Exact Discrete Compact-like Traveling Kinks and Pulses in ϕ^4 Nonlinear Lattices.

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We show that by properly choosing the analytical form of a solitary wave solution of discrete ϕ^4 models we can calculate the parameters of the potential which allows the propagation of compact (kink and pulses) solutions. Our numerical simulations show that narrow kinks and pulses with finite extent can propagate freely, and that discrete breathers with finite but long lifetime, can emerge from their collisions. Moveover, our numerical simulations, reveal that the propagation of two successive pulses at a relative distance of two lattice spacings propagate freely, i.e. without interaction.

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I. INTRODUCTION

In recent years, the dynamics of kinks in hamiltonian (non dissipative or Klein-Gordon) systems [1] has attracted considerable attention. It becomes clear that continuous propagation equations with linear coupling provides an inadequate description of the behavior of weakly coupled lattices where the interplay between nonlinearity spatial discreteness can lead to novel effects not present in the continuum models. For instance, lattices such as ferromagnetic chains [2], hydrogen bonded chains [3], or chains of base pairs in DNA [4], kink solitons or domain walls, whose width is of the order of few lattice spacings, may pin in the lattice owing to discreteness effects. On the other hand, classical equations which describe the behavior of the previously cited systems possesses extended spatial solutions what may be incorrect from a physical point of view.
In order to gain understanding of wave motion in discrete systems, where exact results are scarce even in one dimension both for linear and nonlinear interaction, it is desirable to investigate lattice models with exact solutions. In this direction, Schmidt [5] pointed out that if a double-well on site potential of a ϕ^4 model is suitably chosen, the single kink soliton becomes an exact solution of the discrete model. Recently, [6, 7] the general problem was considered of finding kink or pulse shaped traveling waves solutions separately in the conservative and dissipative case with a linear interaction coupling, giving place to infinite extent solution (tanh-shaped). However, observed patterns in nature whether stationary or traveling are of finite extent. Indeed, it was recently shown by Rosenau and Hyman [12–14], that solitary-wave solutions may be compactify under the influence of nonlinear dispersion which is capable of causing deep qualitative changes in the nature of nonlinear phenomena. Such robust soliton-like solutions, characterized by the absence of an infinite tail or wings and whose width is velocity independent, have been called compactons [14–16]. One might therefore wonder if it is possible to construct a discrete model including nonlinear coupling, allowing the propagation of compact-like wave fronts and pulses.
The purpose of this work is to make some progress in the understanding of the effects of discreteness and nonlinear interactions on the dynamical behavior of one dimensional nonlinear ϕ^4 lattices.
The paper is organized as follow. First, we present our specific lattice model and show analytically that it can admit exact compact-like kink solutions if parameters of the ϕ^4 potential is adequately chosen. Then, in Sec. III, we study numerically the propagation and the collisions of such compact-like kinks and antikinks, in the discrete case and in the continuous limit. In Sect. IV, we show that compact-like pulses may be solutions of our system. In Sect. V, we study their propagation and their. Finally, Sect. VI is devoted to concluding remarks.

II. MODEL AND EQUATION OF MOTION

We consider, a lattice model where a system of atoms with unit mass, are coupled anharmonically to their nearest neighbors and interact with a nonlinear substrate potential $V(u_n)$. The Hamiltonian of the system is given by

$$H = \sum_n \left(\frac{1}{2}\, \dot{u}_n^2 \;+\; \frac{K}{(\alpha+1)}\, (u_{n+1}-u_n)^{\alpha+1} \;+\; V(u_n) \right), \tag{1}$$

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where u_n is the scalar dimensionless displacement of the nth atom. Constants K and α are respectively the stiffness coupling term and the strength interaction law between nearest neighbors atoms. In the specific case $\alpha = 3$ (which will considered in this paper), the corresponding equation of motion of the nth atom is

$$\ddot{u}_n = K \left[(u_{n+1} - u_n)^3 - (u_n - u_{n-1})^3\right] - \frac{dV(u_n)}{du_n}, \quad (2)$$

Let us introduce $u_n = u_0\ \psi_n$, where u_0 is a constant, and setting $\omega_0^2 = K\ u_0^2$, and $\Omega_0^2 = 1/u_0$, equation (2) becomes,

$$\ddot{\psi}_n = \omega_0^2\left[(\psi_{n+1} - \psi_n)^3 - (\psi_n - \psi_{n-1})^3\right] - \Omega_0^2\ F(\psi_n), \quad (3)$$

Finally, dividing the two members of (3) by ω_0^2, and setting $t' = \omega_0\ t$ (dimensionless time), and $\Gamma = \Omega_0^2/\omega_0^2$, we get:

$$\frac{d^2\psi_n}{dt'^2} = \left[(\psi_{n+1} - \psi_n)^3 - (\psi_n - \psi_{n-1})^3\right] - \Gamma\ F(\psi_n). \quad (4)$$

Assuming that, a traveling compact-like kink or compacton solution has the following kink shape:

$$\begin{aligned} \psi_n &= sin(s), && if \quad s \in [-\pi/2, +\pi/2], \\ \psi_n &= -1, && if \quad s \in]-\infty, -\pi/2[, \\ \psi_n &= +1, && if \quad s \in]+\pi/2, +\infty[, \end{aligned} \quad (5)$$

where $s = \omega\ t' - kna$. Here, a is the lattice spacing, and ω and k are two constants such that the ratio ω/k represents the velocity of the font wave. Contrary to the linear coupling models proposed [5–7] for the description of the dynamic behavior of such systems, where the tanh-shaped wave front solution extends asymptotically to infinity, solution (5) has the advantage to taking into account the finite spatial extent of a physical or real wave front.

Now, following an inverse procedure, we first insert (5) in (3), in order to calculate the expression of $F(\psi_n)$. Thus,

$$\frac{d^2\psi_n}{dt'^2} = -\ \omega^2\ \psi_n. \quad (6)$$

$$\begin{aligned} (\psi_{n+1} - \psi_n)^3 = \ & (\sin(s - \xi) - sin(s))^3 \\ & (\sin s \cos\xi + \sin\xi \cos s - \sin s)^3 \end{aligned} \quad (7)$$

$$\begin{aligned} (\psi_n - \psi_{n-1})^3 = \ & (\sin(s) - sin(s + \xi))^3 \\ & (\sin s - \sin s \cos\xi - \sin\xi \cos s)^3, \end{aligned} \quad (8)$$

with $\xi = ka$. Setting $A = -\sin\xi\cos s$ and $B = \sin s(\cos\xi - 1)$, the cubic difference becomes:

$$\Delta = (\psi_{n+1} - \psi_n)^3 - (\psi_n - \psi_{n-1})^3 = 2B(B^2 + 3A^2) \quad (9)$$

That is,

$$\Delta = 2\ (\tau - 1)^2\ \psi_n \left(4\ (\tau + 1/2)\ \psi_n^2 - 3(1 + \tau)\right), \quad (10)$$

with $\tau = cos(\xi)$. Using the previous expressions we deduce that the substrate force is,

$$F(\psi_n) = \frac{1}{\Gamma}\left(\alpha\ \psi_n + \beta\ \psi_n^3\right), \quad (11)$$

with,

$$\begin{aligned} &\alpha = \omega^2 - 6(\tau + 1)(\tau - 1)^2,\ and \\ &\beta = 8(\tau + 1/2)(\tau - 1)^2. \end{aligned} \quad (12)$$

Finally the total equation becomes:

$$\frac{d^2\psi_n}{dt'^2} = \left[(\psi_{n+1} - \psi_n)^3 - (\psi_n - \psi_{n-1})^3\right] - \beta\psi_n(\psi_n^2 + \frac{\alpha}{\beta}). \quad (13)$$

This last equation presents a ϕ^4 substrate potential structure given by (14) with two degenerated minima if the ratio α/β is negative (see fig.1).

$$V(\psi_n) = \beta\ (\frac{\psi_n^4}{4} - \frac{\alpha}{\beta}\ \frac{\psi_n^2}{2}) \quad (14)$$

Since we have assumed that the solution of (13) has the

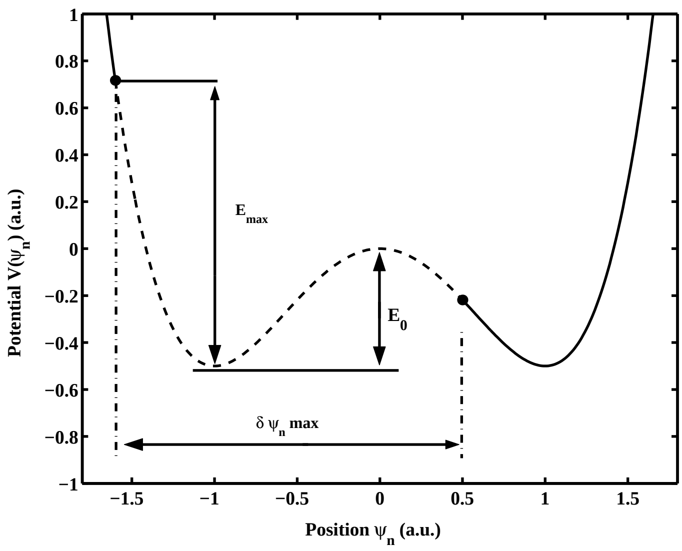

FIG. 1: Symmetric potential $V(\psi_n)$, with its two degenerated minima. The shape is obtained with the parameters $\tau = \cos(\pi/3)$, and $\omega = 0.5$. The dashed line represents the asymmetric oscillations of the central particles of the breather (with an amplitude $\delta\psi_n max = 2.1$) created by the kink-antikink collision. E_{max} represents the maximum of energy of the particles during the oscillations while $E_0 = 0.5$ is the barrier height.

form (5), the two minima must be located respectively at $\psi_n = -1$ and $\psi_n = +1$, which corresponds to a ratio $\alpha/\beta = -1$. This, gives us the existence condition of our compact kink solution, and then define the value of parameter ω, for a fixed constant discrete parameter τ. Therefore, the front wave velocity is then given by,

$$V_\phi = \frac{\sqrt{2\ (1 - \tau)^3}}{\arccos(\tau)} = \frac{\sqrt{2(1 - \cos(ka))^3}}{ka}. \quad (15)$$

We note that, the velocity of the wave font is associated to discrete parameter ka.

III. NUMERICAL RESULTS: FRONT DYNAMICS

A. Compact-like kink propagation

We have checked by numerical simulations that an exact discrete compact kink solution given by (5) can propagate freely, that is without experiencing any discreteness effects for the parameter range $ka \le \pi/3$. From this value on, some discreteness effects appears owing to the fact that it is very difficult to describe a sine function only with three points or two lattice spacing (see fig.2.a). Figures (2.a) and (2.b) show the spatio-temporal dynamics of compact-like kinks respectively for $ka = \pi/2$ and $ka = \pi/8$.

One can remark fig.(2.a) (discrete parameter $ka = \pi/2$) that, kink velocity decrease strongly with time until reaching a speed limit corresponding to a solution which is different to the predicted one. This means that there exists other exact compact solution in a such system. Indeed, as shown in fig.(2.c), the profile of this numerical solution is also a compact-like solution of (13).

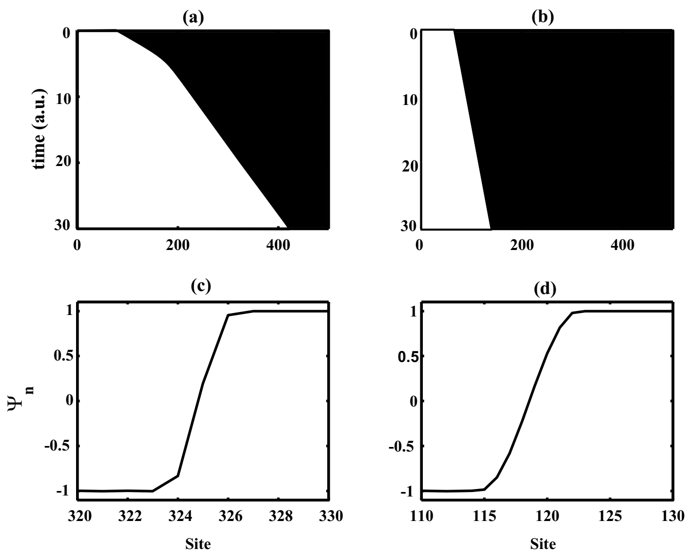

FIG. 2: Compact kinks propagation and shape: (a) Spatio-temporal evolution for a solution with discrete parameter $ka = \pi/2$. (b) Spatio-temporal evolution for a solution with discrete parameter $ka = \pi/8$. (c) Structure of the solution after a time $t' = 20$ (expressed in arbitrary unit) for discrete parameter $ka = \pi/2$. (d) Structure of the solution after a time $t' = 20$ (expressed in arbitrary unit) for discrete parameter $ka = \pi/8$.

Unlike to the very discrete case discussed previously, kink compacton with discrete parameter $ka = \pi/8$ propagates freely, i.e. without emission of radiation, confirming thus the exact character of solution (5). Figure (2.d) shows the profile solution after a time $t' = 20$ (expressed in arbitrary units). This profile is identical to high accuracy to the initial condition. A systematic investigation of the velocity and the emission of radiation reveals, that the critical value of parameter ka over which a solution of type (5) radiates and consequently reduces its velocity is $ka = \pi/3$.

Note that, this value of discrete parameter ($ka = \pi/3$) already corresponds to a very discrete situation, since the construction of the corresponding solution require only three lattice spacings.

B. Breather generation.

We have also studied the possible generation of nonlinear localized modes or compact-like breathers via kink (K) and antikink ($\bar{K}$) collisions, respectively in the discrete and continuous regime. This interesting type of nontopological excitations appears in a large variety of nonlinear lattices and their existence related to energy localization [8, 9]. Here, we studied numerically a K-$\bar{K}$ collision in the discrete ($ka = \pi/3$) and the continuous limit ($ka = \pi/8$) cases respectively. First, in the discrete case the two entities travel with velocity $v_\phi \simeq 0.478\ cells^{-1}$ and $-v_\phi$, respectively. As shown in Fig.3.(a), a discrete stationary breather and small amplitude nonlinear oscillation background emerge from the weakly inelastic K-$\bar{K}$ collision. The asymmetric breather amplitude oscillations (see fig.1) decrease slowly with time (see fig.3.(c)). Although the breather appears to be stable, after time $t = 60$ (a.u.) the breather sink to chaotic oscillations of small amplitude. Nevertheless, in spite of these weak nonlinear radiation losses (which propagate away), this discrete breather has a significant lifetime and presents a genuine physical interest. Note that, the interaction between these two compact entities is very different compared to the case of *tanh*-shaped or spatially extented solutions which interact at long distances. Indeed, their collision may be compared to that of two hard spheres, i.e. without long distance interaction.

IV. COMPACT-LIKE PULSE SOLUTIONS

As seen in section II, solutions of (13) are strictly localized sine functions $\psi_n = \pm sin(s)$ defined on interval $s \in [-\pi/2, +\pi/2]$, and ± 1 otherwise (see fig.2.d). Taking into account the symmetry of these previous solutions, a straightforward calculation shows that,

$$\begin{aligned} \psi_n &= (-1)^\lambda \cos(s), \qquad &if\ s \in [-\pi, +\pi], \\ \psi_n &= (-1)^{\lambda+1}, \qquad &otherwise, \end{aligned} \tag{16}$$

are also solutions of (13). The parameter λ is an integer equal to zero or one. If $\lambda = 0$ the solution corresponds to a bright type compact-like pulse (see fig.4.a), and if $\lambda = 1$ the solution corresponds to a dark type compact-like pulse (see fig.4.b). Note that, the pulses velocity is

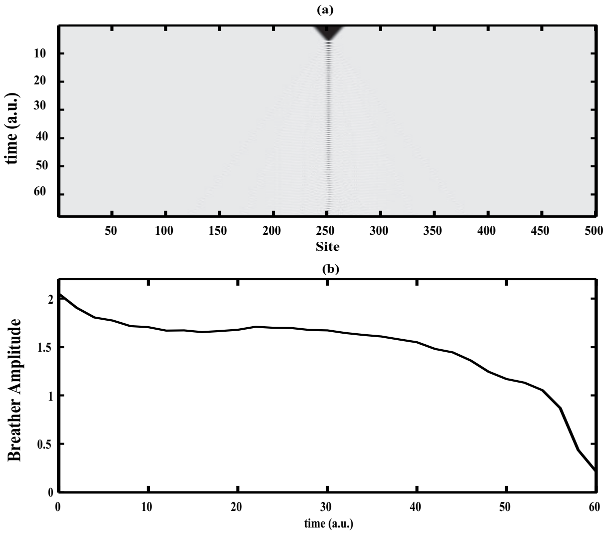

FIG. 3: (a) Creation of a discrete stationary breather with nonlinear oscillation background generated by a $K-\bar{K}$ collision. The oscillations of the central particle are asymmetric with an amplitude $\delta\psi_n max = 2.1$ (see Fig.1) and a period $T_B = 0.7$ (a.u.). (b) Breather amplitude decreasing versus time (in arbitrary unit).

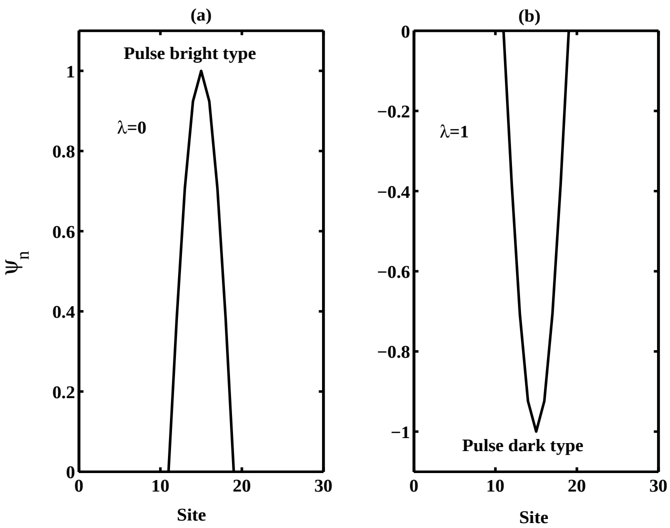

FIG. 4: Pulse shape solutions of equation (13). Left: a bright type compact-like pulse, corresponding to $\lambda = 0$ in eq.(16). Right: a dark type compact-like pulse, corresponding to $\lambda = 1$ in eq.(16). Both solutions have discrete parameter $ka = \pi/8$.

also given by eq.(15). Therefore, in the following, each pulse will associated we discrete parameter ka.

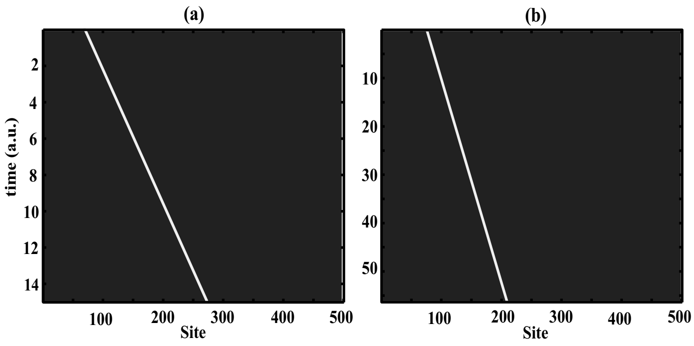

FIG. 5: (a) Pulse propagation for discrete parameter $ka = \pi/3$ (width: 6 lattice spacings). (b) Pulse propagation for discrete parameter $ka = \pi/8$ (width: 8 lattice spacings).

V. NUMERICAL RESULTS: PULSE DYNAMICS

A. Compact-like pulse propagation

We have checked numerically the stability of the solutions given by (16) and their exact discrete compact character for discrete parameter $ka \leq \pi/3$. As shown in fig.(5.a) and fig.(5.b) the solutions propagate freely, that is without emission of radiation or nonlinear oscillations. Likewise with the front dynamics, a systematic investigation of emission of radiation and velocity, reveals that the critical value of the discrete parameter ka over which a solution of type (16) radiates or emits nonlinear oscillations is $ka \leq \pi/3$. Note that, from a numerical point of view, it is very important to describe correctly the horizontal asymptote on the pulse top (when $ka \simeq \pi/3$). Indeed, nonlinear oscillations occur if this condition is not respected. The specific case (not shown here), corresponding to a discrete parameter $ka = \pi/2$, leads to a unstable pulse, that tends to widen along the propagation until it reacher a stable width. This pulse is then composed of two complementary fronts ($K - \bar{K}$) as seen in sect. III (see fig.2.c) and traveling in the same direction. The final width after widening is equal to 17 lattice spacings. This effect stems from the fact that, it is very difficult to define a sine function and its horizontal asymptote with only three points or two lattice spacings. Therefore, to obtain and propagate compact-like pulses in a such system, it is necessary to define the solution on 6 lattice spacings at least, as well as define correctly its horizontal asymptote.

B. Compact-like pulse collisions

As in sect. III, we have investigated the collisions between two pulses in the discrete regime and in the continuous limit. As shown in fig.(6), in the two cases, the collision leads to a localized mode, and to counter propagating compact-like kinks (see fig.6.a and 6.b).
In the discrete regime this mode is unstable (see fig.6.a).

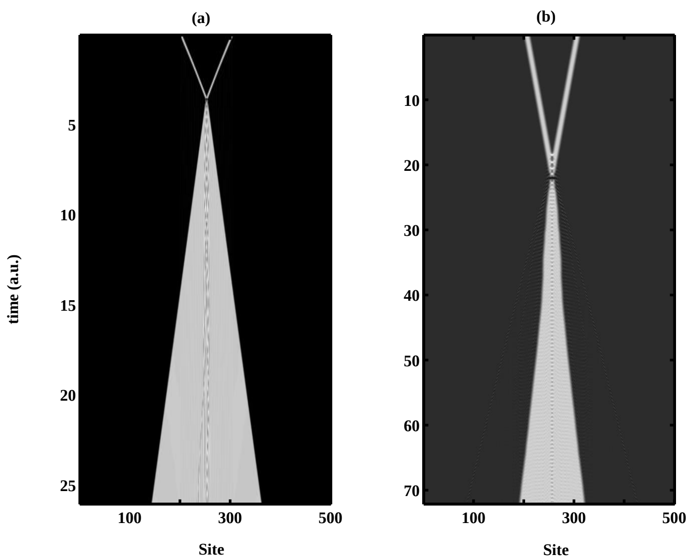

FIG. 6: Compact-like collision. (a) collision between two pulses in discrete regime: discrete parameter $ka = \pi/3$. (b) collision between two pulses in the continuous limit: discrete parameter $ka = \pi/8$.

Indeed, its interaction with the nonlinear oscillation background split it in two modes which move erratically and disappear in small amplitude chaotic oscillations.
On the other hand, in the continuous limit (see fig.6.b), the generated mode is very stable in amplitude, time and position, and therefore presents a physical interest. Moreover, we have verified that two adjacent pulses spaced of two lattice spacing can propagate freely, that is without any interaction. A systematic study reveals that the discrete parameter must be lower than $\pi/3$. Indeed, for values higher than this critical value, any interactions occur between the two successive pulses because of the nonlinear oscillation background that is generated during the propagation by the exceedingly discrete solutions.

VI. CONCLUDING REMARKS

We have explored the dynamics of a ϕ^4 lattice model with nonlinear coupling interaction between nearest neighbor atoms. We have first shown that by properly choosing the analytical form of a discrete solitary wave or compact-like solution of the model we can calculate analytically the parameters of the ϕ^4 potential. The compact-like kink solutions are sine-shaped and therefore strictly localized, that is without wings or tails. We have checked numerically that discrete compact-like kink (antikink) solutions can propagate freely without experiencing any discreteness effects if the discrete parameter ka is lower or equal to $\pi/3$. Kink-antikink collisions reveal that static breather with finite but with physically interesting lifetimes can be generated. Moreover, we have shown that compact-like pulses can be also solutions of such systems, and propagate also freely. Their collisions are pseudo-elastic and give birth to localized modes which are unstable in the discrete regime, but very stable in the continuous limit, and consequently are able to play a role in physical processes. We have also studied, but not presented the propagation of two consecutive pulses spaced of two lattice spacing and seen that no interaction between them occurs if the discrete parameter ka is smaller than $\pi/3$. We would like to point out again that our model and results are relevant for physical systems in which lattice discreteness is important. Obviously, further studies are necessary especially by including a linear coupling and a dissipative term, to determine all the properties of these compact-like kinks and pulses with exceptional mobilities. In conclusion, we believe that the understanding of discrete nonlinear models is an active and attractive topic of the current research. Since realistic physical systems are rather complicated, it is extremely important to develop the basic concepts with help of simple lattice models with exact solutions.

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