Chapter 6

Integrable Systems

Up to now we mainly tried to explain the reasons leading to stochastic dynamics of various physical systems, and described different methods of investigation of the chaotic equilibrium state with the help of a computer. Now we consider the opposite class of systems, namely the systems where the nonlinearity leads not to a chaos, but to the regular motion.

6.1 Fermi-Pasta-Ulam paradox

Perhaps, during all development of physics up to recent times, when a wide employing of computer modeling has been started, the harmonic approximation for solution of physical problems was used as the main approach. Namely, the potential energy of the system was expanded into Taylor series with respect to small displacements of atoms from their equilibrium positions up to square terms, so that the force acting on a given atom occurs to be a linear function of the displacements. In this case the system evolution is governed by a system of linear equations, and the latter always has an exact solution at least in principle. In a general case this solution can be expressed as a sum over independent normal modes, i.e. the system is described by a set of harmonic oscillators.

When the total energy of the system increases, the amplitude of vibrations rises, and this leads to an anharmonicity of the vibrations as well as to a nonlinear interaction of different modes. In other words, the set of harmonic oscillators may be interpreted as a set of quasiparticles (phonons, magnons, plasmons, *etc.*). Then, with increasing of the system total energy, the number of these quasiparticles increases too, and they begin to interact between themselves. In a classical approach these anharmonic (or nonlinear) effects are assumed to be small, and they are taken into account with the help of one or another variant of the perturbation theory. However, it turns out that, as a rule, such a perturbation series diverges and, consequently, the corresponding physical system is nonintegrable usually. In the result, practically in all systems a chaos emerges, and the statistical mechanics laws start to work leading the system to thermal equilibrium.

However, observing nature and life surrounding us, we see that real systems are often very far from the chaotic equilibrium state. This phenomenon is caused by two reasons. First, a majority of systems are open, i.e. an energy and/or particles constantly enter into the system and/or are taken away from it, and that causes the system to be in a nonequilibrium state. Second, in some "special" systems the nonlinearity leads not to a chaos, but, on the contrary, to an "ordering" of their state. In the result of co-action of both reasons, in some systems the processes, which are reverse to chaotization ones, the so-called *self-organizing processes*, take place. Such processes are studied by a new science called *sinergetics* [155, 156]. And, although a number of self-organized systems is rather small, their role in science is extremely high, because namely such systems surround us and, moreover, we present an example of such a system ourselves.

In the present Chapter we give a brief introduction to the theory of "special" nonlinear systems, where the existence of nonlinearity results in appearing of specific "solitonic" solutions. In developing of this

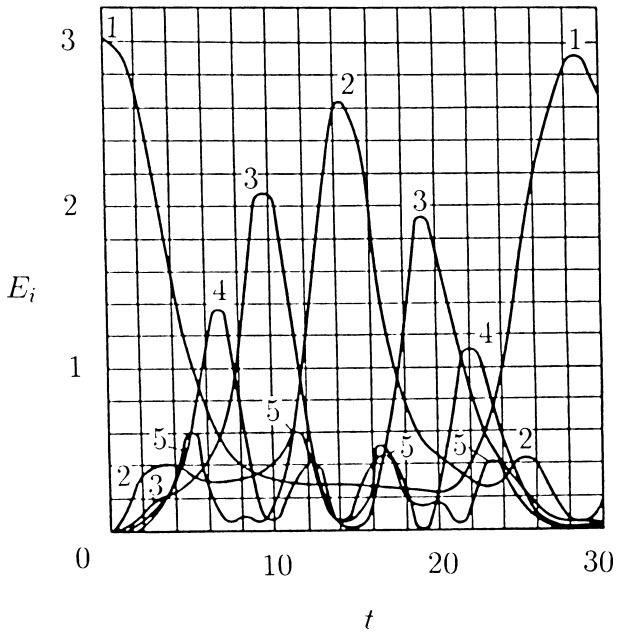

Figure 6.1: Fermi-Pasta-Ulam paradox. Energies of different linear modes E_i versus time t (after [157]).

theory the computer modeling played one of main roles as it did also in developing of the stochastic theory discussed in the previous chapters of this book.

Fermi, Pasta and Ulam [157] were the first who have met with such a problem. They tried to answer on the following question stated long time ago: why do the laws of statistical physics and thermodynamics operate, i.e. why does the kinetic energy is equally shared among the system degrees of freedom? The problem has being solved with the help of one of the first computers "MANIAC" by the method which now is known as the molecular dynamics method.

Fermi *et al.* [157] have considered a chain consisting of N_p atoms (it was taken $N_p = 32$ or 64), both chain's ends (i.e., the atoms with the numbers $n = 0$ and $n = N_p + 1$) were kept fixed. The anharmonic interaction (between the nearest neighbors only) was accounted with the help of two types of potentials, the potential with cubic anharmonicity,

$$v(x) = \frac{1}{2}g(x - a_0)^2 + \frac{1}{3}\alpha(x - a_0)^3, \tag{6.1}$$

and the potential with quadric anharmonicity,

$$v(x) = \frac{1}{2}g(x - a_0)^2 + \frac{1}{4}\beta(x - a_0)^4, \tag{6.2}$$

where g is the elastic constant, a_0 is the mean interatomic distance, and α and β are small coefficients. At $t = 0$ the chain was taken to be in rest, but the initial atomic displacements $u_n = x_n - na_0$ were taken as the following,

$$u_n(0) \propto \sin\left[\pi n/(N_p + 1)\right], \tag{6.3}$$

i.e. only the lowest linear mode was excited. It was expected that for a some time the thermalization should take place, i.e. the initial energy would be equally shared among all modes. In computer experiment, however, nothing similar to the thermodynamical behavior have been observed. An example of variation of the energies E_i versus time t for different linear modes is shown in Fig. 6.1. As seen, a part of the initial energy is transferred from E_1 to E_2, then to E_3 and so on, but after a certain time almost the whole energy comes back to the first mode. Moreover, the displacement of each atom returns to the initial value too. This recurrence phenomenon was called the *Fermi-Pasta-Ulam* (FPU) *paradox*.

To anticipate, we have to note that such a result was obtained because of a small capacity of early computers. In fact, the system described above is nonintegrable, so that a chaos will be arised after a long enough time interval [158]–[161]. Namely, the recurrence state does not exactly coincide with the initial state, and with each recurrence period the measure of chaos slowly increases. But the thermalization time is very long, so that the simulation of such problems need a more high-speed computer. That means that the given system is "close" to the exactly integrable one.

The attempts to resolve the FPU paradox have led to a drastic acceleration of the rate of development of the theory of nonlinear systems and to discovery of exactly integrable nonlinear systems exhibiting solitonic solutions. Zabusky and Kruskal [162] were the first who have done this with the help of computer simulation.

6.2 Solitons

6.2.1 Boussinesq's equation

First let us deduce the motion equation for the FPU chain. To do this, let us take the potential energy of the infinite atomic chain in the following form,

$$V = \sum_n v\left(u_{n+1} - u_n\right), \tag{6.4}$$

so that in accordance with the second Newton law we obtain the motion equations

$$m_a \ddot{u}_n = -\frac{\partial V}{\partial u_n} = v'(u_{n+1} - u_n) - v'(u_n - u_{n-1})\,. \tag{6.5}$$

Further we put $m_a = 1$ for the atomic mass.

Let us expand the interaction potential $v(\Delta u)$ into Taylor series and restrict ourselves by accounting of cubic anharmonicity only as, e.g., in Eq. (6.1),

$$v'(\Delta u) \approx v'(0) + v''(0)\,\Delta u + \frac{1}{2} v'''(0)\,\Delta u^2. \tag{6.6}$$

Now let us consider long-wave disturbances only, that allows to use the so-called continuum approximation. Namely, if we suppose that

$$|u_{n+1} - u_n| \ll a_0\,, \tag{6.7}$$

we may turn of from the discrete variable n to a continuous variable x ($x = na_0$), $u_n(t) \to u(x,t)$. Then, it is easy to deduce the following expressions,

$$u_{n\pm1} = u_n \pm a_0 u' + \frac{1}{2} a_0^2 u'' \pm \frac{1}{3!} a_0^3 u''' + \frac{1}{4!} a_0^4 u'''' + \cdots, \tag{6.8}$$

$$u_{n+1} - u_n = a_0 u' + \frac{1}{2} a_0^2 u'' + \frac{1}{3!} a_0^3 u''' + \frac{1}{4!} a_0^4 u'''' + \cdots, \tag{6.9}$$

$$u_n - u_{n-1} = a_0 u' - \frac{1}{2} a_0^2 u'' + \frac{1}{3!} a_0^3 u''' - \frac{1}{4!} a_0^4 u'''' + \cdots, \tag{6.10}$$

$$(u_{n+1} - u_n)^2 = a_0^2 u'^2 + a_0^3 u' u'' + \cdots, \tag{6.11}$$

$$(u_n - u_{n-1})^2 = a_0^2 u'^2 - a_0^3 u' u'' + \cdots\,. \tag{6.12}$$

Further, we will exploit the following notations commonly used for nonlinear equations:

$$\frac{\partial u(x,t)}{\partial x} \equiv u_x\,, \quad \frac{\partial u(x,t)}{\partial t} \equiv u_t\,, \quad \frac{\partial^2 u(x,t)}{\partial^2 x} \equiv u_{xx}\,, \quad etc. \tag{6.13}$$

Substituting Eqs. (6.6), (6.8–6.12) into Eq. (6.5), we obtain the equation

$$u_{tt} = s^2 u_{xx} + B^2 u_{xxxx} - \Lambda u_x u_{xx} \,, \tag{6.14}$$

where s is the sound velocity in the chain,

$$s^2 = a_0^2 v''(0) \,, \tag{6.15}$$

the constant B characterizes the dispersion of linear waves,

$$B^2 = \frac{1}{12} a_0^4 v''(0) \,, \tag{6.16}$$

the coefficient Λ describes the nonlinearity of interaction,

$$\Lambda = -a_0^3 v'''(0) \,, \tag{6.17}$$

and usually $v'''(0) < 0$ so that $\Lambda > 0$.

Next, we have to turn to dimensionless variables. For this, let us introduce new variables

$$\tilde{t} = t/t_0 \,, \;\; \tilde{x} = x/x_0 \,, \;\; \text{and} \;\; \tilde{u} = u/u_0 \,, \tag{6.18}$$

and rewrite Eq. (6.14) in the form

$$\tilde{u}_{\tilde{t}\tilde{t}} - \frac{s^2 t_0^2}{x_0^2} \, \tilde{u}_{\tilde{x}\tilde{x}} - \frac{B^2 t_0^2}{x_0^4} \, \tilde{u}_{\tilde{x}\tilde{x}\tilde{x}\tilde{x}} + \frac{\Lambda u_0 t_0^2}{x_0^3} \, \tilde{u}_{\tilde{x}} \tilde{u}_{\tilde{x}\tilde{x}} = 0 \,. \tag{6.19}$$

It is natural to choose the values t_0, x_0 and u_0 in the following way:

$$x_0 = s t_0 = B/s \,, \;\; t_0 = B/s^2, \;\; \text{and} \;\; u_0 = sB/\Lambda \,. \tag{6.20}$$

Then Eq. (6.19) takes the canonical form,

$$u_{tt} - u_{xx} - u_{xxxx} + u_x u_{xx} = 0 \,, \tag{6.21}$$

where we have omitted all tildes in order to reduce the notations. Equation (6.21) is just the *Boussinesq equation* which we were looking for.

6.2.2 Competition of dispersion and nonlinearity

First let us investigate Eq. (6.21) on a qualitative level. If we will keep in Eq. (6.21) the two first terms only, we obtain the simplest wave equation,

$$u_{tt} - u_{xx} = 0 \,. \tag{6.22}$$

This equation is solved with the help of Fourier transform, and the solutions correspond to the plane waves,

$$u(x,t) \propto \exp\left[i\,\omega(k) t - i\,kx\right] , \tag{6.23}$$

with the wave length $\lambda = 2\pi/|k|$ and the frequency $\omega(k) = |k|$. These waves may propagate in both directions, and the phase velocity of all waves is the same, $s = 1$ in the chosen system of units.

Now let us take into account the third term in Eq. (6.21), i.e. let us consider the equation

$$u_{tt} - u_{xx} - u_{xxxx} = 0 \,. \tag{6.24}$$

This is the linear equation too, and its solutions are again the plane waves (6.23), but now with the dispersion law

$$\omega(k) = \pm k \sqrt{1 - k^2} . \tag{6.25}$$

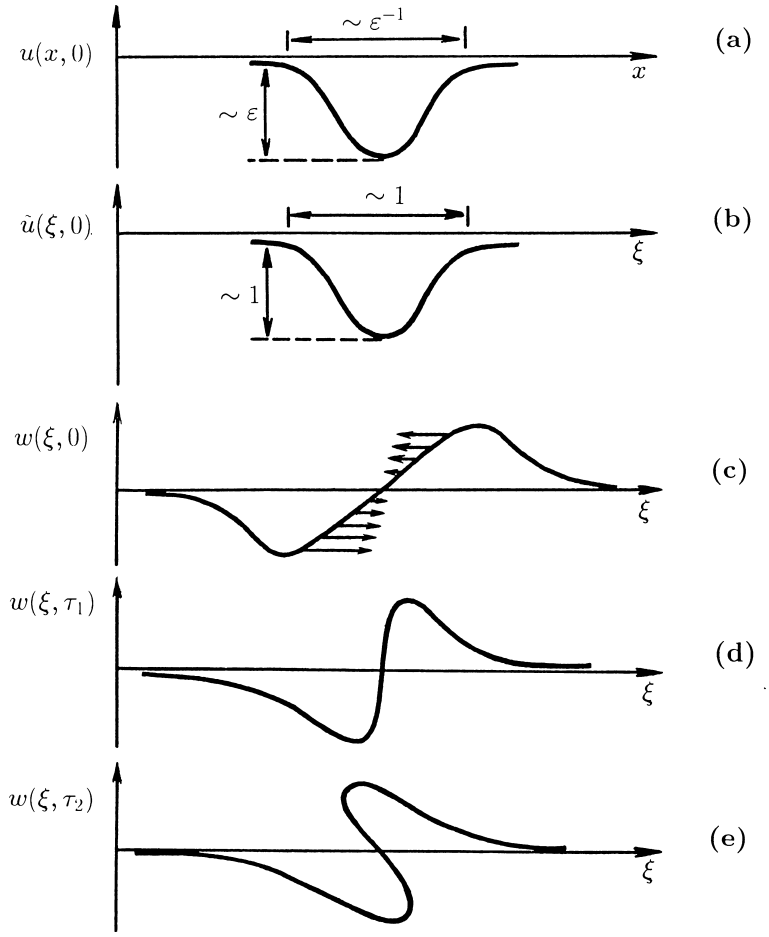

Figure 6.2: Evolution of the localized region of compression ($\tau_2 > \tau_1 > 0$) (from [164]).

Thus, now the phase velocity $v_{\rm ph}$ of the waves depends on the wave momentum,

$$v_{\rm ph} = \frac{\omega(k)}{k} = \pm\sqrt{1-k^2}. \tag{6.26}$$

Consequently, a lower is the wave length, the lower is its velocity. Therefore, if at the initial time moment we have created a localized wave packet constructing of the harmonics (6.23) with different k, then the packet will spread (delocalize) during its evolution. Namely due to this fact the dispersed linear systems are inappropriate for transmission of information.

Now let us investigate a role of the last term in Eq. (6.21) which is connected with the chain's nonlinearity. For this, let us neglect for a moment by the dispersion, and consider the equation

$$u_{tt} - u_{xx} + u_x u_{xx} = 0\,. \tag{6.27}$$

For the sake of simplicity, let us consider the waves propagating in one direction only, for instance, from the left-hand to the right-hand side. In this case it is convenient to turn to the moving reference frame, the center of which moves with the sound speed $s = 1$, i.e. to change from the coordinate x to the new coordinate $\xi \propto x - st$.

Let us suppose that at the initial time moment we had a wave packet with a small amplitude of the order ε ($\varepsilon \ll 1$), which was localized in a wide region of extension $\sim \varepsilon^{-1}$ as is shown in Fig. 6.2a. To describe the evolution of the packet, it is convenient to turn to the so-called Gardner variables introduced according to the following relations,

$$x \to \xi = \varepsilon\,(x - t)\,, \tag{6.28}$$

$$t \to \tau = \frac{1}{2}\,\varepsilon^3 t\,, \tag{6.29}$$

$$u \to \tilde{u} = \frac{1}{\varepsilon}\,u\,. \tag{6.30}$$

In these new variables the packet will be localized in a region of extension ~ 1, and it will have an amplitude ~ 1 (see Fig. 6.2b). Then, according to standard differential rules, we have

$$\frac{\partial}{\partial x}\cdots = \frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi}\cdots + \frac{\partial \tau}{\partial x}\frac{\partial}{\partial \tau}\cdots, \tag{6.31}$$

$$\frac{\partial}{\partial t}\cdots = \frac{\partial \xi}{\partial t}\frac{\partial}{\partial \xi}\cdots + \frac{\partial \tau}{\partial t}\frac{\partial}{\partial \tau}\cdots, \tag{6.32}$$

and from Eqs. (6.28) and (6.29) it follows that

$$\frac{\partial \xi}{\partial x} = \varepsilon\,,\ \ \frac{\partial \tau}{\partial x} = 0\,,\ \ \frac{\partial \xi}{\partial t} = -\varepsilon\,,\ \ \frac{\partial \tau}{\partial t} = \frac{1}{2}\varepsilon^3. \tag{6.33}$$

Substituting Eqs. (6.28–6.33) into Eq. (6.27) and keeping the terms up to $\sim \varepsilon^5$ inclusively, we get the equation

$$\tilde{u}_{\xi\tau} - \tilde{u}_\xi \tilde{u}_{\xi\xi} = 0\,. \tag{6.34}$$

Introducing the variable

$$w = \tilde{u}_\xi\,, \tag{6.35}$$

which describes the chain's deformation in the moving frame, we finally obtain the following equation for the variable w:

$$w_\tau - w w_\xi = 0\,. \tag{6.36}$$

Emphasize ones more that Eq. (6.36) approximately describes the evolution of the wave packet of small amplitude which translates in one spacial direction only. The procedure of turning from the original equation (6.27) to the approximate equation (6.36) is called the method of coordinate extension, or the many–scale method. This method is described in more detail in, e.g., the book [163], where, in particular, it is explained why we have to introduce the coefficient ε^3 in Eq. (6.29).

Using the direct substitution, we may check that in an implicit form the solution of Eq. (6.36) is given by the expression

$$w(\xi, \tau) = f(\xi + w\tau)\,, \tag{6.37}$$

where $f(z)$ is an arbitrary function. For example, if $f(z) = az$, so that at the initial time moment the deformation w had a linear section,

$$w(\xi, 0) = a\xi\,, \tag{6.38}$$

then during the evolution the slope of this section will increase,

$$w(\xi, \tau) = a\xi/(1 - a\tau)\,. \tag{6.39}$$

For a qualitative analysis of evolution of a perturbation with an arbitrary shape, let us suppose that the variables ξ and τ depend on some parameter α, so that $\xi = \xi(\alpha)$ and $\tau = \tau(\alpha)$. Then we may write

$$\frac{dw}{d\alpha} = \frac{\partial w}{\partial \xi}\frac{d\xi}{d\alpha} + \frac{\partial w}{\partial \tau}\frac{d\tau}{d\alpha}\,. \tag{6.40}$$

Let us follow now for evolution of points of a constant profile. For this, we have to find a solution of the equation

$$w(\tilde{\xi}, \tilde{\tau}) = \mathrm{Const}\,. \tag{6.41}$$

Substituting Eq. (6.41) into Eq. (6.40) and using Eq. (6.36), we get

$$\frac{d\tilde{\xi}}{d\tilde{\tau}} = \frac{\xi_\alpha}{\tau_\alpha} = -\frac{w_\tau}{w_\xi} = -w\,. \tag{6.42}$$

Consequently, evolution of a nonlinear wave is reduced to that the points on the graph of the solution moves horizontally with a speed equal to the value of the deformation taken with the opposite sign. In a result, the profile of translating wave is modified as time increases. For example, if at the initial instant a localized region of compression existed in the chain as shown in Fig. 6.2a, then during the evolution this region is being narrowed (Fig. 6.2d) and, after some time, the front of the wave will be overturned (Fig. 6.2e) [164]. At the same time, the linear section at the center of the wave will behave in accordance with Eq. (6.39).

Note that if the parameter of the interaction's nonlinearity has the another sign, i.e. if $v'''(0) > 0$, then in Eqs. (6.21), (6.27), (6.34) and (6.36) we have to change the sign in the front of the nonlinear term. In this case the theory predicts the analogous behavior for a localized region of the chain's extension.

Now we may predict the behavior of a solution of Boussinesq's equation (6.21). Namely, the dispersion term leads to smoothing of a wave packet which was localized at the beginning, while the nonlinear term, on the contrary, leads to the narrowing of the region of chain's compression and to increasing (sharping) of the wave front. Thus, we expect that during the evolution of the localized compressed region, a balance between these two processes would be achieved, and in a result some localized pulse with a permanent shape will translate. Computer modeling of Zabusky and Kruskal [162] confirmed this prediction and also showed that although the wave may become very sharp, it will never be overturned if the dispersion term is taken into account.

6.2.3 Waves of stationary shape

If we apply the method of coordinate extension to the full Boussinesq equation (6.21), then instead of Eq. (6.36) we obtain the equation

$$w_\tau \mp 6ww_\xi + w_{\xi\xi\xi} = 0\,. \tag{6.43}$$

Equation (6.43) is called the *Korteweg-de Vries* (KdV) *equation* [165]. The sign "minus" ("plus") in the front of the nonlinear term emerges at the description of waves of compression (expansion) in the case of $v'''(0) < 0$ $(v'''(0) > 0)$, when the deformations $w(\xi, \tau)$ as a function of ξ at a fixed time τ has a shape with one or several hollows (humps). The numerical factor 6 before the nonlinear term is introduced for convenience, and it may be changed by scaling the variable w.

Equation (6.43) is the equation with partial derivatives. Let us try to find one of its particular solutions, namely the solution which may be presented in the form

$$w(\xi, \tau) = \Phi(z)\,, \quad z = \xi - c\tau\,. \tag{6.44}$$

The solutions of the type (6.44) is called the *wave of stationary shape* (WSS), and it describes a wave which propagates without changing its shape. Note that the speed c in Eq. (6.44) corresponds to the WSS's speed in moving reference frame, so that in the rest frame the WSS's speed is equal to $(s+c)$, where s is the sound velocity in the chain (for our system of units $s = 1$).

Substituting Eq. (6.44) into Eq. (6.43), we obtain an ordinary differential equation (further for the sake of definiteness we will consider only the upper sign in Eq. (6.43)):

$$-c\Phi' - 6\Phi\Phi' + \Phi''' = 0\,, \tag{6.45}$$

which may be rewritten in the form

$$(-c\Phi - 3\Phi^2 + \Phi'')' = 0\,. \tag{6.46}$$

Integration of Eq. (6.46) yields

$$\Phi'' = c\Phi + 3\Phi^2 + C_1\,. \tag{6.47}$$

Multiplying Eq. (6.47) by Φ' and then integrating it, we get

$$\frac{1}{2}\Phi'^2 = \frac{1}{2}c\Phi^2 + \Phi^3 + C_1\Phi + C_2\,. \tag{6.48}$$

Equation (6.48) may be rewritten in the form

$$\Phi'(z) \equiv \frac{d\Phi}{dz} = \pm\sqrt{c\Phi^2 + 2(\Phi^3 + C_1\Phi + C_2)}\,, \tag{6.49}$$

and after that it may be integrated ones more:

$$z = z_0 \pm \int d\Phi \Big/ \sqrt{c\Phi^2 + 2(\Phi^3 + C_1\Phi + C_2)}\,. \tag{6.50}$$

Here C_1, C_2 and z_0 are the integration constants. The integral in Eq. (6.50) is the *elliptic integral*. Equation (6.50) presents the WSS solution in an implicit form. In order to get the explicit solution, we have to find the corresponding inverse function (such functions are called the elliptic functions too).

Now let us choose the integration constants in such a way that Eq. (6.44) would describe the spatially localized wave packet. For this, let us impose additionally the following boundary conditions,

$$\Phi(z),\ \Phi'(z) \to 0 \ \text{ at } \ z \to \pm\infty\,, \tag{6.51}$$

that leads to the values $C_1 = C_2 = 0$ (the constant z_0 called the phase of the WSS, may be easily removed by an appropriate choice of the beginning of coordinates). Then the function (6.44), (6.51) will describe the so-called *solitary* WSS (SWSS). In this case the integral (6.50) may be expressed through elementary functions, and the solution has the form

$$\Phi(z) = -w_0\,\mathrm{sech}^2\left(z\sqrt{w_0/2}\right), \tag{6.52}$$

where w_0 is the amplitude of the SWSS which is coupled with its speed c by the relationship

$$c = 2w_0\,. \tag{6.53}$$

Emphasize that $c > 0$, i.e., the SWSS of the KdV equation propagates with the faster-than-sound speed, and a higher is the amplitude of a single translating pulse, the higher is its speed.

Note that the original Boussinesq equation (6.21) has a solution of a SWSS form too:

$$u(x,t) = -6\sqrt{c^2-1}\left\{1 + \tanh\left[\frac{1}{2}\sqrt{c^2-1}\,(x-ct)\right]\right\}. \tag{6.54}$$

The displacement field for the SWSS of the Boussinesq equation is shown in Fig. 6.3a, and the deformation which follows the SWSS, in Fig. 6.3b. The deformation within the SWSS is described by the expression

$$w(x,t) \equiv \frac{\partial u(x,t)}{\partial x} = -3(c^2-1)\,\mathrm{sech}^2\left[\frac{1}{2}\sqrt{c^2-1}\,(x-ct)\right]. \tag{6.55}$$

As seen, the deformation is bell–shaped with a width $\sim (c^2-1)^{-1/2}$ and an amplitude $\sim (c^2-1)$ similarly to the SWSS (6.52) of the KdV equation. As for the field of displacements itself, it undergoes a jump $\Delta u(t) \equiv u(+\infty,t) - u(-\infty,t) = -12\sqrt{c^2-1}$. Contrary to the SWSS of the KdV equation, the SWSS (6.54) may propagate from the left-hand to the right-hand side ($1 < c < \infty$) as well as in the opposite direction ($-\infty < c < -1$).

Finally, for the FPU chain of atoms with the quadric anharmonicity (6.2), the method described above leads to the so-called *modified Korteweg-de Vries equation*,

$$w_\tau + 6w^2 w_\xi + w_{\xi\xi\xi} = 0\,, \tag{6.56}$$

which has the SWSS-type solution too:

$$w(\xi,\tau) = \pm\sqrt{c}\,\mathrm{sech}\left[\sqrt{c}\,(\xi - c\tau)\right],\ \ c > 0\,. \tag{6.57}$$

Emphasize that the modified Korteweg-de Vries equation allows both types of the SWSS's, the compression waves as well as the expansion ones.

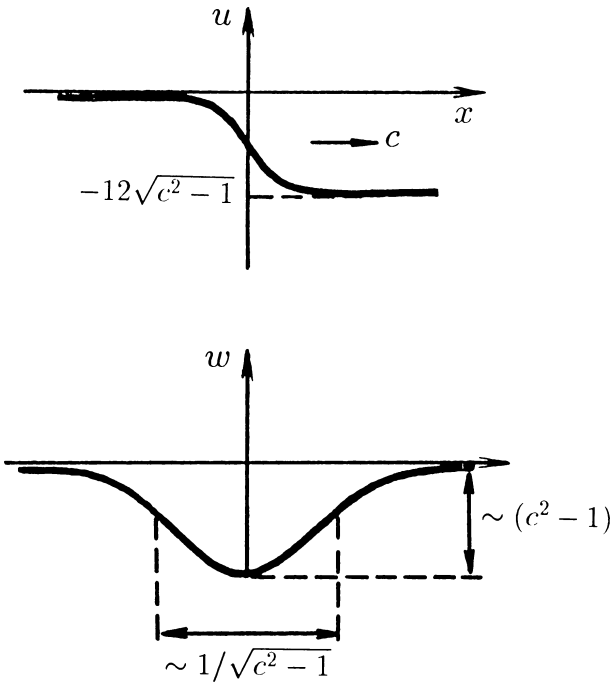

Figure 6.3: (a) Displacements $u(x,t)$ and (b) deformations $w(x,t) \equiv \partial u(x,t)/\partial x$ of the wave of stationary shape at a fixed time moment t for Boussinesq's equation (6.21) (c is the wave velocity) (from [164]).

6.2.4 Atomic chain in an external periodic potential

Let us consider now another characteristic example — a chain of interacting atoms, where each of the atoms is subjected to some external potential $v_{\rm sub}(x)$. Let for the sake of simplicity the interaction between the atoms is harmonic,

$$v(\Delta x) = \frac{1}{2}\, g\,(\Delta x - a_0)^2, \;\; \Delta x = x_{n+1} - x_n\,, \tag{6.58}$$

and let the external potential depends only on the displacement $u_n = x_n - x_n^{(0)}$ of a given atom with respect to its equilibrium position $x_n^{(0)} = na_0$ in a free chain. Assuming also that $v'_{\rm sub}\left(x_n^{(0)}\right) = 0$, let us write the potential $v_{\rm sub}(x)$ in the form

$$v_{\rm sub}(x_n) = \omega_0^2\, v_s(u_n)\,, \tag{6.59}$$

where the function $v_s(u)$ is normalized in such a way that $v_s''(0) = 1$, so that ω_0 corresponds to the frequency of vibrations of an isolated atom in the external potential. Then the motion equations take the form ($m_a = 1$):

$$\ddot{u}_n = g\,(u_{n+1} + u_{n-1} - 2u_n) - \omega_0^2\, v_s'(u_n)\,. \tag{6.60}$$

When all displacements are small, $|u_n| \ll a_0$, Eq. (6.60) may be linearized, $v'(u_n) \approx u_n$. In this case it has solutions in a form of plane waves, $u_n(t) \propto \exp\left[i\omega(k)t - ikna_0\right]$, with an optical dispersion law,

$$\omega(k) = \sqrt{\omega_0^2 + 2g\,(1 - \cos a_0 k)} \approx \sqrt{\omega_0^2 + s^2k^2}, \tag{6.61}$$

where $s = a_0\sqrt{g}$ is the sound velocity in the free chain.

Otherwise, if only the relative displacements are small, $|u_{n+1} - u_n| \ll a_0$, we may use the continuum approximation described above, $u_n(t) \to u(x,t)$. Substituting Eqs. (6.8–6.10) into Eq. (6.60), in this case we obtain the equation

$$u_{tt} - s_0^2\, u_{xx} + \omega_0^2\, v_s'(u) = 0\,. \tag{6.62}$$

In the linear case, when $v_s'(u) = u$, Eq. (6.62) is reduced to the so-called *Klein-Gordon equation*.

Analogously to the method used above, let us try to find one of particular solutions of Eq. (6.62), namely the solution of the WSS form,

$$u(x,t) = \Phi(z)\,, \quad z = x - ct\,. \tag{6.63}$$

In the present case, substituting Eq. (6.63) into Eq. (6.62) and then making the simple transformations,

$$\gamma^2\Phi'' = g\,v_s'(\Phi)\,, \tag{6.64}$$

$$\frac{1}{2}\gamma^2\Phi'^2 = g\,[v_s'(\Phi) + C_1]\,, \tag{6.65}$$

$$\Phi' \equiv \frac{d\Phi}{dz} = \pm\frac{1}{\gamma d}\sqrt{2[v_s'(\Phi) + C_1]}\,, \tag{6.66}$$

where

$$\gamma = \sqrt{1 - c^2/s^2} \tag{6.67}$$

and

$$d = s/\omega_0\,, \tag{6.68}$$

leads to the implicit solution in the form of the integral

$$z = z_0 \pm \gamma d \int d\Phi/\sqrt{2[v_s'(\Phi) + C_1]}\,. \tag{6.69}$$

Further, let us assume that the potential $v_{\rm sub}(x)$ has at least two equivalent absolute minima. Then the ground state of the system will be doubly degenerated, because two ground states will be possible: the state GS_1, where all atoms are situated in one minimum, and the state GS_2, where the atoms occupy the another minimum. Impose now on the function (6.63) the following boundary conditions: let the left-hand section of the chain (at $z \to -\infty$) is in the GS_1, while the right-hand section (at $z \to +\infty$), in the GS_2 (to satisfy these conditions, we have to choose the integration constants and the integration limits in Eq. (6.69) in an appropriate way). In a result, we obtain a solitary WSS called the *kink*. Contrary to the SWSS of the KdV equation, the kink is topologically stable, so that it can exist in an immobile state too.

The following three variants of choice of the external potential are used most often:

(a) the model with the piecewise parabolic potential

$$v_s(u) = \frac{1}{2}\,(|u| - 1)^2\,; \tag{6.70}$$

in this case the kink has the following shape:

$$\Phi(z) = \pm\,[1 - \exp\,(-|z|/\gamma d)]\,\operatorname{sign} z\,; \tag{6.71}$$

(b) the ϕ^4-model, where

$$v_s(u) = \frac{1}{4}\,(u^2 - 1)^2, \tag{6.72}$$

$$\Phi(z) = \pm\tanh\,(z/\gamma d\sqrt{2})\,; \tag{6.73}$$

(c) the *sine-Gordon* (SG) *model*, where

$$v_s(u) = 1 - \cos u\,, \tag{6.74}$$

$$\Phi(z) = 4\tan^{-1}\,\exp\,(\pm z/\gamma d) + 2\pi n\,, \tag{6.75}$$

n being an integer. The signs + or − in Eqs. (6.71), (6.73) and (6.75) describe the kink (which links GS_1 with GS_2) or the antikink (that links GS_2 with GS_1) correspondingly.

As one can see, in all cases the kink is localized within the region of extension of the order d (d is called the kink width), and the kink can move with the subsonic velocity only, $|c| < s$. When the kink moves, its width is equal to γd, i.e. the faster is the kink, the more narrow is it (the "relativistic" narrowing).

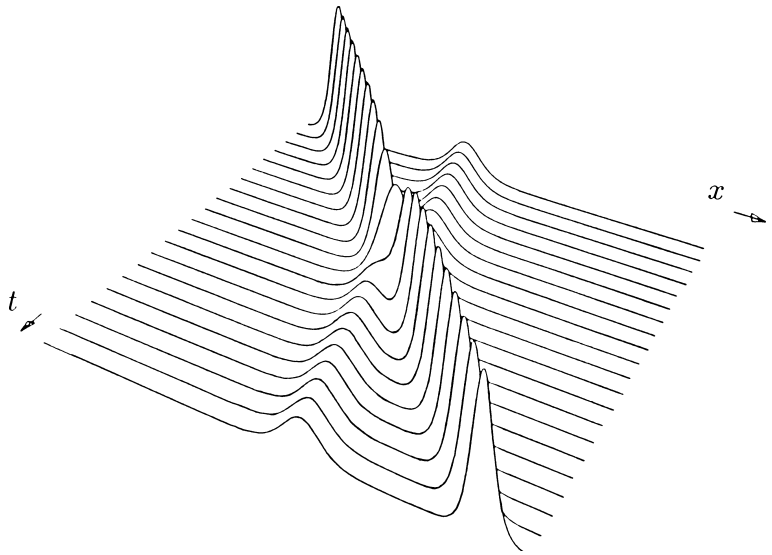

Figure 6.4: Collision of two waves of the stationary shape for the Korteveg-de-Vris equation (from [163]).

6.2.5 Solitonic solutions

Thus, some partial differential equations admit particular solutions of the SWSS form. Such a solution describes the spatially localized perturbation which propagates through the system without changing the shape. But this solution describes an isolated SWSS, i.e. it corresponds to the case when there are no other perturbations in the system except the SWSS. From the physical viewpoint, however, the question about a behavior of the SWSS in a general case, i.e. when other perturbations are present in the system, appears.

A stability of the SWSS with respect to small perturbations may be clarified with the help of the standard perturbation technique. For this, we have to substitute the expression

$$u(x,t) = \Phi(x - ct) + \delta u(x,t) \tag{6.76}$$

into the original equation with partial derivatives, and then to linearize the obtained equation in small perturbation $\delta u(x,t)$. In a result we get the linear equation for the function $\delta u(x,t)$, which has the same form as the Schrödinger equation for a fictitious particle moving in the potential determined by the function $\Phi(x)$. The SWSS stability is then determined by the eigenvalues λ_k of this Schrödinger equation: if even one of the eigenvalues is negative, then the given SWSS is unstable. For the examples described above, it occurs that $\lambda_k \geq 0$, and it exists only a single zero eigenvalue which corresponds to the so-called *Goldstone mode* which describes the possibility of a spacial displacement of the SWSS as a whole for an arbitrary distance.

It is very important, however, to investigate the stability of the SWSS not only with respect to small perturbations, but also for a more general case, for example, to check the SWSS stability when it collides with a large-amplitude wave packet or with another SWSS. The simplest and the most reliable method of solution of this problem is to use computer simulation. For this, we have to take an appropriate initial state, and then to investigate its evolution with the help of the MD method. Characteristic examples of such experiments are presented in Figs. 6.4 to 6.6. Each wave profile in these figures describes the graph of the function $u(x,t)$ on x for some fixed time t. As a whole, the figures correspond to the superpositions of a number of such profiles for the increasing sequence of times separated by equal intervals.

Figure 6.4 demonstrates the collision of two SWSSs of the KdV equation, when one SWSS overtakes the another SWSS, the latter having the smaller amplitude (and, therefore, the smaller speed), and passes throughout it. Figure 6.5a shows the collision of two SWSSs of the SG equation with different polarities (the kink-antikink collision), while Fig. 6.5b, the collision of two kinks of the same polarity. As seen, in all these cases the solitary waves of stationary shape come out from the collision region, completely preserving

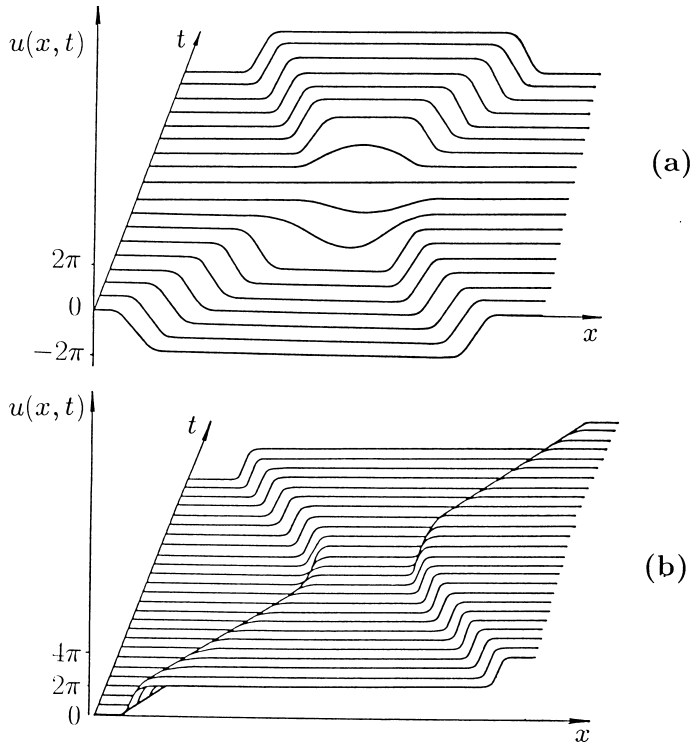

Figure 6.5: Collision of kinks for the sine-Gordon equation: (a) kink-antikink collision, (b) collision of two kinks of the same polarity (from [164]).

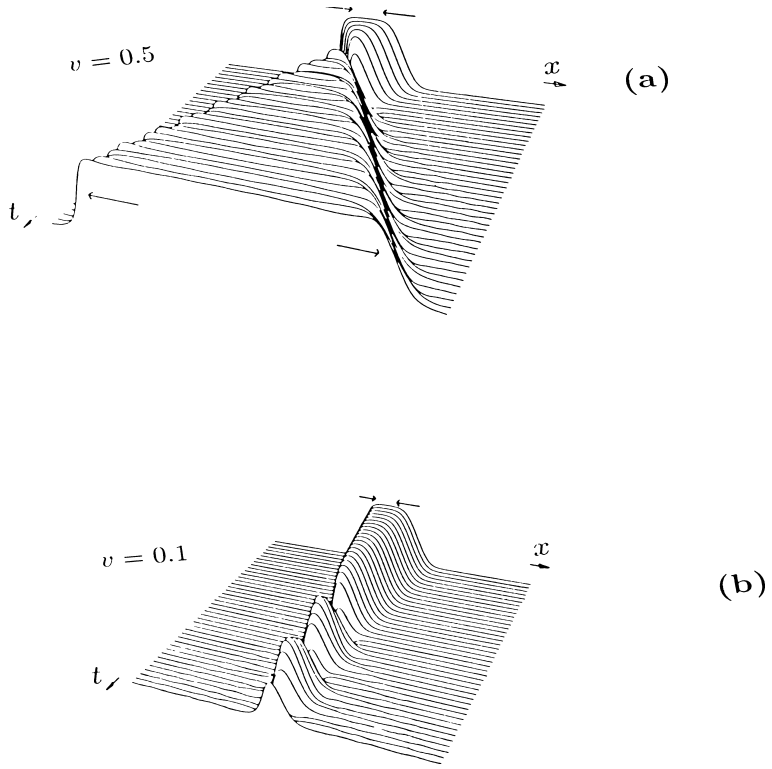

Figure 6.6: Collision of kinks for the ϕ^4-model: (a) collision of fast kinks, and (b) slow kinks' collision (v is the difference of kinks' velocities) (from [163]).

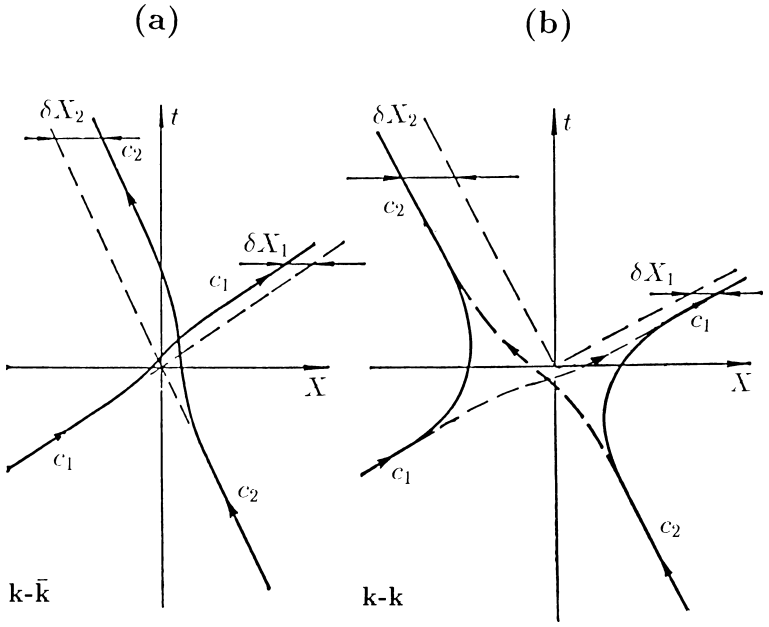

Figure 6.7: The kink center coordinates versus time for (a) the kink-antikink collision, and (b) the kink-kink collision in the SG model (schematically) (from [164]).

their identity (i.e. the shapes, speeds, *etc.*), so that these SWSSs behave like real particles. Zabusky and Kruskal [162] have named such SWSSs by *solitons*. Each soliton may be assigned with some energy, speed, effective mass (and also with the topological charge $\sigma = \pm 1$ in order to distinguish the kink from the antikink in the case of the SG model), which remain unchanged at the collisions. At the same time, the soliton trajectories on the (x,t)-plane before and after the collision do not coincide. This fact indicates that the solitons during the collision undergo a phase shift, i.e. the soliton centers occur to be slightly shifted from their positions for the case when the interaction of solitons would be completely absent. For example, Fig. 6.7b describes the coordinates of centers of two colliding SG kinks of the same polarity. This process may be interpreted as the "elastic" collision of two quasiparticles which repel each other and exchange by their momenta during the collision. The another process, the collision of the kink and the antikink of the SG model shown in Fig. 6.7a, may be interpreted as the "elastic" interaction of two quasiparticles which effectively attract each other. During the collision, they "accelerate" and "pass through" one another "shifting" in the direction to each other. Note that we may think that during the collision the solitons pass through each other, as well as we may think that the solitons exchange by their identities; both the interpretations are true. The only important fact is that in all the cases the solitons completely preserve their characteristics.

However, the collision scenario described above, is observed not for all SWSSs. For example, Fig. 6.6 shows the kink-antikink collision for the ϕ^4-model. When the relative velocity of the colliding kinks is high, the kinks pass through each other analogously to the SG model (Fig. 6.6a). But, opposite to the SG model, now the collision is "inelastic", a part of the kink kinetic energy is converted into the radiation, so that after the collision it appears a "ripple" (oscillating tails) behind the kinks. On the other hand, when two slow kinks collide (Fig. 6.6b), they annihilate during the collision, i.e. they lose such amount of the kinetic energy that they cannot go away for an infinite distance, and they create a coupled oscillating state (the so-called *breather*) which continues to radiate waves (phonons) and finally disappears. Therefore, the behavior of the SWSSs of the ϕ^4-model is not completely the same as those of the SG solitons, although they remind each other in many features.

6.3 Exactly integrable systems

Computer simulation shows a surprising stability of SWSSs for some nonlinear systems. This fact has been served as a prompt that these systems may be completely integrable, i.e. that their solution may be found in an analytical form. Indeed, soon it has been found by Gardner *et al.* [166] and Zahkarov and Shabat [167] that under very weak restrictions (namely, in a class of functions which approach sufficiently fast to a finite limit as $|x| \to \infty$), a general solution of some nonlinear equations may be found with the help of the *inverse scattering transform* method which is the canonical transformation to generalized variables of the action–angle type. These variables correspond to possible types of elementary excitations of the system ("nonlinear normal modes"), namely phonons and solitons, which have an infinite lifetime, and preserve their identity in collisions with other excitations. A solution of the problem with an arbitrary initial condition may be presented with the help of the extended Fourier transform as a "set" of phonons and solitons, the interaction of which is asymptotically reduced to simple additive phase shifts. Because the systems described by partial differential equations are the systems with an infinite degrees of freedom, they must have the infinite set of conservation laws (integrals of motion) in order to be completely integrable. At the same time, contributions of different nonlinear normal modes into the Hamiltonian (as well as into other integrals of motion) are completely separated.

The number of exactly integrable nonlinear equations is relatively small. Among the examples described above, the KdV equation (as well as the modified KdV equation) and the SG equation are the exactly integrable ones. Besides, the exactly integrable *nonlinear Schrödinger* (NLS) *equation* found a wide application in physics too. It is very surprising that problems from various branches of physics such as hydrodynamics, plasma physics, nonlinear optics, low temperature physics, solid state physics, surface physics, elementary particles physics, astrophysics, biophysics, *etc.* are very often reduced to one among namely these three equations.

Below we briefly describe the area of application of the KdV, NLS and SG equations. The detailed description of methods of solution of these equations may be found, e.g., in the books [163, 168, 169].

6.3.1 Korteweg-de Vries equation

The soliton of the KdV equation (6.43) is given by the expression (6.52). The shape of the KdV soliton is described by a single parameter only, by its speed c. The soliton amplitude is proportional to c, and the spacial localization, to $1/\sqrt{c}$, so that the faster is the KdV soliton, the "higher" and "narrower" it is. The KdV soliton is the dynamical one, i.e. it can exist with a faster-than-sound velocity c only; it delocalizes and disappears as c approaches to the sound velocity $s = 1$.

The structure of solutions of the modified KdV equation (6.56) is more rich. First, it has solutions of the type of one–parameter solitons (6.57) which are similar to the KdV solitons. Contrary to the latter, however, the modified KdV solitons may have two different signs describing a local compression or extension of the system. Besides, the modified KdV equation admits solutions of the form of two–parameter solitons, the so-called *breathers*. The latter has the following shape [164],

$$w(\xi,\tau) = 2\frac{\partial}{\partial\xi}\tan^{-1}\left\{\frac{\kappa}{k}\frac{\sin(k\xi-\omega\tau)}{\cos[\kappa(\xi-c\tau)]}\right\}, \tag{6.77}$$

where

$$\kappa = \sqrt{(k^3-\omega)/3k} \tag{6.78}$$

and

$$c = 3k^2 - \kappa^2. \tag{6.79}$$

The solution (6.77) corresponds to the localized (in the region $\sim \kappa^{-1}$) perturbation with the amplitude $\sim \kappa$ moving with the speed c. If we turn to the frame moving with the speed c,

$$\tilde{\xi} = \xi - c\tau\,, \tag{6.80}$$

and put

$$k\xi - \omega\tau = k\tilde{\xi} - \Omega\tau\,,\ \ \Omega = \omega - kc\,, \tag{6.81}$$

then one can see that the breather oscillates with the frequency Ω. In the limit $\kappa \to 0$ the solution (6.77) is transformed into weakly localized small–amplitude linear waves, while in the limit $\Omega \ll 1$ the breather (6.77) may be interpreted as a coupled state of two one–parameter solitons (6.57) with opposite signs which oscillate with respect to the common center of mass with the frequency Ω and the amplitude $\sim -\ln|\Omega|$ in the moving frame.

The KdV equation has been deduced by Korteweg and de Vries [165] in order to describe long surface waves on shallow water without friction effects. However, from the deduction of the KdV equation given above, one can see that the KdV equation (or its modifications) will always emerge in description of propagation of a small (but finite) amplitude plane wave in a homogeneous medium with dispersion and nonlinearity. The variable w describes in this case the deviation of some physical quantity such as height, velocity, density, *etc.* from the corresponding equilibrium value. This class of problems include the ion–acoustic and hydro–magnetic waves in plasma [170], the Rossbi waves in homogeneous rotated liquid [163], *etc.*

6.3.2 Nonlinear Schrödinger equation

The nonlinear Schrödinger (NLS) equation

$$i\psi_t + \psi_{xx} - \omega_0\psi + g|\psi|^2\psi = 0 \tag{6.82}$$

is the exactly integrable equation too. This equation is called in such a way because its form coincides with the quantum Schrödinger equation for the potential $\omega_0 - g|\psi|^2$, so that the constant $g \quad (g > 0)$ may be interpreted as the "intensity of attraction".

In Eq. (6.82) the function $\psi(x,t)$ takes complex values. If we represent it in the following form [164],

$$\psi(x,t) = \Phi(x,t)\ \exp\left[i\varphi(x,t)\right], \tag{6.83}$$

where $\Phi(x,t)$ and $\varphi(x,t)$ are real functions ($\Phi(x,t) > 0$), then the NLS equation is reduced to the set of two real equations,

$$\begin{cases} \Phi_{xx} - (\omega_0 + \varphi_t + \varphi_x^2 - g\Phi^2)\,\Phi = 0\,, \\ (\Phi^2)_t + 2\,(\Phi^2\varphi_x)_x = 0\,. \end{cases} \tag{6.84}$$

The second equation of the set (6.84) may be interpreted as the local conservation law for the quantity

$$N = \int \Phi^2\,dx \equiv \int |\psi|^2\,dx\,, \tag{6.85}$$

which has a meaning of the number of particles in non-ideal bose gas described by the self-consistent equation (6.82). In this case $\Phi^2 = |\psi|^2$ is the density of particles, and $J = 2\Phi^2\varphi_x$ is the density of the particles' flux.

The NLS soliton has the following shape,

$$\psi(x,t) = A\,\frac{\exp\left(ikx - i\omega t\right)}{\cosh\left[\kappa(x - ct)\right]}\,, \tag{6.86}$$

where the soliton amplitude is equal to

$$A = \kappa\sqrt{2/g}\,, \tag{6.87}$$

and the "filling" of the soliton is determined by the parameters

$$k = \frac{1}{2}\,c \tag{6.88}$$

and

$$\omega = \omega_0 + k^2 - \kappa^2. \tag{6.89}$$

The NLS soliton (6.86) is the dynamical two–parameter soliton which describes the localized (in the region $\sim \kappa^{-1}$) perturbation with the amplitude A given by Eq. (6.87), translating with the speed c, and at the same time oscillating with the frequency $\Omega = \omega - \frac{1}{2}\,c^2$. The soliton (6.86) corresponds to the density of the particles' flux $J = c\,|\psi|^2$. In the limit $\kappa \to 0$ the amplitude of the soliton (6.86) decreases and it delocalizes transforming into a linear wave. In the opposite, extremely nonlinear case of $\kappa \to \infty$, the soliton solution transforms into a moving singularity,

$$\psi(x,t) \to \pi\sqrt{2/g}\;\delta(x-ct)\;\exp(-i\Omega t)\,. \tag{6.90}$$

The NLS equation and its modifications play a significant role in the theory of wave propagation in physical systems with dispersion which admit solutions in the form of harmonic wave packets,

$$\psi(x,t) = a(x,t)\;\exp\{i[kx - \omega(x)t]\}\,. \tag{6.91}$$

The change of the amplitude $a(x,t)$ of such spacial–temporal sinusoidal oscillations occurs owing to nonlinear effects, namely due to the reverse action of higher harmonics created by nonlinear terms, on the primary wave.

The well known example of the wave packet (6.91) is, e.g., the amplitude–modulated radio waves which carry out the usual radio communication. Another important area of application, where a carrier wave is modulated by a slowly varying envelope pulse, corresponds to the coherent laser optics. For example, a coherent optical pulse of one nanosecond duration in, say, the region of blue light, has about 10^6 vibrations of the carrier in the envelope pulse. In nonlinear optics there exist methods which allow to obtain the evolution equation for the slowly–varying amplitude and phase of the envelope from the original motion equations. For this, one typically neglects by high-order derivatives for the envelope as well as by higher harmonics of the carrier wave in the original motion equations. These ideas may be applied to a number of areas such as plasma physics, hydrodynamics and optics; the key idea is to find a slowly nonlinear expansion for vibrations of the system under consideration (see detail in [163]).

Above it was noted that dispersive linear systems are not suitable for the transmission of information, because localized pulses in these systems are smoothed. But if we will use a nonlinear system, for example, if we will transmit signals through a fibre with the parameters chosen in such a way that this system will be described by the NLS equation, and instead the pulses we will use the NLS solitons, then we get an ideal system for transmission of information (Hasegawa and Tappert [171], Mollenauer *et al.* [172]).

Also, we should note very interesting applications of the NLS equation for description of biological molecules (the so-called *Davydov solitons*) [173].

6.3.3 Sine-Gordon equation

The sine-Gordon (SG) equation

$$u_{tt} - u_{xx} + \sin u = 0 \tag{6.92}$$

is the exactly integrable equation too. The SG equation admits two types of solitons: one–parameter solitons (kinks) and two–parameter solitons (breathers). The SG kink moving with the velocity c ($|c| < 1$), is described by the expression

$$u(x,t) = 4\tan^{-1}\exp\left[\sigma(x-ct)/\gamma\right], \tag{6.93}$$

where $\sigma = \pm 1$ is the topological charge of the kink, and $\gamma = \sqrt{1-c^2}$ describes the Lorentz narrowing of the moving kink. The SG kink is the topological soliton. The principal difference of topological solitons from dynamical ones consists in the following [164]. The properties of dynamical solitons are determined by the type of dispersion and the sign (and character) of nonlinear terms of the equation, i.e. by local properties of differential equations. On the other hand, the existence of topological solitons is determined only by the

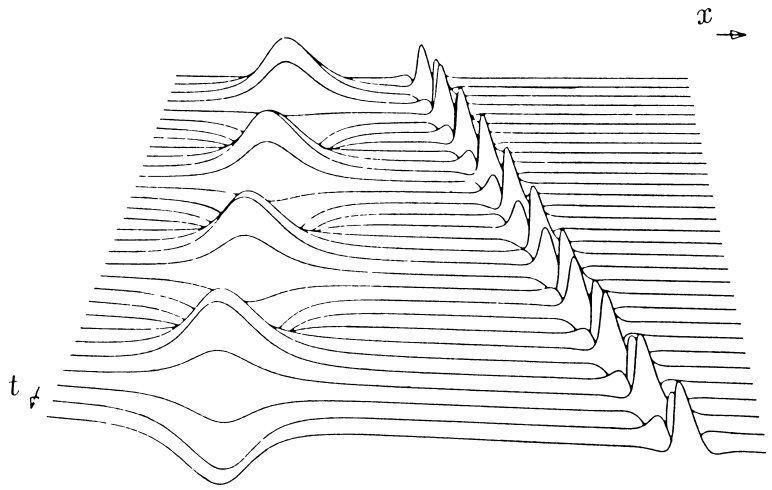

Figure 6.8: Two breathers (immobile and moving ones) for the SG equation (from [163]).

character of the ground state, namely by the existence of the discrete degeneration of the GS, while the type of nonlinearity is not essential. A single topological soliton may be inserted into the system (or be removed from it) only through a free end of the system (which lies at an infinity). In the "bulk" of the system the topological solitons may appear or disappear (annihilate) by kink-antikink pairs only.

The SG breather moving with the velocity c ($|c| < 1$), is described by the expression

$$u(x,t) = 4\tan^{-1}\left\{\frac{\sqrt{1-\nu^2}}{\nu}\ \operatorname{sech}\left[\frac{\sqrt{1-\nu^2}}{\gamma}(x-ct)\right]\sin(\omega t - kx)\right\}, \tag{6.94}$$

where the parameter ν gives the frequency of internal vibrations of the breather,

$$0 < \nu < 1\,, \tag{6.95}$$

while the "filling" of breather is determined by the parameters

$$\omega = \nu/\gamma \tag{6.96}$$

and

$$k = c\omega\,. \tag{6.97}$$

The SG breather is the dynamical soliton which may be considered as a quasiparticle with an internal degree of freedom (see Fig. 6.8). It is similar to the breather of the modified KdV equation or to the NLS soliton. In the case $(1-\nu) \ll 1$ the SG breather is the high–frequency small–amplitude one; in the limit $\nu \to 1$ it may be interpreted as a coupled state of two phonons which attract one another owing to anharmonic effects. In the opposite case of $\nu \ll 1$ the frequency of internal breather's vibrations is small, and it may be considered as a coupled state of kink and antikink vibrating with respect to the common center of mass with the amplitude $\Delta x \sim -\ln|\Omega|$ and the frequency $\Omega = \omega - ck = \gamma\nu$. In the limit $\nu \to 0$ the amplitude of vibrations logarithmically increases, and the breather breaks down into free kink and antikink.

The area of application of the SG equation in physics is large. First of all, the SG equation naturally emerges in systems which may be described with the help of the Frenkel-Kontorova (FK) model [174]. The classical FK model describes a harmonic chain of atoms subjected to the external sinusoidal potential. As has been shown in Sec. 6.2.4, motion equations for such a model reduce to the SG equation. With the help of the FK model we may describe dislocations in solids, and also crowdions (crowdion describes a structure which emerges when an extra atom is inserted into a closely packed atomic row in a metal) [175].

The FK model is widely used in investigation of adsorption systems [87]. In this case the adsorbed atoms play the role of particles, while the external potential is created by the surface atoms of the substrate. One among interesting physical phenomena described by the FK model in adsystems, is the transition from commensurate to incommensurate structure of adatoms.

Starting from the classical work of Frank and van der Merwe [176], the FK model is used to describe the epitaxial crystal growth. Because in a general case the lattice periods of the substrate and the growing crystal do not coincide, their matching at the interface boundary results in a large mismatch energy. To lower this energy, the first layer of the growing crystal adjusts to the substrate, and in order to compensate the difference of the lattice periods, the so-called *misfit dislocations* are created in this layer, and the latter are described by the FK model.

The FK model and its modifications are widely used to describe the proton transport in biological molecules [173].

The next application of the SG equation lies in the description of superionic conductors, where the conductivity is carried out by charge density waves.

The SG model is used also to describe Bloch's walls which separate domains in ferromagnetics (e.g., see [163]).

Interesting effects emerge for ultra–short coherent optical pulses (duration of $10^{-9} \div 10^{-12}$ sec) traversing a quantum two-level system with a large relaxation time. In this case the leading edge of the pulse excites the system atoms, while the trailing edge regenerates the pulse energy owing to stimulated radiation. Dynamics of such a process is described by the SG equation [177].

The SG equation is used also to describe the Josephson junction, i.e. the sandwich consisting of two layers of superconducting metals separated by thin dielectric tunnel barrier. In this case a physical object corresponding to soliton is the quantum of the magnetic flux called *fluxon*. Fluxons are surprisedly stable, they can be kept, be displaced in a given direction, and they can interact with electronic devices. Therefore, in principle the fluxon may be used as a bit in electronic information systems, and the operations with fluxons may be carried out with an extremely high speed and low energy expenses (e.g., see [178]).

Last, note the using of the SG equation in nonlinear field theory [179], where kinks owing to their topological stability claim to a role of fundamental elementary particles.

6.3.4 Toda chain

The exactly integrable KdV, NLS and SG equations describe continuous systems. On the other hand, real physical systems are discrete usually. As a rule, the accounting of discreteness effects destroys the complete integrability of the system. However, there exist two models, which describe a discrete atomic chain and, at the same time, they are exactly integrable (note that there are a number of other discrete exactly integrable systems which, unfortunately, have no direct correspondence to physical objects).

First, the motion equation for an atomic chain where the potential energy of interaction between the atoms is described by the law $\propto x^{-2}$, is exactly integrable [180]. Unfortunately, there are no solitonic solutions in this model.

A more interesting is the second exactly integrable model, the so-called *Toda chain* [181]. In this model only the adjacent atoms interact between themselves, and the interaction is carried out with the help of the exponential law

$$v(x) = \frac{a}{b}\,\exp\left[-b(x-a_0)\right] + a\,(x-a_0)\,. \tag{6.98}$$

The graph of this potential is shown in Fig. 6.9. If we expand $v(x)$ into Taylor series in small $(x-a_0)$, we obtain

$$v_{\rm int}(x) \approx \text{Const} + \frac{1}{2}\,(ab)\,(x-a_0)^2\left[1-\frac{1}{3}\,b\,(x-a_0)\right]. \tag{6.99}$$

Thus, at sufficiently small deviations of the interatomic distances from the equilibrium distance a_0, $|x-a_0| \ll b^{-1}$, the Toda potential is close to the harmonic one with the elastic constant $g = ab$. For higher deviations,

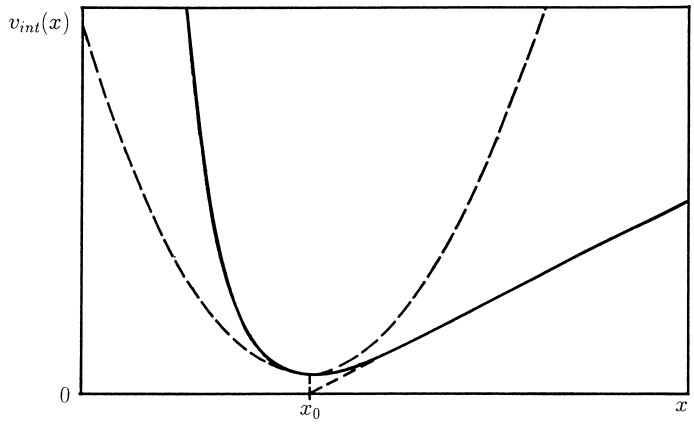

Figure 6.9: The Toda potential.

a measure of nonlinearity of interaction is determined by the parameter b. On the other hand, in the limit $b \to \infty$ the Toda potential reduces to the hard-core potential (3.2) with the core diameter a_0.

Dynamics of the atomic chain is described by the following set of equations ($m_a = 1$),

$$\ddot{u}_n = v'(u_{n+1} - u_n + a_0) - v'(u_n - u_{n-1} + a_0)\,, \tag{6.100}$$

where u_n is the displacement of the n-th atom from the equilibrium position $x_n^{(0)} = na_0$. It is more convenient to write the solution of Eq. (6.100) through the relative displacements

$$w_n \equiv u_{n+1} - u_n\,, \tag{6.101}$$

which are the discrete analog of the deformation $w = \partial u/\partial x$ used above in the long-wave limit.

The Toda soliton has the following shape,

$$w_n(t) = -\frac{1}{b}\,\ln\left\{1 + \sinh^2(\kappa a_0)\,\mathrm{sech}^2[\kappa(na_0 - ct)]\right\}, \tag{6.102}$$

where the parameter κ is coupled with the soliton velocity c by the relationship

$$c = s\,\frac{\sinh(\kappa a_0)}{\kappa a_0}\,, \tag{6.103}$$

and $s = a_0\sqrt{g/m_a}$ is the sound velocity in the chain. From Eq. (6.102) one can see that the Toda soliton is the one–parameter dynamical soliton localized within a region $\sim \kappa^{-1}$ and translating with a faster–than–sound speed. The atomic displacements u_n for the Toda soliton are equal to [164]

$$u_n = \frac{1}{b}\,\ln\left[\frac{1 + \exp\left[2\kappa((n-1)a_0 - ct)\right]}{1 + \exp\left[2\kappa(na_0 - ct)\right]}\right]. \tag{6.104}$$

From this equation it follows that the Toda soliton describes a local compression of the chain which is characterized by a jump of displacements

$$\Delta u \equiv u(+\infty) - u(-\infty) = -2\kappa a_0/b\,. \tag{6.105}$$

The limit $\kappa a_0 \ll 1$ corresponds to small–amplitude Toda solitons; in this case the motion equation (6.100) may be reduced to the KdV equation, and the Toda soliton is reduced to the KdV soliton. In the opposite case of $\kappa a_0 \gg 1$, the region of localization of the Toda soliton is $\kappa^{-1} \ll a_0$, so that at each instant the Toda soliton actually consists of only one atom. Thus, the atoms move in a relay–race fashion, and the compressed bond number consequently changes during the soliton motion.

The Toda solitons are stable not only with respect to collisions with each other and phonons, but also with respect to collisions with impurities. This property yields a possibility to suppose that the Toda solitons play a significant role in thermal conductivity of crystals. Besides, the Toda model may be used to describe long transmission lines constructed of nonlinear capacitors and inductances.

It is interesting to mention the important role of system dimensionality for its integrability. One-dimensional chain of hard balls which corresponds to the limiting case of the Toda model, is the completely integrable system. On the other hand, two-dimensional system of hard balls corresponds to Lorentz-gas model described above in Chapter 2, and this model is characterized by the "maximum chaos" (i.e., there are no islands of stability in this model).

6.4 Systems close to integrable

6.4.1 General remarks

Evidently that behavior of real physical systems may be described by exactly integrable equations approximately only. Often, however, a physical system occurs to be close to the exactly integrable one. In this case it is convenient to describe its behavior in terms of the corresponding exactly integrable system. Namely, it is convenient to present the system state as a superposition of nonlinear normal modes, phonons and solitons. Now, however, these modes are not independent, but they interact between themselves, and the quasiparticles (solitons) themselves are "soft" ("deformable") and may have a finite lifetime. Besides, the nonintegrable systems are characterized by nonzero Kolmogorov-Sinai entropy, so that there always exists some "small" chaos in these systems.

When a deviation of the system from the exactly integrable one is "small", it may be taken into account with the help of one or another variant of the perturbation theory. Unfortunately, to proceed beyond the second-order expansion of the perturbation theory is too difficult usually. Therefore, it remains open the question on a reliability of the results obtained with the help of the perturbation theory. Moreover, in many cases the perturbation can not be considered as a small one, so that the employing the perturbation technique becomes problematic at all. In these cases the computer simulation becomes practically the unique reliable method of investigation.

Methods of computer simulation of systems close to integrable ones, in principle are not different from those described in the previous chapters. If the original physical system is discrete (so that it corresponds to a set of interacting particles), it may be investigated by standard methods of molecular dynamics. When the model under investigation is described by partial differential equations, a natural method of its solution is the converting to difference equations (the description of the corresponding methods as well as the bibliography on this question may be found, for example, in the last chapter of the book [163]). Note that in construction of the model, one has to give a care to the choice of boundary conditions, because they play an essential role in soliton behavior near the system boundary. For example, in the SG model the kink is elastically reflected by the fixed chain's end (and the kink repels from the fixed end). On the other hand, when the chain's end is free, the SG kink is attracted to the end, and during the elastic reflection from the free end, the kink is converted into the antikink. When the periodic boundary conditions are used, the kink will run over the circle, making a whole run for a time $T = Na_0/c$. Therefore, when we want to get rid of the influence of boundary conditions, the most preferable would be the using of damped boundary conditions.

The main questions that emerge in investigation of systems close to integrable ones, are the following.

First, we have to find "nonlinear normal modes", i.e. to find a shape of the SWSS. For this, we have to guess the initial configuration which is the most close to the "true" SWSS for the given system (by taking, for example, the soliton's shape for the most close integrable system and "correcting" it with the help of the perturbation theory), and then we have to follow for the relaxation of the SWSS to the stationary shape. At the same time we are solving the questions about the stability of the SWSS and the character of its motion, i.e. either the motion is freely (without friction) or the SWSS motion is permanently followed by radiation of phonons, which leads to decreasing of the SWSS's speed and its stop or disappearing.

The next important question is about the character of interaction of the given mode with other modes (phonons and other SWSSs). Usually the following scenarios may be observed: **(a)** collisions are quasielastic (i.e., at the collision of quasiparticles a part of their kinetic energy is transferred into phonon radiation), **(b)** collisions lead to creation of new quasiparticles (for example, the creation of a breather at the soliton-antisoliton collision), and **(c)** in the result of the collision the primary quasiparticles are totally destroyed.

A more complex is the question about the evolution of the initial state which corresponds to excitation of a few nonlinear modes (i.e., the search of many-soliton solutions). Finally, the investigation of evolution of some important initial states has a large interest from the practical viewpoint, for example, the decay of the initial rectangular pulse into a set of stable normal modes (SWSSs and phonons). Also a large interest has the study of the SWSS motion in a "thermalized" chain, i.e. the situation when in the initial state there exist, additionally to the SWSS, phonons distributed according to the Maxwell–Boltzmann law.

Let us list now main perturbations which most often occur in modeling of physical objects.

(1) At deduction of Boussinesq's equation and then the KdV equation (see Sec. 6.2) we have used the expansion into Taylor series, and then we have neglected by terms with higher derivatives. Naturally it arises a question of the influence of these neglected terms on the solution of the original problem.

(2) All exactly integrable systems considered in Sec. 6.3 were infinite, while real physical objects are usually finite. Except the something artificial case of using the periodic boundary conditions, the transition from an infinite system to the finite one destroys, as a rule, the exact integrability of the system.

(3) Real physical systems always contain various defects, for example, irregularities of the ideal structure, impurity atoms, *etc.* Naturally it emerges the question of the interaction of phonons and SWSSs with the defects. This problem may be reduced to motion equations with variable coefficients. In some cases (for example, in investigation of disordered systems) the model may be described by nonlinear equations with random coefficients.

(4) A large practical interest has the investigation of systems subjected to some external field. If this field is "weak", it leads to polarization of the soliton, i.e. to small deviation of its shape and, consequently, its parameters too. "Strong" external fields may lead to creation of an instability, for example, to spontaneous creation of new solitons in the system. A more complex is the question of action of variable fields, which may lead either to chaotization of system dynamics, or, on the contrary, to its self–organization.

(5) As a rule, physical systems are not isolated, but they are in contact with some "thermostat". In this case, two questions appear. On the one hand, we have to clarify the influence of dissipation on the soliton dynamics. On the other hand, it emerges a problem about the soliton behavior under the action of a random force. The accounting of both factors leads to equations of the Langevin type, which describe the system behavior at a finite temperature.

(6) Finally, physical systems are discrete usually. Except the Toda chain, the accounting of discreteness effects destroys the exact integrability of the system. Below we consider in more detail one interesting example of such type, namely the Frenkel-Kontorova model which is the discrete analog of the SG model.

6.4.2 The Frenkel-Kontorova model and its generalizations

Recall (see Sec. 6.2.4) that the Frenkel-Kontorova (FK) model describes a linear chain of atoms interacting with the help of the potential $v_{\rm int}(x)$ and subjected to the external periodic potential $v_{\rm sub}(x)$. In the standard FK model it is assumed that only the nearest neighboring atoms interact, and that this interaction is described by the harmonic potential

$$v_{\rm int}(x) = \frac{1}{2}\, g\,(x - a_0)^2, \tag{6.106}$$

and also that the external potential is sinusoidal,

$$v_{\rm sub}(x) = \frac{1}{2}\,\varepsilon_s(1 - \cos 2\pi x/a_s)\,. \tag{6.107}$$

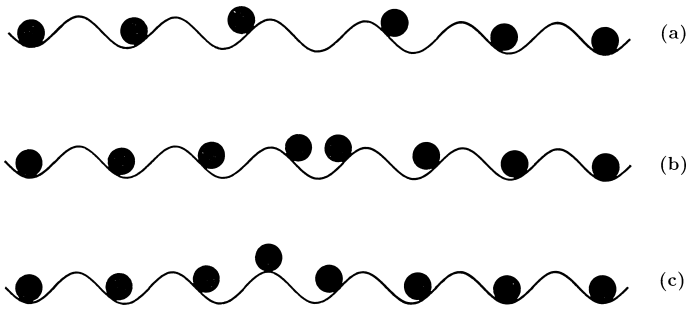

Figure 6.10: Structure of kinks in the Frenkel-Kontorova model: (a) the antikink configuration, (b) the kink at the minimum of the Peierls-Nabarro potential, and (c) the saddle kink configuration.

If, besides, the period of the chain a_0 and that of the external potential a_s are close to one another, $a_0 \approx a_s$ (or $a_0 \approx qa_s$, where q is an integer), then in the case of $ga_0^2 \gg \varepsilon_s$ ("strong" springs) we may use the continuum approximation, where the system motion equations reduce to the SG equation. Recall that nonlinear normal modes of the SG equation correspond to phonons, kinks (topological solitons) and breathers (dynamical solitons).

The main difference of the FK model from the exactly integrable SG model is connected with the discreteness of the former. It occurs, however, that it is still convenient to describe dynamics of the FK model in terms of the SG quasiparticles, i.e. phonons, kinks and breathers. The role of discreteness effects in this case reduces to the following factors.

The structure of phonon modes in the FK model remains practically the same as it was in the SG model, the only difference appears in the dispersion law for large wave vectors k (see Eq. (6.61)).

Kinks in the FK model are topologically stable objects too, and they are characterized by an infinite lifetime. But the kink shape is slightly changed (the FK kink is narrower than the SG kink). Besides, the free motion of the SG kink is changed to the motion of the FK kink in the external periodic potential of the height $\varepsilon_{\rm PN}$ (the so-called Peierls-Nabarro (PN) potential) [182]. Namely, the SG system is characterized by the continuous symmetry group of translations, while the FK model is characterized by the discrete group, i.e. the FK model is invariant under displacement of all atoms only for discrete distances multiple of a_s. In a result the shape and parameters of the isolated FK kink depend on the coordinate of its center. In particular, there exist discrete kink positions where the kink potential energy is minimal (the corresponding kink and antikink configurations are shown in Fig. 6.10a and Fig. 6.10b respectively). To move the kink over the distance a_s to the nearest equivalent state, we have to pass through the "saddle" configuration shown in Fig. 6.10c, overcoming the activation barrier $\varepsilon_{\rm PN}$. In the result, a moving with a velocity c kink will "breathe", i.e. its shape will slightly oscillate with the frequency ω_c ($\omega_c = 2\pi/t_c$, $t_c = a_s/c$) leading to phonon radiation. Evidently that the intensity of this radiation is maximal, when the frequency ω_c or its higher harmonics comes into resonance with phonon frequencies of the chain. Therefore, during the motion of the FK kink in the PN relief, the kink losses its energy for the phonon radiation, and after some time it will be "pinned" at one of minima of the PN relief. Then the kink will vibrate with the frequency ω_{PN} still radiating phonons, and finally it will stop. From the mathematical point of view, the discreteness of the chain removes the Goldstone zero-frequency mode of the SG model.

The collisions of the FK kinks are quasielastic, i.e. phonons are always radiated at the collisions. If the losses of the kinetic energy of the colliding kink and antikink are sufficiently large, then in the collision process they create their coupling state, i.e. breather.

Finally, the dynamical soliton, or breather, in the FK model has a finite lifetime, because it constantly radiates phonons thus losing its energy, and finally it disappears. However, contrary to quasilocal vibrations in the linear chain with impurities, the decay of the breather's amplitude is described by a power law instead of the exponential one.

The applications of the FK model were described above in Sec. 6.3.3. Note, however, that in order to describe real physical objects, the FK model is in need of generalizations. Below we briefly list the important from the physical viewpoint generalizations of the standard FK model (in more detail these questions are considered in, e.g., the review article [183]).

(1) An interesting generalization of the FK model consists in consideration of incommensurate systems, i.e. the case when the ratio a_0/a_s is an irrational number. In this case the investigation of stationary states is of the main interest. The equations describing the stationary states correspond to the Chirikov map, which, together with the logistic map (Sec. 2.3), is the classical model exhibiting the transition from regular to chaotic behavior. Namely, with decreasing of the parameter g (the spring elasticity) at a fixed ratio a_0/a_s the so-called Aubry transition takes place, i.e. the transition from regular trajectories of the Chirikov map to chaotic ones. Simultaneously the nature of the ground state of the FK model changes (the so-called "sliding mode" disappears).

(2) In modeling of real systems, the external periodic potential $v_{\rm sub}(x)$ is usually non-sinusoidal. This leads to changing of kink parameters, in particular, to changing of the shape and amplitude of the PN relief. For example, in some cases the minimum of the kink potential energy is achieved not for the configuration of Fig. 6.10b, but for the configuration shown in Fig. 6.10c or even for a more complicated configuration. For some shape of the function $v_{\rm sub}(x)$ the kink may have one or more the so-called "shape modes", i.e. the shape of the kink may vibrate while its center remains immobile. If the potential $v_{\rm sub}(x)$ has, besides the absolute minima, additional local minima, then the kink is characterized by a complex structure (the kink consists of "sub-kinks"). Finally, if the function $v_{\rm sub}(x)$ has more than one absolute minimum over the period a_s, then the model admits the existence of kinks of different types. In the latter case, a consequence of kinks must satisfy some topological constrains.

(3) Evidently that the interatomic interaction in a real chain may be described by the harmonic law (6.106) approximately only. The main effect which emerges in the FK model with anharmonic interatomic interaction, is the violation of the kink-antikink symmetry, so that now the kink and the antikink are characterized by different parameters.

(4) Various generalizations of the FK model to more than one spacial dimension are very important also. First, we may still consider one-dimensional atomic chain, but to assume that the atoms may move not only along the chain but also in the transverse direction. Second, we may consider two-dimensional (2D) model, which describes two-dimensional array of atoms. In the latter case there exist two modifications of the model. In the *scalar* 2D FK model it is assumed that only a single variable (which describes, for example, the atomic displacements in a single direction only) is coupled with each atom. This model may be interpreted as the system of parallel FK chains which interact between themselves. On the other hand, in the *vector* 2D FK model two variables (which describes, for example, the atomic displacements in both directions) are coupled with each atom. Note that 2D models may differ also by a type of the 2D lattice formed by the minima of the external potential (e.g., square, triangular, *etc.* lattices).

(5) At last, it is interesting to study the effects of finiteness of the system, the role of defects, external fields, contact with a thermostat, *etc.*

Note that the kink describes the system configuration with the inserted extra atom (Fig. 6.10b), while the antikink configuration describes the chain with the extra vacancy (Fig. 6.10a). The amplitude of the PN relief $\varepsilon_{\rm PN}$ is always lower than the amplitude of the original external potential $\varepsilon_{\rm sub}$, so that kinks move along the chain more freely than isolated atoms (i.e., kink's motion is characterized by a lower activation energy). Because kinks transfer mass during their motion along the chain, it is clear that namely the kinks are responsible for diffusivity and conductivity of the system.