac{1}{\sqrt{2}} - \frac{3\mu}{16\lambda}\, e^{-1/2\lambda\sqrt{2}},$$
$$\Delta E_0^{(0)} = E_{0-}^{(0)} - E_{0+}^{(0)} \simeq \frac{3}{8\lambda}\, e^{-1/2\lambda\sqrt{2}}. \tag{2.23}$$

Thus, the OM zeroth approximation permits us to estimate the exponentially small level splitting [73].

According to the accepted procedure now we consider the OM capabilities in using it for the exact calculation of the Hamiltonian (2.15) eigenvalues. It should be noted that such a problem solution on the basis of ordinary numerical methods is rather sophisticated, especially within the range of small λ [74]. Generally speaking one can use the iteration scheme of the OM in two ways in solving Eq. (2.19). On the one hand, one can transform operator $\hat{H}$ into the secondary quantization representation by canonical transformation (1.2) which does not break the parity and contains only one arbitrary parameter ω. In this representation the Hamiltonian $\hat{H}$ has a simple polynomial form with respect to a, a^+:

$$\hat{H} = \frac{1}{4}\left(\omega - \frac{1}{\omega}\right)(2a^+a + 1) - \frac{1}{4}\left(\omega + \frac{1}{\omega}\right)(a^2 + a^{+2}) + \frac{\lambda}{4\omega^2}(6\hat{n}^2 + 6\hat{n} + 3 + a^{+4} + a^4 + 4a^{+2} + 4a^+a^2 + 6a^{+2} + 6a^2). \quad (2.24)$$

Nothing prevents us now from applying the OM calculation procedure directly. Its essence is the use of recurrent relations (2.10) with Hamiltonian (2.24) matrix elements in this problem. For this the eigenfunction $|\Psi_{ns}\rangle$ expansion over states with definite excitation number,

$$\hat{n}\,|n\rangle = n\,|n\rangle,$$
$$|\Psi_{n\mu}\rangle = |n\rangle + \sum_{n \neq k} C_{nk}^{(\mu)}\,|k\rangle, \quad (2.25)$$

has to include only state vectors with even k at $\mu = +1$ and with odd k at $\mu = -1$. Such an approach was used in [36]. It was shown there that despite the tangible difference between zeroth approximation wave function $|n\rangle$ and exact state vectors $|\Psi_s\rangle$ especially at small λ, the OM iteration sequence converges to the exact SE solution and permits the calculation of level splitting with any precision. However, the convergence rate happens to be very slow in the range of exponentially small distance ΔE between levels corresponding to symmetrical and nonsymmetrical states. For example, it takes about 300 iterations to compute $\Delta E \leqslant 10^{-5}$. This means that the use of the mentioned form of OM for systems similar to (2.14), but with several degrees of freedom it becomes too complicated. It is easy to understand that this problem arises because of the qualitative change of the system wave function at $\lambda \to 0$, in comparison with ordinary HO wave functions.

In connection with this let us consider a certain modification of the recurrent relations (2.10) which allows us to use more accurate zeroth approximation wave functions and to provide the conservation of state parity at the same time. First we consider the iteration procedure of the SE solution

$$\hat{H}\,|\Psi_0^{(\mu)}\rangle = E_0^{(\mu)}\,|\Psi_0^{(\mu)}\rangle \quad (2.26)$$

for the lowest symmetrical $|\Psi_0^{(+)}\rangle$ and nonsymmetrical $|\Psi_0^{(-)}\rangle$ states. According to above-mentioned results of the OM zeroth approximation calculation, the normalized state vectors

$$|\Psi_0^{(\mu)}\rangle \simeq |\varphi_0^{(s)}\rangle \equiv C(1+\mu\hat{P})\,|u\rangle = C(|u\rangle - u\rangle),$$
$$C = \frac{1}{\sqrt{2(1+|\langle u|-u\rangle|^2)}} \tag{2.27}$$

provide sufficiently exact representation of Eq. (2.25) solutions with respect to parity of the system. State vector $|u\rangle$ is defined by formula (2.17) with the given parameters ω and u. The difference between state vectors $|\Psi_0^{(\mu)}\rangle$ and $|\varphi_0^{(\mu)}\rangle$ is small at every λ and can be found in the form of an expansion into a series over the full set of states $|n\rangle$,

$$|\Psi_0^{(+)}\rangle = |\varphi_0^{(+)}\rangle + \sum_{k=0}^{\infty} C_{2k}^{(+)}\,|2k\rangle, \qquad C_{2k+1}^{(+)} = 0,$$
$$|\Psi_0^{(-)}\rangle = |\varphi_0^{(-)}\rangle + \sum_{k=0}^{\infty} C_{2k}^{(-)}\,|2k\rangle, \qquad C_{2k}^{(-)} = 0. \tag{2.28}$$

Substituting these expansions into Eq. (2.26) we obtain nonlinear algebraic equations for eigenvalues E and coefficients C_n:

$$E_0^{(\mu)} = \left\{E_{00}^{\mu} + \sum_{k=0}^{\infty} C_k^{\mu}\langle k|\,\hat{H}\,|\varphi_0^{(\mu)}\rangle\right\}\left\{1 + \sum_{k=0}^{\infty} C_k^{\mu}\langle\varphi_0^{(\mu)}\,|k\rangle\right\}^{-1},$$
$$E_{00}^{\mu} = \langle\varphi_0^{(\mu)}|\,\hat{H}\,|\varphi_0^{(\mu)}\rangle, \tag{2.29}$$

$$C^{(\mu)} = -[H_{ll} - E_{00}^{(\mu)}]^{-1}\left\{E_0^{(\mu)}\langle l\,|\varphi_0^{(\mu)}\rangle - \langle l|\,H\,|\varphi_0^{(\mu)}\rangle - \sum_{p\neq l} C_p^{(\mu)} H_{pl}\right\},$$
$$H_{kl} = \langle k|\,\hat{H}\,|l\rangle. \tag{2.30}$$

However, if we try to solve these equations by means of ordinary iterations like in (2.10), we have to face the problem mentioned in Section 1.2. Due to the nonorthogonality of approximate state vector $|\varphi_0^{(\mu)}\rangle$ and basis set functions $\langle n\,|\varphi_0^{(\mu)}\rangle \neq 0$ the number of intermediate states to be taken into account in Eqs. (2.29) and (2.30) becomes infinite despite the polynomial nature of the Hamiltonian. Let us note that the problem is not simplified by choosing basis functions in the form

$$|n, u\rangle = \frac{(b^+)^n}{\sqrt{n!}}\,|0, u\rangle, \qquad b = a - u, \qquad b\,|0, u\rangle = 0,$$

corresponding to the excited states of a shifted HO without a definite parity. In order to simplify the solution of Eqs. (2.29), (2.30) we use the fact that the diagonal

matrix element of Hamiltonian $\langle \varphi_0^{(\mu)} | \hat{H} | \varphi_0^{(\mu)} \rangle$ defines the OM zeroth approximation evenly valid at any λ for the corresponding choice of parameters ω and u. Therefore, in the given problem we can apply the procdure of successive inclusion of matrix elements $\langle k | \hat{H} | \varphi_0^{(\mu)} \rangle$ into the iteration scheme which was described in Section 1.2 with respect to the nonpolynomial Hamiltonian (Eq. (1.55)). As a result the OM recurrent relation system for a SE solution might be presented in the form

$$E_0^{(s)} = \left[E_0^{(\mu)} + \sum_{n=n_0-s}^{n_0+2} C_n^{(s-1)} \langle n | H | \varphi_0^{(\mu)} \rangle \right] \left[1 + \sum_{k=n_0-s}^{n_0+s} C_k^{(s-1)} \langle k | \varphi_0^{(\mu)} \rangle \right]^{-1}, \quad (2.31)$$

$$C_l^{(s)} = -[E_0^{(\mu)} - E_0^{(s)}]^{-1} \left\{ E_0^{(s)} \langle l | \varphi_0^{(\mu)} - \langle l | H | \varphi_0^{(\mu)} - \sum_{n=n_0-s}^{n_0+s} C_n^{(s)} \langle n | H | n_0 \rangle \right\}, \quad (2.32)$$

where

$$E_0^{(\mu)} = \lim_{s \to \infty} E_0^{(s)}, \qquad C_l^{(\mu)} = \lim_{s \to \infty} C_l^{(s)}, \qquad E_0^{(0)} = E_0^{(\mu)}, \qquad C_l^{(0)} = 0. \quad (2.33)$$

Let us pay attention to the fact that in general, due to the nonorthogonality of functions $|n\rangle$ and $|\varphi_0^{(\mu)}\rangle$, the main contribution to correction of the zeroth approximation wave function in expansions (2.28) is defined by state vector $|n_0\rangle$ with quantum number n_0 which does not equal zero even for the basic state. Therefore, in contrast to recurrent formulas used before, the sequence (2.32) is calculated, starting from the coefficient C_{n_0}. Value n_0 might be considered as an additional parameter and its optimal choice permits us to increase the convergence rate of iteration schem (2.32). Specific estimation of this parameter might be found from the fact that in the first iteration the coefficients C_n are defined by overlap integral $\langle n | \varphi_0^{(\mu)} \rangle$. Therefore the maximum value of C_n is reached at n_0 found by the extremum condition

$$\frac{\partial}{\partial n} \langle n | \varphi_0^{(\mu)} \rangle = 0. \quad (2.34)$$

It is obvious that the given scheme of the SE solution is not connected with specificity of the given system and it can be used for other quantum systems, where one manages to construct the exact symmetry of zeroth approximation wave functions. Passing over to the description of numerical results obtained for Hamiltonian (2.15) we list first the closed expressions of matrix elements contained in Eqs. (2.31), (2.32),

$$\langle n | \varphi_0^{(\mu)} \rangle = e^{-u^2/2} \frac{u^2}{n!} [1 + \mu(-1)^n],$$

$$\langle \varphi_0^{(\mu)} | \hat{H} | \varphi_0^{(\mu)} \rangle = \frac{1}{4} \left(\omega - \frac{1}{\omega} \right) + \frac{3\lambda}{4\omega^2} + (1 + \mu e^{-2u^2})^{-1}$$

$$\times\left[\frac{\lambda u^2}{\omega^2}(4u^2+6)-\frac{u^2}{\omega}-\mu\omega u^2 e^{-2u^2}\right], \tag{2.35}$$

$$\langle l|\,H\,|k\rangle=\sqrt{k(k+1)}\,\delta_{k+2,l}+\sqrt{k(k+1)(k+2)(k+3)}\,\delta_{l,k+4}.$$

The curve shown in Fig. 10 illustrates the influence of parameter n_0 on the iteration convergence rate. It presents the n_0 choice dependence on the number of iterations s_0 which are to be carried out in calculating the basic state energy of the considered system at $\lambda=0.10$ to obtain the given accuracy ($\sim 10^{-7}$) of the energy calculation. The value $(n_0)_{\text{opt}}$ at which the convergence rate is a maximum corresponds to the estimation which derives from formula (2.34). Table XI shows the results of the system basic state energy $E_0^{(\pm)}$ calculation at different values of λ. The same table lists the values of parameters ω and u at which calculations are carried out, the value $(n_0)_{\text{opt}}$ for every λ, and the number of iterations s_0 required to obtain the mentioned number of exact figures in energy calculating. The comparison of the obtained results with the results of [36] shows that the OM iteration scheme modification defined by (2.31) permits us to considerably decrease a number of iterations for calculation of the eigenvalues with the given accuracy.

In conclusion we consider the problem of wave function choice in describing the excited states. The best approximation for them is obtained by a symmetrized linear combination of the excited state wave function of the shifted HO as was done in the case of the basic state. In particular, symmetrical and non-symmetrical functions of the $n$the excited state might be presented in the form

$$|\tilde{\varphi}_n^{(\mu)}\rangle=\frac{1}{\sqrt{n!}}[(a^+-u)^n\,|0,u\rangle+(-1)^n\mu(a^++u)^n\,|0,-u\rangle]. \tag{2.36}$$

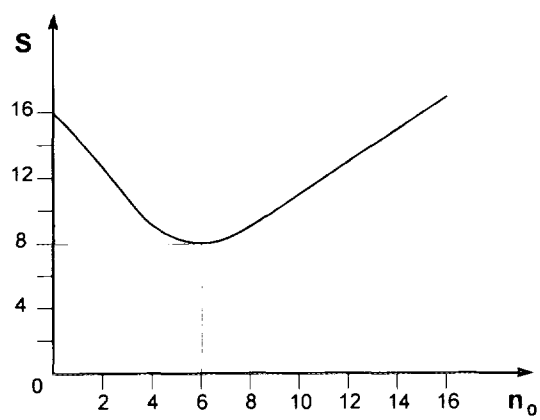

FIG. 10. The optimal choice of the OM zeroth approximation state in the double-well potential.

TABLE XI

The Energies of Symmetric and Antisymmetric States of the System with Hamiltonian (2.15)

λ	n_0	s_0	ω	u	$E_0^{(-)(0)}$	$E_0^{(-)(s \geq s_0)}$	$E_0^{(+)(s \geq s_0)}$
0.005	20	34	0.4	3.05	−11.1965301	−11.7979755	−11.7979755
0.012	15	19	0.6	2.35	−4.2749434	−4.5137280	−4.5137283
0.016	11	19	0.6	1.98	−2.9896903	−3.2160644	−3.2160702
0.02	9	14	0.6	1.73	−2.2255034	−2.4393456	−2.4394387
0.05	7	10	0.9	1.2	−0.5170587	−0.5765296	−0.6327464
0.5	3	10	2.0	0.2	1.5697561	1.4172688	0.3288265
10	0	12	5.5	0.02	5.2279415	4.9895186	1.2836945
					$E_1^{(-)(0)}$	$E_1^{(-)(s \geq s_0)}$	$E_1^{(+)(s \geq s_0)}$
0.01	15	48	1.5	4.25	−4.1287797	−4.2039848	−4.2039848

This approximation might be improved if one provided the orthogonality of this function to the wave functions of all the lower lying states in calculating the state vector $|\varphi_n^{(\mu)}\rangle$ by the formula

$$|\varphi_n^{(\mu)}\rangle = |\tilde{\varphi}_n^{(\mu)}\rangle - \sum_{k=0}^{n-1} \langle \varphi_n^{(\mu)}| \, |\tilde{\varphi}_n^{(\mu)}\rangle \, |\varphi_k^{(\mu)}\rangle. \tag{2.37}$$

Substitution of this function in the iteration scheme defined by formulas (2.30), (2.31) permits us to construct the SE solution for the system of excited states. To exemplify the above, Table XI shows the results of such calculations for the two closest excited states.

2.3. *The Operator Method of the Uniformly Fitted Estimation of Integrals and Sums*

The development of computing machinery does not lessen the significance of the physical process analytical description. Usually analytical calculations permit us to understand the problems qualitative peculiarities and to choose a sufficiently good initial approximation for further numerical calculation. From this point of view the significance of analytical results is defined, not by their absolute precision, but by the possibility to describe correctly the physical value and functional dependence on the problem parameters in the entire range of their variation. As we have seen from the examples above, the OM zeroth approximation satisfies this condition in many cases. But this methods possibilities prove to be not limited in their use only to approximate the solution of differential equations.

The thing is, that very often a physical problem's solution is expressed by some special functions or is reduced to calculating integrals and sums having no exact analytical form. In such cases one can use the modification below of the OM, permitting us to obtain the analytical approximation of corresponding expressions, even at such parameter values, when ordinary methods of integral and sum asymptotic estimation become not applicable and not valid [75, 76].

Let us consider a calculation algorithm of the method, using the example of the following integral [77]:

$$J(\lambda)=\int_{-\infty}^{\infty} e^{-x^2-\lambda x^4}\,dx. \tag{2.38}$$

It is easy to construct the function $J(\lambda)$ expansions in the ranges of large or small values λ,

$$\begin{aligned} J(\lambda) &\simeq \sqrt{\pi}\left\{1-\frac{3}{2}\lambda+\cdots\right\}, && \lambda \ll 1, \\ J(\lambda) &\simeq \frac{1}{2}\lambda^{-1/4}\left\{\Gamma\left(\frac{3}{4}\right)-\frac{1}{\sqrt{\lambda}}\Gamma\left(\frac{5}{4}\right)+\cdots\right\}, && \lambda \gg 1, \end{aligned} \tag{2.39}$$

where $\Gamma(x)$ is the gamma function.

An essentially different analytical structure of both expansions shows that they are asymptotic and cannot describe function $J(\lambda)$ in the whole range $0<\lambda<\infty$.

To use the OM in calculating the integral (2.38) we introduce the normalized state vector

$$|\omega\rangle=\left(\frac{\omega}{\pi}\right)^{1/4} e^{-(1/2)\omega x^2} \tag{2.40}$$

with parameter ω, which is to be defined below. Then the initial integral is transformed identically to quantum mechanical averaging of some exponential operator

$$J(\lambda)=\sqrt{(\pi/\omega)}\langle\omega|\, e^{(\omega-1)\hat{x}^2-\lambda\hat{x}^4}\,|\omega\rangle \equiv \sqrt{(\pi/\omega)}\langle\omega|\, e^{\hat{H}(\omega,\lambda)}\,|\omega\rangle. \tag{2.41}$$

The main idea of using the OM in calculating such an average is in choosing the parameter ω in such a way that the state vector $|\omega\rangle$ becomes an approximate eigenfunction of the operator $\hat{H}$, i.e.,

$$\hat{H}(\omega,\lambda)\,|\omega\rangle \simeq \varepsilon(\omega,\lambda)\,|\omega\rangle, \qquad \omega=\omega(\lambda). \tag{2.42}$$

Then the integral estimation is obvious:

$$J(\lambda)\simeq\sqrt{(\pi/\omega)}\, e^{\varepsilon(\omega,\lambda)}. \tag{2.43}$$

Thus the problem of integral calculation is reduced to the approximate solution of Eq. (2.42), which we should find by the OM. Let us pass over (2.42) to the secondary quantization representation of the ordinary way

$$x=\frac{1}{\sqrt{2\omega}}(a+a^+), \qquad [aa^+]=1,$$

so that

$$a\,|\omega\rangle=0.$$

By the definition, we extract the zeroth approximation operator $\hat{H}_0$ and the perturbation operator $\hat{H}_1$ from $\hat{H}$,

$$\hat{H} = \hat{H}_0 + \hat{H}_1,$$

$$\hat{H}_0 = \frac{\omega - 1}{2\omega}(2a^+a + 1) - \frac{3\lambda}{4\omega^2}[1 + 4a^+a + 2a^{+2}a^2], \tag{2.44}$$

$$\hat{H}_1 = \frac{1}{2\omega^2}[\omega(\omega - 1) - 3\lambda][a^{+2} + a^2] - \frac{\lambda}{\omega^2}[a^{+3}a + a^+a^3] - \frac{\lambda}{4\omega^2}[a^{+4} + a^4].$$

Then in the OM zeroth approximation, the state vector $|\omega\rangle$ should be the approximate eigenfunction of operator $\hat{H}$ if the matrix element of transition in the closest excited state, i.e., the addend proportional to $a^{+2}|\omega\rangle$ in the expression of $\hat{H}_1|\omega\rangle$, becomes zero. This condition results in the following equation for the parameter ω definition

$$\omega(\omega - 1) - 3\lambda = 0. \tag{2.45}$$

It should be noted that the same equation arises from applying the Bogoliubov inequality [78] to identity (2.41),

$$J(\lambda) = \sqrt{(\pi/\omega)}\langle\omega| e^{\hat{H}} |\omega\rangle \geqslant J_0(\lambda, \omega) \equiv \sqrt{(\pi/\omega)}\, e^{\langle\omega|\hat{H}|\omega\rangle}, \tag{2.46}$$

and obtaining the parameter ω from the condition of the extremum of the right part of inequality (2.46),

$$\frac{\partial}{\partial\omega} J_0(\lambda, \omega) = 0. \tag{2.47}$$

Substituting the solution of Eq. (2.45) in formula (2.43), we find the following analytical approximation of the initial integral:

$$J(\lambda) \simeq J(\lambda, \omega)|_{\omega = \omega(\lambda)} = \frac{\sqrt{2\pi}}{[1 + \sqrt{1 + 12\lambda}]^{1/2}} \exp\left[\frac{3\lambda}{(1 + \sqrt{1 + 12\lambda})^2}\right]. \tag{2.48}$$

It is easy to check up that three initial terms of this function expansion at $\lambda \ll 1$ coincide exactly with analogous ones in (2.39). The main expansion term in (2.48) at $\lambda \gg 1$ is

$$J_0(\lambda) \simeq \frac{\sqrt{2\pi}\, e^{1/4}}{(12\lambda)^{1/4}} \simeq \frac{1.73}{\lambda^{1/4}}, \qquad \lambda \gg 1, \tag{2.49}$$

and it can be compared with the exact asymptotic expansion from (2.39)

$$J(\lambda) \simeq \frac{1.81}{\lambda^{1/4}}, \qquad \lambda \ll 1.$$

Thus, the simple formula (2.48) defines correct functional dependence $J(\lambda)$, and numerical calculation shows that it differs from the exact values of integral by less than 5% within the entire range $0 \leqslant \lambda < \infty$.

To investigate a problem analytically in specific applications it is usually enough to confine oneself to zeroth approximation in the integral estimation. However, the considered method permits to find a correction to the zeroth approximation if it is necessary. Let us suppose that we know not the approximate but the exact eigenfunctions of the above introduced operator $\hat{H}$ (2.41),

$$\hat{H}\,|\psi_n\rangle = E_n\,|\psi_n\rangle. \tag{2.50}$$

Then, formally, Eq. (2.50) solutions might be presented by a series over HO eigenfunctions,

$$|\psi_n\rangle = \sum_{k=0}^{\infty} C_{nk}\,|k\omega\rangle, \qquad |k\omega\rangle = \frac{(a^+)^k}{\sqrt{k!}}\,|\omega\rangle$$

and formula (2.41) transforms as

$$J(\lambda) = \sqrt{(\pi/\omega)} \sum_{n=0}^{\infty} C_{n0}^2 e^{E_n}. \tag{2.51}$$

To construct the full set of the eigenvalues E_n and eigenvectors we can solve Eq. (2.50) by using OM, taking the expansion over perturbation operator $\hat{H}_1$ from (2.44). Then in zeroth approximation we find

$$\begin{aligned} &|\psi_n^{(0)}\rangle \simeq |n\omega\rangle, \qquad C_{n0} = \delta_{n0}, \\ &E_n^{(0)} \simeq \varepsilon_n = \frac{\omega - 1}{2\omega}(2n+1) - \frac{3\lambda}{4\omega^2}(2n^2+4n+1). \end{aligned} \tag{2.52}$$

and the first-order correction to the wave function has the form

$$\begin{aligned} |\psi_n^{(1)}\rangle = -(\hat{H}_0 - E_n^{(0)})^{-1}\,\hat{H}_1\,|n\omega\rangle = \frac{\lambda}{8\omega^2}\frac{\omega^2}{[2\omega(\omega-1)-3\lambda(2n+5)]} \\ \times\sqrt{\frac{(n+4)!}{n!}}\,|n+4,\omega\rangle - \frac{1}{2}\frac{\omega(\omega-1)\,\lambda(2n+3)}{[2\omega(\omega-1)-3\lambda(2n+3)]}\sqrt{\frac{(n+2)!}{n!}}\,|n+2,\omega\rangle. \end{aligned} \tag{2.53}$$

In this approximation the equation for parameter ω does not coincide with extremum condition (2.47) because now we choose it from the condition of turning the coefficient at $(a^+)^2$ to zero in the expression $\hat{H}_1(|\psi_0^{(0)}\rangle + |\psi_0^{(1)}\rangle)$ which appears when the perturbation operator impacts the basic state vector. This condition results in

$$\omega^2 - \omega - 3\lambda + \frac{3\lambda}{2}\frac{\omega(\omega-1)-7\lambda}{2\omega(\omega-1)-15\lambda} = 0, \tag{2.54}$$

which has analytical solution as before,

$$\omega = \frac{1}{2}(\sqrt{1+4\xi}+1), \qquad \xi = \frac{\lambda}{8}(39-\sqrt{39^2-16\cdot 69}).$$

By using the function $|\psi_n^{(0)}\rangle + |\psi_n^{(1)}\rangle$ in formula (2.51) we find the expression

$$J(\lambda) \simeq J_1(\lambda) = \sqrt{\frac{\pi}{\omega}}\left\{\left[1 - \frac{3\lambda^2}{8(2\xi-15\lambda)} - \frac{1}{2}\left(\frac{\xi-3\lambda}{2\xi-9\lambda}\right)^2\right] e^{E_0^{(0)}+E_0^{(2)}} + \frac{1}{2}\left(\frac{\xi-3\lambda}{2\xi-9\lambda}\right)^2 e^{E_2^{(0)}+E_2^{(2)}} + \frac{3}{8}\frac{\lambda^2}{(2\xi-15\lambda)^2} e^{E_4^{(0)}+E_4^{(2)}}\right\}, \tag{2.55}$$

where

$$\begin{aligned} E_n^{(2)} = &-\frac{\lambda^2}{32\omega^2}\frac{(n+1)(n+2)(n+3)(n+4)}{[2\xi-3\lambda(2n+5)]} \\ &-\frac{[\xi-\lambda(2n+3)]^2(n+1)(n+2)}{4\omega^2[2\xi-3\lambda(2n+3)]} \\ &+\frac{[\xi-\lambda(2n-1)]^2 n(n-1)}{4\omega^2[2\xi-3\lambda(2n-1)]} \\ &+\frac{\lambda^2}{32\omega^2}\frac{(n-1)(n-2)(n-3)(n-4)}{[2\xi-3\lambda(2n-3)]}, \end{aligned}$$

and parameters ω and ξ are defined by the solution of Eq. (2.54). Formula (2.55) provides a sufficiently more exact approximation of function $J(\lambda)$ as compared with (2.48). As, for example, in the limit of $\lambda \gg 1$ we find

$$J_1(\lambda) \simeq \frac{1.80}{\lambda^{1/4}},$$

which means a relative error of less than 0.5%.

In calculating some types of integrals one should use a canonical transformation of the operators which is more general than in (2.44). As an example we consider the integral representation of the Γ function,

$$\Gamma(x) = \int_0^\infty t^{x-1} e^{-t}\, dt = \frac{1}{x}\int_0^\infty t^x e^{-t}\, dt. \tag{2.56}$$

In this case the operator form of $\Gamma(x)$, the same as (2.41), can be obtained by expanding the interval of integration over the whole-number axis:

$$t = e^\rho, \qquad dt = e^\rho d\rho, \qquad -\infty < \rho < \infty, \tag{2.57}$$

Now the transition to a secondary quantization representation has to be connected with extracting a classical component from the operators because the maximum of the integrand is not in the origin of coordinates:

$$\rho = u + \frac{1}{\sqrt{2\omega}}(a + a^+), \qquad [aa^+] = 1. \tag{2.58}$$

As a result of these transformations we obtain

$$\Gamma(x) = \frac{e^{u(x+1)}}{x}\sqrt{(\pi/\omega)}\,\langle\omega|\, e^{\hat{H}}\,|\omega\rangle, \tag{2.59}$$

where

$$\hat{H} = \frac{x+1}{\sqrt{2\omega}}(a + a^+) - e^{u+1/4\omega}e^{a^+/\sqrt{2\omega}} + \frac{1}{2}[a^{+2} + a^2 + 2a^+a + 1], \qquad a\,|\omega\rangle = 0.$$

According to the above-considered recipe of the OM zeroth approximation one should choose paremeters ω and u in such a way that the operators a^{+^2} and a^+ coefficients defining transitions to the closest excited states should become zero. This results in the equation

$$e^{u+1/4\omega} = x + 1, \qquad e^{u+1/4\omega} = 2\omega. \tag{2.60}$$

By substituting Eq. (2.60) solutions in $\hat{H}$ and using the Bogoliubov inequality for estimation of (2.59), we find the following approximate analytical formula for the Γ function:

$$\begin{aligned} \Gamma(x) &\simeq \Gamma_1(x) = \frac{e^{u(x+1)}}{x}\sqrt{\frac{\pi}{\omega}}\,e^{\langle\omega|\hat{H}|\omega\rangle} \\ \Gamma_1(x) &= \sqrt{2\pi}\,\frac{(x+1)^{x+1/2}}{x}\,e^{-(x+1)}. \end{aligned} \tag{2.61}$$

Although the $\Gamma_1(x)$ is expressed by elementary functions it differs from $\Gamma(x)$ by not more than 8% in the whole range $0 < x < \infty$. For example,

$$\Gamma_1(x) \simeq \frac{0.922}{x}, \qquad x \ll 1, \qquad \Gamma_1(1) \simeq 0.960, \qquad \Gamma_1(2) \simeq 0.972,$$

$$\Gamma(x) \simeq 1/x, \qquad x \ll 1, \qquad \Gamma(1) = 1, \qquad \Gamma(2) = 1,$$

$$\Gamma_1(x) \simeq \sqrt{2\pi}\,x^{x-1/2}e^{-x}, \qquad x \gg 1,$$

which coincides with the asymptotic Stirling formula in the given limit.

Some difficulties in evaluating integrals might be encountered in the cases, when equations for variational parameters do not provide analytical solutions. Let us

consider, in particular, two special functions which can be often encountered in different applications. One of them is the error function [63]

$$\operatorname{erfc} z = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2}\, dt, \tag{2.62}$$

which is applied in solving problems of the probability theory; and another one is the function $H(b, a)$, which describes spectrum line broadening with respect to the radiation attenuation and the Doppler effect [79]:

$$H(b, a) = \frac{a}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{(t-b)^2 + a^2}\, dt. \tag{2.63}$$

We obtain the error function approximation by means of the transformation similar to (2.58):

$$\begin{aligned} \operatorname{erfc} z &= \frac{2}{\sqrt{\omega}} \langle \omega |\, \exp\{\omega \hat{y}^2 + u + \hat{y} - (e^{u+\hat{y}} + z)^2\}\, | \omega \rangle \\ y &= \frac{1}{\sqrt{2\omega}} (a + a^+). \end{aligned} \tag{2.64}$$

Confining to the OM zeroth approximation to estimate (2.64) we use the Bogoliubov inequality,

$$\operatorname{erfc} z \simeq J(\omega, u, z) = \frac{1}{\sqrt{\omega}} \exp[u + \omega - z^2 - 1], \tag{2.65}$$

and the condition of the function $J(\omega, u, z)$ extremum, concerning the parameters ω and u,

$$z^2 = \frac{(1-\omega)^2}{\omega - 1/2} e^{1/2\omega}, \qquad u = \frac{1}{2}\left[\ln\left(\omega - \frac{1}{2}\right) - \frac{1}{\omega} \right]. \tag{2.66}$$

In this case the equation for ω does not have analytical solution. However, it is not necessary to find ω in a specific calculation because one can consider the dependencies

$$z = \varphi(\omega), \qquad J = f(\omega),$$

as the parametric definition of an approximating function $J(z)$.

In the above examples the function $J(z)$ provides evenly valid estimation for $\operatorname{erfc} z$. Particularly in the asymptotic limits

$$\begin{aligned} &z \ll 1, \qquad \operatorname{erfc} z \simeq 1, \qquad J(z) \simeq \sqrt{2/e} \\ &z \gg 1, \qquad \operatorname{erfc} z \simeq \frac{1}{\sqrt{\pi}} \frac{e^{-z^2}}{z}; \qquad J(z) \simeq \frac{\sqrt{2}}{e} \frac{e^{-z^2}}{z}. \end{aligned} \tag{2.67}$$

TABLE XII

The Comparison of the Results Obtained by the OM Integral Estimation with the Exact Values of Special Functions

ω		$\sqrt{e/2}J(z)$	erfc z
0.04		0.7726	0.7679
0.25		0.4878	0.4804
0.92		0.1802	0.1751
1.0		0.1620	0.1573
3.68		0.0070	0.0067
a	b	$W(a, b)$	$H(a, b)$
0.5	0.2	0.5331	0.6015
1.0	10	0.0028	0.003
1.0	0.4	0.3835	0.4038
1.0	1.0	0.2745	0.3047
10	2.0	0.0539	0.0541
10	40	0.0033	0.0033

As one can see, $J(z)$ provides a one-sided error concerning the exact value in the both cases. Therefore, the approximation results might be improved, essentially by multiplying the function $J(z)$ by $\sqrt{e/2} \simeq 1.167$, taken from the condition of functions erfc z and $J(z)$ asymptotic coincidence at $z \to 0$. Table XII shows that with respect to this correction the function $J(z)$ permits us to calculate the error function with sufficiently high accuracy at all z.

Without going into the calculation detail we list the function $H(b, a)$ approximation in the OM zeroth approximation,

$$H(b, a) \simeq W(b, a, u, \omega) = \frac{a}{\sqrt{\pi\omega}} \frac{\exp(1/2 - b^2 - 1/2\omega)}{(u-b)^2 + a^2 + 1/2\omega}, \tag{2.68}$$

parameters ω and u are the solutions to the equations

$$\omega = \frac{b}{b-u}, \qquad \frac{1}{2}\left(1 - \frac{u}{b}\right) = \frac{b}{u} - 1 - a^2 - (u-b)^2.$$

In the limit cases formula (2.68) provides good coincidence with the exact formulas

$$b \gg 1, \quad a \gg 1, \qquad W \simeq \frac{1}{2a\sqrt{\pi}}, \qquad H \simeq \frac{1}{2a\sqrt{\pi}};$$

$$b \gg 1, \quad a \ll 1, \qquad W \simeq \frac{1}{\sqrt{\pi}} \frac{a}{b^2}, \qquad H \simeq \frac{1}{\sqrt{\pi}} \frac{a}{b^2};$$

$$b \ll 1, \quad a \ll 1, \qquad W \simeq \sqrt{e/2\pi}\, e^{-b^2}, \qquad H \simeq \left(1 - \frac{2a}{\sqrt{\pi}}\right) e^{-b^2+a^2};$$

$$b \ll 1, \quad a \gg 1, \qquad W \simeq \frac{1}{a\sqrt{\pi}}, \qquad H \simeq \frac{1}{a\sqrt{\pi}};$$

The functions H and W are compared at intermediate arguments in the Table XII as well. In conclusion we note that Feynman and Kleinert [80, 81] have recently proposed an approximate method of estimation of the partition functions in the form of path integrals for systems with nonquadratic Lagrangian. As the analytis shows, the results of this method coincide exactly with the OM ones.

Tangible expansion of the OM possibilities arises from its generalization for functions represented by different sums, especially in application to the quantum statistics problems. For example, let us obtain evenly valid interpolation of Θ-function which is one of the Weiersstrass' functions which frequently appears in solving equations of diffusion equation type and in calculating partition functions for certain quantum systems. The canonical form of this function has the form [63]

$$\Theta_3(\lambda, v) = \sum_{n=-\infty}^{\infty} e^{-\pi\lambda n^2 + i2\pi v n}. \tag{2.69}$$

In order to obtain the estimation by analogy with (2.41), we represent the Θ-function in the form of a quantum mechanical average, using the following normalized state vector

$$|u\rangle = \sqrt{1-u^2} \sum_{n=0}^{\infty} u^n |n\rangle. \tag{2.70}$$

Here u is an arbitrary parameter and $|n\rangle$ is an eigenvector of the excitation number operator. With this state vector $\Theta(\lambda, v)$ transforms identically into the form

$$\Theta_3(\lambda, v) = \frac{2}{1-u^2} \langle u| \exp[2\pi i v\hat{n} - \pi\lambda\hat{n}^2 - 2\hat{n} \ln u^2] |u\rangle - 1, \tag{2.71}$$

$\hat{n}$ being an excitation number operator. By using the Bogoliubov inequality in (2.72) and the average calculation result,

$$\langle u| \hat{n} |u\rangle = \frac{u^2}{2(1-u^2)}, \qquad \langle u| \hat{n}^2 |u\rangle = \frac{u^2(1+u^2)}{(1-u^2)^2},$$

we obtain

$$\Theta_3(\lambda, v) \geqslant S(\alpha) \equiv 2 \exp\left\{\frac{2\pi v\alpha}{1-\alpha} i - \pi\lambda \frac{\alpha(1+\alpha)}{(1-\alpha)^2} - \frac{\alpha}{1-\alpha} \ln \alpha - \ln(1-\alpha)\right\} - 1, \qquad \alpha = u^2. \tag{2.72}$$

Estimation (2.72) should be the best for the given class of the trial functions if parameter α is defined by the condition of extremum $S(\alpha)$:

$$\ln \alpha = 2\pi v i + \pi\lambda \frac{1+3\lambda}{\alpha - 1}. \tag{2.73}$$

Eventually we come to a simple analytical formula,

$$S = \frac{2}{1-\alpha} \exp\left[2\pi\lambda \frac{\alpha^2}{(1-\alpha)^2}\right], \tag{2.74}$$

with α satisfying Eq. (2.73). Different extreme cases in this formula coincide with well-known asymptotic behaviour of Θ-function:

$$\begin{aligned}
&\lambda \gg 1, && \alpha \simeq e^{2\pi v i - \pi\lambda}, && S \simeq 1 + e^{2\pi v i - \pi\lambda};\\
&\lambda \ll 1, \quad v = 0 && \alpha \simeq 1 - 2\sqrt{\pi\lambda}, && S \simeq \sqrt{(e/\pi)}\,\lambda - 1;\\
&\lambda \ll 1, && \alpha \simeq e^{2\pi v i}, && S \simeq [1 - e^{2\pi v i}]^{-1}.
\end{aligned}$$

Besides, Table XIII shows that one can calculate Θ-function values by this formula with the accuracy of $\sim 5\%$ at any argument.

The same method might be applied to the analytical calculation in quantum statistics. Consider, for example, the partition function defining thermodynamic characteristics of ideal gas of two-atom molecules which spectrum consists of n bound states,

$$Z = \sum_{k=0}^{n} \exp(-\beta E_k) = \sum_{k=0}^{n} \langle \psi_k | \exp(-\beta \hat{H}) | \psi_k \rangle, \qquad \beta = \frac{1}{vT}, \tag{2.75}$$

where $|\psi_k\rangle$ are the state vectors of a molecule Hamiltonian $\hat{H}$,

$$\hat{H} |\psi_k\rangle = E_k |\psi_k\rangle, \tag{2.76}$$

v is the Boltzmann's constant; T is the system temperature.

TABLE XIII

The Comparison of the OM Zeroth Approximation of Θ-Function with Its Exact Values

v	λ	Θ_3	S
0	1.6	1.007	1.013
0	0.74	1.098	1.195
1	1.6	0.993	0.987
1	1.0	0.957	0.914

Let us introduce the normalized state vector

$$|v\rangle = C^{1/2} \sum_{k=0}^{n} v^{k/2} |\psi_k\rangle, \qquad 0 \leqslant v \leqslant 1,$$

$$\langle v|v\rangle = 1, \qquad C(v) = \frac{1-v}{1-v^{n+1}}, \tag{2.77}$$

which permits us to present the partition function without any approximation in the form

$$Z(\beta) = \langle v| \exp(-\hat{R}) |v\rangle;$$
$$\hat{R} = \beta\hat{H} + \hat{k} \ln v + \ln C(v), \tag{2.78}$$

where the operator $\hat{k}$ is defined by

$$\hat{k} |\psi_k\rangle = k |\psi_k\rangle.$$

In order to calculate the partition function approximately in the entire range of T we use the Bogoliubov inequality to estimate the operator average in formula (2.78),

$$Z \geqslant \exp[-\varphi(\beta, v)], \tag{2.79}$$

$$\varphi(\beta, v) = \beta C \sum_{k=0}^{n} v^k E_k + \left[\frac{v}{1-v} - \frac{(n+1)\, v^{n+1}}{1-v^{n+1}}\right] \ln v - \ln \frac{1-v}{1-v^{n+1}}.$$

The accuracy of estimation (2.79) depends on two factors. The first one is connected with the precision of the Hamiltonian eigenvalue calculation and the second one deals with the accuracy of inequality (2.79) for the optimal choice of the parameter v. Particularly, if we substitute in formula (2.79) the QAO eigenvalues (1.22) found in the OM zeroth approximation, and the parameters ω and v chosen from the condition of function $\varphi(\beta, v)$ extremum, the approximation function $Z(\beta)$ coincides with the results of the partition function calculation by means of the path integrals [80]. However, now we discuss only the influence of the second one of the mentioned factors for the system with a finite number of bound levels, as it is in real molecules. Therefore, we use the Morse model [82] for the interatomic potential which permits us to find the exact eigenvalues E_n with respect to unharmonicity and the upper bound of the spectrum

$$E_n = \left[\kappa\sqrt{\frac{2D}{m}} - \frac{\kappa^2}{2m}\left(n+\frac{1}{2}\right)\right]\left(n+\frac{1}{2}\right), \tag{2.80}$$

where D and κ are the parameters of the Morse potential ($\hbar = c = 1$)

$$u(x) = D(1 - e^{-\kappa x})^2$$

and the coordinate $x = R - R_0$ is counted from the point of equilibration R_0 of atoms with mass m.

In this case the function $\varphi(\beta, v)$ in (2.79) is calculated analytically,

$$\varphi(\beta, v) = \beta\kappa\sqrt{\frac{2D}{m}}\left[\frac{v}{1-v} - \frac{(n+1)v^{n+1}}{1-v^{n+1}+1/2}\right]$$
$$-\beta\frac{\kappa^2}{2m}\left[\frac{2v}{(1-v)^2} - \frac{1+v}{1-v}\frac{(n+1)v^{n+1}}{1-v^{n+1}} - \frac{(n+1)^2 v^{n+1}}{1-v^{n+1}} + \frac{1}{4}\right]$$
$$+\left[\frac{v}{1-v} - \frac{(n+1)v^{n+1}}{1-v^{n+1}}\right]\ln v - \ln\left(\frac{1-v}{1-v^{n+1}}\right), \tag{2.81}$$

and the parameter v is defined from the condition of the extremum of the right side of this inequality,

$$\frac{\partial}{\partial v}\varphi(\beta, v) = 0. \tag{2.82}$$

Generally speaking, Eqs. (2.81) and (2.83) define the unknown function $Z(\beta)$ approximation in parametric form. However, direct calculation shows that at $n \geqslant 5$, as it is in real molecules, the solution of this equation coincides with the accuracy of less than 1% when solving the same equation corresponding to the limit $n \to \infty$ when it takes the form

$$\varphi(\beta, v) = \frac{1}{2}\beta\kappa\sqrt{\frac{2D}{m}}\left(\frac{1+v}{1-v}\right) - \beta\frac{\kappa^2}{2m}\left[\frac{2v}{(1-v)^2} + \frac{1}{4}\right] - \frac{v}{1-v}\ln v - \ln(1-v);$$
$$\kappa\sqrt{\frac{2D}{m}} + \frac{1}{\beta}\ln v = \frac{\kappa^2}{m}\frac{1+v}{1-v}. \tag{2.83}$$

Within the limits of the given approximation one can obtain the evenly valid analytical approximation for other thermodynamical characteristics of the gas. For example, we find the formula

$$E = \frac{\partial\varphi}{\partial\beta} = \frac{\kappa}{2}\sqrt{\frac{2D}{m}}\frac{1+v}{1-v} - \frac{\kappa^2}{2m}\left[\frac{2v}{(1-v)^2} + \frac{1}{4}\right] \tag{2.84}$$

for the average molecular energy ($n \gg 1$) and the specific heat of the same system is

$$C_v(\beta) = \left[\kappa\sqrt{\frac{2D}{m}} - \frac{\kappa^2}{m}\frac{1+v}{1-v}\right]\frac{v\ln v}{2(\kappa^2/m)\,v - (1-v^2)/\beta}, \tag{2.85}$$

parameter v being defined by the solution of the second of Eq. (2.83).

It is of great interest to calculate the mean deviation of an atom from equilibrium distance $\langle x \rangle$, caused by the potential anharmonicity

$$\langle x \rangle = \sum_{k=0}^{n} x_k e^{-\beta E_k} Z^{-1}, \tag{2.86}$$

where x_k is the diagonal matrix element of coordinate operator. To estimate such sums one has to use the trial state vector $|v_x\rangle$ having a more general form than in (2.76),

$$|v_x\rangle = C_x^{1/2} \sum_{k=0}^{n} (x_k v^k)^{1/2} |\psi_k\rangle. \tag{2.87}$$

In particular, for the Morse potential

$$x_k = \frac{1}{\kappa}\left[\psi\left(2\frac{\sqrt{2mD}}{\kappa}\right) - \psi\left(2\frac{\sqrt{2mD}}{\kappa} - k\right)\right],$$

where $\psi(z)$ is the logarithmic derivative of the Γ-function [63], however, for real molecules $\sqrt{2mD}/\kappa \gg 1$, the expression for x_k is simplified:

$$x_k \simeq \frac{\kappa}{2\sqrt{2mD}}\left(k + \frac{1}{2}\right).$$

It permits us to find the estimation of $\langle x \rangle$,

$$\langle x \rangle = \frac{1}{4\sqrt{2mD}} \frac{1+v}{1-v}. \tag{2.88}$$

TABLE XIV

Thermodynamical Characteristic of the Ideal Gas of N_2 Molecules

$T°k$	1000	2000	5000	10000	20000
$v(n \to \infty)$	0.035	0.189	0.521	0.732	0.868
Z	0.191	0.529	1.474	3.053	6.243
Z_e	0.191	0.529	1.474	3.053	6.431
Z_0	0.190	0.525	1.447	2.935	5.891
$E-0.5$	0.035	0.228	1.059	2.608	5.977
$E_e-0.5$	0.035	0.228	1.059	2.607	5.987
$E_0-0.5$	0.035	0.225	1.031	2.477	5.410
C_v	0.424	0.807	1.002	1.081	1.253
C_{ve}	0.414	0.807	1.004	1.091	1.254
C_{v0}	0.362	0.791	0.963	0.990	0.997
$\langle x \rangle \cdot 10^3 Å$	9.287	12.696	27.610	57.462	135.120

Table XIV compares the results of the calculation of thermodynamic characteristics of molecules of an ideal gas of N_2 found in the OM zeroth approximation [83] with the corresponding exact values (noted by sign "e") and with the approximation frequently used for the same values calculated in the limits of the harmonic interatomic potential (sign "o"). The Morse potential parameters for these molecules are chosen according to [84]. The same approximation used in Ref. [85] for a two-atom gas with double-well interatomic potential is allowed to describe the phase transition in such system.

Conclusion

In this paper we have carried out the detailed analysis of the partial problem of quantum anharmonic oscillator on the basis of the operator method of the Schrödinger equation solution. Similar ideas have already been applied for description of systems with several number and the infinite number of degrees of freedom. The detailed consideration of such applications of the OM is out of the framework of the paper and we confine ourselves to references of the main results obtained in this field.

The quantum systems in the extremal fields that are periodic in space or time were considered in papers [29, 30] and it was shown that the Bloch band spectrum or quasi-energy spectrum can be calculated by means of the OM for any value of the field amplitude. This algorithm was used for the calculation of the radiation spectrum from the particles channeled in a crystal [87].

The equivalency of the Coulomb problem and the problem of the harmonic oscillator in two-dimensional complex space was proven in [26] and it allowed us to use the OM for calculation of the energies and the width of the hydrogen atom levels in the magnetic and electric fields with arbitrary amplitudes [26, 28, 30]. As was shown in [25] the OM zeroth-order approximation in this problem permits one to find the analytical expressions for energies and widths of Rydberg states of the hydrogen atom.

The eigenfunctions of the Hamiltonian of two coupled anharmonic oscillators and the energy levels of the particle in the Yukawa potential and other potentials used in the quark models were calculated in [30, 36]. It was shown that the OM zeroth approximation ensures good analytical evaluation of this problem solution and the OM iteration scheme allows us to find the solutions with any accuracy.

Besides, the OM was also used for consideration of the systems with an infinite number of degrees of freedom. We mentioned the analysis of the phase transition in the gas of the anharmonic oscillators above [85]. Besides, a number of peculiarities of the "polaron" problem were considered in the OM zeroth approximation [21, 27]. It is a well-known problem of interaction between electron and optical phonons of the ionic crystal. It was shown that the OM allowed us to describe in the usual way the regimes of weak, strong, and intermediate coupling constants in this problem.

All these results confirm that the OM provides an effective way for both qualitative and accurate descriptions of various physical problems and, therefore, it is of interest for further applications and may require a more strict mathematical grounding.

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