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New perturbation theory for the nonstationary anharmonic oscillator

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Abstract. The new perturbation theory for the problem of the nonstationary anharmonic oscillator with polynomial nonstationary perturbation is proposed. As a zeroth-order approximation, the exact wavefunction of the harmonic oscillator with variable frequency in external field is used. Based on some intrinsic properties of unperturbed wavefunctions, the variational–iterational method is proposed, which makes it possible to correct both the amplitude and phase of the wavefunction. As an application, the first-order corrections are proposed for both the wavefunction and S-matrix elements for asymmetric perturbation potential of the type $V(x,\tau) = \alpha(\tau)x^3 + \beta(\tau)x^4$. The transition amplitude 'ground state–ground state' $W_{00}(\lambda;\rho)$ is analysed in detail depending on the perturbation parameter λ (including the strong coupling region $\lambda \sim 1$) and the one-dimensional refraction coefficient ρ.

1. Introduction

Every successful effort in the investigation of some physical problem in the strong interaction region usually brings new insight into the behaviour of a corresponding system. Thus, the outstanding results, obtained in the solution of one-dimensional model problems in quantum field theory, molecular and solid-state physics [1–3], are of great interest. But the investigation becomes much more complicated when many-dimensional problems are approached. In such a situation contradictory results are possible even in calculations of the system eigenenergy [4].

The situation becomes even more dramatic when dealing with nonstationary problems with eigenfunctions basis, changing in time. The most important example of it is given by the model of the two-dimensional scattering problem, which is called the collinear model for rearrangement [5]. It is one of the simplest and still realistic descriptions of the three-body reaction of $A + (B, C)_n \to (A, B)_m + C$ type.

This problem can be of principle importance both for the practical applications in the theory of chemical reaction for moderate energies and for illuminating the mechanisms of the rearrangement in the multichannel scattering theory. It can also be regarded as a good test bed for the application of the nonperturbative method in the realistic few-body problem with all reaction channels involved.

In our previous paper [6] it was shown, that in the limit $\bar{h} \to 0$ this problem is effectively reduced to that for one-dimensional anharmonic oscillators with the frequency $\Omega(\tau)$, changing in the field of external force $F(\tau)$. Numerous quantum-chemical calculations

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of the potential energy surface for the most popular three-particle systems have shown strong anharmonism in normal coordinates even for principle quantum numbers as low as $n \geqslant 3$–4.

Here we propose a method that seems to be a natural development of the ideas of stationary perturbation theory of [3] for the case of nonstationary coefficients of a zeroth-order equation. The method is of variational/iteration type and is essentially backed by the main ideas of the singular perturbation theory—one can expand only such parts of the solution, that do not bring singularities, and if one cannot find a pattern for the singular part of the solution it is possible to expand it in the exponential.

Our final aim would be the derivation of the scattering matrix representation, which makes the computation of simulations of the probabilities for all pertinent scattering mechanisms possible, taking into account close coupling of many channels, resonance effects and chaotic behaviour in the intermediate state.

The perturbation theory proposed might be especially interesting for the calculation of the wavepacket of the scattering system, since harmonic approximation, that exactly propagates Gaussian wavepackets, is a natural starting point of that theory [7].

The suggested development also covers two of the principle questions of the quantum theory. First, one is connected to the possibility of studying the quantum system behaviour in the region of close coupling. For that purpose it is necessary to build up a perturbation theory, that does not need to know about the spectrum of the unperturbed system. Also, there are several such approaches (see, e.g. [3]), which are not generalized to nonstationary case and so are not suited for scattering problems. Our method exactly serves for that purpose.

The second question is closely connected to the limits of the quasiclassical description of the quantum system evolution. The traditional WKB approach, as it is well known, is limited for scattering applications. At the same time there is the famous path integral approach that makes it possible to describe exactly quantum dynamics in terms of classical trajectories. So the basic question is how to improve the WKB approximation to describe all the effects, for which the traditional approach fails. Our investigations make it possible to develop the representation of the scattering theory via the classical trajectories and so build up the intermediate approximate solutions between exact and primitive WKB forms.

It is well known, that the nonstationary form can be reduced by a transformation to the stationary form [10], that can be solved exactly. In our case unfortunately the use of such approach is not very effective, since after such transformation the perturbation becomes so complicated, that analytic computation of the perturbation matrix elements would be unrealistic.

2. Formulation of the problem

Let us consider the Schrödinger equation for the one-dimensional nonstationary anharmonic oscillator

$$\hat{L}\Psi + \lambda V(x,\tau)\Psi = 0 \qquad -\infty < x \qquad \tau < +\infty \tag{2.1}$$

$$\hat{L} = \mathrm{i}\partial_\tau + \tfrac{1}{2}\partial_x^2 - (\tfrac{1}{2}\Omega^2(\tau)x^2 - F(\tau)x) \tag{2.2}$$

with Ψ being the oscillator wavefunction, λ being the dimensionless coupling parameter, and the perturbation potential $V(x,\tau)$, oscillator frequency $\Omega(\tau)$ and the external force $F(\tau)$ having the following asymptotic behaviour

$$V_\pm(x) = \lim_{\tau\to\pm\infty} V(x,\tau) \qquad \Omega_{\mathrm{in(out)}} = \lim_{\tau\to\pm\infty}\Omega(\tau) \qquad \lim_{\tau\to\pm\infty} F(\tau) = 0. \tag{2.3}$$

Let us assume that the solution of (2.1) satisfies the following boundary and initial conditions

$$\lim_{x\to\pm\infty}\Psi(x,\tau)=0 \qquad \lim_{x\to\pm\infty}\Psi(x,\tau)\partial_x\Psi(x,\tau)=0$$
$$\lim_{\tau\to-\infty}\Psi(x,\tau)=\Psi_{\rm in}(n;\Omega_{\rm in},x)\exp[-{\rm i}(n+\tfrac{1}{2})\Omega_{\rm in}\tau] \tag{2.4}$$

where $\Psi_{\rm in}(n;\Omega_{\rm in},x)$ is a function of the stationary anharmonic oscillator of the initial channel.

The physical meaning of these conditions is obvious—the decay of probability and its flow at infinity—and it corresponds to the formulation of the physical problems, discussed in the introduction. When perturbation is absent, i.e. with $V=0$, the equation

$$\hat{L}\Psi_0(n;x,\tau)=0 \tag{2.5}$$

with boundary conditions (2.3), (2.4) has an exact solution (see, e.g. [8])

$$\Psi_0(n;x,\tau)=f_0(n;x,\tau)=K(n;\tau)\exp(a_1(\tau)y+a_2(\tau)y^2)H_n(y)$$
$$K(n;\tau)=\left(\frac{(\Omega_{\rm in}/\pi)^{1/2}}{2^n n!|\zeta(\tau)|}\right)^{1/2}\exp\left({\rm i}\int_{-\infty}^{\tau}L_{cl}(\tau)\,{\rm d}\tau-{\rm i}\int_{-\infty}^{\tau}E(n;\tau)\,{\rm d}\tau\right) \tag{2.6}$$
$$a_1(\tau)={\rm i}\frac{\dot\eta|\zeta|}{(\Omega_{\rm in})^{1/2}} \qquad a_2(\tau)=\frac{1}{2}\left({\rm i}\frac{|\zeta\|\dot\zeta|}{\Omega_{\rm in}}-1\right) \qquad \dot\eta={\rm d}\eta/{\rm d}\tau$$
$$y=(\Omega_{\rm in})^{1/2}\frac{x-\eta(\tau)}{|\zeta(\tau)|} \qquad |\dot\zeta|=\frac{{\rm d}|\zeta|}{{\rm d}\tau} \tag{2.7}$$
$$L_{cl}=\tfrac{1}{2}(\dot\eta)^2-\tfrac{1}{2}\Omega^2\eta^2+F\eta \qquad E(n;\tau)=\frac{\Omega_{\rm in}}{|\zeta(\tau)|^2}(n+\tfrac{1}{2})$$

with the constant $\Omega_{\rm in}$ being the initial frequency, n being the principle quantum number, $E(n;\tau)$ being the adiabatically changing nth energy level and the functions $\zeta(\tau)$, $\eta(\tau)$ satisfies the equations

$$\ddot\zeta+\Omega^2(\tau)\zeta=0 \qquad \ddot\eta+\Omega^2(\tau)\eta=F(\tau) \tag{2.8}$$

with the following asymptotic and initial conditions

$$\zeta_+(\tau)=\lim_{\tau\to\infty}\zeta(\tau)=c_1\exp({\rm i}\Omega_{\rm out}\tau)-c_2\exp(-{\rm i}\Omega_{\rm out}\tau)$$
$$\zeta_-(\tau)=\lim_{\tau\to-\infty}\zeta(\tau)=\exp({\rm i}\Omega_{\rm in}\tau) \qquad |c_1|^2-|c_2|^2=1 \tag{2.9}$$
$$\eta(-\infty)=\dot\eta(-\infty)=0.$$

It is well known that the solution of the second equation (2.8) can be constructed on the base of the solution of the corresponding homogeneous equation

$$\eta(\tau)=\frac{1}{\sqrt{2\Omega_{\rm in}}}[\zeta(\tau)d^*(\tau)+\zeta^*(\tau)d(\tau)] \qquad d(\tau)=\frac{\rm i}{\sqrt{\Omega_{\rm in}}}\int_{-\infty}^{\tau}{\rm d}\tau'\,\zeta(\tau')F(\tau'). \tag{2.10}$$

A semiclassical-type analysis gives the following form of the solution of (2.1)

$$\Psi^{(+)}(n;x,\tau)=f(n;x,\tau)\exp(-\Phi(n;x,\tau)) \tag{2.11}$$

with $\Psi^{(+)}$ being the total wavefunction, that is developed from the nth asymptotic excited state at $\tau\to-\infty$.

Substitution of (2.11) into (2.1) gives the following equation for unknown functions Φ and f

$$({\rm i}\partial_\tau\Phi-\tfrac{1}{2}(\partial_x\Phi)^2+\tfrac{1}{2}\partial_x^2\Phi-\lambda V(x,\tau))f-(\hat{L}f-(\partial_x\Phi)(\partial_x f))=0. \tag{2.12}$$

For further investigation of equation (2.12) it is convenient to expand functions $f(n;x,\tau)$ and $\Phi(n;x,\tau)$ into power series over λ

$$\Phi(n;x,\tau)=\sum_{k=0}^{\infty}\lambda^k\Phi_k(n;x,\tau)\qquad \Phi_0(n;x,\tau)=0 \tag{2.13}$$

$$f(n;x,\tau)=\sum_{k=0}^{\infty}\lambda^k f_k(n;x,\tau). \tag{2.14}$$

As in all exponential approximation approaches, one term of the expansion of $\Phi(n;x,\tau)$ takes into account an infinite number of terms of standard perturbation theory. But the more we try to take into account within the exponential, the more difficult the equations for individual members would be. In our case there is an optimal choice, that makes it possible to formulate additional conditions for (2.13), (2.14), and so to determine both functions Φ and f_{in} without ambiguity. Let us start from the equation from the kth correction

$$\mathrm{i}\partial_\tau\Phi_k+\tfrac{1}{2}\partial_x^2\Phi_k+q_k^{(1)}(x,\tau)-f_0^{-1}(\hat{L}f_k-(\partial_x\Phi_k)(\partial_x f_0)+q_k^{(2)}(x,\tau))=0 \tag{2.15}$$

with

$$q_k^{(1)}=-\tfrac{1}{2}\sum_{m=1}^{k-1}(\partial_x\Phi_m)(\partial_x\Phi_{k-m})\qquad k\geqslant 2$$

$$q_k^{(2)}(x,\tau)=-\sum_{m=1}^{k-1}\Bigg[f_m(\mathrm{i}\partial_\tau\Phi_{k-m}+\tfrac{1}{2}\partial_x^2\Phi_{k-m}-\delta_{k-m,1}V \tag{2.16}$$

$$-\tfrac{1}{2}\sum_{l=1}^{k-m-1}(\partial_x\Phi_l)(\partial_x\Phi_{k-m-l}))-(\partial_x\Phi_m)(\partial_x f_{k-m})\Bigg]\qquad k\geqslant 2.$$

In case of $k=1$ one has the simple relations

$$q_1^{(1)}(x,\tau)=-V(x,\tau)\qquad q_1^{(2)}(x,\tau)=0. \tag{2.17}$$

Note, that the eigenenergies are not preserved in our problem and so the corrections to them in general give no useful information about the system. Thus, the problem is reduced to the solution of equation (2.15), i.e. to determine the correction to the wavefunction of the anharmonic oscillator.

3. Construction of the solution

Before solving equation (2.15) let us note two important points.

(a) The equation is not correctly formulated as there are two unknown functions in one equation.

(b) There is, in general, at least one singular member in this equation. It can be explained most easily from the analysis of (2.16), taking into account that $f_0(n;x,\tau)$ includes the Hermitian polynomial. This difficulty is readily solved if the perturbation is of polynomial form, as we would suppose in the future.

Such form of perturbation does not seriously influence our discussion, as any smooth perturbation can be approximated by a finite part of its Taylor expansion.

As in every exponential perturbation theory one can solve both above problems by choosing an additional condition for equation (2.15). Let us start from equations of the first order in perturbation. It is convenient to choose

$$\mathrm{i}\partial_\tau\Phi_1+\tfrac{1}{2}\partial_x^2\Phi_1+q_1^{(1)}(n;x,\tau)+Q_1(n;x,\tau)=0 \tag{3.1}$$

$$\hat{L}f_1=(\partial_x\Phi_1)(\partial_x f_0)-Q_1(n;x,\tau)f_0 \tag{3.2}$$

with $Q_1(n;x,\tau)$ being an unknown function. With the additional condition of $\Phi_1(n;x,\tau)$ being a nonsingular correction, one has $\Phi_1(n;x,\tau)$, $Q_1(n;x,\tau)$ and all the terms in (3.2) are polynomials of the same order, as $q_1^{(1)}(n;x,\tau)$. By expanding the functions of equation (3.2) in a series of Hermitian polynomials and supposing the absence of the members of an order, higher than n, one can correctly determine the coefficients of polynomial $Q_1(n;x,\tau)$. So, it is clear that both above difficulties are thus overcome and the system of equations (3.1), (3.2) is quite correct. The procedure is readily generalized to any order. As for $k \geqslant 2$, $q_k^{(2)}(n;x,\tau) \neq 0$, so one has

$$\begin{aligned} Q_k(n;x,\tau) = \Bigg\{ & (\partial_x \Phi_k)(\partial_x f_0) - \hat{L} f_k \\ & - \sum_{m=1}^{k-1} \Bigg(f_m \Bigg[(\mathrm{i}\partial_\tau \Phi_{k-m}) + \tfrac{1}{2}\partial_x^2 \Phi_{k-m} - \delta_{k-m,1} V - \tfrac{1}{2} \sum_{l=1}^{k-m-1} (\partial_x \Phi_l)(\partial_x \Phi_{k-m-l}) \Bigg] \\ & - (\partial_x f_{k-m})(\partial_x \Phi_m) \Bigg) \Bigg\} f_0^{-1}. \end{aligned} \tag{3.3}$$

Taking into account the fact that the expression in square brackets is equal to Q_{k-l}, equation (3.3) is written in the following form

$$Q_k(n;x,\tau) = \left\{ (\partial_x \Phi_k)(\partial_x f_0) - \hat{L} f_k - \sum_{m=1}^{k-1} (f_m Q_{k-m} - (\partial_x f_m)(\partial_x \Phi_{k-m})) \right\} f_0^{-1} \tag{3.4}$$

and for the determination of f_k one has the equation

$$\hat{L} f_k = \sum_{m=1}^{k-1} ((\partial_x f_m)(\partial_x \Phi_{k-m}) - f_m Q_{k-m}). \tag{3.5}$$

And again if one supposes that f_m, Φ_m and Q_m for $m \leqslant k$ are polynomials, then Q_k and f_k are easily determined and it is possible to find the equation for Φ_k

$$\mathrm{i}\partial_\tau \Phi_k + \tfrac{1}{2}\partial_x^2 \Phi_k + q_k^{(1)}(n;x,\tau) + Q_k(n;x,\tau) = 0. \tag{3.6}$$

Note that for the polynomial $Q_k(n;x,\tau)$ the solution of (3.6) is also a polynomial and only high-order terms of perturbation potential $V(x,\tau)$ are important for the determination of Φ_m and f_m.

4. Calculation of the wavefunction to the first order of perturbation theory

Let us study, in more detail, the case of asymmetric polynomial perturbation

$$V(x,\tau) = \alpha(\tau)x^3 + \beta(\tau)x^4 = \sum_{m=0}^{4} b_m(\tau) y^m \tag{4.1}$$

with coefficients $b_m(\tau)$ of the form

$$\begin{aligned} & b_0(\tau) = \eta^3(\beta\eta + \alpha) \qquad b_1(\tau) = \Omega_{\mathrm{in}}^{-1/2}\eta^2|\zeta|(4\beta\eta + 3\alpha) \\ & b_2(\tau) = 3\Omega_{\mathrm{in}}^{-1}\eta|\zeta|^2(2\beta\eta + \alpha) \qquad b_3(\tau) = \Omega_{\mathrm{in}}^{-3/2}|\zeta|^3(4\beta\eta + \alpha) \\ & b_4(\tau) = \Omega_{\mathrm{in}}^{-2}\beta|\zeta|^4 \end{aligned} \tag{4.2}$$

and the assumption that $\alpha(\tau)$ and $\beta(\tau)$ are slowly varying functions of τ.

Before passing to the solution of (3.1) and (3.2), in accordance with previous discussion, let us rewrite Φ_1 and Q_1 in the following form

$$\Phi_1(n;x,\tau)=\sum_{k=0}^{4}v_k(n;\tau)y^k \qquad Q_1(n;x,\tau)=\sum_{k=0}^{4}\sigma_k(n;\tau)y^k. \tag{4.3}$$

Thus, the additional conditions, introduced for regularization of perturbation approach, can be expressed in the form

$$f_0(n;x,\tau)\sum_{k=0}^{4}\sigma_k(\tau)y^k=\kappa_0((2a_2(\tau)y+a_1(\tau))f_0(n;x,\tau)+2nK(n;\tau)$$
$$\times K^{-1}(n-1;\tau)f_0(n-1;x,\tau))\sum_{k=1}^{4}kv_k(\tau)y^{k-1}-\hat{L}f_1 \qquad \kappa_0=\frac{\Omega_{\rm in}}{|\zeta(\tau)|^2}. \tag{4.4}$$

Writing $f_0(n;x,\tau)$ in an explicit form and equating coefficients of the polynomials of the same order on both sides of (4.4) we may determine the coefficients in the polynomial $Q_1(n;x,\tau)$:

$$\sigma_0(n;\tau)=\kappa_0(a_1v_1+2nv_2+2n(n-1)v_4) \qquad \sigma_1(n;\tau)=2\kappa_0(a_2v_1+a_1v_2+\tfrac{3}{2}nv_3)$$
$$\sigma_2(n;\tau)=4\kappa_0(a_2v+\tfrac{3}{2}a_1v_3+nv_4) \qquad \sigma_3(n;\tau)=6\kappa_0(a_2v_3+\tfrac{2}{3}a_1v_4) \tag{4.5}$$
$$\sigma_4(n;\tau)=8\kappa_0a_2v_4.$$

Substituting (4.5) into (3.1) one obtains a system of nonuniform linear differential equations for the determination of coefficients in the correction $\Phi_1(n;x,\tau)$:

$$\mathrm{i}\dot{v}_j-c_j(\tau)v_j-d_j(\tau)=0 \qquad \dot{v}_j=\mathrm{d}v_j(\tau)/\mathrm{d}\tau \qquad j=0,1,2,3,4 \tag{4.6}$$

with functions $c_j(\tau)$ and $d_j(\tau)$ given by

$$c_4(\tau)=4\kappa_0 \qquad c_3(\tau)=3\kappa_0 \qquad c_2(\tau)=2\kappa_0 \qquad c_1(\tau)=\kappa_0 \qquad c_0(\tau)=0$$
$$d_4(\tau)=b_4 \qquad d_3(\tau)=b_3 \qquad d_2(\tau)=b_2+2(2n+3)\kappa_0v_4 \tag{4.7}$$
$$d_1(\tau)=b_1+3(n+1)\kappa_0v_3 \qquad d_0(\tau)=b_0+(2n+1)\kappa_0v_2+2n(n-1)\kappa_0v_4.$$

Initial conditions for system (4.5) are

$$v_0^-=0 \qquad \dot{v}_0^-=-\mathrm{i}d_0 \qquad v_j^-=-\frac{d_j^-}{c_j^-} \qquad j=1,2,3,4. \tag{4.8}$$

Note that '$-$' parameters correspond to the limit $\tau\to-\infty$. It is clear that the solution of (4.6) must start from $j=4$. In such a way, the solution of each equation is presented in the following form

$$v_j(\tau)=G_j(\tau,-\infty)\left[v_j^- -\mathrm{i}\int_{-\infty}^{\tau}G_j(-\infty,\tau')d_j(\tau')\,\mathrm{d}\tau'\right] \qquad j=0,\ldots,4 \tag{4.9}$$

with $G_j(\tau,\tau')$ being the evolution operator of the pertinent homogeneous equation

$$G_j(\tau,\tau')=G_j^{-1}(\tau',\tau)=\exp\left[-\mathrm{i}j\int_{\tau'}^{\tau}\kappa_0(\tau'')\,\mathrm{d}\tau''\right]. \tag{4.10}$$

Taking into account conditions (4.5), equation (4.4) can be represented in the following form

$$\hat{L}f_1(n;x,\tau)-\sum_{j=1}^{4}\bar{e}_j(n;\tau)f_0(n-j;x,\tau)=0 \tag{4.11}$$

with

$$\begin{aligned}
\bar{e}_4(n;\tau) &= 2\kappa_0 v_4 \left[\frac{n!}{(n-4)!}\right]^{1/2} G_4(-\infty,\tau) \\
\bar{e}_3(n;\tau) &= 3\kappa_0 v_3 \left[\frac{n!}{2(n-3)!}\right]^{1/2} G_3(-\infty,\tau) \\
\bar{e}_2 &= \kappa_0[2(2n-3)v_4 + v_2]\left[\frac{n!}{(n-2)!}\right]^{1/2} G_2(-\infty,\tau) \\
\bar{e}_1(n;\tau) &= \kappa_0[3(n-1)v_3 + 2v_1]\left[\frac{n!}{2(n-1)!}\right]^{1/2} G_1(-\infty,\tau).
\end{aligned} \tag{4.12}$$

In all cases, when $n - j \prec 0$, $\bar{e}_j$ are equal to zero. The solution of (4.11) is naturally represented in such a way

$$f_1(n;x,\tau) = \sum_{j=1}^{4} \bar{w}_j(n;\tau) f_0(n-j;x,\tau) \qquad \bar{w}_j(n;\tau) = G_j(-\infty,\tau) w_j(n;\tau). \tag{4.13}$$

Substituting (4.13) into (4.11) one obtains the linear first-order equations for coefficients $w_j(\tau)$

$$\mathrm{i}\dot{w}_j - j\kappa_0(\tau) w_j - e_j(n;\tau) = 0 \qquad e_j(n;\tau) = \bar{e}_j(n;\tau) G_j(\tau,-\infty) \tag{4.14}$$

with initial conditions

$$w_j^- = \lim_{\tau\to-\infty} w_j(n;\tau) = -\frac{e_j(n,-\infty)}{j\kappa_0(-\infty)} \qquad j = 1,\ldots,4. \tag{4.15}$$

The solution of this equation is obvious,

$$w_j(\tau) = G_j(\tau,-\infty)\left[w_j^- - \mathrm{i}\int_{-\infty}^{\tau} \mathrm{d}\tau' G_j(-\infty,\tau') e_j(\tau')\right]. \tag{4.16}$$

Solutions for expansions of higher orders are constructed in the same way.

5. Calculation of the transition S-matrix for nonstationary anharmonic oscillator

The fact that unharmonic oscillator wavefunctions, determined above, are nonstationary, opens new possibilities in view of our previous result [6]. It was shown there that scattering in the three-body collinear system is effectively reduced to the evolution of the anharmonic oscillator in the external field, and so the above wavefunctions can be used for the computation of the scattering matrix. It is not evident how to calculate the scattering matrix elements via the oscillator functions. It is possible to show, using the development of [5], that S-matrix elements for scattering problems can be represented in one-dimensional integral in the form, similar to standard representation [9] of the nonstationary S-matrix:

$$S_{mn} = \lim_{\tau\to+\infty} \langle \psi_f^*(m;x,\tau)\psi^+(n;x,\tau)\rangle \qquad \langle\ldots\rangle = \int_{-\infty}^{\infty} \ldots \mathrm{d}x \tag{5.1}$$

with $\psi_f(m;x,\tau)$ being the asymptotic wavefunction of the final state. Let us examine the approximations of exact and asymptotic wavefunctions. For the nonstationary wavefunction $\psi^{(+)}(n;x,\tau)$ with the help of (2.11) to the first order of perturbation theory over λ one has

$$\begin{aligned}
\psi^{(+)}(n;x,\tau) &= [f_\lambda(n;x,\tau) + \lambda f_\lambda^1(n;x,\tau)]\exp\left[-\lambda\sum_{l=1}^{4} v_l(\tau) y^l\right] + \mathrm{O}(\lambda^2) \\
f_\lambda(n;x,\tau) &= \exp[-\lambda v_0(\tau)] f_0(n;x,\tau) \qquad f_\lambda^1(n;x,\tau) = \exp[-\lambda v_0(\tau)] f_1(n;x,\tau).
\end{aligned} \tag{5.2}$$

Note that functions $f_0(n;x,\tau)$ and $f_1(n;x,\tau)$ are determined by formulae (2.6), (2.7) and (4.13). Expanding the exponential function in (5.2) one has

$$\psi^{(+)}(n;x,\tau)=f_\lambda(n;x,\tau)+\lambda\left[f^1_\lambda(n;x,\tau)-f_\lambda(n;x,\tau)\sum_{l=1}^{4}v_l(\tau)y^l\right]+\mathrm{O}(\lambda^2). \tag{5.3}$$

Now one can use the well known formula for Hermitian polynomials $xH_m(x)=1/2H_{m+1}(x)+mH_{m-1}(x)$ and expand in (5.3) the expressions of the type $y^j f_\lambda(n;x,\tau)$ into the series over the Hermit polynomials. One obtains

$$\psi^{(+)}(n;x,\tau)=f_\lambda(n;x,\tau)+\lambda\left[\sum_{j=1}^{4}\bar w_l(n;\tau)f_\lambda(n-l;x,\tau)\right.$$
$$\left.-\sum_{p=-4}^{4}\bar u_p(n;\tau)f_\lambda(n-p;x,\tau)\right]+\mathrm{O}(\lambda^2) \tag{5.4}$$

with

$$\bar u_p(n;\tau)=G_p(\tau,-\infty)u_p(n;\tau)\qquad u_p(n;\tau)=\left[\frac{(n-p)!}{2^p n!}\right]^{1/2}\chi_p(n;\tau). \tag{5.5}$$

In view of $\chi_p(n;\tau)$ functions, they are given by the following expressions

$$\begin{aligned}
&\chi_{-4}(n;\tau)=\frac{1}{2^4}v_4(\tau)\qquad \chi_{-3}(n;\tau)=\frac{1}{2^3}v_3(\tau)\\
&\chi_{-2}(n;\tau)=\tfrac12(n+\tfrac32)v_4(\tau)+\frac{1}{2^2}v_2(\tau)\qquad \chi_{-1}(n;\tau)=\tfrac34(n+1)v_3(\tau)+\tfrac12 v_1(\tau)\\
&\chi_0(n;\tau)=\tfrac32(n^2+n+\tfrac12)v_4(\tau)+(n+\tfrac12)v_2(\tau)\\
&\chi_4(n;\tau)=n(n-1)(n-2)(n-3)v_4(\tau)\qquad \chi_3(n;\tau)=n(n-1)(n-2)v_3(\tau)\\
&\chi_2(n;\tau)=3n(n-1)^2v_4(\tau)+n(n-1)v_2(\tau)\qquad \chi_1(n;\tau)=\tfrac32 n^2v_3(\tau)+nv_1(\tau).
\end{aligned} \tag{5.6}$$

In the same way we can obtain the representations for asymptotic states of the anharmonic oscillator. So for (out) states one has

$$\psi_f(m;x,\tau)=\varphi^0_f(m;x,\tau)+\lambda\left[\sum_{l=1}^{4}\bar w^f_l(m;\tau)\varphi^0_f(m-l;x,\tau)\right.$$
$$\left.-\sum_{p=-4}^{4}\bar u^f_p(m;\tau)\varphi^0_f(m-p;x,\tau)\right]+\mathrm{O}(\lambda^2). \tag{5.7}$$

The function $\varphi^0_f(m;x,\tau)$ in the above expression is an (out) asymptotic state of the harmonic oscillator

$$\varphi^0_f(m;x,\tau)=\varphi^0_f(m;\Omega_{\mathrm{out}};x)\exp[-\mathrm{i}(m+\tfrac12)\Omega_{\mathrm{out}}\tau] \tag{5.8}$$

$$\varphi^0_f(m;\Omega;x)=\left[\frac{(\Omega/\pi)^{1/2}}{2^m m!}\right]^{1/2}\exp(-\tfrac12\Omega x^2)H_m(\sqrt{\Omega}x). \tag{5.9}$$

In the above expressions the functions $\bar w^f_l(m;\tau)$ and $\bar u^f_p(m;\tau)$ are given by

$$\bar w^f_l(m;\tau)=w^f_l(m)\exp(-\mathrm{i}l\Omega_{\mathrm{out}}\tau) \tag{5.10}$$

$$\bar u^f_p(n;\tau)=u^f_p(n)\exp(-\mathrm{i}p\Omega_{\mathrm{out}}\tau). \tag{5.11}$$

In view of coefficients $w_l^f(m)$ and $u_p^f(n)$, they can immediately be obtained from (4.16), (5.7) and (5.8) in the limit $\tau \to -\infty$ after the substitution of $w_j^- \to w_j^f$ and $v_j^- \to v_j^f$. Now, taking into account (5.5) and (5.10) and using (5.3) and (5.6) in (5.1) one obtains

$$S_{mn}(\lambda) = (S^0_{mn} + \lambda[S^1_{mn} + S^2_{mn}]) \exp[-\lambda v_0^{(+)}] + O(\lambda^2) \tag{5.12}$$

with

$$S^1_{mn} = \sum_{l=1}^{4} w_l^f(m) S^0_{(m-l)n} - \sum_{p=-4}^{4} u_p^f(m) S^0_{(m-p)n} \tag{5.13}$$

$$S^2_{mn} = \sum_{l=1}^{4} w_l^{(+)}(m) S^0_{m(n-l)} - \sum_{p=-4}^{4} u_p^{(+)}(n) S^0_{m(n-p)} \tag{5.14}$$

$$S^0_{mn} = \lim_{\tau\to+\infty} \langle (\varphi_f^0(m; x, \tau))^* f_0(n; x, \tau)\rangle. \tag{5.15}$$

Now, starting from (5.12)–(5.15), it is not difficult to obtain the analytic expressions for transition probabilities for the anharmonic oscillator,

$$W_{mn}(\lambda) = \exp[-2\lambda v_0^{(+)}] \left[1 + 2\lambda \,\mathrm{Re}\left(\frac{S^1_{mn} + S^2_{mn}}{S^0_{mn}}\right)\right] W^0_{mn} + O(\lambda^2) \tag{5.16}$$

$$W^0_{mn} = |S^0_{mn}|^2 = \lim_{\lambda\to 0} W_{mn}(\lambda). \tag{5.17}$$

In the above expressions, the value S^0_{mn} is a matrix element of the S-matrix for transitions in the harmonic oscillator with variable frequency $\Omega(\tau)$ in the external field. The matrix element in (5.15) is calculated via the generating function [6] (see also [10]). So we can only give here the final result

$$W^0_{mn} = \left(\frac{1-\rho}{m!n!}\right)^{1/2} |H_{mn}(y_1, y_2)|^2 \exp[-\nu(1 - \sqrt{\rho}\cos 2\theta)]. \tag{5.18}$$

Here $H_{mn}(y_1, y_2)$ is the Hermitian polynomial of two variables [10] with

$$y_1 = \sqrt{\nu(1-\rho)}\mathrm{e}^{\mathrm{i}\theta} \qquad y_2 = -\sqrt{\nu}(\mathrm{e}^{-\mathrm{i}\theta} - \sqrt{\rho}\mathrm{e}^{\mathrm{i}\theta}) \qquad \theta = \tfrac{1}{2}(\delta_1 + \delta_2) - \beta. \tag{5.19}$$

The parameters ν, ρ, δ_j and β are determined from the solution of the classical problem for harmonic oscillator (2.3), (2.9) and are given by the following expressions:

$$\begin{aligned} &c_1 = \mathrm{e}^{\mathrm{i}\delta_1}\sqrt{\frac{\Omega_{\mathrm{in}}}{\Omega_{\mathrm{out}}}}\frac{1}{(1-\rho)^{1/2}} \qquad c_2 = \mathrm{e}^{\mathrm{i}\delta_2}\sqrt{\frac{\Omega_{\mathrm{in}}}{\Omega_{\mathrm{out}}}}\left(\frac{\rho}{1-\rho}\right)^{1/2} \\ &\rho = \left|\frac{c_2}{c_1}\right|^2 \qquad d = \lim_{\tau\to+\infty} d(\tau) = \sqrt{\nu}\mathrm{e}^{\mathrm{i}\beta}. \end{aligned} \tag{5.20}$$

Note that in the expression proposed both for S-matrix (5.1) and transition probability W_{mn} (5.16) we only used the first members of the expansion of exponentials in Taylor series over the coordinate y. Such approximations for the wavefunction and transition probability are effectively used for many interesting applications. In some cases, when anharmonic perturbation substantially changes the spectrum of the problem and thus our expansion bases, the leading terms of perturbation must be taken into account.

It is clear that for scattering problems unharmonic perturbation is very important for higher excited states, especially for rearrangement processes. At the same time in some situations for rearrangement processes even for the ground state, the effect of perturbation can be substantial. To show it let us discuss one particular case.

6. Application to the 'ground state–ground state' transition

We shall demonstrate an application of the method proposed to the most simple situation—the perturbation of the parametric harmonic oscillator by symmetric potential $\beta(\tau)x^4$, with $\beta(\tau)$ being adiabatically changing functions with boundary values $\beta(-\infty) = 0$ and $\beta(\infty) = \beta^+ \neq 0$. Note that the transition probability for the unperturbed oscillator can be obtained from (5.16) with $\nu = 0$, or by Taylor expansion of the generating function of corresponding S-matrix [10]

$$W^{(0)}_{mn} = |S^{(0)}_{mn}|^2 = \frac{n_<!}{n_>!}\sqrt{1-\rho}\left|P^{(n_>-n_<)/2}_{(n_<+n_>)/2}\left(\sqrt{1-\rho}\right)\right|^2 \tag{6.1}$$

$$S^{(0)}_{mn}(\rho) = \frac{1}{\sqrt{m!n!}}\{\partial^m_{z_1}\partial^n_{z_2} I(z_1, z_2; \rho)\}_{z_1=z_2=0} \tag{6.2}$$

where the generating function I is equal to

$$I(z_1, z_2; \rho) = (1-\rho)^{1/4}\exp\left\{\tfrac{1}{2}\left[\sqrt{\rho}(z_1^2 - z_2^2) + 2\sqrt{1-\rho}z_1 z_2\right]\right\} \tag{6.3}$$

with $n_< = \min(m, n)$, $n_> = \max(m, n)$, and $P^m_n(x)$ being the associated Legendre polynomial.

For many reasons one of the most important parameters of the problem is $W_{00}(\lambda; \rho)$, which measures the probability of the change of the initial ground state to the final ground state. So we shall discuss it in more detail. From (6.1–(6.3) one obtains

$$W_{00}(\lambda; \rho) = \exp[-\lambda v^{(+)}_0][1 - 2\,\mathrm{Re}\,\Lambda(\rho)]W^{(0)}_{00}(\rho) \tag{6.4}$$

$$\Lambda(\rho) = [S^{(0)}_{00}]^{-1}\sum_{k=0}^{2}(u^f_{-2k}S^{(0)}_{2k,0} + u^{(+)}_{-2k}S^{(0)}_{0,2k}) \tag{6.5}$$

with matrix elements $S^{(0)}_{2k,0}$ and $S^{(0)}_{02,k}$ given by (6.2) and (6.3),

$$S^{(0)}_{00} = (1-\rho)^{1/4} \qquad S^{(0)}_{20} = -S^{(0)}_{02} = \frac{1}{\sqrt{2!}}\sqrt{\rho}S^{(0)}_{00} \qquad S^{(0)}_{40} = S^{(0)}_{04} = \frac{1}{\sqrt{4!}}\rho S^{(0)}_{00}. \tag{6.6}$$

For the determination of the u^f_{-2k} and $u^{(+)}_{-2k}$ coefficients, that are important for the $\Lambda(\rho)$ dependence and also the dependence of scattering amplitude, one must find coefficients v^f_j and $v^{(+)}_j = v_j(\infty)$. After integrating (4.9) by parts and taking into account the adiabatic dependence $\beta(\tau)$ one obtains

$$v_j \simeq -\frac{d_j}{jk_0(\tau)} + \frac{1}{j}G_j(\tau; -\infty)\int_{-\infty}^{\tau}\mathrm{d}\tau' G_j(-\infty, \tau')\frac{\dot{d}_j(\tau')}{k_0(\tau')} \qquad j = 1, 2, 3, 4. \tag{6.7}$$

Now the coefficients $v^{(+)}_j$ are determined from (6.7) by taking into account (4.7) and (4.8) by using integration by parts and averaging over fast oscillations

$$\begin{aligned} &v^{(+)}_4 \simeq -\frac{\beta^+}{4\bar{k}_0^3} \qquad v^{(+)}_2 \simeq \frac{3\beta^+}{4\bar{k}_0^3} \qquad v^{(+)}_0 \simeq \frac{3\beta^+}{8\bar{k}_0^3} \\ &\bar{k}_0 = \Omega_{\mathrm{in}}/(|c_1|^2 + |c_2|^2). \end{aligned} \tag{6.8}$$

In the same way, for the coefficients v^f_j one has

$$\begin{aligned} &v^f_4 = -\frac{d^f_4}{c^f_4} = -\frac{1}{4}\frac{\beta^+}{\Omega^3_{\mathrm{out}}} \qquad v^f_2 = -\frac{d^f_2}{c^f_2} = \frac{3}{4}\frac{\beta^+}{\Omega^3_{\mathrm{out}}} \qquad v^f_0 = 0 \\ &c^f_j = j\Omega_{\mathrm{out}}. \end{aligned} \tag{6.9}$$

Now using (5.5)–(5.7) from (6.8), (6.9) one obtains the expressions for coefficients u^{+}_{-2k} and u^{f}_{-2k} in the form

$$u^{f}_{0} = \frac{3}{16}\left(\frac{\beta^{+}}{\Omega^{3}_{\mathrm{out}}}\right) \qquad u^{+}_{0} = \frac{3}{16}\frac{\beta^{+}}{\Omega^{3}_{\mathrm{out}}}\left(\frac{1+\rho}{1-\rho}\right)^{3}$$
$$u^{f}_{-2} = u^{+}_{-2} = 0 \qquad u^{f}_{-4} = -\frac{1}{4}\sqrt{\frac{3}{2}}\frac{\beta^{+}}{\Omega^{3}_{\mathrm{out}}} \qquad u^{+}_{-4} = -\frac{1}{4}\sqrt{\frac{3}{2}}\frac{\beta^{+}}{\Omega^{3}_{\mathrm{out}}}\left(\frac{1+\rho}{1-\rho}\right)^{3}. \tag{6.10}$$

Formula (6.4) with the above results gives the final expression for W_{00}

$$W_{00}(\lambda;\rho) \simeq \sqrt{1-\rho}\{1-\lambda[1-v^{+}_{0}(\rho)](1-\tfrac{1}{3}\rho)\}\exp[-\lambda v^{+}_{0}(\rho)] \tag{6.11}$$

with new notations

$$v^{+}_{0}(\rho) = \frac{\Omega^{3}_{\mathrm{out}}}{\beta^{+}}v^{(+)}_{0} = \left(\frac{1+\rho}{1-\rho}\right)^{3} \qquad \lambda \to \frac{3\beta^{+}}{8\Omega^{3}_{\mathrm{out}}}\lambda.$$

As it was shown in [10], parameter ρ, that measures the excitation of classical oscillator, corresponds to quantum mechanical reflection coefficient of the particle with momentum $k(x) = \Omega(x)$. That makes it possible to use the well known results from quantum mechanics for ρ.

As can be seen from figure 1, the anharmonic oscillator, unlike the harmonic parametric one, in the limit $\rho \to 0$ has a transition probability that is not equal to 1. Not only that, as it is seen from (6.11), the dependence of transition probability over λ is regular, which makes it possible to use the proposed formula up to the values of λ of the order of unity.

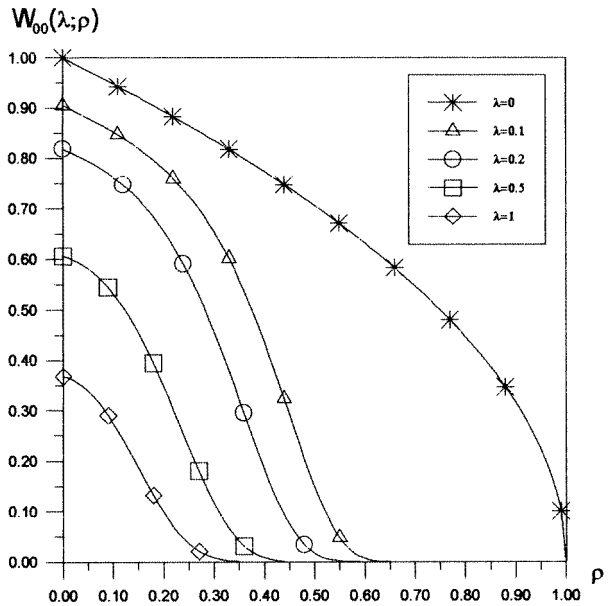

Figure 1. The dependence of the 'ground state–ground state' transition probability on the reflection coefficient ρ and dimensionless constant λ.

7. Conclusions

Many important problems in theoretical and mathematical physics are reduced to the solution of the equation of the nonstationary unharmonic oscillator with different sets of (in) and (out) states. The use of standard approaches to such a problem meets the following two basic difficulties.

(a) Opposite to the stationary situation, we do not have the fixed basic set for the perturbed wavefunction.

(b) In nonstationary situations the dimensionless perturbation parameter changes with time and can become large in the strong coupling region.

In this paper, as a generalization of nonlinearization method [3], we propose a way to overcome the above difficulties. The perturbation theory is constructed on exact wavefunctions for the quantum harmonic oscillator with variable frequency in external field as a basis state. This makes it possible, due to some unique intrinsic properties of those solutions, to work out the system of two linear equations, that determine the first corrections both to the amplitude and to the phase of the total wavefunction. It should also be noted that the nth-order correction is also determined by two independent differential equations, that are obtained after n iterations.

A very important computational property of our approach is connected to the fact that any order correction is constructed on the basis of a finite number of wavevectors. This will allow one to calculate the corrections to the transition operator.

The possibility of a simultaneous correction of the phase and amplitude of the wavefunctions, as in the case of the stationary problem, gives a regular method of investigation of the strong coupling region, where perturbation is strong and the small parameter is absent.

The use of this approach is well suited in numerous applications, of which we point out only some of the most important:

- corrections to path integral representations of the propagator in field and scattering theories;
- account of kinetics in some problems of solid-state and condensed matter physics;
- anharmonic corrections for scattering matrix in collinear model of rearrangement collisions;
- anharmonic corrections for the propagator in the wavepacket dynamics approach to molecular scattering.

We shall discuss these problems in detail in our future publications.

Note that analysis of the proposed expressions shows that taking account of antisymmetric terms in potential expansion can cause nonadiabatic behaviour and also cause nonanalytic dependence of $W_{00}(\lambda;\rho)$ over λ. Depending on the form of the perturbation, 'ground state–ground state' transition probability might have several maxima in such a case.

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References

[1] Hioe F T, McMillen D and Montroll E W 1978 *Phys. Rep.* **43** 306
[2] Klinger M I 1983 *Phys. Rep.* **94** 183
[3] Turbiner A V 1984 *Sov. J. Usp. Fiz. Nauk.* **144** 79–112

[4] Dolgov A D and Turbiner A V 1980 *Phys. Lett.* **77A** 15
[5] Gevorkyan A S 1995 *Rep. NAS Armenia* **95** 146–51
[6] Bogdanov A V, Gevorkyan A S and Dubrovskii G V 1994 *Pis. Zh. Tekh. Fiz.* **20** 39–45
[7] Henriksen N E and Heller E J 1988 *Chem. Phys. Lett.* **148** 567–71
[8] Popov V S and Perelomov A M 1970 *Sov. J.–Teor. Mat. Fiz.* **3** 377
Popov V S and Perelomov A M 1970 *Teor. Mat. Fiz.* **4** 48
[9] Newton R G 1966 *Scattering Theory of Waves and Particles* (New York: McGraw-Hill)
[10] Baz' A I, Zel'dovich Ya B and Perelomov A M 1971 Scattering reactions and decays *Nonrelativistic Quantum Mechanics* (Moscow: Nauka) (in Russian)