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# Operator method for coupled anharmonic oscillators

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**Abstract.** Two coupled anharmonic oscillators are considered as a model for a nonperturbative description of the correlation and nonadiabatic effects which are typical for many-dimensional quantum systems. The eigenvalues and eigenfunctions for this model are found by means of the operator method, modified for the case of degenerate solutions of the Schrödinger equation. It is shown that the zeroth approximation of the method allows one to find the analytical and uniformly suitable approximation for the energy levels and their splitting in the entire range of Hamiltonian parameters and quantum numbers. Numerical calculations demonstrate the convergence of the successive approximations, even for quasistationary states of the system. The results are of interest for applied problems of spectroscopy and solid state physics.

## 1. Introduction

It is well known that, in spite of the increase in computer facilities, direct *ab initio* calculations for complicated atomic and molecular systems are impossible at present, and some approximations should be used in order to separate the variables in the Schrödinger equation. The most commonly used approximations are Born–Oppenheimer, or adiabatic, approximations (AA) and one-particle (OPA) approximations. However, for many physical problems nonadiabatic and correlation (i.e. essentially multiparticles) effects are very significant and should be taken into account in zeroth approximations. It is especially important for the correct classification of energy levels and the qualitative analysis of the system characteristics near to the points where the approximate eigenvalues with different quantum numbers are intersected.

Therefore, it is of great interest that these methods allow one to find an approximate solution of the Schrödinger equation in the entire range of system parameters, and also to define the correct sequence of energy levels in the initial approximation, without considering nonadiabaticity and correlation as the perturbation effects. One such approach was introduced in [1] as the operator method (OM) for obtaining a solution of the Schrödinger equation. This method had generalized the variational-scaling approach, proposed by Caswell [2], to the ground state of the anharmonic oscillator. It proved to be useful for both the ground and excited states of a number of specific physical systems. The main advantage of the method is the fact that the OM zeroth approximation is suitable uniformly for all considered systems. It means that the corresponding analytical formulae interpolate the energy levels for any quantum numbers and parameters of the systems with rather high accuracy. As a result, the subsequent

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approximations converge uniformly to the exact values. The history of the problem and its connection with other methods were discussed in our review [3].

In the present paper we analyse the OM capabilities for the model of two coupled anharmonic oscillators (CAO). In spite of its simplicity, this model includes many properties typical for many-dimensional quantum systems and often used for development of non-perturbative methods [4]. The model allows us to compare the results of various methods and consider the mathematical nature of their distinctions.

The main purpose of the paper is to show that the OM zeroth approximation leads to analytical and uniformly suitable formulae for the collective energy levels of the system and their classification for any quantum number and Hamiltonian parameter. It is essential that the standard perturbation, adiabatic or strong-coupling expansions can be obtained considering the corresponding limits in our algebraic approximation. We also consider the second-order corrections which essentially improve the accuracy of the formulae.

In the last section we consider the convergence of the OM high-order corrections calculated numerically by means of the rather simple iteration algorithm. In contrast to the asymptotic series of usual perturbation theory the OM successive approximations are proved to be convergent and permit one to calculate the energies and wavefunctions of the system with any necessary accuracy, even in the case of quasistationary states.

## 2. Coupled harmonic oscillators

Firstly, let us consider this simple quantum model being solved exactly in order to illustrate some specific problems connected with the application of approximate methods to many-particle systems. The dimensionless form of the corresponding Hamiltonian is

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

where  $M$  is the ratio of the oscillator masses and  $\lambda$  is the interaction parameter.

In spite of its simplicity, this Hamiltonian is often used for approbation of various approximate methods [5]. It is well known that the classical trajectories of the system are described by rather complicated Lissajous figures which correspond to the essential dependence of its quantum levels on the interaction and mass parameters. The exact eigenvalues of the Hamiltonian can be found easily:

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

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

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

One can see from formula (2) that the system energy has singularities if it is considered as an analytical function in the complex plane of the parameters  $\lambda$  and  $M$ . This means that the series in terms of powers of these parameters have the finite convergence radii. This is the mathematical reason for the restrictions on various approximate methods as discussed earlier for the one-dimensional system [3, 6].

The analogous restrictions appear here when the interactions between oscillators are considered by some approximate methods. In fact, let us consider the results of a one-particle approximation used for the Hamiltonian (1). The wavefunctions of the system in the zeroth order (Hartree approximation) are chosen as the product of one-particle functions

(the symmetrization of the function in the case of  $M = 1$  is not essential for our discussion):

$$\begin{aligned} \Psi_{\text{OPA}}(x, y) &= \varphi_n(x) \chi_m(y) \\ \int \varphi_n(x) \varphi_m(x) dx &= \int \chi_n(x) \chi_m(x) dx = \delta_{mn}. \end{aligned} \quad (3)$$

The system of approximate equations for the one-particle functions follows from the exact Schrödinger equation

$$\begin{aligned} \left\{ \frac{1}{2} \hat{p}_x^2 + \frac{1}{2} x^2 + \lambda x y_{mm} - \epsilon_n \right\} \varphi_n(x) &= 0 \\ \left[ \frac{1}{2M} \hat{p}_y^2 + \frac{1}{2} y^2 + \lambda y x_{nn} - \epsilon_m \right] \varphi_m(y) &= 0. \end{aligned} \quad (4)$$

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

$$\bar{x} = -\lambda y_{mm} \quad \bar{y} = -\lambda x_{nn}.$$

The energy spectrum of the system in this approximation is

$$E_{nm}^{(\text{OPA})} = n + \frac{1}{2} + \frac{1}{\sqrt{M}} \left( m + \frac{1}{2} \right) - \frac{1}{2} \lambda^2 (y_{mm}^2 + x_{nn}^2) - \lambda x_{nn} y_{mm}. \quad (5)$$

One can see that it is actually the power series of parameter  $\lambda$ . Taking into account the conditions of self-consistency for the parameters  $\bar{x}$ ,  $\bar{y}$ ,

$$\bar{x} = -\lambda \bar{y} \quad \bar{y} = -\lambda \bar{x} \quad (6)$$

one finds

$$\bar{x} = \bar{y} = 0 \quad (7)$$

for an arbitrary value of  $\lambda$ .

Thus, the zeroth-order approximation  $E_{mn}^{\text{OPA}}$  differs essentially from the corresponding exact value. Certainly, the consequent corrections take into account the particle correlations, but in any case the OPA fails to describe the energy levels  $E$  over the entire range of parameters  $\lambda$  and  $M$ .

Let us show now that the adiabatic approximation applied to the Schrödinger equation with Hamiltonian (1) leads to an analogous problem. A similar calculation has also been considered by Fernandez [5] in order to illustrate the general method for calculation of the AA high-order corrections.

In the AA zeroth-order approximation ( $M \gg 1$ ) the operator  $\hat{p}_y^2$  should be neglected and the ‘adiabatic’ terms  $\epsilon_n(y)$  are defined by the energy levels of that part of the Hamiltonian which depends on the ‘quick’ variable  $x$

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

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

$$E_{nm}^{(\text{AA})} = n + \frac{1}{2} + \sqrt{\frac{1 - \lambda^2}{M}} \left( m + \frac{1}{2} \right). \quad (8)$$

Comparing this expression with formula (2) one can see that the Born–Oppenheimer approximation also does not lead to the uniformly suitable estimation for the energy levels, even for such a simple system (compare with the result of Fernandez [5]).

Certainly, the same restrictions of the considered methods appear for the more complicated model when the anharmonicity of the oscillators is included. In any case, the singularities of

the energy, considered as an analytical function of the Hamiltonian parameters, define the finite radii of convergence for the power series in these parameters and do not allow one to find the uniformly suitable approximation.

In contrast, let us show now that the OM zeroth approximation takes into account the above-mentioned singularities and defines the eigenvalues over the entire range of the Hamiltonian parameters similarly to a number of other systems [6–8]. Certainly, the considered simple system is of methodical interest only (compare with the paper [6]). However, it will be shown in later sections that the OM also leads to analogous results for the nontrivial system.

In accordance with the OM, let us introduce the creation  $a^+$ ,  $b^+$  and annihilation operators  $a$ ,  $b$  by means of the following canonical transformation:

$$\begin{aligned} x &= x' \cos \alpha + y' \sin \alpha & y &= y' \cos \alpha - x' \sin \alpha \\ \hat{p}_x &= \hat{p}'_x \cos \alpha + \hat{p}'_y \sin \alpha & \hat{p}_y &= -\hat{p}'_x \sin \alpha + \hat{p}'_y \cos \alpha \\ x' &= \frac{a + a^+}{\sqrt{2\omega_1}} & y' &= \frac{b + b^+}{\sqrt{2\omega_2}} \\ \hat{p}'_x &= -i(a - a^+) \sqrt{\frac{\omega_1}{2}} & \hat{p}'_y &= -i(b - b^+) \sqrt{\frac{\omega_2}{2}}. \end{aligned} \quad (9)$$

In formulae (9) the variational parameters  $\omega_{1,2}$  for both coordinates are introduced for analogy to the one-dimensional case [1], and the parameter  $\alpha$  for the operator phase transformation is connected with the additional degree of freedom for the two-dimensional system. In the linear case considered the transformation (9) leads to the same result as the well known Bogoliubov–Tyablikov transformation [9], but our algorithm for choice of the optimal values of the parameters is suitable for nonlinear systems as well.

The Hamiltonian (1) in the new representation has the form

$$\begin{aligned} \hat{H} &= \frac{1}{4} \left\{ (a^2 + a^{+2}) \left( \frac{1}{\omega_1} - \omega_1 \right) + (b^2 + b^{+2}) \left( \frac{1}{\omega_2} - \omega_2 \right) \right. \\ &\quad \left. + (2a^+a + 1) \left( \frac{1}{\omega_1} + \omega_1 \right) + (2b^+b + 1) \left( \frac{1}{\omega_2} + \omega_2 \right) \right\} \\ &\quad + \frac{\lambda}{2} \left\{ \frac{\cos 2\alpha}{\sqrt{\omega_1\omega_2}} (ab + a^+b^+ + a^+b + ab^+) \right. \\ &\quad \left. + \frac{\sin 2\alpha}{2} \left[ -\frac{1}{\omega_1} (a^2 + a^{+2} + 2a^+a + 1) + \frac{1}{\omega_2} (b^2 + b^{+2} + 2b^+b + 1) \right] \right\} \\ &\quad + \frac{1}{4} \left( 1 - \frac{1}{M} \right) \left[ (a^+ - a)^2 \omega_1 \sin^2 \alpha + (b^+ - b)^2 \omega_2 \cos^2 \alpha \right. \\ &\quad \left. - (a^+ - a)(b^+ - b) \sqrt{\omega_1\omega_2} \sin 2\alpha \right]. \end{aligned} \quad (10)$$

The OM zeroth approximation corresponds to that part of the Hamiltonian which commutes with the excitation number operators  $a^+a = \hat{n}$  and  $b^+b = \hat{m}$

$$\begin{aligned} \hat{H}_0 &= \frac{1}{4} \left[ \left( \frac{1}{\omega_1} + \omega_1 \right) (2\hat{n} + 1) + \left( \frac{1}{\omega_2} + \omega_2 \right) (2\hat{m} + 1) \right] \\ &\quad + \frac{\lambda \sin 2\alpha}{4} \left[ \frac{1}{\omega_2} (2\hat{m} + 1) - \frac{1}{\omega_1} (2\hat{n} + 1) \right] \\ &\quad + \frac{1}{4} \left( \frac{1}{M} - 1 \right) \left[ \omega_1 (2\hat{n} + 1) \sin^2 \alpha + \omega_2 (2\hat{m} + 1) \cos^2 \alpha \right]. \end{aligned} \quad (11)$$

One can show by analogy with the one-dimensional case [3] that the perturbation series in the operator  $\hat{V} = \hat{H} - \hat{H}_0$  is uniformly suitable in that it converges over the entire range of

$\lambda$ ,  $M$  and auxiliary parameters  $\alpha$ ,  $\omega_{1,2}$ . However, the best zeroth approximation corresponds to choosing these parameters such that the eigenvalues are independent of them, because they define only the eigenfunction representation [3].

Therefore,

$$\frac{\partial E_{mn}}{\partial \omega_1} = \frac{\partial E_{mn}}{\partial \omega_2} = \frac{\partial E_{mn}}{\partial \alpha} = 0 \quad (12)$$

where  $E_{mn}(\omega_1, \omega_2, \alpha)$  is defined by formula (11) where the operators are changed to the numbers  $m, n$ .

Two equations in formulae (12) allow one to find  $\omega_{1,2}(\alpha)$  and exclude them from the expression for energy

$$\begin{aligned} E_{mn}^{(\text{OM})}(\alpha) &= v_1(\alpha)(n + \frac{1}{2}) + v_2(\alpha)(m + \frac{1}{2}) \\ v_{1,2}^2 &= \frac{1}{2M}(1 \pm \lambda \sin 2\alpha)[(M+1) \mp (M-1) \cos 2\alpha]. \end{aligned} \quad (13)$$

The energy (13) has an extremum when the transformation parameter  $\alpha$  is equal to

$$z_{1,2} = \frac{1}{2M\lambda}[(M-1) \pm \sqrt{(M-1)^2 + 4M\lambda^2}] \quad (14)$$

where  $z = \tan \alpha$ .

Substitution of the values (14) to the equation (13) shows that the energy levels  $E_{mn}^{(\text{OM})}$  found in the OM zeroth approximation coincide with the exact ones (2).

### 3. Analytical approximation for the CAO energy levels

Let us now consider the general form of the nonsymmetrical CAO Hamiltonian [10]

$$\hat{H} = \frac{1}{2}\hat{p}_x^2 + \frac{1}{2}\hat{p}_y^2 + \frac{1}{2}(x^2 + \Omega^2 y^2) + \lambda xy + Ax^4 + By^4 + Cx^2 y^2. \quad (15)$$

Here  $A$ ,  $B$  and  $C$  are the dimensionless parameters ( $A, B > 0, C > -2\sqrt{AB}$ ) and we have introduced not only a quadratic interaction between the oscillators but a linear one as well, because it is essential for the modelling of some molecular or lattice potentials [11].

As mentioned previously, we use the same transformation (9) in order to put the Hamiltonian (15) into the second quantized form. Then it is necessary to separate the zeroth-order Hamiltonian  $\hat{H}_0$  as the part of  $\hat{H}$  which commutes with the particle number operators  $\hat{n}_a$  and  $\hat{n}_b$ . In the considered case,  $\hat{H}_0$  is defined by the following expression:

$$\begin{aligned} \hat{H}_0 &= \frac{1}{2} \left( \omega_1 + \frac{u^2 + \Omega^2 v^2}{\omega_1} \right) (\hat{n}_a + \frac{1}{2}) \\ &+ \frac{1}{2} \left( \omega_2 + \frac{v^2 + \Omega^2 u^2}{\omega_2} \right) (\hat{n}_b + \frac{1}{2}) + \frac{\lambda uv}{\omega_1 \omega_2} [\omega_1 (\hat{n}_b + \frac{1}{2}) - \omega_2 (\hat{n}_a + \frac{1}{2})] \\ &+ \frac{3}{2\omega_1^2} (\hat{n}_a^2 + \hat{n}_a + \frac{1}{2}) (Au^4 + Bv^4 + Cu^2 v^2) \\ &+ \frac{3}{2\omega_2^2} (\hat{n}_b^2 + \hat{n}_b + \frac{1}{2}) (Av^4 + Bu^4 + Cu^2 v^2) \\ &+ \frac{1}{\omega_1 \omega_2} (\hat{n}_a + \frac{1}{2}) (\hat{n}_b + \frac{1}{2}) [2u^2 v^2 (3A + 3B - 2C) + C(u^4 + v^4)] \end{aligned} \quad (16)$$

where

$$u = \cos \alpha \quad v = \sin \alpha.$$

Now, by definition the eigenfunctions of the operator (16) are defined by the eigenvectors of the particle number operators

$$\hat{n}_a|N, M\rangle = N|N, M\rangle \quad \hat{n}_b|N, M\rangle = M|N, M\rangle \quad (17)$$

with the eigenvalues  $E_{NM}^{(0)}(\omega_1, \omega_2, \alpha)$ , which can be found from formula (16) by substituting the quantum numbers  $N$  and  $M$  instead of the corresponding operators.

However, these eigenvalues play only an intermediate role, and they lead us to the proper OM zeroth approximation only when we calculate the parameters  $\omega_1, \omega_2$  and  $\alpha$  for any quantum state from the conditions (12). Obviously, they prove to be rather complicated functions of the quantum numbers and Hamiltonian parameters, and just these functions ensure the uniform suitability of the OM approximation [3]. We use the same algorithm for the considered system and find a quite simple analytical approximation for the energy levels of the coupled anharmonic oscillators

$$E_{NM}^{(OM)} = \frac{1}{4} \left( 3\omega_1 + \frac{u^2 + \Omega^2 v^2}{\omega_1} \right) \left( N + \frac{1}{2} \right) + \frac{1}{4} \left( 3\omega_2 + \frac{v^2 + \Omega^2 u^2}{\omega_2} \right) \left( M + \frac{1}{2} \right) + \frac{\lambda uv}{2\omega_1 \omega_2} \left[ \omega_1 \left( M + \frac{1}{2} \right) - \omega_2 \left( N + \frac{1}{2} \right) \right]. \quad (18)$$

Of course, the nontrivial dependence of the energy on the quantum numbers is defined by the parameters  $\omega_1, \omega_2, \alpha$  being solutions of the following algebraic equations:

$$\omega_1^3 - \omega_1 \left\{ u^2 + \Omega^2 v^2 - 2\lambda uv + \frac{4}{\omega_2} \left( M + \frac{1}{2} \right) \left[ (3A + 3B - 2C) u^2 v^2 + \frac{1}{2} C (u^4 + v^4) \right] \right\} - \frac{6(2N^2 + 2N + 1)}{2N + 1} (Au^4 + Bv^4 + Cu^2 v^2) = 0 \quad (19)$$

$$\omega_2^3 - \omega_2 \left\{ v^2 + \Omega^2 u^2 + 2\lambda uv + \frac{4}{\omega_1} \left( N + \frac{1}{2} \right) \left[ (3A + 3B - 2C) u^2 v^2 + \frac{1}{2} C (u^4 + v^4) \right] \right\} - \frac{6(2M^2 + 2M + 1)}{2M + 1} (Av^4 + Bu^4 + Cu^2 v^2) = 0 \quad (20)$$

$$\begin{aligned} & \left[ \omega_1 \left( M + \frac{1}{2} \right) - \omega_2 \left( N + \frac{1}{2} \right) \right] (1 - \Omega^2 + 2\lambda \cot 2\alpha) \\ & + \frac{3\omega_2}{\omega_1} (2N^2 + 2N + 1) \left[ B - (A + B) \cos^2 \alpha + \frac{1}{2} C \cos 2\alpha \right] \\ & + \frac{3\omega_1}{\omega_2} (2M^2 + 2M + 1) \left[ A - (A + B) \cos^2 \alpha + \frac{1}{2} C \cos 2\alpha \right] \\ & + 12 \left( N + \frac{1}{2} \right) \left( M + \frac{1}{2} \right) (A + B - C) \cos 2\alpha = 0. \end{aligned} \quad (21)$$

These formulae should be modified in order to take into account the additional degeneracy of the energy levels caused by the permutative symmetry of the system in the case of identical oscillators ( $A = B, \Omega = 1$ ). If we do not make the modification in the OM zeroth approximation, the high-order corrections will have pseudo-singularities typical for any perturbation theory in the case of the levels close to the degeneracy [12].

Partly, this degeneracy is removed because of the rotation of the coordinates due to the transformation parameter  $\alpha$  (9). This leads to asymmetry relative to the permutation  $N \leftrightarrow M$  term in formula (19), but it is proportional to the parameter  $\lambda$  of linear coupling, and in the important case of only quadratic interaction of the oscillators [10] the degeneracy remains.

There is a well known algorithm to solve this problem in the general case. We should construct 'the right linear combinations' of the degenerate zeroth-order wavefunctions and take

into account the perturbation operator on this finite basis [12]. The operator method allows one to use this idea for obtaining the uniformly suitable approximation and the example of a two-level system in a quantum field was considered [13].

The modification of the OM zeroth-order approximation in our case means that the following wavefunctions of the ‘collective’ states

$$|\Psi_{NM}^{(0)}\rangle = C_1|N, M\rangle + C_2|M, N\rangle \quad N \neq M \quad (22)$$

should be used, instead of eigenfunctions of the operators  $\hat{n}_a$  and  $\hat{n}_b$ , in order to calculate the energy levels of the system. The coefficients  $C_{1,2}$  for any set of quantum numbers are considered as additional linear variational parameters.

Then, the degeneracy is removed because those terms in the perturbation operator  $\hat{V} = \hat{H} - \hat{H}_0$  which are proportional to

$$\hat{V}_{ab} = a^{+2}b^2 + a^2b^{+2} \quad (23)$$

commute with the total particle number operator

$$\hat{n} = \hat{n}_a + \hat{n}_b$$

but mix the states with the reverse order of the quantum numbers  $N$  and  $M$ .

As usual the condition of existence of nonzero coefficients  $C_{1,2}$  leads to the following expression for the energy levels of CAO instead of formula (18):

$$E_{NM}^{\pm} = \frac{1}{2}(E_{NM}^{(OM)} + E_{MN}^{(OM)}) \pm \sqrt{\frac{1}{4}(E_{NM}^{(OM)} - E_{MN}^{(OM)})^2 + |\langle N, M | \hat{V}_{ab} | M, N \rangle|^2} \quad (24)$$

with matrix elements

$$\langle N, M | \hat{V}_{ab} | M, N \rangle = \frac{C}{4\omega_1\omega_2} [(N+1)(N+2)\delta_{N,M-2} + (M+1)(M+2)\delta_{N,M+2}] \quad (25)$$

where  $\delta_{N,M}$  is the Kronecker delta.

It is important to note that the transformation parameters  $\omega_1, \omega_2, \alpha$  are defined by the same equations (19)–(21).

Generally speaking, formulae (18)–(21) and (24) realize the main purpose of our paper because they give the approximate algebraic presentation for the energy levels of CAO in the entire range of the Hamiltonian parameters and quantum numbers. These formulae can essentially complete the asymptotic and numerical calculations when the CAO are used for qualitative simulation of real physical systems.

#### 4. Comparison with known results

In this section we will consider the obtained formulae in various limit cases when the exact analytical series can also be found by other known methods. Besides, a number of the values  $E_{NM}^{(OM)}$  are compared with the numerical results  $E_{NM}^{(acc)}$  for the intermediate range of the oscillator parameters in order to prove the uniform suitability of the OM zeroth approximation. Finally, the second-order correction is calculated to analyse the convergence of the OM successive approximations.

It is important to stress here the point [3] that most of the above-mentioned series are asymptotic and make sense only in the range of small values of the corresponding parameters. At the same time, the OM zeroth approximation is written in the form of the analytical function over the entire range of variation for all parameters and quantum numbers. As a result, this function is expanded into the convergent power series and their coefficients cannot coincide completely with the analogous coefficients of the asymptotic divergent series. The differences between them are the same order of magnitude as the accuracy of the OM zeroth approximation for the intermediate values of the parameters.



#### 4.1. Small anharmonicity

( $AN, CM \ll 1$  and, for simplicity, we put  $\Omega = 1, B = \lambda = 0$ ).

The usual perturbation series, in terms of powers of  $A$  and  $C$ , with second-order accuracy, has the following form:

$$E_{NM}^{(PT)} \simeq N + M + 1 + \frac{3}{4}(2N^2 + 2N + 1)A + \frac{1}{4}[(2N + 1)(2M + 1) \pm (N^2 + 3N + 2)\delta_{N,M-2} \pm (M^2 + 3M + 2)\delta_{N,M+2}]C - \frac{1}{8}(34N^3 + 51N^2 + 59N + 21)A^2 - \frac{3}{4}(2M + 1)(2N^2 + 2N + 1)AC - \frac{3}{16}[3NM(N + M + 2) + \frac{3}{2}(N^2 + M^2) + \frac{5}{2}(N + M) + 1]C^2. \quad (26)$$

In order to consider formula (24) in the corresponding limit one should find the approximate solutions of the equations (19)–(21):

$$\begin{aligned} \omega_1 &\simeq 1 + \frac{1}{2}p_1 - \frac{1}{8}p_1^2 - \frac{1}{4}p_1p_2 - \frac{1}{2}p_1q + \frac{1}{2}q - \frac{1}{8}3q^2 \\ \omega_2 &\simeq 1 + \frac{1}{2}p_2 - \frac{1}{8}p_2^2 - \frac{1}{4}p_1p_2 - \frac{1}{4}p_2q \\ \alpha = 0 \quad p_1 &= (2M + 1)C \quad p_2 = (2N + 1)C \quad q = 6A \frac{2N^2 + 2N + 1}{2N + 1}. \end{aligned} \quad (27)$$

Substitution of these solutions into formula (24) shows that the expansion of the value  $E_{NM}^{(\pm)}$  in the case of small anharmonicity has almost the same form as  $E_{NM}^{(PT)}$  in formula (26), with only two distinctive terms of second order:

$$-\frac{9}{4} \frac{(2N^2 + 2N + 1)^2}{2N + 1} A^2 - \frac{1}{8}[4NM(N + M + 2) + 2(N^2 + M^2) + 3N + 3M + 1]C^2. \quad (28)$$

#### 4.2. Strong anharmonicity

Essentially, almost equivalent simplifications of the OM formulae can be made both in *strong coupling* ( $A, B, C \gg 1$ ) and *quasiclassical* ( $N, M \gg 1$ ) limit cases. As usual, even asymptotical formulae in the strong-coupling limit remain quite unwieldy in the general case, and we write them out only for the most interesting set of parameters ( $A = B; \Omega = 1; \lambda = 0$ )

As before we should begin from the equations for the OM parameters

$$\begin{aligned} \alpha = 0 \quad u = 1 \quad v = 0 \\ \omega_1 &\simeq \left[ Cz(2M + 1) + 6A \frac{2N^2 + 2N + 1}{2N + 1} \right]^{1/3} \\ \omega_2 &\simeq \left[ \frac{C}{z}(2N + 1) + 6A \frac{2M^2 + 2M + 1}{2M + 1} \right]^{1/3} \end{aligned} \quad (29)$$

where the value  $z$  is the positive solution of the following algebraic equation:

$$z^3 6A \frac{2M^2 + 2M + 1}{2M + 1} + z^2 C(2N + 1) - zC(2M + 1) - 6A \frac{2N^2 + 2N + 1}{2N + 1} = 0.$$

Then, one can find the approximate formula for the energy

$$E_{NM}^{(\pm)} \simeq \frac{3}{8}\omega_1(2N + 1) + \frac{3}{8}\omega_2(2M + 1) \pm \frac{C}{4\omega_1\omega_2} [(N + 1)(N + 2)\delta_{N,M-2} + (M + 1)(M + 2)\delta_{N,M+2}]. \quad (30)$$

It easy to verify that in the case of noninteracting systems ( $C = 0$ ) formula (30) leads to the same expression for the energy of each oscillator

$$\epsilon_N \simeq \frac{3}{8} [6A(2N+1)^2(2N^2+2N+1)]^{1/3}$$

as found previously [3] and proved to be quite a good approximation of the leading asymptotic term for the energy of the one-dimensional anharmonic oscillator.

Unfortunately, we do not know the accurate asymptotic formulae for interacting oscillators, but comparison of formula (29) with numerical results (see below) shows that the functional dependence of the energy levels on the Hamiltonian parameters in the considered range is correct with rather small errors ( $\sim 3\text{--}5\%$ ) in the coefficients of the corresponding series.

#### 4.3. Adiabatic approximation ( $\Omega \ll 1$ )

We simplify and transform the Hamiltonian (15) in such a way that one is able to find accurately the asymptotic series and compare with the OM results. Let us put  $A = B = \lambda = 0$ ;  $\Omega_Y = Y$ . This means that actually the following Hamiltonian is considered

$$\hat{H}_{ad} = \frac{1}{2} \hat{p}_x^2 + \frac{1}{2} \Omega^2 \hat{p}_Y^2 + \frac{1}{2} (x^2 + Y^2) + \frac{C}{\Omega^2} x^2 Y^2. \quad (31)$$

The adiabatic terms of the ‘quick’ oscillator ( $x$ ) can be found easily and corresponds to the zeroth-order Born–Oppenheimer approximation

$$\epsilon_N(Y) = \sqrt{1 + 2 \frac{C}{\Omega^2} Y^2} (N + \frac{1}{2}) \simeq \frac{\sqrt{2C}}{\Omega} |Y| (N + \frac{1}{2}).$$

Then the vibration spectrum of the ‘slow’ oscillator ( $Y$ ) in the considered limit can be found in the quasiclassical approximation. In the result, the leading term of the adiabatic series is defined as follows:

$$E_{NM}^{(AD)} \simeq \left(\frac{3}{4}\pi\right)^{2/3} [C(N + \frac{1}{2})^2 (M + \frac{1}{2})^2]^{1/3}. \quad (32)$$

**Table 1.** The ground state energy  $E_{00}$  for CAO,  $\lambda = 0$ ,  $\Omega = 1$ ,  $A = \mu a_{11}$ ,  $B = \mu$ ,  $C = 2\mu a_{12}$ .

$a_{11}$	$\mu$	E	$a_{12} = 1.0$	$a_{12} = 0.0$	$a_{12} = -0.6$
		$E^{(0)}$	1.1432	1.1103	1.0889
	0.1	$E^{(2)}$	1.1410	1.1083	1.0862
		$E^{(A)}$	1.1409	1.1082	1.0861
		$E^{(0)}$	1.7066	1.5852	1.5003
0.8	1.0	$E^{(2)}$	1.6923	1.5712	1.4776
		$E^{(A)}$	1.6913	1.5689	1.4740
		$E^{(0)}$	3.2641	2.9620	2.7444
	10	$E^{(2)}$	3.2240	2.9208	2.6739
		$E^{(A)}$	3.2200	2.9118	2.6572
		$E^{(0)}$	1.1226	1.0874	1.0643
	0.1	$E^{(2)}$	1.1206	1.0859	1.0621
		$E^{(A)}$	1.1206	1.0859	1.0621
		$E^{(0)}$	1.6263	1.4859	1.3824
0.4	1.0	$E^{(2)}$	1.6130	1.4743	1.3575
		$E^{(A)}$	1.6123	1.4725	1.3545
		$E^{(0)}$	3.0597	2.6979	2.4175
	10	$E^{(2)}$	3.0207	2.6616	2.3266
		$E^{(A)}$	3.0175	2.6538	2.3057

The analogous expansion can also be found for the OM zeroth approximation by means of the corresponding limit transition in the formulae (18)–(21). It leads to

$$E_{NM}^{(\text{OM})} \simeq \left(\frac{6}{4}\sqrt{3}\right)^{2/3} \left[C\left(N + \frac{1}{2}\right)^2 \left(M + \frac{1}{2}\right)^2\right]^{1/3} \quad (33)$$

which is in good agreement with formula (32).

#### 4.4. Numerical results

It is of interest to compare our analytical approximation with the accurate numerical results calculated for intermediate values of the Hamiltonian parameters in the series of papers [4, 10]. Table 1 shows the results of such a comparison for some specific values of the Hamiltonian parameters and quantum numbers.

In this table,  $E^{(0)}$  are calculated by means of the OM zeroth-order approximation,  $E^{(A)}$  are the same values from the above-mentioned papers. Besides, we have shown the values  $E^{(2)} = E^{(0)} + \Delta E$  with the OM next correction  $\Delta E$  calculated by means of the second-order perturbation theory in the operator  $\hat{V} = \hat{H} - \hat{H}_0$  with the Hamiltonians  $\hat{H}$  and  $\hat{H}_0$  defined by formulae (15) and (16). The details of the OM high-order corrections are considered in our paper [3]. For example, we write out the analytical formula for this correction in the considered case

$$\begin{aligned} \Delta E_{MN} = & X_1 \left[ \frac{1}{4} \left( \frac{1}{\omega_1} - \omega_1 \right) + 2a(2N - 1) + c(2M + 1) \right]^2 \\ & + X_2 \left[ \frac{1}{4} \left( \frac{1}{\omega_1} - \omega_1 \right) + 2a(2N + 3) + c(2M + 1) \right]^2 \end{aligned}$$

**Table 2.** The collective state energies  $E_{02}^{\pm}$  for CAO  $\lambda = 0$ ,  $\Omega = 1$ ,  $A = 1$ ,  $B = 1$ .

$C/2$	$E$	$E_{02}^+$	$E_{02}^-$
1.0	$E^{(0)}$	6.527	6.249
	$E^{(2)}$	6.526	6.248
	$E^{(A)}$	6.549	6.214
0.8	$E^{(0)}$	6.434	6.199
	$E^{(2)}$	6.435	6.201
	$E^{(A)}$	6.454	6.173
0.4	$E^{(0)}$	6.227	6.096
	$E^{(2)}$	6.233	6.102
	$E^{(A)}$	6.242	6.083
0.0	$E^{(0)}$	5.985	5.985
	$E^{(2)}$	5.993	5.993
	$E^{(A)}$	5.983	5.983
−0.4	$E^{(0)}$	5.687	5.868
	$E^{(2)}$	5.688	5.869
	$E^{(A)}$	5.657	5.879
−0.8	$E^{(0)}$	5.297	5.752
	$E^{(2)}$	5.260	5.715
	$E^{(A)}$	5.174	5.759
−1.0	$E^{(0)}$	5.046	5.698
	$E^{(2)}$	4.958	5.610
	$E^{(A)}$	4.775	5.690

$$\begin{aligned}
 &+X_3 \left[ \frac{1}{4} \left( \frac{\Omega^2}{\omega_2} - \omega_2 \right) + 2b(2M - 1) + c(2N + 1) \right]^2 \\
 &+X_4 \left[ \frac{1}{4} \left( \frac{\Omega^2}{\omega_2} - \omega_2 \right) + 2b(2M + 3) + c(2N + 1) \right]^2 + X_5 a^2 + X_6 b^2 + X_7 c^2.
 \end{aligned}
 \tag{34}$$

Here

$$\begin{aligned}
 a &= \frac{A}{4\omega_1^2} & b &= \frac{B}{4\omega_2^2} & c &= \frac{C}{4\omega_1\omega_2} \\
 X_1 &= \frac{N(N - 1)}{Z_{N-2,M}} & X_2 &= \frac{(N + 1)(N + 2)}{Z_{N+2,M}} \\
 X_3 &= \frac{M(M - 1)}{Z_{N,M-2}} & X_4 &= \frac{(M + 1)(M + 2)}{Z_{N,M+2}} \\
 X_5 &= \frac{N(N - 1)(N - 2)(N - 3)}{Z_{N-4,M}} + \frac{(N + 1)(N + 2)(N + 3)(N + 4)}{Z_{N+4,M}} \\
 X_6 &= \frac{M(M - 1)(M - 2)(M - 3)}{Z_{N,M-4}} + \frac{(M + 1)(M + 2)(M + 3)(M + 4)}{Z_{N,M+4}} \\
 X_7 &= \frac{N(N - 1)M(M - 1)}{Z_{N-2,M-2}} + \frac{(N + 1)(N + 2)(M + 1)(M + 2)}{Z_{N+2,M+2}} \\
 Z_{KL} &= -E_{KL}^{(OM)} + E_{NM}^{(OM)}.
 \end{aligned}
 \tag{35}$$

**Table 3.** The collective state energies  $E_{13}^{\pm}$  for CAO ( $\hat{H} = \hat{p}_x^2 + \hat{p}_y^2 + x^2 + y^2 + Cx^2y^2$ ).

$C$	$E$	$E_{13}^+$	$E_{13}^-$
0.1	$E^{(0)}$	10.3495	10.5943
	$E^{(2)}$	10.3440	10.5888
	$E^{(A)}$	10.3439	10.5883
1.0	$E^{(0)}$	12.4137	13.5932
	$E^{(2)}$	12.3339	13.5134
	$E^{(A)}$	12.3323	13.4505
5.0	$E^{(0)}$	16.8013	19.3336
	$E^{(2)}$	16.5758	19.1080
	$E^{(A)}$	16.5965	18.7387
20	$E^{(0)}$	24.1062	28.4908
	$E^{(2)}$	23.6777	28.0622
	$E^{(A)}$	23.7604	27.1386
100	$E^{(0)}$	39.1704	46.9931
	$E^{(2)}$	38.3734	46.1960
	$E^{(A)}$	38.582	44.249
1000	$E^{(0)}$	82.5140	99.6842
	$E^{(2)}$	80.7340	97.9042
	$E^{(A)}$	81.29	93.2
5000	$E^{(0)}$	140.5087	169.9703
	$E^{(2)}$	137.4448	166.9065
	$E^{(A)}$	138.39	158.8

One can see from table 1 that the OM zeroth approximation allows one to calculate the ground-state energy of the system with quite good accuracy for any parameters. Tables 2 and 3 are of particular interest because they show that OM is also effective when calculating the energies of the excited collective states and their splitting.

### 5. Iteration algorithm for the OM consequent approximations

In spite of the numerical calculation of the accurate energy spectrum for CAO not being the main purpose of our paper, we consider here the equations for the OM high-order corrections in order to illustrate the convergence of the method for the system with several degrees of freedom.

The full algorithm for calculation of the OM successive approximations was described in detail earlier [3] so we discuss it here very shortly. We find the solution of the Schrödinger equation

$$\hat{H}|\Psi_{NM}\rangle = E_{NM}|\Psi_{NM}\rangle \quad (37)$$

with Hamiltonian (15), in the following form:

$$|\Psi_{NM}\rangle = |N, M\rangle + \sum_{K, L \neq N, M} C_{NM}^{KL} |K, L\rangle. \quad (38)$$

Here,  $|N, M\rangle$  are the eigenvectors defined by equations (17). It is important to note that, in the general case, the operators  $\hat{n}_{a,b}$  and their eigenfunctions depend on the parameters of the transformation (9) and on the quantum numbers  $N, M$  because of equations (19)–(21). In the result, the state vectors  $|\Psi_{NM}^{(0)}\rangle \simeq |N, M\rangle$  are nonorthogonal in the OM zeroth-order approximation. But in the expansion (38) we use the full and orthogonal set of the state vectors referring to the quantum numbers  $N, M$  of the unknown wavefunction.

One can substitute the expansion (38)–(37) and obtain the system of infinite number of algebraic but nonlinear equations for the energy  $E_{NM}$  and coefficients  $C_{NM}^{KL}$  using the normalization condition in the form typical for perturbation theory in the Wigner–Brillouin form [3]

$$\langle N, M | \Psi_{NM} \rangle = 1.$$

If we suppose that the Hamiltonian (16) of the OM zeroth-order approximation defines the main contribution to the exact eigenvalue the above-mentioned equations can be solved by means of simple iteration considering the operator  $\hat{V} = \hat{H} - \hat{H}_0$  as a small value. It leads to the following system of recursion equations:

$$\begin{aligned} E_{NM}^{(s)} &= E_{NM}^{(0)} + \sum_{K, L \neq N, M} C_{NM}^{KL}(s-1) \langle N, M | \hat{V} | K, L \rangle \\ C_{NM}^{KL}(s) &= [E_{NM}^{(s)} - \langle K, L | \hat{H}_0 | K, L \rangle]^{-1} \\ &\quad \times \left\{ \langle N, M | \hat{V} | K, L \rangle + \sum_{P, Q \neq N, M} \langle N, M | \hat{V} | P, Q \rangle C_{KL}^{PQ}(s-1) \right\}. \end{aligned} \quad (39)$$

Here  $s = 0, 1, 2, \dots$  and the initial terms of the recursion sequence are

$$C_{NM}^{KL}(0) = 0 \quad E_{NM}^{(0)} = E_{NM}^{(OM)}.$$

It is well known that, in usual perturbation theory, the eigenvalue is calculated as the sum of the series of the corrections in a power of some parameter and this series is diverged for

**Table 4.** Convergence of the iterations  $E_{NM}^{(s)}$  for CAO,  $\lambda = 0, \Omega = 1, A = B, C = \mu A$ .

$A$	0.1	0.1	1.0	1.0	10	10
$\mu$	1.0	-1.0	1.0	-1.0	1.0	-1.0
$E_{00}^{(0)}$	1.152 760	1.085 516	1.765 877	1.492 155	3.108 030	2.770 058
$E_{00}^{(8)}$	1.150 188	1.081 282	1.724 184	1.443 776	3.301 210	2.557 740
$E_{00}^{(A)}$	1.150 2	1.081 3	1.724 2	1.443 8	3.301 2	2.557 7
$E_{10}^{(0)}$	2.419 662	2.231 765	3.835 767	3.105 372	7.610 856	5.924 771
$E_{10}^{(8)}$	2.414 341	2.221 196	3.830 324	3.066 649	7.527 043	5.487 183
$E_{10}^{(A)}$	2.414 3	2.211 2	3.830 4	3.066 6	7.527 1	5.488 1

**Table 5.** Complex-valued energies  $\text{Re } E_{NM}^{(s)} - i \text{Im } E_{NM}^{(s)}$  for the CAO quasistationary states  $\lambda = 0, \Omega = 1, A = B, C = \mu A$ .

$A$	-0.1	-0.1	-0.2	-0.2	-0.4	-0.4
$\mu$	1.0	-1.0	1.0	-1.0	1.0	-1.0
$\text{Re } E_{00}^{(10)}$	0.753 411	0.864 702	0.719 257	0.798 733	0.752 215	0.768 634
$\text{Im } E_{00}^{(10)}$	0.159 099	0.046 916	0.379 077	0.163 381	0.642 765	0.340 915
$\text{Re } E_{10}^{(12)}$	1.439 368	1.663 981	1.458 860	1.627 066	1.596 000	1.651 425
$\text{Im } E_{10}^{(12)}$	0.571 692	0.252 742	1.070 673	0.540 111	1.646 405	0.884 010

anharmonic oscillators. In contrast, the accurate values for the energy and coefficients of the wavefunction are calculated as the limits of the recursion sequences

$$C_{NM}^{KL} = \lim_{s \rightarrow \infty} C_{NM}^{KL}(s) \quad E_{NM} = \lim_{s \rightarrow \infty} E_{NM}^{(s)} \tag{40}$$

which are proved to converge rather rapidly.

The numerical results in table 4 show that, in many cases, eight iterations calculated by our method lead to more precise eigenvalues than found in [10] by means of a more complicated algorithm.

In conclusion, we would like to discuss one more important application of the operator method. The matter is that, in accordance with the analysis considered in our paper [3] for a one-dimensional system, the optimal choice of artificial parameters in the transformation (9) is essential for uniformly suitable zeroth approximation. However, in the OM successive approximations these parameters define only the rate, not the convergence, of the iterations which exist in the complex-valued plane of  $\omega$ . The same result proved to be correct for the CAO system. Moreover, the recursion sequence (40) also converges for the complex-valued parameters  $\omega_{1,2}$ . It allows one to use the method of complex rotation of the coordinates when calculating the energies and widths of the quasistationary states [14]. In our case, such a problem appears when the parameters  $A, B$  in Hamiltonian (15) are negative. Also, table 5 shows the real parts  $E_{NM}^{(s)}$  of the energy for the quasistationary levels and their imaginary parts  $(-\Gamma_{NM}^{(s)}/2)$  calculated by means of the equations (39) in the result of  $s$  iterations. One can see that 12 iterations were enough in order to find six exact figures for unknown values and this confirms the high rate of convergence for the OM algorithm.

## 6. Conclusions

Thus, the quantum system of two coupled anharmonic oscillators was investigated by means of the operator method for the solution of the Schrödinger equation. Analysis of this model allows us to emphasize the two most essential aspects of the considered approach.

On the one hand, it was shown that the OM, as the nonperturbative method for the description of quantum systems, remained effective in the case of several degrees of freedom with strong interaction. It means that the OM zeroth approximation interpolates the exact eigenvalues in the entire range of the system parameters and its subsequent approximations converge rather rapidly to the exact solution of the Schrödinger equation.

More applied results of our paper are defined by formulae (18)–(22) which describe analytically the quantum levels of the system with arbitrary values of anharmonicity and coupling constant. Formulae (18) can be considered as the generalization for the nonlinear system the conception of the normal coordinates. Of course, there is no full separation of variables in this case because of the parameters  $\omega_{1,2}$ , but nevertheless it can be a good basis for classification of the vibration spectra for the molecules with strong anharmonicity and for analysis of nonadiabatic and correlation effects in solid state physics.

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