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WAVES IN QUANTUM SYSTEMS WITH NONLINEARITY AND WALLS

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Abstract. The nonlinear cubic Shrödinger equation is integrated numerically for quantum systems confined by potential walls of a well. If nonlinear potential describing nonlinearity is distributed on the whole width of the well, soliton generation is possible. For the nonlinear potential distributed on the right half of the well with free motion on the left one the propagation of waves occurs. Solutions for the probability density, expectation positions and velocities of the wave were analyzed under different initial conditions including the Gaussian and specified wave packets.

1. Introduction

Soliton problem was intriguing and promising in during the 20th century. Great interest to the investigations is supported also at the present time. In those investigations, much attention is given to unbounded in length systems. There different types of waves have been investigated analytically as well as numerically [1, 2]. At the same time, the problem of solitons in the bounded quantum systems with impenetrable walls remained open. In our paper, we investigated one-dimensional quantum system, bounded by potential walls including nonlinearity on the total width or only in its half.

2. Basic equations and assumptions

The dynamic of spatially bounded quantum system is considered in domain

$$-L \le x \le L\,, \tag{1}$$

where x is the coordinate located in $[-L; L]$. On the domain boundaries the wave function $\Psi(x,t)$ satisfies to the condition

$$\Psi(\pm L,\, t) = 0\,, \tag{2}$$

where boundaries are of the walls of an impenetrable well, t is the time. To set Cauchy's problem it is necessary to specify the corresponding initial condition

$$\Psi(x, t=0) = \Psi_0(x)\,. \tag{3}$$

Below, we consider two types of these conditions. In the first case, we use the Gaussian packet, in the second one the solution of the nonlinear cubic Shrödinger equation. The wave function $\Psi(x, t)$ satisfies the normalization condition

$$\int_{-L}^{L} \Psi^* \Psi \, dx = 1. \tag{4}$$

To describe the wave packet dynamics at conditions (2), (3), the time dependent Schrödinger equation is used

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \Psi + U\Psi , \tag{5}$$

where $U = K|\Psi|^2$ is the nonlinear potential; $\hbar$ is the reduced Plank constant; i, m are imaginary unit and mass, respectively. The transition to the non-dimensional quantities and operators in Eq. 5 can be obtained by means of the basic units of length Δl, time Δt, and energy U_0 as follows

$$\Delta l = \sqrt{\frac{\hbar}{m\omega}} , \qquad \Delta t = \omega^{-1} , \quad U_0 = \frac{\hbar^2}{m(\Delta l)^2} .$$

As results, we have

$$\zeta = x / \Delta l , \; \zeta_L = L / \Delta l , \; \tau = t / \Delta t , \; \tilde{U} = U / U_0 ,$$

$$\frac{\partial^2}{\partial x^2} = \frac{1}{(\Delta l)^2} \frac{\partial^2}{\partial \zeta^2} , \; \frac{\partial}{\partial t} = \frac{1}{\Delta t} \frac{\partial}{\partial \tau} , \; \tilde{\Psi} = \Psi / (\Delta l)^{-1/2} ,$$

and the Schrödinger equation is rewritten as

$$i \frac{\partial \tilde{\Psi}}{\partial \tau} = -\frac{1}{2} \frac{\partial^2}{\partial \zeta^2} \tilde{\Psi} + \tilde{U} \tilde{\Psi} . \tag{6}$$

The quantity $\tilde{U}$ becomes non-dimensional and equal to

$$\tilde{U} = k|\Psi|^2 , \; k = \frac{K}{\hbar \omega \Delta l} . \tag{7}$$

The normalization condition (4) can be rewritten as

$$\int_{-\zeta_L}^{\zeta_L} |\tilde{\Psi}|^2 \, d\zeta = 1 . \tag{8}$$

The nonlinear potential (7) in Eq. 6 plays the fundamental role in dynamical properties of the quantum system.

By using the standard formulae for the probability density and probability stream density, in the next analysis we introduce the non-dimensional velocity of the probability fluid V determined as follows

$$N = \tilde{\Psi}^* \tilde{\Psi}\,,\ V = \frac{1}{2i}\left(\tilde{\Psi}^* \frac{\partial \tilde{\Psi}}{\partial \zeta} - \tilde{\Psi} \frac{\partial \tilde{\Psi}^*}{\partial \zeta} \right) \Big/ N\,. \tag{9}$$

The non-dimensional velocity operator can be defined as $\tilde{V} = -i\,\partial / \partial\zeta$. For the dynamical analysis we shall also calculate the mean values of the position and velocity by means of the formulae

$$\begin{aligned} <\zeta> &= \int_{-\zeta_L}^{\zeta_L} \tilde{\Psi}^*(\zeta,\tau)\ \zeta\ \tilde{\Psi}(\zeta,\tau)\,d\zeta, \\ <V> &= \int_{-\zeta_L}^{\zeta_L} \tilde{\Psi}^*(\zeta,\tau) \left(-i\frac{\partial}{\partial \zeta} \right) \tilde{\Psi}(\zeta,\tau)\,d\zeta. \end{aligned} \tag{10}$$

The next sections will be devoted to the soliton solutions and propagating waves.

3. Soliton waves

Firstly, we discuss the solutions of Eq. (6) at $k = 2$ for the potential U distributed on the whole width $[-8\pi, 8\pi]$ of the well. For preparation of the initial packet we used the soliton solution (1.62) from [1] satisfying to the condition $\tilde{\Psi}_0 \to \infty$ at $|\zeta| \to \infty$; it can be presented as

$$\tilde{\Psi}_0 = \frac{1}{\sqrt{2}} \cdot \mathrm{sech}(\zeta) \exp(i \cdot 0.5\zeta)\,. \tag{11}$$

Initial packet is located in the vicinity of the point $\zeta = 0$ and has the initial velocity $V_0 = 0.5$. The extension in length of the packet is very small in comparison with the well width. The numerical calculations are shown in Figs. 1-3. In Fig. 1 we see the picture of the probability density values on the plane (ζ,τ). It demonstrates the motion similar a classical particle with the constant velocity between the well walls. After collisions the particle reflects from the wall and changes the sign of velocity. The mean position $<\zeta>$ and velocity $<V>$ are shown in Figs. 2, 3. The derivative $d<\zeta>/d\tau$ is consistent satisfactorily with $<V>$. The accuracy of calculations was not very high and became worse with time due to collisions. The normalization integral increases jump and then returns to unity. The numerical calculations of probability stream density were also carried out, they agree with the results of other calculations. The width of trajectories is thin and does not enlarge (see Fig. 1). This property allows declaring that nonlinearity caused by $\tilde{U}_0 \neq 0$ plays self-organizing role in the formation of a soliton.

If $k = 2$ and the potential $\tilde{U}$ is distributed on the whole width of the well, but the initial condition is Gaussian packet

$$\tilde{\Psi}_0(\zeta) = 0.751126 \exp\left(-\frac{\zeta^2}{2} \right) \exp\left(i \cdot 0.5\zeta \right) \tag{12}$$

the dynamical picture is changed. Here, the wave-packet solutions are not similar to ones in the previous regime. The trajectories on the plane (ζ, τ) become broader than in Fig. 1 and amplitude $<\zeta>$ is decreased. It is believed that soliton solutions are destroyed or do not exist at large times.

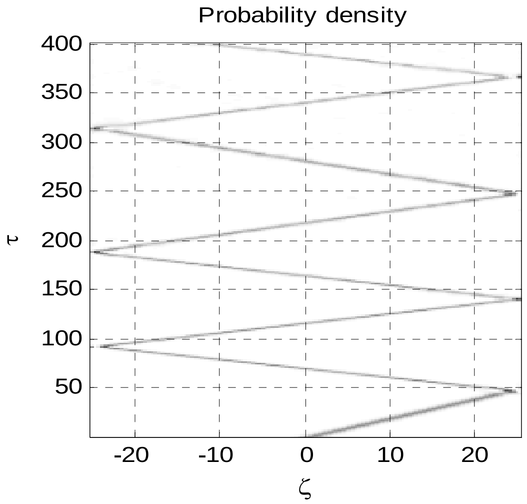

Fig. 1. Map of probability density values at $k = 2$ in $[-\zeta_L, \zeta_L]$, $\zeta_0 = 0$, $V_0 = 0.5$ (regime *a*).

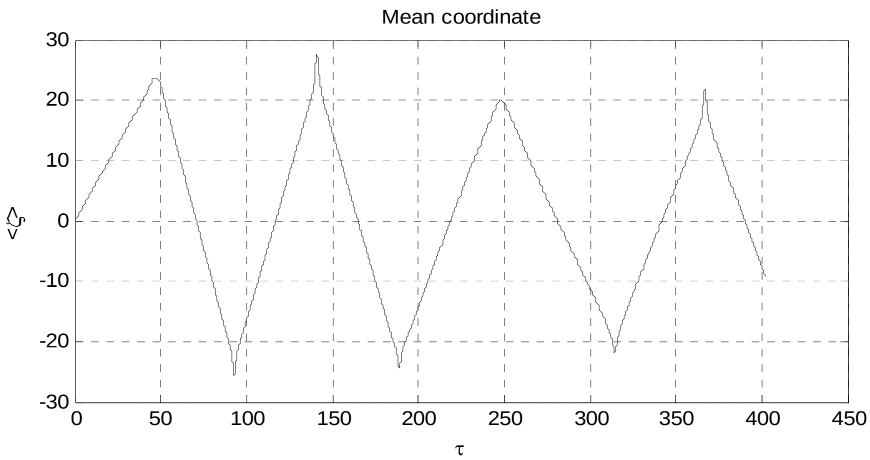

Fig. 2. Mean position as a function of time in regime (*a*).

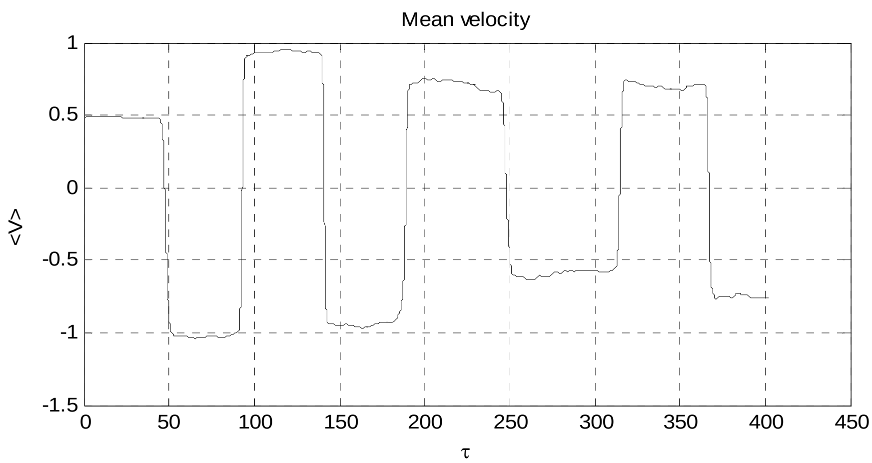

Fig. 3. Mean velocity as function of time in regime (a).

4. Constituent quantum system

In this section we consider the quantum system having properties $k=0$ for $\zeta \in [-8\pi, 0]$ and $k=2$ in $[0, 8\pi]$. Differently, in the domain $[-8\pi, 0]$ the potential $\tilde{U}=0$ and the quantity $\tilde{U} \neq 0$ for $[0, 8\pi]$. The initial wave packet has a form

$$\tilde{\Psi}_0 = \frac{1}{\sqrt{2}} \cdot \operatorname{sech}(\zeta - 3)\exp(-i \cdot 0.5\zeta) . \tag{13}$$

In Fig. 4 the probability density is presented on plane (ζ, τ). The initial velocity $< V_0 >$ is directed to the left and equal -0.5; initial position $< \zeta_0 >= 3$ and displayed to the right form $\zeta = 0$. The wave packet is moving to the left, then, in point $\zeta = 0$ the main part of the probability fluid is reflected and remains in domain $[0, 8\pi]$ during a prolonged time (see Fig. 4). The very small portion of probability fluid is not reflected and passes through $\zeta = 0$ into domain $[-8\pi, 0]$, then it is spreading.

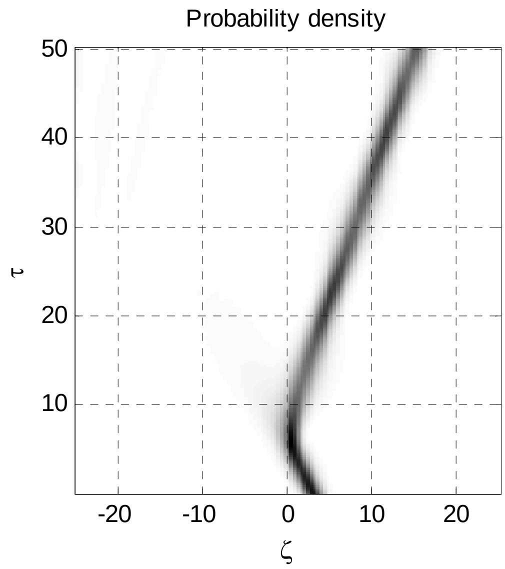

Fig. 4. Map of probability density at $k=2$ in $[0, \zeta_L]$, $\zeta_0 = 3$, $V_0 = -0.5$ (regime *b*).

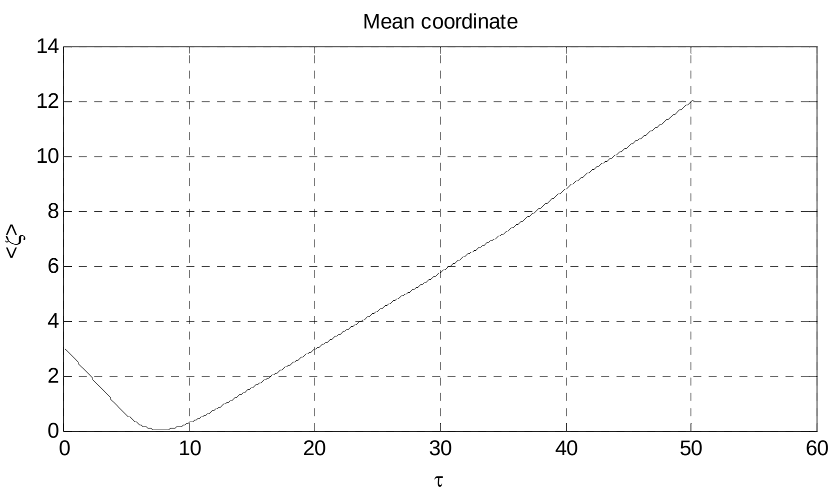

Fig. 5. Mean position as function of time in regime (*b*).

In Figs. 5, 6 we see the sequence of this process. The accuracy of calculations becomes worse at times when the wave packet collides with walls. Normalization integral increases at instant of time collision to $3 \cdot 10^{-3}$, after a short impulse returns to unity, and the process repeats. In spite of its limits, we have a good qualitive, although crude quantitative model of the dynamical process. Contrary to the previous case with $k = 2$ on the whole width of well, here the wave packet becomes more broad and spreading. The mean position in Fig. 5 tends to zero and then increases while mean velocity (Fig. 6) increases and then the growth is slowing down. For comparison, consider the dynamical regime with the opposite initial velocity $V_0 = 0.5$, but the remaining parameter being the same as in the previous regime. The map of probability density values on plane (ζ, τ) is presented in Fig. 7. It shows the quick change of the dynamical process. The quantities $<\zeta>$, $<V>$ are plotted in Figs. 8, 9. If $k = 0$ and respectively $\tilde{U} = 0$, then for both initial conditions we have the known solutions for the packets in the well with impenetrable walls.

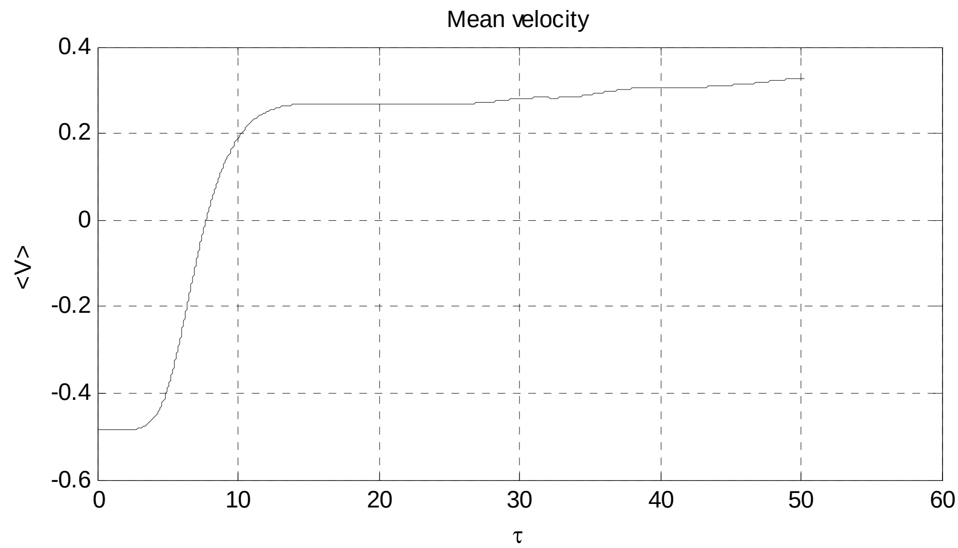

Fig. 6. Mean velocity as function of time in regime (b).

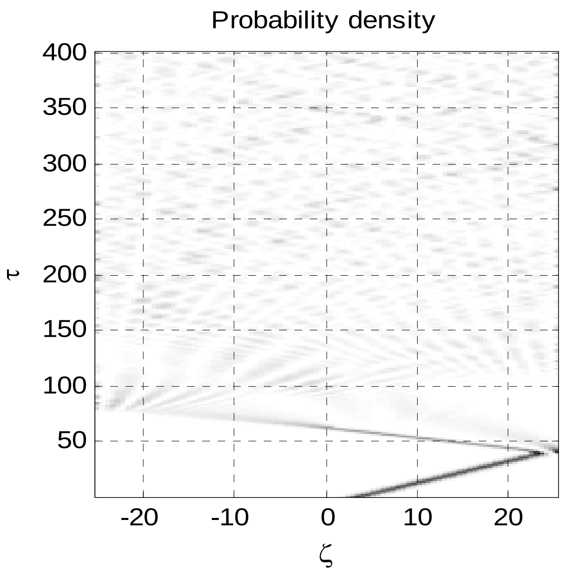

Fig. 7. Map of probability density at $k = 2$ in $[0, \zeta_L]$, $\zeta_0 = 3$, $V_0 = 0.5$ (regime c).

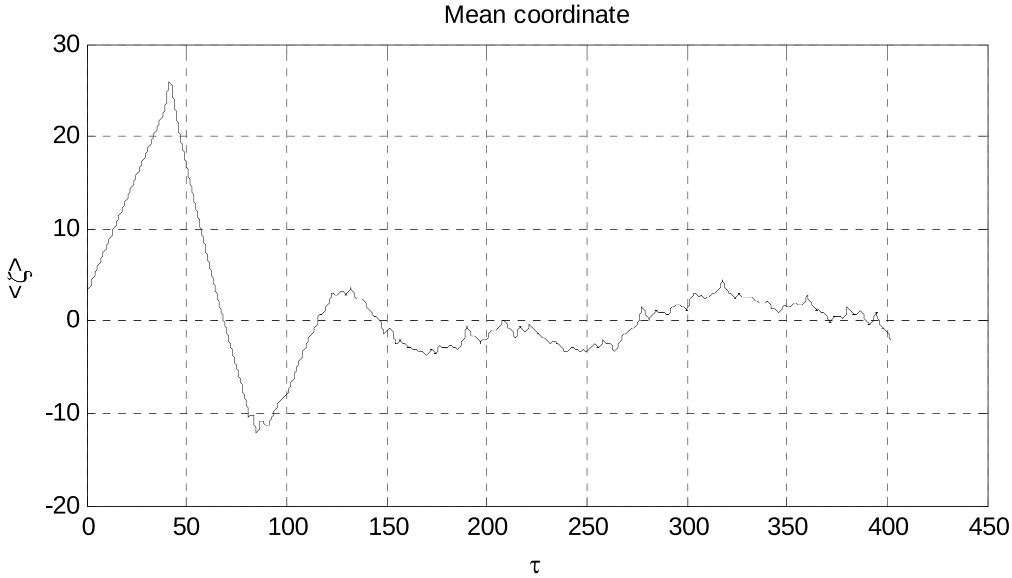

Fig. 8. Mean position as a function of time in regime (*c*).

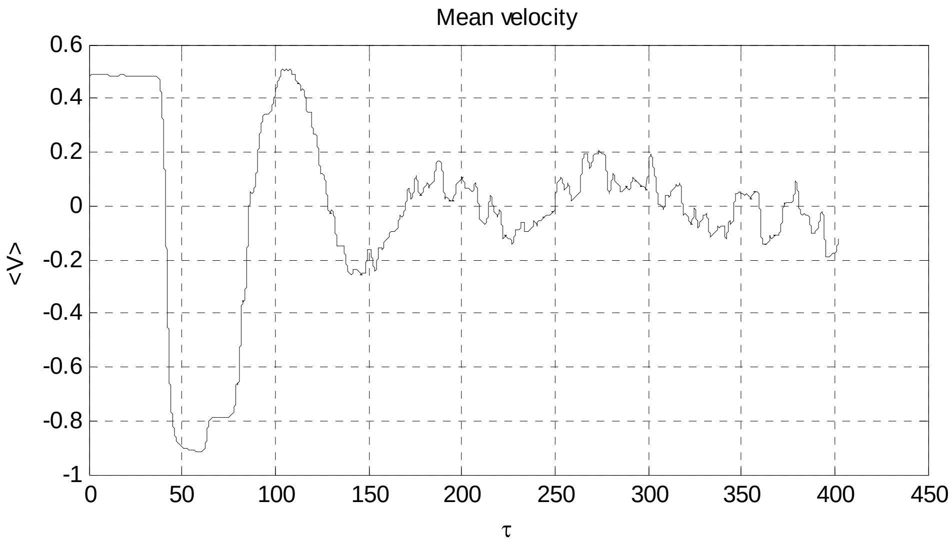

Fig. 9. Mean position as function of time in regime (*c*).

5. Conclusion

In the context of the nonlinear cubic Schrödinger equation, it has been investigated the wave problem for concrete parameters and initial conditions. The influence of sharp transition from linear properties to nonlinear ones on wave propagation was found. Solitons and spreading waves were discussed.

References

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[2] A. Scott, *Nonlinear Science, Emergence and Dynamics of Coherent Structures* (Oxford University Press, 2003).