Canonical averaging of the equations of quantum mechanics

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The representation of a Schrödinger equations as a classic Hamiltonian system allows to construct a unified perturbation theory both in classic, and in a quantum mechanics grounded on the theory of canonical transformations, and also to receive asymptotic estimations of affinity of the precise approximated solutions of Schrodinger equations.

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I. INTRODUCTORY REMARKS

The very possibility of applying the modern methods of the classical theory of non-linear oscillations to quantum mechanics is based upon the representation of the non-stationary Schrödinger’s equation as a classical Hamiltonian system. From this perspective it is quite natural to construct a special asymptotic perturbation theory which utilises the advantages of the Hamiltonian formalism, that is to apply canonical transformations. Special and sufficiently efficient approaches [1], [2] and [3] were developed by mathematicians for canonical systems. However, the generality of these approaches makes them very cumbersome whereas the first two non-trivial approximations are ordinarily sufficient for practical application.

Traditionally, mathematicians use the methods of spectral analysis of operators for constructing perturbation theory in non-relativistic quantum mechanics, see [4], [5]. However, it is necessary to take into account that, in practice, physicists do not distinguish between the concepts of self-adjoint and symmetric operators. This gives rise to two unpleasant things: firstly, the domain of definition of the operator in Hilbert space remains unclear which does not allow one to apply the methods of spectral theory, and secondly, the domain of definition of the operator includes all functions for which analytical operations are meaningful regardless of the fact whether these functions (and the result of applying an operator to them) belong to Hilbert space. A rigorous consideration of the latter case requires the introduction of an equipped Hilbert space, see [6], [7].

For this reason it is not possible to prove even the conditions for applicability of the regular perturbation theory developed by Kato-Relih [8], [9] providing us with the criterion for the Rayleigh-Schrödinger formal series to have a non-zero radius of convergence.

It is well known that orthodox perturbation theory is not applicable to many cases since the corresponding series diverge. The asymptotic character of the series used in perturbation theory was first proved by Titchmarsh [10]. A rigorous proof of the divergence of this series for an anharmonic oscillator \( V \sim x^4 \) is given by Bender and Woo [11].

In addition to the associated complexity, the above-mentioned methods possess another shortcoming, namely they do not allow one to obtain the wave function which plays an important role in the investigation of physical systems.

In the present chapter we suggest another approach which is based upon the representation of the non-stationary Schrödinger’s equation as a classical Hamiltonian system. This representation enables one to make use of the powerful, modern, rigorously substantiated methods of the classical theory of non-linear oscillations (asymptotic perturbation theory) and indicate simple conditions for justifying the applicability of the results obtained.

An important part for the transition from the hypotheses of Planck and Einstein to quantum mechanics was played by the adiabatic hypothesis by Ehrenfest. Born and Fock showed in 1928, [11], that Ehrenfest’s hypothesis is a consequence of the postulates of quantum mechanics. A rigorous mathematical proof of the adiabatic theory was given by Kato in 1949, [12]. Later on, the adiabatic Landau-Dykhne approximation, [13], [14], [15], was built on the analogy between the adiabatic and quasi-classical approximations.

The Born-Fock adiabatic approximation is actually not an approximation since all of the terms of the adiabatic Born-Fock series have the same order of smallness, [15], [16], which, in turn, does not allow us to construct a post-adiabatic approximation. The Born-Fock condition, which implies real-valued wave functions, does not allow us to use this approximation in problems involving magnetic fields.

The results of the Landau-Dykhne adiabatic approximation relate to the results of non-stationary perturbation theory only approximately. In addition to this, both approximations yield an incorrect factor in front of the exponential function, see [14].

The problem of the time interval, within which the difference between the approximated and exact solutions is small, plays an important part in the non-stationary case. In the above works, this problem is not discussed at all.

In the present chapter, the adiabatic and the post-
II. STATIONARY SCHRODINGER’S EQUATION AS A CLASSICAL HAMILTONIAN SYSTEM

In this section the classical canonical perturbation theory is applied to constructing asymptotic solutions of Schrödinger’s equation with a discrete spectrum. The main subject of analysis of the non-relativistic quantum theory is Schrödinger’s equation, 13,

\[ i\hbar \frac{\partial \Psi(q,t)}{\partial t} = \hat{H} \Psi(q,t), \]  

where \( i^2 = -1, \; \hbar = 1.054 \times 10^{-34} \text{Js} \) denotes Planck’s constant, \( q = (q_1, q_2, ..., q_n) \) denotes a point of the configuration space of the corresponding classical system, \( t \) is time and \( \Psi(q,t) \) denotes a complex-valued function with integrable square of the absolute value. Further, \( \hat{H} \) denotes a self-adjoint (symmetric) operator in Hilbert space, which in Cartesian coordinates, in Schrödinger’s representation for one particle, has the form, 12,

\[ \hat{H} = \hat{T} + \hat{V} = -\frac{\hbar^2}{2m} \Delta + \hat{V}(x,y,z), \]  

where \( \hat{T} \) and \( \hat{V} \) designate operators of the kinetic and potential energies, respectively, \( \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \), and \( m \) is mass of the particle. Schrödinger’s equation 13 is subject to an initial condition \( \Psi(q,0) = \Psi_0(q) \) and some boundary conditions.

The case studied in the framework of perturbation theory appears when operator \( \hat{H} \) can be cast as the sum

\[ \hat{H} = \hat{H}_0 + \varepsilon \hat{V}, \; 0 < \varepsilon << 1, \]  

of two self-adjoint operators, the corresponding problem 14 for operator \( \hat{H}_0 \) being assumed to have an exact solution and the second operator (perturbation) being small in some sense, 3, 5, 13.

The majority of the physically interesting problems turn out to be mathematically incorrect, since the perturbation operators are usually not bounded and not even self-adjoint. The latter is related to the fact that physicists never distinguish between the concepts of self-adjoint and symmetric operators. This leads to the operator space in Hilbert space being unclear, which in turn does not allow one to apply the methods of spectral theory 3, 5. For this reason, it is difficult to indicate the conditions for the applicability of perturbation theory and estimate the discrepancy between the exact and an approximate solution for practical problems.

However, it is possible to reduce Schrödinger’s equation to a form of classical Hamiltonian system, which is well-developed in non-linear mechanics. This allows one to apply the methods of classical dynamics which are rigorously substantiated and simpler from the perspective of application.

Let us consider eq. 11 with Schrödinger’s operators 3, i.e. the problem

\[ i\hbar \frac{\partial \Psi(q,t)}{\partial t} = (\hat{H}_0 + \varepsilon \hat{V}) \Psi(q,t), \]  

\[ \Psi(q,0) = \Psi_0(q). \]  

(4)

where operator \( \hat{H}_0 \) does not depend on time and \( \varepsilon \) is a formal small parameter. The question of choosing the small parameters is discussed below.

Along with the problem we consider, the generating approximation, which is obtained from eq. 4 at \( \varepsilon = 0 \)

\[ i\hbar \frac{\partial \Psi^0(q,t)}{\partial t} = \hat{H}_0 \Psi^0(q,t), \]  

\[ \Psi^0(q,0) = \Psi_0(q). \]  

(5)

Assuming the spectrum to be discrete, we can apply Fourier’s method and set the general solution of problem 5 in the form

\[ \Psi^0(q,t) = \sum_{n=0}^{\infty} \psi_n^0(q) \exp(-i\omega_n^0 t), \]  

\[ \psi_n^0(q) = \int \Psi_0(q) \psi_n^0(q) dq, \; \omega_n^0 = E_n^0 / \hbar, \]  

(6)

where \( \psi_n^0(q) \) and \( E_n^0 \) denote respectively the eigenfunctions and eigenvalues of the following problem

\[ \hat{H}_0 \psi_n^0(q) = E_n^0 \psi_n^0(q) \]  

and an asterisk denotes the complex conjugate.

The self-adjoint character of operator \( \hat{H}_0 \) means that for \( \Psi(q,t) \in L^2 \) the following expansion is valid

\[ \Psi(q,t) = \sum_{n=0}^{\infty} c_n(t) \psi_n^0(q) \exp(-i\omega_n^0 t). \]  

(8)

Inserting expansion 5 into eq. 4 yields the following equations for the coefficients of the expansion \( c_n(t), c_n^*(t) \)

\[ \dot{c}_n(t) = -i \varepsilon \sum_{m=0}^{\infty} v_{nm} c_m(t) \exp(-i\omega_m^0 t), \]  

\[ \dot{c}_n^*(t) = i \varepsilon \sum_{m=0}^{\infty} v_{mn} c_m^*(t) \exp(i\omega_m^0 t), \]  

(9)
\[
v_{mn}(t) = \frac{1}{\hbar} \int \psi_m^0(q)V(q,t)\psi_n^0(q)dq, \tag{10}\]

where a dot implies time derivative and \(\omega_{mn}^0 = \omega_m^0 - \omega_n^0\).

The system of equations (3) is Hamiltonian (in the classical sense) with the following Hamilton function

\[
\epsilon H_1(c, c^*, t) = -\epsilon \sum_{n,m=0}^{\infty} v_{nm} c_n^* c_m \exp(i\omega_{nm}^0 t), \tag{11}\]

and describes a classical distributed system with an infinite number of internal resonances. The system is Hamiltonian as matrix \(v_{nm}\) is Hermitian, that is the perturbation operator is self-adjoint. By separating the principal resonance \(\omega_m^0 = \omega_n^0\), we can cast Hamilton’s function (11) as follows

\[
\epsilon H_1(c, c^*, t) = -\epsilon \sum_{n,m=0}^{\infty} v_{nm} c_n^* c_m \exp(i\omega_{nm}^0 t), \tag{12}\]

where a prime denotes the sum without the term with \(n = m\). Transformation of variables \(c_n, c_n^*\) to the real-valued “action-angle” variables \(I_n, \psi_n\) by means of the formulae

\[
c_n = \sqrt{I_n} \exp(-i\psi_n), \quad I_n = c_n c_n^*, \]
\[
c_n^* = \sqrt{I_n} \exp(i\psi_n), \quad \psi_n = -\arctan \left(\frac{c_n - c_n^*}{i(c_n + c_n^*)}\right) \tag{13}\]

we can set system (10) in the form

\[
\dot{I}_n = \epsilon^2 \sum_{m=0}^{\infty} \sqrt{I_n I_m} \times \text{Im}\{v_{nm} \exp[-i(\psi_m - \psi_n + \omega_{mn}^0 t)]\} \tag{14}\]
\[
\dot{\psi}_n = \epsilon v_{nn} + \epsilon \sum_{m=0}^{\infty} \sqrt{I_n I_m} \times \text{Re}\{v_{nm} \exp[-i(\psi_m - \psi_n + \omega_{mn}^0 t)]\}
\]

and Hamilton’s function (12) as follows

\[
\epsilon H_1(I, \psi, t) = \epsilon \sum_{m,n=0}^{\infty} v_{nm} \sqrt{I_n I_m} \times \exp[-i(\psi_m - \psi_n + \omega_{mn}^0 t)] \tag{15} \]

Systems (3) and (14) do not contain Planck’s constant explicitly and are the classical Hamiltonian systems with an infinite number of internal resonances. Estimates of the norm of discrepancy between the exact and approximate solutions as well as the conditions for applicability of the averaging method for these systems are given by the Los theorem, see [17] and [18], which is a generalisation of Bogolyubov theorem for the case of an infinite-dimensional coordinate Hilbert space.

The canonical form of systems (9) and (14) allows us to consider the evolutionary equations by operating only with Hamilton’s functions (12) and (15), i.e. by calculating an averaged Hamilton’s function. For example, for eqs. (9) and (14) the second approximation \(\tilde{H}^{(2)}\) for the help of the following formulae

\[
\tilde{H}^{(2)}(\tilde{c}, \tilde{c}^*) = \epsilon \tilde{H}_1(\tilde{c}, \tilde{c}^*) + \epsilon^2 \tilde{H}_2(\tilde{c}, \tilde{c}^*),
\]
\[
\tilde{H}_1 = \langle H_1 \rangle, \quad \tilde{H}_2 = -\left\langle \frac{\partial H_1}{\partial \tilde{c}^*} \frac{\partial \{H_1\}}{\partial \tilde{c}^*} \right\rangle, \tag{16}\]

where \(\tilde{c}_n\) and \(\tilde{c}_n^*\) denote the evolutionary components of variables \(c_n\) and \(c_n^*\). In the latter equation the following notation is used

\[
\langle f \rangle = \lim_{T \to \infty} \frac{1}{T} \int_{t_0}^{t_0 + T} f(\tilde{c}, \tilde{c}^*, t)dt,
\]
\[
\hat{f}(\tilde{c}, \tilde{c}^*, t) = f(\tilde{c}, \tilde{c}^*, t) - \langle f \rangle,
\]
\[
\{ f \} = \int \hat{f}(\tilde{c}, \tilde{c}^*, t)dt, \tag{17}\]

the arbitrary function of slow variables \(\tilde{c}\) and \(\tilde{c}^*\) being set to zero while estimating the last integral.

Let us notice that \(\tilde{H}\) is an integral of the averaged equations of motion, i.e. an adiabatic invariant [20, 21].

The first approximation \(\tilde{c}_n^{(1)}\) to expansion coefficient \(c_n\) is given by the formula \(\tilde{c}_n^{(1)} = \tilde{c}_n\), where \(\tilde{c}_n\) satisfies the following equation

\[
\bullet \quad \tilde{c}_n = \epsilon \frac{\partial \tilde{H}_1}{\partial \tilde{c}_n^*}. \tag{18}\]

The second approximation \(\tilde{c}_n^{(2)}\) to expansion coefficient \(c_n\) is given by

\[
\tilde{c}_n^{(2)} = \tilde{c}_n + \epsilon \frac{\partial \{H_1\}}{\partial \tilde{c}_n^*}, \tag{19}\]

where the second approximation to evolutionary component \(\tilde{c}_n\) is obtained from the equation

\[
\bullet \quad \tilde{c}_n = \epsilon \frac{\partial \tilde{H}_1}{\partial \tilde{c}_n} + \epsilon^2 \frac{\partial \tilde{H}_2}{\partial \tilde{c}_n^*}. \tag{20}\]

### III. GENERAL PROPERTIES OF THE CANONICAL FORM OF SCHRODINGER’S EQUATION

Representation of Schrödinger’s equation in canonical form (9) or (14) allows us to draw a number of conclusions without performing any calculations.
1. The original formulation of the problem of perturbation theory for the non-stationary Schrödinger’s equation results in formulae enabling us to study all cases: stationary (non-degenerate and degenerate), non-stationary, resonant, adiabatic etc.

2. In the stationary case, for which matrix elements \(v_{mn}\) are independent of time, in the absence of degeneracy and the internal resonances \(\omega_{mn} \neq O(\varepsilon), m \neq n\) except for the selected principal resonance \((m = n)\), systems \([9]\) or \([13]\) admit direct averaging. The equation for the evolutionary components of phase \(\psi_n\) has the form \(\psi_n = \varepsilon v_{nn} t + \psi_{n0}\). In turn, this means that the first correction to the energy appears due to the principal internal resonance. This conclusion remains valid for any order of the perturbation theory since the corrections to the eigenvalues of the unperturbed operator \(H_0\) are basically determined by the principal internal resonance.

3. It is obvious that the first-order contribution to the averaged Hamilton function are the corrections to the energy.

Let us notice that direct averaging without introducing the resonant terms would lead to the appearance of divergent terms which are proportional to \(1/(E_m - E_n)\) \((m \to n)\). Thus, separation of the resonant terms eliminates the divergent terms in the perturbation theory series.

4. Contributions from these sums are not zero if the perturbation is stationary and the unperturbed levels contain close levels for which \(\omega_{nn} = O(\varepsilon)\). Thus, the problem of close levels should be solved only in a non-stationary form. It is evident that the problem for degenerate levels is a particular case of the previous one for which, along with the principal quantum number \(n\), there is a multiindex \(\alpha\) characterising the unperturbed eigenvalue, so that the relationship \(\omega_{\alpha n, n\beta} = O(\varepsilon)\) holds. All these cases are manifestations of the resonances additional to the principal internal resonance.

5. Generally speaking, a general analysis is not applicable for time-dependent perturbations because it is necessary to know the spectrum of the perturbation so as to take correct account of the possible resonances. Only general analysis of periodic (in particular, single-frequency) perturbation is feasible.

6. For the sake of simplicity, let us consider the case of single-frequency perturbation \((v_{mn} \sim \exp(\pm i\omega t))\). Clearly, the problem in this case is reduced to the stationary one, for which the expansion is performed for wave functions of the stationary states with the new frequencies \(\omega_{mn} = \omega_m - \omega_n\) such that \(\omega_m = \omega_m^0 - \omega/2, \omega_n = \omega_n^0 + \omega/2\) (for \(\omega \sim \exp(i\omega t)\)) and \(\omega_m = \omega_m^0 + \omega/2, \omega_n = \omega_n^0 - \omega/2\) (for \(\omega \sim \exp(-i\omega t)\)).

Thus, the corresponding quantities \(E_m,n = \hbar \omega_{mn}\) are energies, that is the energy of the system: unperturbed system (atom) and a field. Their interaction is absent, the original interaction being included into the definition of the quasi-energy. This gives rise to the concept of the system dressed by a field (dressed atom, \([21]\)).

Traditionally, this conclusion is obtained in a rather sophisticated way by means of Floquet theorem and the conclusion on the level splitting is obtained only in the resonant approximation, see \([17], [20]\). Let us notice that the results of this point are valid for any value of parameter \(\varepsilon\), that is regardless of the perturbation theory.

7. The exact eigenfrequencies of the perturbed system are given by the relationship \(\omega_n = \omega_n^0 + \psi_n\). Thus, the second equations in \([14]\) determine corrections to the eigenfrequencies caused by perturbation. In principle, these corrections can be removed by a canonical transformation of the phase which can serve as a distinctive procedure of renormalisation which allows one to remove the secular terms from the series of the perturbation theory. It is obvious that in the non-stationary case (even for \(v_{mn} = 0\) there exists a non-zero contribution of the first order stemming from the sum. The presence of this contribution is not possible using orthodox perturbation theory. The coherent interaction with the external field is realised under the condition of constant phase difference (the condition of equality of the original frequencies is only a necessary condition) and has the form \(\dot{\psi}_2 - \dot{\psi}_1 - \omega = \omega_2^0 + \dot{\psi}_2 - \omega_1^0 + \dot{\psi}_1 = \omega_{21}^0 - \omega + \dot{\psi}_2 - \dot{\psi}_1 = 0\),

where \(\omega\) denotes the frequency of the external field satisfying the condition that \(\omega_{21}^0 = \omega = O(\varepsilon)\).

One usually uses the condition that the transition frequency is close to that of the external field. It follows from the form of the equations for \(\psi_n\) that the type of problem for resonant interaction coincides with the type considered in point 4 above.

The exact frequencies \(\omega_{n}\) the system are anisochronous which is a characteristic of the non-linear classical system and leads to bounded solutions at resonance even in the case of no damping, in spite of the linearity of Schrödinger’s equation.

Thus, Schrödinger’s equation is equivalent to some classical non-linear distributed system whereas representations \([9]\) or \([13]\) are expansions in terms of normal forms of the unperturbed system.

To some extent, it is the picture to which Schrödinger tended and which is most close to the classical one. "There is no need to explain that the representation of the energy transformation from one oscillatory form to another under a quantum energy transition is much more satisfactory than that of electron jump"\(^{1}\), \([22]\).

8. It is evident that no specific "quantum-mechanical"

\[1\] Translation from Russian
properties of the generating operator $\hat{H}_0$, but being self-adjoint, is used. Nevertheless, this technique allows us to analyse other self-adjoint problems of mathematical physics with a discrete spectrum. Taking into account the particular structure of the generating operator $\hat{H}_0$ we can construct a more efficient theory [24].

An attempt to apply the averaging method to quantum mechanics was undertaken in [23]. However, as follows from the above, the absence of resonances (the main assumption of the authors) is not correct. Besides, despite the title of this article, the authors did not succeed in a proof of the theorem of convergence of the constructed perturbation theory.

9. All formulae remain valid for the case of adiabatic perturbation, i.e. under the additional dependence of perturbation on the slow time $\tau = \varepsilon t$ ($\varepsilon V = \varepsilon V(\vec{r}, t, \tau)$). In this case, equations for the evolutionary components become non-stationary and require more sophisticated integration methods.

10. Small parameter $\varepsilon$ is introduced in systems [21] and [14] in a formal way. Generally speaking, the question of a rigorous introduction into equations should be considered individually for each particular problem. Let us point out some general ideas.

Let us introduce some characteristic values $[E]$ and $[V]$ for the eigenvalues $E$ and matrix elements $V_{nm}$ respectively. Then $[E]/\hbar = \omega_0$ and $[V]/\hbar = \Omega_0$ can be referred to as a characteristic eigenfrequency and the generalised Rabi frequency (for a dipole interaction $V \sim \vec{d}\vec{E}_0$ and $V/\hbar \sim \Omega$ is called the Rabi frequency). Further study depends on the relationship between frequencies $\omega_0$ and $\Omega_0$. Let $\omega_<$ and $\omega_>$ denote respectively the smaller and the larger of frequencies $\omega_0$ and $\Omega_0$. Entering a non-dimensional time $t_n = \omega_<> t$ into dimensional systems [19] and [14] we obtain the following value $\varepsilon = \omega_< / \omega_>$. Three cases are possible:

a) the case of a weak field $\omega_0 >> \Omega_0$, $t_n = \omega_0 t$, $\varepsilon = \Omega_0/\omega_0$,
b) the case of a strong field $\omega_0 << \Omega_0$, $t_n = \Omega_0 t$, $\varepsilon = \omega_0/\Omega_0$,
c) the case in which the frequencies are of the same order, that is, $\omega_0 \sim \Omega_0$. In this case an additional resonance occurs in the system and the small parameter is absent. This situation requires special consideration.

Clearly, both $[E]$ and $[V]$ are, in general, functions of $n$ and $m$ which should be taken into account while carrying out estimates.

11. In problems with initial conditions, the values of the coefficients $c_n^{(1)} |_{t=0}$ in the expansions of the initial functions have order of unity, whilst those which do not appear ($c_n^{(1)} |_{t=0} = 0$) are of order of $\varepsilon$. As follows from Parseval’s equality $\left( \sum_n |c_n|^2 = 1 \right)$ coefficient $c_n$ must rapidly decreases with the growth of $n$, thus, the first order approximation in [3] contains a finite sum with terms having non-zero coefficients $c_n$ of the expansion of the initial function.

It becomes clear from the above that an accurate account of all possible internal and external resonances in the system, i.e. the analysis of the phase relationships, plays a crucial part for obtaining a correct result. For this reason, it is natural to refer to this perturbation as the phase perturbation theory.

IV. STATIONARY PERTURBATION OF A NON-DEGENERATE LEVEL OF THE DISCRETE SPECTRUM

Let us consider a perturbation of a non-degenerate level of the discrete spectrum, i.e. the case $\hat{V} = \hat{V}(\vec{r})$. The canonical procedure of averaging is carried out by using Hamilton’s function (12) under the condition $\omega_{mn}^0 \neq O(\varepsilon)$ implying no degeneracy and no close energy levels. Simple calculation by means of eq. (10) yields

$$\{ \hat{H}_1 \} = \sum_{n,m} v_{nm} \bar{c}_m c_n \exp(-i\omega_{mn}^0 t)$$

$$\hat{H}_1 = -i \sum_k v_{kk} \bar{c}_k c^*_k$$

The second approximation to the averaged Hamilton’s function (12) is given by

$$\bar{H}^{(2)} = \varepsilon \bar{H}_1 + \varepsilon^2 \bar{H}_2 = -i \sum_k \Delta \omega_k \bar{c}_k c^*_k,$$

$$\Delta \omega_k = \varepsilon v_{kk} + \varepsilon^2 \sum_l \frac{|v_{kl}|^2}{\omega_{kl}^0}$$

Both first and second terms on the averaged Hamilton function can be renormalised by the phase (frequency) renormalisation in the original expansion [5], i.e. by replacing $\omega_{kl}^0$ by $\Omega_{kl}^0 = \omega_{kl}^0 + \Delta \omega_k$. In addition to this, $H^{(2)} \equiv 0$. This procedure can be performed in any order of calculations. This means in turn that, instead of a standard time interval $\Delta t \sim 1/\varepsilon$, this approximation is valid for exponentially large time intervals which is in full agreement with the general theorems of mechanics on the behaviour of Hamiltonian systems close to integrable systems [21].

The Hamilton function has a diagonal form and the coefficients of the quadratic form are corrections to the phase (energy) of the unperturbed wave function.

Equation (20) of the second approximation for the evolutionary component $\bar{c}_k^{(2)}$ has the form

$$\bar{c}_k = \frac{\partial \bar{H}^{(2)}}{\partial \bar{c}_k} = -i \Delta \omega_k \bar{c}_k .$$

Then we easily obtain

$$\bar{c}_k^{(2)} = A_k \exp(-i\Delta \omega_k t).$$
Coefficients $A_k$ are determined from the initial conditions.

The second approximation to coefficients $c_k$ in expansion (3), obtained by means of formula (13), is as follows

$$c_k^{(2)} = A_k^{(2)} \exp(-i\epsilon \Delta \omega t)$$

$$+ \varepsilon \sum_m \frac{\varepsilon km}{\omega_{mk}^0} A_m^{(1)} \exp(-i\Omega_{mk} t),$$

(25)

where $\Omega_{mk} = \Omega_m - \Omega_k$, $\Omega_k = \omega_k^0 + \Delta \omega_k$, and $A_k^{(1)}, A_k^{(2)}$ denote the first and the second approximations to coefficients $A_k$ (it is sufficient to substitute only the first approximation to $A_k$ into the second term in eq. (25)).

The second approximation to wave function $\Psi^{(2)}$ is constructed with the help of coefficients $c_k^{(2)}$

$$\Psi^{(2)} = \sum_k \left[ A_k^{(2)} - \varepsilon \sum_m \frac{\varepsilon km}{\omega_{km}^0} A_m^{(1)} \right] \exp(-i\Omega_{km} t)$$

$$\times \Psi_0^k \exp(-i\Omega_k t),$$

(26)

where $\Omega_k = \omega_k^0 + \Delta \omega_k$, i.e. it is sufficient to restrict the consideration by the first correction to the eigenfrequency.

Provided that the system is in the $n$-th stationary state of the discrete spectrum, then $A_k = \delta_{kn}$ and we obtain from eq. (26) that

$$\Psi_n^{(2)} = \left[ \Psi_n^0 + \varepsilon \sum_k \frac{\varepsilon kn}{\omega_{nk}^0} \Psi_k^0 \right] \exp(-i\Omega_n t).$$

(27)

In the case of Cauchy’s problem, the system at the initial time instant is in a certain stationary state of the discrete spectrum, in the $s$-th state say, that is $\Psi(q, t)|_{t=0} = \Psi_s^0$ and $c_n|_{t=0} = \delta_{ns}$. Coefficients $A_n^{(1)}, A_n^{(2)}$ are obtained from the relationship

$$\delta_{ns} = A_n^{(2)} + \varepsilon \sum_m \frac{\varepsilon nm}{\omega_{mn}^0} A_m^{(1)}.$$  

(28)

From this relationship we obtain $A_n^{(1)} = \delta_{ns}$ and $A_n^{(0)} = \delta_{ns} - \varepsilon \omega_{n s}^0$. The second approximation to the wave function has the form

$$\Psi^{(2)} = \left[ \Psi_s^{(0)} + \varepsilon \sum_k \frac{\varepsilon ks}{\omega_{sk}^0} \Psi_k^0 \right] \exp(-i\Omega_s t)$$

$$+ \varepsilon \sum_k \frac{\varepsilon ks}{\omega_{sk}^0} \Psi_k^0 \exp(-i\Omega_k t).$$

(29)

This formula is absent in the standard textbooks on quantum mechanics. It is important to mention that it is adopted in courses on quantum mechanics that the probability of transition to this problem is determined by the square of the absolute value of the first correction to the expansion coefficients $c_n$, that is, by the second term in eq. (25), see for example [13]. The relationships in eq. (26) show that it is not correct. This term determines the correction to the unperturbed wave function of the initial state. The transition probability is determined by the second terms in $\Delta \Omega_n^{(1)}$ which is completely absent in the standard perturbation theory. This is due to the fact that initial condition $c_n|_{t=0} = \delta_{ns}$ is not satisfied. The whole coefficient $c_n^{(2)}$, rather than a part of it, as in the standard theory, must satisfy this initial condition. In the case under consideration, coincidence is occasional because the coefficients are independent of time. But these coefficients are different in the non-stationary theory.

As an example of applying formula (26), we consider the problem of the excitation of a charged oscillator by an abruptly applied homogeneous electric field $\varepsilon$, directed along the oscillation axis, [13], [20].

In this case it is necessary to solve the problem

$$i\hbar \frac{\partial \Psi(x,t)}{\partial t} = (\hat{H}_0 + \hat{V})\Psi(q,t) = \left( \hat{p}^2/2m + kx^2/2 - e\varepsilon x \right)\Psi,$$

$$\Psi|_{t=0} = \Psi_0^0, \quad \Psi|_{x=\pm\infty} = \text{bounded},$$

(30)

where $\hat{p}^2 = -\hbar^2 \Delta$, $m$ denotes the oscillator mass, $k$ is the rigidity coefficient, $e$ is the electron charge and $\hat{V} = -e\varepsilon x$.

Let us introduce into eq. (30) a non-dimensional variable $\xi = x/a$, ($a = \sqrt{\hbar/m\omega_0}$) and the eigenfrequency $\omega = \sqrt{\hbar/m}$. The eigenfrequency $\omega$ (with $\omega = \omega_0$) is taken as a characteristic frequency $\omega_0$ and the generalised Rabi frequency is $\Omega_0 = e\varepsilon a/\hbar$. Assuming the external field to be weak, we enter a small parameter $\varepsilon$ by the relationship $\varepsilon = \Omega_0/\omega = e\varepsilon a/\hbar \omega = \varepsilon/ka < 1$.

An exact solution of the problem of eigenfunctions and eigenvalues in terms of the non-dimensional units is given by

$$\Psi_n(x,t) = (2^n \sqrt{\pi} an)^{-1/2} \exp\left[-(\xi - \varepsilon)^2/2\right]$$

$$\times H_n(x) \exp\left[-i(n + 1/2 - \varepsilon^2/2)\right],$$

$$\omega_n = \omega_0 - \varepsilon^2/2 = n + 1/2 - \varepsilon^2/2,$$

(31)

where $H_n(z)$ denotes Hermite polynomials, [13], [28].

The general solution of problem (30) constructed by means of eigenfunctions (31), has the form

$$\Psi(x,t) = \sum_{n=0}^{\infty} c_n \Psi_n(x,t).$$

(32)

Using the initial condition we obtain the following expansion coefficients $c_n$ in eq. (32)

$$c_n = \varepsilon^n (2^n n!)^{-1/2} \exp(-\varepsilon^2/4),$$

(33)
so that the final result is as follows

\[ \Psi(x, t) = \sum_{n=0}^{\infty} \frac{\varepsilon^n \exp(-\varepsilon^2)}{\sqrt{2^n n!}} (2^n \sqrt{\pi n!})^{-1/2} \times \exp \left[ -\frac{(\xi - \varepsilon)^2}{2} \right] H_n(\xi - \varepsilon) \times \exp \left[ -i \left( n + 1/2 - \varepsilon^2/4 \right) \right] \]

Performing expansion with accuracy up to terms of order of \( \varepsilon^2 \) yields

\[ \Psi^{(2)}(x, t) = \left\{ \Psi_0 + \varepsilon \frac{1}{\sqrt{2}} \Psi_1 \right. \\
+ \left. \varepsilon \frac{1}{\sqrt{2}} \Psi_1 \exp(-it) \right\} \exp(-it/2) \]

where \( \Psi_n^0 \) denotes the eigenfunctions of the unperturbed problem.

Let us now construct the solution of problem \( \Psi \) by means of the canonical theory of perturbation. The matrix elements of the perturbation operator are

\[ \varepsilon v_{nm} = -\varepsilon \left[ \frac{n}{2} \right]^{-1/2} \delta_{m,n-1} \\
+ \left( \frac{(n + 1/2)}{2} \right)^{-1/2} \delta_{m,n+1} \]

the corrections to the eigenfrequencies are \( \Delta \omega_k = -\varepsilon^2/2 \), the eigenfrequencies of the unperturbed system are \( \omega_0^0 = 1/2 \), \( \omega_1^0 = 3/2 \), and eq. \( 24 \) takes the form

\[ \Psi^{(2)}(x, t) = \left\{ \Psi_0 + \varepsilon \frac{1}{\sqrt{2}} \Psi_1 \right. \\
+ \left. \varepsilon \frac{1}{\sqrt{2}} \Psi_1 \exp(-it) \right\} \exp(-it/2) \]

As expected, the solution constructed by the perturbation theory coincides with the series expansion of the exact solution. Let us notice that obtaining solution \( 34 \) is simpler than expanding the exact solution in the series.

The probability of transition to the first excitation state is the square of the absolute value of the coefficient of \( \Psi_1^{(1)} \exp(-i\Delta t/2) \) and is equal to \( \varepsilon^2/2 \).

**V. STATIONARY EXCITATION OF TWO CLOSE LEVELS**

In the case of stationary perturbation, it is expedient to take into account the principal resonance by renormalisation of the frequency in the original expansion, i.e. to present expansion \( 8 \) as follows

\[ \Psi(q, t) = \sum_n c_n(t) \psi_n^0(q) \exp(-i\Omega_n^0 t), \]
it is easy to find that the probability of being in the state become unity \( |v_0 = 1 \) after the time interval \( \tau^* = 2\pi/\Delta \). Thus, the oscillations between the levels \( \alpha \) and \( \beta \) have period \( T = 2\pi/\Delta \) or frequency \( \omega = \Delta \).

Substituting coefficients \( \alpha, \beta \) into expansion \( c_{\alpha, \beta} \), we obtain that the wave function is a superposition of two stationary states with

\[
\omega_{\alpha, \beta} = \frac{\Omega^0_\alpha + \Omega^0_\beta}{2} \pm \frac{1}{2} \sqrt{(\Omega^0_\alpha - \Omega^0_\beta)^2 + 4|g|^2}. \quad (42)
\]

In the case of a degenerate level \( \delta_0 = 0 \) and from eq. \( \alpha, \beta \), we obtain the correction \( \Delta \omega \) to the frequency of the stationary state \( \omega_\alpha^0 = \omega_\beta^0 = \omega^0 \)

\[
\Delta \omega = \varepsilon \left( v_{\alpha \alpha} + v_{\beta \beta} \right) \pm \frac{1}{2} \sqrt{(v_{\alpha \alpha} - v_{\beta \beta})^2 + 4|v_{\alpha \beta}|^2}. \quad (43)
\]

Therefore, all three problems, namely the problems on close levels, two-fold degenerate level and resonant interaction with an external single-frequency field, are all solved in the framework of the same approach and yield the results coinciding with the traditional one with first order accuracy.

While solving the problem, we determine the conditions under which the quantum system with a discrete spectrum can be modelled, in the first approximation, by a two-level system. The main point of this procedure is the possibility of averaging Hamilton’s function \( \psi(q,t) \). The condition of weakness of the external field is needed for this. Then, the non-trivial initial conditions are required, at least for one of the coefficients \( c_{\alpha, \beta} \), otherwise the solutions of the homogeneous equations in \( c_{\alpha, \beta} \) are trivial.

Nowadays, the procedure of solving these problems is performed backwards. A two-level systems is first taken, then a so-called resonant approximation (rotating wave approximation), \( \alpha, \beta \), is applied to it. At this stage it is incorrectly assumed that the resonant approximation is also applicable in the cases where the perturbation theory is invalid, see for example \( \alpha, \beta \).

VI. NON-STATIONARY SCHRÖDINGER’S EQUATION AS A HAMILTONIAN SYSTEM

The situation studied in the non-stationary perturbation theory occurs when operator \( \hat{H} \) can be represented as sum \( \hat{H} = \hat{H}_0 + \varepsilon \hat{V}(q,t) \) \( (0 < \varepsilon << 1) \) of two self-adjoint operators. In the adiabatic approximation the perturbation operator \( \hat{V}(q,t) \) is not small and depends on slow time \( \tau = \varepsilon t \) such that \( \hat{V}(q,t) = \hat{V}(q,\tau) \). The solution should be constructed within the asymptotically large time interval \( \tau \sim 1/\varepsilon \) when change in the perturbation operator is large. In this case splitting the total Schrödinger’s operator \( \hat{H} \) into two operators, namely the generating (unperturbed) operator and a perturbation operator makes no sense. In order to embrace both possibilities we consider problem \( \alpha, \beta \) with the time-dependent Schrödinger operator \( \hat{H} = \hat{H}(q,t) \).

Let us assume that the stationary problem corresponding to \( \alpha, \beta \) is solvable for a parametric dependence of Schrödinger’s operator on time and has a discrete spectrum. This means that the eigenfunctions and the eigenvalues of the problem are given by

\[
\hat{H}(t) \psi_n(q,t) = E_n(t) \psi_n(q,t), \quad (44)
\]

with time \( t \) being fixed. The eigenfunctions are assumed to be orthonormalised as follows

\[
\int_{-\infty}^{\infty} \psi_m(q,t) \psi_n(q,t) dq = \delta_{mn}, \quad (45)
\]

where a bar denotes the complex conjugate.

The existing approximations of Born-Fock \( \alpha, \beta \) and Landau-Dykhne \( \alpha, \beta \) suggest that the eigenfunctions can be chosen as being real-valued (i.e. no magnetic field is assumed) which essentially reduces the applicability of the method. In the present study this assumption is not needed.

In the case of weak fields the results of the adiabatic approximation of Landau-Dykhne do not coincide with the results of perturbation theory \( \alpha, \beta \). The approximation of Born-Fock is actually not an approximation at all since all higher approximations turn out to be of the order of the first approximation \( \alpha, \beta \). In addition to this, both approximations yield an incorrect factor in front of the exponential function \( \alpha, \beta \).

Let us look for the solution of the exact problem in the form

\[
\Psi(q,t) = \sum_n c_n(t) \psi_n(q,t) \exp \left\{ -i \int_0^t \Omega_n(z) dz \right\}, \quad (46)
\]

where

\[
\Omega_n(t) = \omega_n(t) + v_{nn}(t), \quad \omega_n(t) = E_n(t), \quad v_{nn} = -i \int_{-\infty}^{\infty} \frac{\partial \psi_n}{\partial t} dq.
\]

The meaning of this choice of the phase becomes clear in what follows.

Inserting eq. \( \alpha, \beta \) into eq. \( \alpha, \beta \) yields the following equation for the expansion coefficients \( c_m(t) \)

\[
\dot{c}_m(t) = -i \sum_{n,m} v_{mn} c_n \exp \left\{ -i \int_0^t \Omega_{mn}(z) dz \right\}, \quad (47)
\]

where a dot denotes a total time derivative and a prime at the summation sign denotes the absence of a diagonal components with \( m = n \). The matrix of coefficients \( v_{mn} \) has the form

\[
v_{mn} = -i \int_{-\infty}^{\infty} \psi_m(q,t) \frac{\partial \psi_n(q,t)}{\partial t} dq. \quad (48)
\]
and is Hermitian, i.e. \( v_{mn} = \bar{v}_{mn} \).

The choice of phase indicated in eq. (46) ensures that the sum has no diagonal component which is responsible for the principal resonance. If eq. (46) had this diagonal component, the sum would have a small resonant denominator.

Indeed, differentiating eq. (46) with respect to time and taking into account that Schrödinger’s operator is self-adjoint, we obtain

\[
v_{mn} = \left( \frac{i}{\hbar \omega_{mn}} \right) \left( \frac{\partial H}{\partial t} \right)_{mn}, \quad m \neq n. \tag{49}\]

It is clear that in the case of the real-valued eigenfunctions \( \bar{\psi}_n = \psi_n \), that is, the diagonal elements \( v_{nn} = 0 \). It is this fact that is the reason for the real-valued normalisation in the Born-Fock approximation.

Similar actions in the case when \( m = n \) leads to the relationship \( \left( \frac{\partial H}{\partial t} \right)_{nn} = \frac{\partial E_n}{\partial t} \) and do not determine the diagonal matrix elements. In the case in which Schrödinger’s operator depends on time \( \tau \) in terms of the set of functions \( \xi_i(\tau) \) \( (i = 1, 2, \ldots) \), elements \( v_{nn} \) determine the topological adiabatic Berry phase \[20\] whose value does not depend on the evolution time and is determined only by a closed contour in the parameter space.

Equation (49) indicates three cases allowing the development of the perturbation theory. In the adiabatic case \( \tilde{H} = \tilde{H}(\xi(\tau)) \), so that \( \frac{\partial \tilde{H}}{\partial t} = \varepsilon \left( \frac{\partial \tilde{H}}{\partial \xi} \right) \left( \frac{\partial \xi}{\partial \tau} \right) \).

In the case of the non-stationary perturbation theory, Schrödinger’s operator has the form \( \tilde{H} = \tilde{H}_0 + \varepsilon \tilde{V}(q, t) \). Finally, in the case of the adiabatic perturbation theory \( \tilde{H} = \tilde{H}_0 + \varepsilon \tilde{V}(q, \tau) \).

The system of equations (47), along with the complex conjugate one, is Hamiltonian (in the classical sense) having the following Hamilton function

\[
H(c, c^*, t) = -i \sum_{n,m} v_{mn}(t) c_n \times c^*_m \exp \left\{ -i \int_0^t \Omega_{mn}(z) dz \right\} \tag{50}
\]

which describes the classical distributed system. The matrix of coefficients \( v_{mn} \) is Hermitian which ensures that this system is Hamiltonian and in turn enables one to apply the phase perturbation theory.

\[\text{VII. ADIABATIC APPROXIMATION}\]

We assume that Schrödinger’s operator has the form \( \tilde{H} = \tilde{H}_0 + \tilde{V}(q, \xi(\tau)) \), where \( \tau = \varepsilon t \) denotes slow time. Then the matrix elements \( v_{mn} \sim \varepsilon \xi' \) and Hamilton’s function (50) can be cast in the form

\[
\varepsilon H_1(c, c^*, t, \tau) = -i \sum_{n,m} v_{mn}(\tau) c_n \times c^*_m \exp \left\{ i \int_0^t \Omega_{mn}(\tau) dt \right\}, \tag{51}
\]

where \( \dot{\tau} = \varepsilon \) and \( \Omega_{mn} = \Omega_{mn} - \Omega_n \).

The canonical form allows us to convert the evolutionary equations by means of the formulae

\[
\tilde{H}_1 = \langle H_1 \rangle, \quad \tilde{H}_2 = -\left( \left. \frac{\partial \tilde{H}_1}{\partial c^*} \right| \left. \frac{\partial \{ H_1 \}}{\partial \bar{c}} \right) \right), \tag{52}
\]

where \( \tilde{H}_2 \) denotes the second approximation to the averaged Hamilton’s function, whilst \( \bar{c} = (\bar{c}_1, \bar{c}_2, \ldots) \) and \( \bar{c}^* = (\bar{c}_1^*, \bar{c}_2^*, \ldots) \) are the evolutionary components of variables \( c \) and \( c^* \).

Averaging expression (51) along the generating solution \( (c_k = \text{const}, \tau = \text{const}) \), we obtain \( \tilde{H}_1 = \langle H_1 \rangle = 0 \) which in turn implies that \( c_k = 0 \). The latter result is the adiabatic theorem of Kato \[12\] which is obtained in fact without calculations, cf. \[30\] for the proof. In the classical sense, the evolutionary components \( \bar{c}_k \) of the original variables \( c_k \) are the adiabatic invariants, see \[8\], \[20\], i.e. they retain the initial values for the asymptotic time interval \( t \sim 1/\varepsilon \). For deriving this result it is necessary to assume that \( \Omega_{mn}(\tau) \neq O(\varepsilon) \), i.e. the system has no degeneracy, there are no close levels and the levels do not intersect during the evolution time.

In the adiabatic (first) approximation, the solution of Schrödinger’s equation has the form

\[
\Psi^{(1)}(q, t) = \sum_{n=0}^{\infty} \varepsilon_n^{(1)} \psi_n(q, t) \times \exp \left\{ -i \int_0^t \Omega_{mn}(z) dz \right\}. \tag{53}
\]

Under rather general assumptions, Los’s theorem \[18\] renders estimates for the difference \( |\Psi(q, t) - \Psi^{(1)}(q)| < C\varepsilon \), where \( C \) is a constant independent of \( \varepsilon \) for time interval \( t \sim 1/\varepsilon \).

\[\text{VIII. POST-ADIABATIC APPROXIMATION}\]

In order to construct the second (post-adiabatic) approximation we make use of relationships in eq. (52).

Simple calculation yields

\[
\tilde{H}_2 = -i \sum_k \Delta \Omega_k(\tau) \bar{c}_k \bar{c}_k^*, \quad \Delta \Omega_k = \sum_l \left| \frac{\langle v_{kl} \rangle}{\Omega_{kl}} \right|^2, \tag{54}
\]

where \( \bar{c}_k \) are the adiabatic invariants and \( \Omega_{kl} \) are the adiabatic transition elements.
so that the second approximation to the averaged Hamilton’s function $H^{(2)}$ has the form

$$H^{(2)} = -i\varepsilon^2 \sum_k \Delta\Omega_k(\tau)\tilde{c}_k\tilde{c}_k^*.$$ (55)

Hamiltonian equations with Hamilton’s function \(H^{(2)}\) for the evolutionary components \(\tilde{c}_k\) are integrated easily, to give

$$\tilde{c}_k = A_k \exp \left\{ -i\varepsilon^2 \int_0^\tau \Delta\Omega_k(z)dz \right\}$$

$$= A_k \exp (-i\alpha_k).$$ (56)

Integration constants \(A_k\) are determined by means of the initial conditions.

Let us notice that the phase of coefficients \(\tilde{c}_k\) could be included into the original expansion (10), then we would obtain \(\tilde{H}_2 = 0, \tilde{H}^{(2)} = 0\).

The second approximation to the expansion coefficients in eq. (10) is constructed by means of formulae (16)

$$c_k^{(2)} = A_k^{(2)} \exp (-i\alpha_k)$$

$$- \varepsilon \sum_m \frac{v_{km}}{\Omega_{km}} A_m \exp (-i\alpha_m + i\Omega_{km}t),$$ (57)

With the help of coefficients \(c_k^{(2)}\) we obtain the second approximation \(\Psi^{(2)}(q, t)\) to the solution of Schrödinger’s equation

$$\Psi^{(2)}(q, t) = \sum_k \left[ A_k \exp (-i\alpha_k) - \varepsilon \sum_m \frac{v_{km}}{\Omega_{km}} A_m \exp (-i\alpha_m - i\Omega_{km}t) \right] \Psi_k \exp \left[-i \int_0^t \Omega_k(z)dz \right].$$ (58)

It is necessary to mention that in eq. (57) we can limit our consideration to the terms in the sum by the first approximation \(A_m^{(1)}\) with respect to \(\varepsilon\).

When Cauchy’s problem is studied, the system at the initial time instant is at a certain stationary state, say \(s\)-th, of the discrete spectrum of the unperturbed problem with Schrödinger’s operator \(\tilde{H}_0\), i.e. \(\Psi(q, t)|_{t=0} = \Psi_s^0\). In contrast to the stationary case we can not take that \(c_n|_{t=0} = \delta_{ns}\), since the expansion is carried out in terms of the eigenfunctions of the perturbed problem \(\psi_n(q, t) = \psi_n(q, \xi(t))\), where \(\xi(t)\) denotes parameters determining the dependence of the perturbation on time. With this in view, we additionally assume that the switch fulfills the conditions \(\xi(0) = \xi(0) = 0\). The problem can be solved under other conditions which implies an instantaneous switching of the perturbation followed by its adiabatic change.

Therefore, we take that the equation for coefficients \(A_k\) has the following form

$$c_k|_{t=0} = \delta_{ks} = A_k - \varepsilon \sum_m \left[ \frac{v_{km}(\tau)}{\Omega_{km}(\tau)} \right]_{t=0} A_m.$$ (59)

Obviously the matrix elements \(v_{km} \sim \tilde{\xi}(\tau)\), thus under the adopted conditions we obtain \(A_{ks} = \delta_{ks}\), that is

$$c_k^{(2)} = \delta_{ks} \exp (-i\alpha_k) - \varepsilon \frac{v_{ks}}{\Omega_{ks}} \exp (-i\alpha_k + i\Omega_{ks}t).$$ (60)

Finally, the second (post-adiabatic) approximation \(\Psi^{(2)}\) for the wave function is as follows

$$\Psi^{(2)}(q, t) = \sum_k \left[ A_k \exp (-i\alpha_k) - \varepsilon \sum_m \frac{v_{km}}{\Omega_{km}} A_m \exp (-i\alpha_m - i\Omega_{km}t) \right] \Psi_k \exp \left[-i \int_0^t \Omega_k(z)dz \right].$$ (61)

It can be proved, see [13], that the estimate \(\left|\Psi(q, t) - \Psi^{(2)}(q, t)\right| < B\varepsilon^2\) is valid for the time interval \(t \sim 1/\varepsilon\). Papers by physicists do not take into account the boundedness of the time interval in which an approximate solution approximates the exact solution. As one can see from the forthcoming examples, this interval, in general, can not be enlarged.

The problem of constructing the adiabatic approximation and taking account of the transition through the virtual levels was posed by Dykhne: "In order to obtain the correct factor of the exponential function it would be necessary to take into account all higher approximations of the perturbation theory, all yielding results of the same order. In practice, this is, of course, not feasible. The obtained formulae give answers to the question of calculating the probability of transition of a quantum system to an "adjacent" level. As for transitions to more remote levels, then the transitions through virtual levels may compete with the considered process of the "direct" transition. However, this question needs an additional investigation", [15]. Nevertheless, this problem has not
been solved so far by the existing methods of perturbation theory.

IX. QUANTUM LINEAR OSCILLATOR IN A VARIABLE HOMOGENEOUS FIELD

In order to compare the obtained results with the known ones, let us study the following problem having an exact solution. The situation considered is the motion of a particle in the field of a parabolic potential subjected to a variable external force, i.e.

\[ i\hbar \frac{\partial \Psi(q,t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} + \frac{m\omega^2q^2}{2} - \varepsilon_0 f(\nu t)q \right] \Psi(q,t) \]

\[ \Psi(q,t)|_{t=0} = \pi^{-1/4} a^{1/2} \exp \left[ -\left( \frac{q}{a\sqrt{2}} \right)^2 \right], \]

\[ \Psi(q,t)|_{q\rightarrow\pm\infty} \text{ bounded}, \tag{62} \]

where \( m \) and \( e \) denote the mass and charge of the oscillator, \( \varepsilon_0 \) is amplitude of the electric field, \( \nu^{-1} \) denotes a characteristic time constant of the field, \( a = (\hbar/m\omega)^{1/2} \) denotes a characteristic length scale. Clearly, the initial state is the main state of the free harmonic oscillator. Let us introduce the non-dimensional time \( t_n = \omega t \), the non-dimensional coordinate \( x = q/a \) and the non-dimensional force amplitude \( \varepsilon_1 = e\varepsilon_0a/\hbar\omega = \Omega/\omega \). Problem \((62)\) in the terms of non-dimensional variables takes the form

\[ i\frac{\partial \Psi(x,t)}{\partial t} = \left[ -\frac{1}{2} \frac{\partial^2}{\partial x^2} + \frac{1}{2} x^2 - \xi(\varepsilon t)x \right] \Psi(x,t), \]

\[ \Psi(x,t)|_{t=0} = \pi^{-1/4} \exp \left( -\frac{x^2}{2} / 2 \right), \]

\[ \Psi(x,t)|_{x\rightarrow\pm\infty} \text{ bounded}, \tag{63} \]

where \( \varepsilon = \nu/\omega, \xi(\varepsilon t) = \varepsilon_1 f(\varepsilon t) \) and the non-dimensional time is denoted by \( t \).

The exact solution of this problem is given by, cf. \(30\),

\[ \Psi_0(x,t) = \pi^{-1/4} \exp \left\{ -\frac{it}{2} + \frac{1}{2} \int_0^t dz \delta^2(z) \exp(-2iz) - \frac{x^2}{2} - \sqrt{2}x\delta(t) \exp(-it) \right\}, \tag{64} \]

\[ \delta(t) = -\frac{i}{\sqrt{2}} \int_0^t \xi(\varepsilon z) \exp(iz) dz \tag{65} \]

In order to construct expansion \(64\) in the adiabatic case \((0 < \varepsilon << 1)\) we integrate eq. \(65\) by parts three times and take into account that \( \xi(0) = \dot{\xi}(0) = \ddot{\xi}(0) = 0 \). The result is

\[ \delta(t) = -\frac{1}{\sqrt{2}} \left[ \xi + i\xi - \dot{\xi} \right] \exp(it) - \frac{i}{2} \int_0^t \exp(iz) \ddot{\xi}(z) dz. \tag{66} \]

Taking \( M = \max |\dot{\xi}(t)| \) in time interval \([0,T]\) we obtain the following estimate

\[ \left| \int_0^T \exp(iz) \ddot{\xi}(z) dz \right| \leq \int_0^T |\ddot{\xi}(z)| dz \leq MT \sim \varepsilon^3 T. \tag{67} \]

It is clear from this equation that one can neglect the latter term in eq. \(66\) within time interval \( \Delta t \sim T \sim 1/\varepsilon \). For this reason, it is necessary to keep the second order term \( \dot{\xi} \) in eq. \(65\) for evaluating integral \(64\) and omit it by substituting without integration.

With the same accuracy we evaluate the following integral

\[ \int_0^t dz \exp(-2iz) \delta^2(z) = \int_0^t \frac{\xi^2}{2} dz - \frac{\xi^2}{2} - i\varepsilon_1 + \int_0^t \frac{i\xi^2}{2} dz \tag{68} \]

and the expansion of the exact solution \(64\) as a series in time interval \( t \sim 1/\varepsilon \)

\[ \Psi_0(x,t) = \left[ \Psi_0(x - \xi) + i\xi \Psi_0(x - \xi) \right] \exp \left\{ -\frac{it}{2} + i \int_0^t \frac{\xi}{2} dz + i \int_0^t \frac{\xi^2}{2} dz \right\} + O(\varepsilon^2). \tag{69} \]

Next, we construct the expansion of the exact solution \(64\) in the case of the harmonic non-resonant perturbation \((\xi(t) = \varepsilon_1 sin \nu t, 0 < \varepsilon_1 << 1, \nu \neq O(\varepsilon_1), \nu \neq 1)\). In this case

\[ \delta(t) = -\varepsilon_1 \frac{i}{\sqrt{2}(\nu^2 - 1)} [(i \sin \nu t - \nu \cos \nu t) \exp(it) + \nu] \tag{70} \]

\[ \int_0^t dz \delta^2(z) \exp(-2it) = -i \varepsilon_1^2 \frac{1}{4(\nu^2 - 1)} t + O(\varepsilon_1^2) \tag{71} \]

The terms omitted in eq. \(71\) are uniformly bound such that approximation \(71\) is valid at any time instant. Inserting eqs. \(70\) and eq. \(71\) into eq. \(64\) yields the following expansion of the exact solution.
\[ \Psi_0(x, t) = \pi^{-1/4} \exp \left\{ \frac{i t}{2} - i \frac{\varepsilon_1^2}{4(\nu^2 - 1)} t - \frac{x^2}{2} + x \frac{i \varepsilon_1}{\nu^2 - 1} (i \sin \nu t - \nu \cos \nu t) + \exp(-i t) \frac{i \varepsilon_1 \nu}{\nu^2 - 1} x \right\} \]

\[ \Psi^{(2)}(x, t) = \left\{ \Psi_0 + \frac{i \varepsilon_1}{\sqrt{2(\nu^2 - 1)}} \Psi_1(i \sin \nu t - \nu \cos \nu t) \right\} \exp \left( \frac{-i t}{2} \right) + \frac{i \varepsilon_1 \nu}{\sqrt{2(\nu^2 - 1)}} \Psi_1 \exp \left( -i \frac{3t}{2} \right) \exp \left[ -i \frac{\varepsilon_1^2}{4(\nu^2 - 1)} t \right] \]

and has the following solution

\[ \Psi_n(x, t) = (2^n \sqrt{n!})^{-1/2} \exp \left[ -(x - \xi(\varepsilon t))^2 / 2 \right] \times H_n (x - \xi(\varepsilon t)) \cdot \omega_n = n + 1/2 - \xi^2 / 2, \]

where \( H_n(z) \) denote Hermite polynomials \([12, 28]\).

Using the recurrent relationships for Hermite polynomials it is easy to calculate the matrix elements \( v_{mn}(t) \) for \( m \neq n \)

\[ v_{mn}(t) = - \left( i \xi / 2 \right) \frac{1}{\sqrt{n + 1}} \delta_{m,n+1} - \frac{1}{\sqrt{n}} \delta_{m,n+1} \]

where a dot denotes the total derivative with respect to time, so that \( \dot{\xi} \) is of order \( \varepsilon \) and \( \delta_{m,n} \) denotes Kronecker’s delta. Since the eigenfunctions \([75]\) are real-valued, the diagonal matrix elements \( v_{nn}(t) = 0 \), i.e. \( \Omega_n = \omega_n = n + 1/2 - \xi^2 / 2 \).

With the help of eq. \([76]\) we can easily calculate values \( \Delta \Omega_k = \Delta \omega_k = -\xi / 2 \) and coefficients \( \bar{c}_k \), see eq. \([70]\)

\[ \bar{c}_k = A_k \exp \left\{ i \int \frac{\xi^2}{2} (\varepsilon z) / 2dz \right\} \]

In the case under consideration \( \langle H_1 \rangle = 0 \) and \( \tilde{H}_1 = H_1 \), then we find \( \langle H_1 \rangle \) and \( \frac{\partial \langle H_1 \rangle}{\partial \bar{c}_k} \)

\[ \langle H_1 \rangle = - \frac{i}{n,m} \frac{v_{mn}(t)}{\omega_{mn}(t)} \bar{c}_n \bar{c}_m \exp \left[ i \omega_{mn}(\tau)t \right], \]

\[ \frac{\partial \langle H_1 \rangle}{\partial \bar{c}_k} = - \sum_n \frac{v_{kn}(t)}{\omega_{kn}(t)} \bar{c}_n \exp \left[ i \omega_{kn}(\tau)t \right]. \]

Making use of relationships \([78]\) we obtain

\[ \bar{c}_k^{(2)} = A_k^{(2)} \exp \left[ i \int \frac{1}{2} \xi^2 dz \right] - \sum_n \frac{v_{kn}(t)}{\omega_{kn}(t)} A_n \exp \left[ i \int \frac{1}{2} \xi^2 dz + i \omega_{kn}t \right]. \]
The equations for determining the integration constants have the form

\[
\dot{c}_k(2)_{t=0} = \delta_{k0} = A_k - \sum_n \frac{v_{kn}(t)}{\omega_{kn}(t)} A_n. \tag{80}
\]

Assuming, as above, that \(\dot{\xi}(0) = v_{kn}(0) = 0\), we obtain \(A_k = \delta_{k0}\) and

\[
\dot{c}_k(2)_{t=0} = \delta_{k0} \exp \left[ i \int_0^t \frac{\dot{\xi}^2}{2} dz \right] = v_{kn}(0) \exp \left[ i \int_0^t \frac{\dot{\xi}^2}{2} dz + i \omega_{k0} t \right]. \tag{81}
\]

As follows from eq. (69) \(v_{kn}(0) = -i \dot{\xi}/\sqrt{2}\), thus

\[
c_k(2) = \left[ \delta_{k0} + i \frac{\xi}{\sqrt{2}} \delta_{k1} \exp(it) \right] \exp \left[ i \int_0^t \frac{\dot{\xi}^2}{2} dz \right]. \tag{82}
\]

Inserting these equalities into expansion (46) yields the post-adiabatic approximation

\[
\Psi^{(2)}(x, t) = \left[ \Psi_0(x - \xi) + i \frac{\xi}{\sqrt{2}} \Psi_1(x - \xi) \right] \exp \left\{ -i \frac{t}{2} + i \int_0^t \frac{\dot{\xi}^2}{2} dz \right\} \tag{83}
\]

which coincides with the expansion of the exact solution (39) within time interval \(\Delta t \sim 1/\varepsilon\), approximation (83) not being applicable for increased times.

As follows from eq. (82), the probability of the oscillator excitation is equal to \(\dot{\xi}^2/2\), i.e. it is zero at extreme points of function \(\xi(t)\). For a Gaussian distribution, \(\xi(t) \sim \exp(-\tau^2)\) and the excitation probability has its only maximum at \(\tau = 1/\sqrt{2}\).

In the traditional Born-Fock approximation, (18), (29), the expansion coefficient corresponding to eq. (74) is given by

\[
c_{kn} = \delta_{kn} + \int_0^t \frac{1}{\omega_{kn}(t')} \left( \frac{\partial V}{\partial t} \right)_{kn} \exp \left[ i \int_0^t \omega_{kn}(t'') dt'' \right] dt', \tag{84}
\]

where \(V(x, t) = -\xi(t)x\). Carrying out simple manipulations we obtain

\[
\dot{c}_{k0} = \delta_{k0} - \frac{\dot{\xi}}{\sqrt{2}} \int_0^t \xi \exp(it') dt'. \tag{85}
\]

Comparing the latter equation with eq. (82) indicates that the factor \(\exp \left[ i \int_0^t \frac{\dot{\xi}^2}{2} dz \right] \) is absent in eq. (83). Equations (84) and (82) coincide at time instant \(t \sim 1\), when a change in \(\dot{\xi}(\varepsilon t)\) in the integrand can be neglected and there are no conditions \(\xi(0) = \dot{\xi}(0) = 0\) under which approximation (82) is valid.

**XI. ADIABATIC PERTURBATION THEORY**

In the case of the adiabatic perturbation theory, Schrödinger’s operator is as follows \(\hat{H} = \hat{H}_0 + \varepsilon \hat{V}(q, \tau)\) which allows us to carry out calculations by using the results of Sec.6.6. However, as mentioned in Sec. 6.2 it is more convenient to apply the formalism of the stationary phase perturbation theory.

Indeed, by casting problem in terms of the eigenfunctions of unperturbed Schrödinger’s operator \(\hat{H}_0\) we find the effective Hamilton function

\[
\varepsilon \hat{H}_1(c, c^*, t, \tau) = -i \sum_{n,m} v_{mn}(\tau) c_n c^*_m \exp(it\Omega_{mn}^0 t), \tag{86}
\]

where \(v_{mn}(\tau)\) denote matrix elements of the perturbation operator which are calculated by means of the unperturbed eigenfunctions, further \(\Omega_{mn}^0 = \omega_n^0 + \varepsilon \int_0^t v_{mn}(\tau) d\tau\) and \(\Omega_{mn}^0 = \Omega_{mn}^0 - \omega_n^0\) denote the eigenvalues of the unperturbed problem.

In this case formulae (82) remain valid since the dependence of the effective Hamilton function on slow time \(\tau\) is observed only in terms of the third order of smallness.

For problem (82) we have

\[
\Psi_c^0(x) = (2^{3/2} \pi n!)^{-1/2} \exp \left[ -x^2/2 \right] H_n(x) \tag{87}
\]

\[
\omega_n^0 = n + 1/2, \quad \Omega_n^0 = \omega_n^0 = n + 1/2
\]

\[
v_{mn}(\tau) = -\varepsilon_1 \dot{\xi}(\tau) \sqrt{\sqrt{n + 1/2} \delta_{m, n + 1} + \sqrt{n/2} \delta_{m, n - 1}}
\]

\[
v_{mn}(\tau) = 0
\]

\[
\Delta \omega_k = -\frac{\varepsilon^2}{2} \dot{\xi}^2(\tau)
\]

with parameter \(\varepsilon_1\) being a small value of order of \(\varepsilon\).

By virtue of the latter relationship in eq. (87) we easily find the second approximation to the expansion coefficients \(c_n(2)\) (under the conditions \(\xi(0) = \dot{\xi}(0) = 0\))

\[
c_n(2) = \exp \left[ i \dot{\xi} \int_0^t \frac{\dot{\xi}^2}{2} dz \right] \delta_{k0} \tag{88}
\]

and the second approximation to the wave function

\[
\psi^{(2)} = \psi_0(x) \exp \left[ -i t / 2 + i \int_0^t \frac{\dot{\xi}^2}{2} dz \right], \tag{89}
\]

which coincides with adiabatic expansion (83) when we take into account a small factor at \(\dot{\xi}\) due to parameter \(\varepsilon_1\).
XII. HARMONIC EXCITATION OF A CHARGED OSCILLATOR. NON-RESONANT CASE

To demonstrate the way of constructing solutions in the case of non-stationary perturbation theory, we consider the case of a harmonic external field which is frequently encountered in practical applications. In this case function \( \xi(t) \) in eq. (62) takes the form \( \xi(t) = \varepsilon_1 \sin \nu t \) and we can adopt that \( \nu \neq 1 \) and \( \nu \neq O(\varepsilon) \).

In other words, we consider the non-resonant case and parameter \( \varepsilon_1 \) is taken as having the order of smallness of parameter \( \varepsilon \).

Let us carry out the corresponding calculations in three ways: first, stationary phase perturbation theory, second, non-stationary phase perturbation theory developed here and finally, traditional method of [13].

In the first case the matrix elements of the perturbation operator, calculated by means of the unperturbed eigenfunctions, have the form

\[
\begin{align*}
\psi_{mn}(t) &= \varepsilon_1 (v_{mn}^0 \exp(i\nu t) - v_{mn}^0 \exp(-i\nu t)), \\
v_{mn}^0 &= \frac{i}{2\sqrt{2}} \left[ \sqrt{n} + 1 \delta_{m,n+1} + \sqrt{n} \delta_{m,n-1} \right].
\end{align*}
\]

The effective Hamilton function is given by

\[
\varepsilon_1 H_1(c, c^*, t) = -i \varepsilon_1 \sum_{n,m} i v_{mn}^0 \exp \left[ i(\omega_{mn}^0 + \nu)t \right] c_n c_m^* + i \sum_{n,m} i v_{mn}^0 \exp \left[ i(\omega_{mn}^0 - \nu)t \right] c_n c_m^*. \tag{91}
\]

\[
\Psi^{(2)}(x, t) = \left\{ \Psi_0 + \frac{i \varepsilon_1}{\sqrt{2(\nu^2 - 1)}} \Psi_1 (i \sin \nu t - \nu \cos \nu t) \right\} \exp \left( -\frac{it}{2} + \frac{i \varepsilon_\nu}{\sqrt{2(\nu^2 - 1)}} \Psi_1 (i \sin \nu t - \nu \cos \nu t) \right) \exp \left( -i \frac{\varepsilon_1^2}{4(\nu^2 - 1)} t \right). \tag{94}
\]

This result suggests that the spectrum remains equidistant and is only subjected to a common shift \( \Delta \omega = \frac{\varepsilon_1^2}{4(\nu^2 - 1)} \). In this case \( \Delta \omega < 0 \) for \( \nu < 1 \) (\( \omega < \omega_0 \), \( \omega \) being the frequency of excitation force), and \( \Delta \omega > 0 \) for \( \nu > 1 \) (\( \omega > \omega_0 \)). The shift \( \Delta \omega \) at \( \omega \rightarrow 0 \) corresponds to effective elevation of the bottom of the potential well. In the case of a high frequency external field (\( \nu >> 1 \)) \( \Delta \omega = \frac{\varepsilon_1^2}{4\nu^2} \) that coincides with the effective potential energy. Hence, the constructed expansion (94) coincides with the expansion of the exact solution (14).

Let us now construct a solution by using formulae of the non-stationary phase perturbation theory. In this case the matrix elements (15) calculated by means of eigenfunctions (16) of the instantaneous Schrödinger’s operator have the form

\[
\psi_{mn}(\tau) = -\frac{i \varepsilon_1}{\sqrt{2}} \left[ \sqrt{n} + 1 \delta_{m,n+1} - \sqrt{n} \delta_{m,n-1} \right]. \tag{95}
\]

In this case \( \bar{H}_1 = \langle H_1 \rangle = 0 \), so that \( H_1 = \bar{H}_1 \). The correction of the second order \( \bar{H}_2 \) to the averaged Hamilton function is as follows

\[
\bar{H}_2 = -i \frac{\varepsilon_1^2}{4(\nu^2 - 1)} \sum_n \bar{c}_n \bar{c}_n^*. \tag{92}
\]

Next we find the second approximation for variables \( \epsilon_n^{(2)} \)

\[
\epsilon_n^{(2)} = \delta_{n0} - i \frac{\varepsilon_1 \nu}{\sqrt{2(1 - \nu^2)}} \delta_{n1} - \frac{\varepsilon_1}{\sqrt{2}} \delta_{n1} \left[ i \sin \nu t - \nu \cos \nu t \right] \exp(it). \tag{93}
\]

Taking into account these relationships we obtain the second approximation \( \Psi^{(2)}(x, t) \) to the solution of the non-stationary problem [92]

\[
\psi_{mn} = v_{mn}^0 \exp(i\nu t) + v_{mn}^0 \exp(-i\nu t), \tag{96}
\]

\[
v_{mn}^0 = -\frac{i \varepsilon_1 \nu}{2\sqrt{2}} \left( \sqrt{n} + 1 \delta_{m,n+1} - \sqrt{n} \delta_{m,n-1} \right).
\]

As the eigenfunctions are real, then \( v_{mn} = 0 \) and \( \Omega_n = \omega_n = n + \frac{1}{2} - \frac{\varepsilon_1^2}{2} \).

The effective Hamilton function is as follows

\[
\varepsilon_1 H_1(c, c^*, t) = -i \varepsilon_1 \sum_{m,n=0}^{\infty} \{ v_{mn}^0 \exp \left[ i(\omega_{mn}^0 + \nu)t \right] + v_{mn}^0 \exp \left[ i(\omega_{mn}^0 - \nu)t \right] \} c_n c_m^*. \tag{97}
\]

It is evident that \( \bar{H}_1 = \langle H_1 \rangle = 0 \), so that \( H_1 = \bar{H}_1 \). The correction \( \bar{H}_2 \) to the averaged Hamilton function, calculated by formulae [92] with the help of eq. (90), is
given by

\[ \hat{H}_2 = -i\frac{\nu^2}{4(\nu^2 - 1)} \sum_k \bar{c}_k c_k^* . \] (98)

The second approximation \( \bar{c}_k \) for the evolutionary components of variables \( c_k \) is found from Hamilton's equations with Hamilton's function \( \hat{H}'(2) = \varepsilon_1 \hat{H}_1 + \varepsilon_1^2 \hat{H}_2 \) and has the form

\[ \bar{c}_k = A_k \exp \left[ -i\frac{\varepsilon_1^2 \nu^2}{4(\nu^2 - 1)} t \right] . \] (99)

Constants \( A_k \) should be obtained from the initial conditions.

The second approximation \( c_k^{(2)} \) to the original variables \( c_k \) is as follows

\[ c_k^{(2)} = \left\{ A_k - \varepsilon_1 \sum_n \nu_n A_n \left[ \exp \left[ i(\omega_{kn} + \nu) t \right] \right] \right. \\
+ \exp \left[ i(\omega_{kn} - \nu) t \right] \left. \right] \exp \left[ -i\frac{\varepsilon_1^2 \nu^2}{4(\nu^2 - 1)} t \right] \right\} (100)

For determining the integration constants \( A_k \) from eq. (100) we obtain the following equation

\[ c_k|_{t=0} = \delta_{k0} = A_k^{(2)} - \varepsilon_1 \sum_n \nu_n A_n \left[ (\omega_{kn} + \nu)^{-1} + (\omega_{kn} - \nu)^{-1} \right] \] (101)

\[ \Psi^{(2)}(x, t) = \left\{ \Psi_0 + \frac{i\varepsilon_1}{\sqrt{2(\nu^2 - 1)}} \Psi_1 (i \sin \nu t - \nu \cos \nu t) \right\} \right. \\
\times \exp \left[ -\frac{it}{2} \right] + \frac{i\varepsilon_1 \nu}{\sqrt{2(\nu^2 - 1)}} \Psi_1 \exp \left( -\frac{3it}{2} \right) \left. \right] \exp \left[ -i\frac{\varepsilon_1^2 \nu^2}{4(\nu^2 - 1)} t \right] \] (105)

coinciding with eqs. (14) and (18).

Finally, taking into account that the second approximation of the present analysis coincides with the first approximation of the traditional approach, we obtain, for the case \( a_k = c_k \), by means of the standard formulae of the non-stationary perturbation theory, that

\[ a_k = a_k^{(0)} + a_k^{(1)} = \delta_{k0} + i\frac{\varepsilon_1 \delta_{k1}}{\sqrt{2(\nu^2 - 1)}} (i \sin \nu t - \nu \cos \nu t) \exp(it) . \] (106)

Comparison of eqs. (103) and (108) allows us to indicate a number of inaccuracies in the standard courses. Firstly, a phase multiplier \( \exp[-i\varepsilon_1^2 \nu^2 t/4(\nu^2 - 1)] \), which is of crucial importance for investigation of the coherent processes, is absent in expression (106). It can be neglected within a non-dimensional time interval \( t \sim 1/\varepsilon \), but not within asymptotical intervals \( t \sim 1/\varepsilon \). Thus, approximation (106) and in turn the whole solution is valid only within this small time interval.

Secondly, only the first approximation \( a_k^{(1)} = \delta_{k0} \) rather than \( a_k \) is subject to the initial condition (100). This explains the absence of the term \( i\varepsilon_1 \nu/\sqrt{2(\nu^2 - 1)} \). Indeed, by assuming \( a_k^{(0)} = \delta_{k0} + \varepsilon_1 \tilde{a}_k^{(0)} \) and subjecting the whole coefficient \( a_k \) to the initial condition \( a_k|_{t=0} = \delta_{k0} \) we find

\[ \tilde{a}_k^{(0)} = i\frac{\nu}{\sqrt{2(\nu^2 - 1)}} \delta_{k1} . \] (107)

Finally, as follows from solution (105) or (18) it is this absent correction (rather than \( a_k^{(1)} \)) that determines the probability of transition to the excited state.
XIII. HARMONIC EXCITATION OF AN OSCILLATOR. TRANSITION THROUGH A RESONANCE

Let us consider excitation of an oscillator by a weak resonant harmonic field \( V(x,t) = -\varepsilon_1 x \cos \nu t \). In this case \( 1 - \nu = \varepsilon \) (\( 0 \ll \varepsilon < 1 \)) and parameter \( \varepsilon_1 \) is a small value.

The effective Hamilton function constructed by means of the eigenfunctions of the unperturbed Schrödinger’s operator has the form

\[
\varepsilon H_1(c,c^*,t) = \frac{i \varepsilon_1}{2 \sqrt{2}} \sum_n \left\{ \sqrt{n} c_n c_{n-1}^* \exp[-i \varepsilon t] + \sqrt{n+1} c_{n+1}^* c_n \exp[i \varepsilon t] \right\} \\
+ \frac{i \varepsilon_1}{2 \sqrt{2}} \sum_n \left\{ \sqrt{n} c_n c_{n-1}^* \exp[-i (\nu + 1) t] + \sqrt{n+1} c_{n+1}^* c_n \exp[i (\nu + 1) t] \right\} .
\]

In the first approximation we obtain the averaged Hamilton function

\[
\varepsilon H_1 = \frac{i \varepsilon_1}{2 \sqrt{2}} \sum_n \left\{ \sqrt{n} c_n c_{n-1}^* \exp[-i \varepsilon t] \right\} \exp \left[ -\frac{\varepsilon_1 t}{2} \frac{2}{\nu} \right] \exp \left( -\frac{\varepsilon_1 t}{2} \frac{\nu}{\nu} \right) \sum_{k=0}^{\infty} \frac{1}{k!} \left( \frac{i \varepsilon t}{2 \sqrt{2}} \right)^k \exp \left[ -\frac{\varepsilon_1 t}{4} \right] \exp \left( -\frac{\varepsilon_1 t}{4} \right) \].
\]

and solution \( \Psi(x,t) \) in the first approximation

\[
\Psi(x,t) = \sum_{k=0}^{\infty} \frac{1}{\sqrt{k!}} \left( \frac{i \varepsilon t}{2 \sqrt{2}} \right)^k \exp \left[ -\frac{\varepsilon_1 t}{4} \right] \exp \left( -\frac{\varepsilon_1 t}{4} \right) \].
\]

Carrying out summation in eq. by means of the generating function for Hermite polynomials [28]

\[
\exp (2xz - z^2) = \sum_{k=0}^{\infty} z^k H_k(x),
\]

we obtain the final solution for the case of exact resonance

\[
\Psi(x,t) = \pi^{-\frac{1}{4}} \exp \left\{ \frac{i t}{2} \frac{x^2}{2} - \left( \frac{\varepsilon_1 t}{4} \right)^2 \right\} \exp \left( -\frac{\varepsilon_1 t}{4} \right) \exp \left( -\frac{\varepsilon_1 t}{4} \right) \].
\]

This solution coincides with the expansion of the exact solution [29]. The probability of excitation of the oscillator has the form of a Poisson distribution

\[
w_n(t) = |c_n(t)|^2 = \frac{\langle \hat{n} \rangle^n}{n!} \exp(-\langle \hat{n} \rangle),
\]

where \( \langle \hat{n} \rangle = (\varepsilon_1 t/2\sqrt{2})^2 \).

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