Sine-Gordon solitons in networks: Scattering and transmission at vertices

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We consider the sine-Gordon equation on metric graphs with simple topologies and derive vertex boundary conditions from the fundamental conservation laws, such as charge, energy and momentum conservation. For a special case we analytically obtain traveling wave solutions in the form of standard sine-Gordon solitons such as kinks and antikinks for star and tree graphs. We show that for this case the sine-Gordon equation becomes completely integrable just as in case of a simple $1D$ chain. This simple analysis provides a cornerstone for the numerical solution of the general case, including a quantification of the vertex scattering. Applications of the obtained results to Josephson junction networks and DNA double helix are discussed.

Introduction. Nonlinear wave dynamics described by the sine-Gordon equation is of importance in a variety of topics in physics, such as as elastic and stress wave propagation in solids, liquids and tectonic plates (see, e.g., [1–7]), transport in Josephson junctions [8], and topological quantum fields [2, 6]. Continuous and discrete forms of the sine-Gordon equation have been used so far for the description of wave transport in different media. However, there are structures for which the wave dynamics cannot be described within the traditional continuous or discrete approaches. These are networks and branched structures where the transmission through a branching point (network vertex) should be described by vertex conditions. Early studies of nonlinear evolution equations in branched structures are [9–11], and in recent few years one can observe rapidly growing interest in nonlinear waves and soliton transport in networks described by nonlinear Schrödinger equation [12–17]. Integrable boundary conditions following from the conservation laws were formulated, and soliton solutions yielding reflectionless transport across the graph vertex were derived in [12], see also [18] for the case of a discrete nonlinear Schrödinger. Other issues of integrability and soliton solutions are discussed in [14, 15]. deleted 1 sentence here, which contained no (or wrong) information

In this paper we address the wave dynamics in networks described by the sine-Gordon equation on metric graphs, which can be used for modeling of soliton transport in DNA double helix, tectonic plates and Josephson junction networks. The latter has attracted much attention in condensed matter physics [19, 20]. Another interesting application of sine-Gordon equations, or, more generally, nonlinear Klein-Gordon equations, on metric graphs can be networks of granular chains [11, 21]. Recently, soliton dynamics in networks was studied by considering the 2D sine-Gordon equation on Y and T junctions [22], and the metric graph limit was also studied numerically. See also [23] for similar results for the 2D Nonlinear Schrödinger equation on "fat" graphs.

Here we focus on the problem of integrability of sine-Gordon equations on metric graphs and soliton transmission at the graph vertex. In particular, using an approach similar to that of [12], we discuss the conditions under which the sine-Gordon equation is completely integrable and allows exact traveling wave solutions which provide reflectionless transmission of sine-Gordon solitons across vertices. Numerical solutions with scattering at a vertex when these conditions are violated are also presented.

Conservation laws and boundary conditions. For evolution equations on graphs, the connections of the bonds at the vertices are provided by vertex boundary conditions. In case of linear wave equations such conditions follow from self-adjointness of the problem [24, 25]. For nonlinear evolution equations one should use such fundamental laws as energy, flux, momentum and (for sine-Gordon model) topological charge conservations [12, 13, 22]. Below we derive such conditions and show the existence of infinitely many conservation laws in our model, which yields the complete integrability of the system.

Most of the 1D sine-Gordon models follow from the Lagrangian density $L = \left[\frac{1}{2}\left(u_t^2 - a^2u_x^2\right) - \beta(1-\cos u)\right]$, where a and β are positive constants. We want to explore

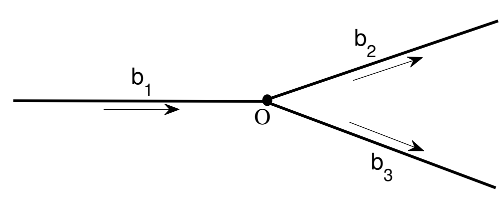

FIG. 1. Sketch of a metric star graph

a sine-Gordon model on networks modeled by graphs, i.e., system of bonds which are connected at one or more vertices (branching points). The connection rule is called the topology of the graph. When the bonds can be assigned a length, the graph is called a metric graph. The sine-Gordon model on each bond b_k, $k = 1,2,3,...,N$ is given by Lagrangian density

$$L_k = \left[\frac{1}{2}\left(u_{kt}^2 - a_k^2 u_{kx}^2\right) - \beta_k(1-\cos u_k)\right],$$

where $a_k, \beta_k > 0$. In the following we consider a star graph with three semi-infinite bonds connected at the point O called vertex of the graph, see Fig. 1. The coordinates are defined as $x_1 \in (-\infty, 0]$ and $x_{2,3} \in [0,\infty)$, where 0 corresponds to the vertex point. The equation of motion derived from the above Lagrangian density leads to the sine-Gordon equation on each bond given as

$$u_{ktt} - a_k^2 u_{kxx} + \beta_k \sin u_k = 0. \tag{1}$$

To formulate physically reasonable vertex boundary conditions (VBC) one can use the continuity of wave function

$$u_1(0,t) = u_2(0,t) = u_3(0,t) \tag{2}$$

and fundamental conservation laws, such as charge, energy and momentum conservations. For the primary star graph in Fig 1, the charge Q is given by

$$2\pi Q = \frac{a_1}{\sqrt{\beta_1}}\int_{-\infty}^{0} u_{1x}dx + \sum_{k=2}^{3}\frac{a_k}{\sqrt{\beta_k}}\int_{0}^{+\infty} u_{kx}dx. \tag{3}$$

From $\dot{Q} = 0$ and (2) we obtain the sum rule

$$\frac{a_1}{\sqrt{\beta_1}} = \frac{a_2}{\sqrt{\beta_2}} + \frac{a_3}{\sqrt{\beta_3}}. \tag{4}$$

The energy for the star graph is defined as

$$E(t) = \sum_{k=1}^{3}\frac{1}{\beta_k}\int_{B_k}\left[\frac{1}{2}\left(u_{kt}^2 + a_k^2 u_{kx}^2\right) + \beta_k(1-\cos u_k)\right]dx, \tag{5}$$

where $B_1{=}(-\infty,0)$, $B_{2,3}{=}(0,+\infty)$, and where for finite E we have $\partial_x u_1(x_1,t), \partial_t u_1(x_1,t) \to 0$ and $u_1(x_1,t) \to 2\pi n_1$ as $x_1 \to -\infty$, and $\partial_x u_k(x_k,t), \partial_t u_k(x_k,t) \to 0$ and $u_k(x_k,t) \to 2\pi n_k$ as $x_k \to \infty, k = 2,3$, for some integer n_k, $k = 1,2,3$. Then

$$\dot{E} = \frac{a_1^2}{\beta_1}u_{1x}u_{1t}\Big|_{x_1=0} - \frac{a_2^2}{\beta_2}u_{2x}u_{2t}\Big|_{x_2=0} - \frac{a_3^2}{\beta_3}u_{3x}u_{3t}\Big|_{x_3=0},$$

and by (2) the energy conservation reduces to

$$\frac{a_1^2}{\beta_1}u_{1x}\Big|_{x_1=0} = \frac{a_2^2}{\beta_2}u_{2x}\Big|_{x_2=0} + \frac{a_3^2}{\beta_3}u_{3x}\Big|_{x_3=0}. \tag{6}$$

Now we consider the momentum defined by

$$P = \sum_{k=1}^{3}\frac{a_k}{\beta_k}\int_{B_k} u_{kx}u_{kt}dx, \tag{7}$$

such that

$$\dot{P} = \frac{a_1}{\beta_1}\left[\frac{1}{2}(u_{1t}^2 + a_1^2 u_{1x}^2) - \beta_1(1-\cos u_1)\right]\Big|_{x_1=0} - \sum_{k=2}^{3}\frac{a_k}{\beta_k}\left[\frac{1}{2}(u_{kt}^2 + a_k^2 u_{kx}^2) - \beta_k(1-\cos u_k)\right]\Big|_{x_k=0}. \tag{8}$$

For $\dot{P} = 0$, we impose was: must impose, but (very unfortunately) I still don't see that we "must"; to me it looks just sufficient, not necessary two conditions. Firstly

$$\beta_1 = \beta_2 = \beta_3 = \beta(>0), \tag{9}$$

which simplifies the sum rule (4) to

$$a_1 = a_2 + a_3. \tag{10}$$

Then (8) becomes

$$\begin{aligned} 2\beta\dot{P} &= a_1^3 u_{1x}^2(0,t) - a_2^3 u_{2x}^2(0,t) - a_3^3 u_{3x}^2(0,t) \\ &= -\frac{a_2 a_3}{a_2 + a_3}(a_2 u_{2x}(0,t) - a_3 u_{3x}(0,t))^2, \end{aligned}$$

where we used (6), (9) and (10) in obtaining the last expression. Thus, $\dot{P} = 0$ yields $a_2 u_{2x}(0,t) = a_3 u_{3x}(0,t)$, which together with (6), (9) and (10) gives

$$a_1 u_{1x}(0,t) = a_2 u_{2x}(0,t) = a_3 u_{3x}(0,t). \tag{11}$$

Conditions on higher-order space-derivatives may be available from higher-order conservations, where the analysis becomes more laborious. However, they can also be obtained directly from (1), (2) via $a_1^2 u_{1xx}\big|_{x_1=0} = (u_{1tt} + \beta\sin u_1)\big|_{x_1=0} = (u_{ktt} + \beta\sin u_k)\big|_{x_k=0} = a_k^2 u_{kxx}\big|_{x_k=0}$ $(k = 2,3)$. Thus,

$$a_1^2 u_{1xx}(0,t) = a_2^2 u_{2xx}(0,t) = a_3^2 u_{3xx}(0,t), \tag{12}$$

and similarly, taking successive $x-$derivatives of (1), for $n \geq 3$,

$$a_1^n \partial_x^n u_1(0,t) = a_2^n \partial_x^n u_2(0,t) = a_3^n \partial_x^n u_3(0,t). \tag{13}$$

Integrability and traveling wave solutions. Let us now introduce two functions defined on the bonds from 1 to $k(=2,3)$ as $v_{1\to k} \equiv u_1(\frac{a_1 x}{\sqrt{\beta}}, \frac{t}{\sqrt{\beta}})$ for $x < 0$ and $\equiv u_k(\frac{a_k x}{\sqrt{\beta}}, \frac{t}{\sqrt{\beta}})$ for $x \geq 0$. Thanks to the vertex boundary conditions (VBC) in (11)-(13), together with the continuity condition in (2), both of $v_{1\to k}$ with $k = 2,3$ $\in C^\infty(-\infty,\infty))$ and satisfy $v_{1\to 2} = v_{1\to 3} = v(x,t)$, where $v(x,t)$ is a solution of the dimensionless sine-Gordon equation

$$v_{tt} - v_{xx} + \sin v = 0 \tag{14}$$

defined on the real line. This fact is identical to the expression of $u_k(x,t)$ in terms of the function v as

$$u_k(x,t) = v\left(\frac{\sqrt{\beta}}{a_k}x, \sqrt{\beta}t\right), x \in B_k \quad (k = 1,2,3). \tag{15}$$

The scaling function v in (15) together with the sum rule (10) guarantees the infinite number of constants of motion and thereby the complete integrablity of the sine-Gordon equation on the network.

In fact, from (15) and the sum rule (10) we find that all the conservation laws [26, 27]

$$\int_{-\infty}^{+\infty} g(v, \partial_x v, \partial_t v, \partial_x^2 v, ..., \partial_x^n \partial_t^l v)dx = const \tag{16}$$

of the sine-Gordon equation (14) on the real line also hold on the star graph, because

$$\begin{aligned}
&\sum_{k=1}^{3}\int_{B_k} g\left(u_k, a_k\beta^{-\frac{1}{2}}\partial_x u_k, \beta^{-\frac{1}{2}}\partial_t u_k, ..., a_k^n\beta^{-\frac{n+l}{2}}\partial_x^n\partial_t^l u_k\right)dx \\
&=a_1\int_{-\infty}^{+\infty} g\left(v, \partial_x v, \partial_t v, \dots, \partial_x^n\partial_t^l v\right)dx \\
&\quad+(a_2+a_3-a_1)\int_{0}^{+\infty} g\left(v, \partial_x v, \partial_t v, \dots, \partial_x^n\partial_t^l v\right)dx \\
&\quad= const.
\end{aligned} \tag{17}$$

The conservation of charge Q, energy E, and momentum P are just special cases.

From now on, we shall prescribe $\beta = 1$ without loss of generality. Eq.(14) has a number of explicit soliton solutions, for instance: kink "+" and anti-kink "-" solutions which can be written as [3, 4]

$$v(x,t) = 4\arctan\left[\exp\left(\pm\frac{x - x_0 - \nu t}{\sqrt{1-\nu^2}}\right)\right], \tag{18}$$

where $|\nu| < 1$ is the velocity of the kink. Other soliton solutions include breathers, kink-kink collisions and kink-antikink collisions [4], to name just a few, see also [28] for further multi-soliton type solutions. If the sum rule in (10) holds, then all these solutions, or, more generally, all solutions of (14), transfer via (15) to solutions on the metric graph. For instance, the kinks then provide reflectionless transmission of energy through the graph vertex, where the speed and energy of a kink traveling in positive direction ($\nu > 0$) split according to the ratios a_2/a_1 and a_3/a_1, respectively. On the other hand, launching two suitably fine tuned kinks on bonds 2 and 3 in negative direction, their joint energy is transmitted to bond 1.

Before entering into the numerical analysis of kink dynamics, we comment on other VBCs originating in the local scattering properties at each vertex. The VBC (2) of continuity and (6) of local flux conservation with $\beta_k = 1 (k = 1, 2, 3)$ are also called δ VBC. They naturally appear ([22], see also [23] for a similar construction for the case of the NLS, and [25, Chapter 8] for an overview of related linear results) by considering the 2D sine–Gordon equation $\partial_t^2 u - \Delta u + \sin u = 0$ on a "fat" graph, i.e., a 2D branched domain with Neumann boundary conditions, where $w_2/w_1 = a_2^2/a_1^2$ and $w_3/w_1 = a_3^2/a_1^2$ are the relative widths of the (fat) bonds.

Similarly, the so–called δ' VBCs [25, Chapter 8] consist of (11) and

$$a_1 u_1(0,t) - a_2 u_2(0,t) - a_3 u_3(0,t) = 0, \tag{19}$$

which conserve charge and energy for all values of the a_k. A simple calculation shows both δ and δ' VBCs can be derived from (10) and (15), but the inverse derivation is not possible. Most importantly, (10) and (15) give the existence of the infinite number of constants of motion (as shown in (16),(17)), which is equivalent to the complete integrability of the sine–Gordon equation on the graph.

Vertex transmission. An important issue for wave dynamics in networks is the scattering at vertices. The sum rule in (10) allows the tuning of the vertex scattering to achieve reflectionless transmission. We now give numerical solutions of (1) with $\beta_k = 1 (k = 1, 2, 3)$, using 2nd order in space and time finite differences, where we first focus on (2) and (6) as VBC, i.e., the δ case. Figure 2 shows the reflectionless propagation of a kink in the special case that the sum rule (10) holds.

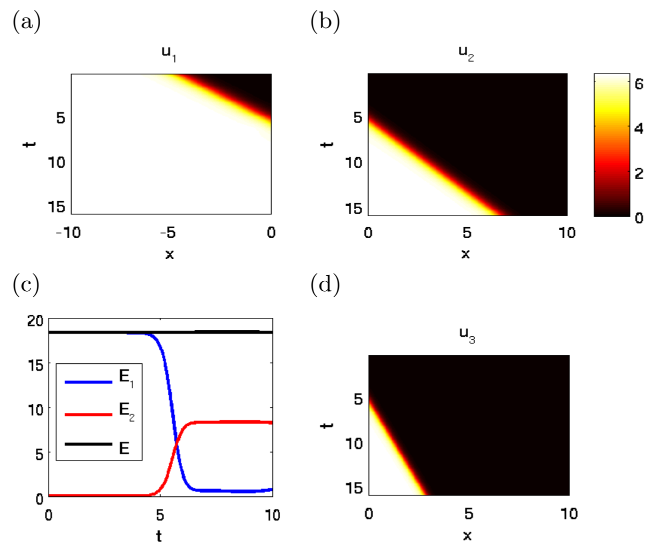

FIG. 2. (Color online). Numerical solution of (1), (2), (6), with $\beta_k = 1$, $k = 1, 2, 3$, and $a_1 = 1$, $a_2 = 0.7$, $a_3 = 0.3$ fulfilling (10). The initial conditions belongs to the kink (18) on bond 1 with $x_0 = -5$ and $\nu = 0.9$, while $u_{2,3} = \partial_t u_{2,3} \equiv 0$. Panels (a),(b),(d) arranged corresponding to Fig. 1, while (c) shows the t–dependence of the energies.

In Fig. 3 we numerically treat the transmission of solitons through the graph vertex when the sum rule (10) is violated. In (a)-(c) we consider the "natural" case a_k=1, $k = 1, 2, 3$, and the same kink initial condition as in Fig.2. The total energy is still conserved (by (6)), but in contrast to the reflectionless case from Fig.2, there now is significant reflection at the vertex. To demonstrate and quantify the dependence of the vertex transmission on the a_k in some more detail, in Fig. 3(d) we essentially return to the situation of Fig. 2. That is, we set $a_1 = 1$, $a_2 = 0.7$, but let a_3 vary and plot the reflection coefficient R, defined as the ratio of the energies in the incoming bond at initial time $t = 0$ and at $t = 15$. At $a_3 = 0.3$, corresponding to Fig. 2, we have $R = 0$, i.e. zero reflection.

Additionally, the red line in Fig. 3(d) shows the analogous simulation for the case of δ' vertex conditions (11) and (19). Again we have zero reflection at $a_3 = 0.3$, while violating the sum rule gives qualitatively similar but slightly stronger reflections than the δ case. Note that the simulations in Figs. 2 and 3 do not use the soliton properties of the kinks, but only the fact that they are traveling wave solutions for which we have formulas for the initial conditions. Thus, these numerical results can be transfered to general nonlinear Klein-Gordon equations that admit travelling wave solutions.

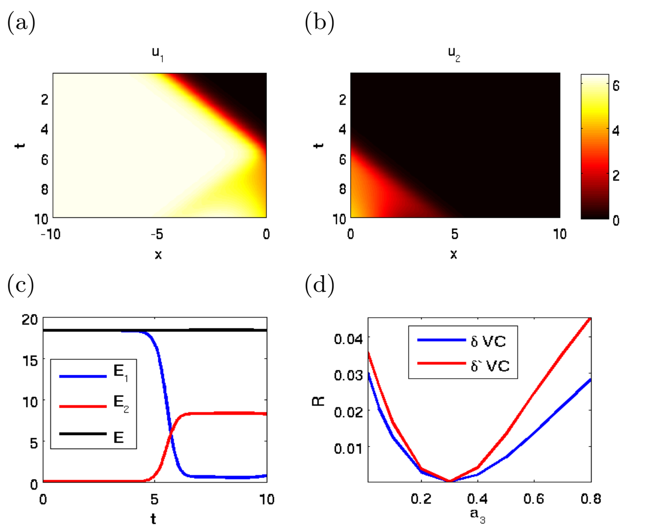

FIG. 3. (Color online). (a)-(c) Numerical solution of (1), (2), (6), with $\beta_k = 1$ for $k = 1, 2, 3$. (a)-(c) Reflection of incoming kink at the vertex in case that $a_1 = a_2 = a_3 = 1$, violating (10), initial conditions as in Fig. 2. u_3 is identical to u_2, and hence u_3 and E_3 in (c) are omitted. (d) (blue line) Dependence of the vertex reflection coefficient $R = E_1|_{t=15}/E_1|_{t=0}$ on a_3, where $a_1 = 1, a_2 = 0.7$, hence $a_3 = 0.3$ corresponding to Fig. 2. The red line is similarly obtained from solving (1) with δ' VBC (11) and (19).

Other graph topologies. Our results can be extended to other simple topologies such as general star graphs, tree graphs, loop graphs and their combinations. Exact traveling wave solutions of sine-Gordon models on such graphs with one incoming semi-infinite bond can be obtained similarly to the above case of a star graph with three bonds, leading to generalizations of the sum rule. We illustrate this for the tree graph from Fig. 4, consisting of three "layers" $b_1, (b_{1i}), (b_{1ij})$, where i, j run over the given bonds.

On each bond b_1, b_{1i}, b_{1ij} we have a sine-Gordon equation given by (1). Setting $\beta_1 = \beta_{1i} = \beta_{1ij} = 1$ for all i, j, the a_{1i} and a_{1ij} have to be determined from the sum rule

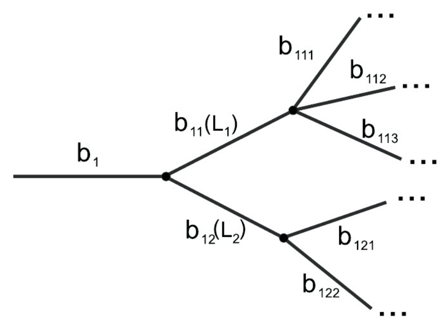

FIG. 4. A tree graph with three layers, $b_1 \sim (-\infty, 0), b_{11}, b_{12} \sim (0, L_k)$, $k = 1, 2$, and $b_{1ij} \sim (0, +\infty)$ with $i, j = 1, 2, \ldots$.

like (10) at each vertex. For instance, at the three nodes in Fig. 4 we need

$$\begin{array}{ll} \text{end of } b_1 : & a_0 = a_{11} + a_{12}, \\ \text{end of } b_{11} : & a_{11} = a_{111} + a_{112} + a_{113}, \\ \text{end of } b_{12} : & a_{12} = a_{121} + a_{122}, \end{array} \tag{20}$$

and this continues through the layers. By (14) and (15) this is based on scalings such as

$$u_1(x, t) = v(x/a_1, t) \text{ and } u_{1i}(x, t) = v(x/a_{1i}, t), \tag{21}$$

where at subsequent bonds we also need to take into account the finite propagation length in the previous bonds, for instance

$$u_{111}(x, t) = v((x + x_0)/a_{111}, t), \; x_0/a_{111} = L_1/a_{11}, \tag{22}$$

i.e. $x_0 = a_{111}L_1/a_{11}$. Necessarily, the speeds and energies of, e.g., an incoming kink, also split according to rules like (20), such that on each final bond we only have slow and small energy kinks. A similar construction has been done and formalized for the propagation of Nonlinear Schrödinger solitons on tree graphs in [12].

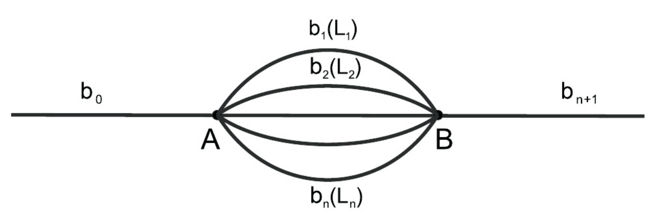

FIG. 5. A graph with a loop. $b_0 \sim (-\infty, 0), b_k \sim (0, L_k)$, $k = 1, \ldots, n$, where $L_k = a_k L$, $b_{n+1} \sim (0, \infty)$.

Another graph for which soliton solutions of sine-Gordon models can be obtained is a graph with a loop (see Fig.5), which consists of two semi-infinite bonds connected by n bonds having finite lengths L_k. Requiring the conditions

$$a_0 = \sum_{k=1}^{n} a_k = a_{n+1} \tag{23}$$

for the coefficients, and $L_k = a_k L$ ($k = 1, 2, ...n$) with a constant L, we can write soliton solutions in a similar way as in (21) and (22).

Finally, it can be shown that the above approach can be applied to obtain exact traveling wave solutions of sine-Gordon models on other (than above) graphs consisting of at least two semi-infinite bonds and any subgraph between them. In this case one needs to impose the pertinent vertex conditions like (21) or (23) at the vertices connecting the semi-infinite bonds with the subgraph.

Conclusions. In this work we studied sine-Gordon equations on simple metric graphs, and derived vertex boundary conditions for charge, energy and momentum conservation, and additionally conditions on parameters, for which the problem has explicit analytical soliton solutions. We find the sum rule (10) for bond-dependent coefficients at each vertex of the graph, which makes the sine-Gordon equation on the graph completely integrable. It is shown that the obtained solutions provide the reflectionless transmission of solitons at the graph vertex. This is also illustrated numerically by quantifying the reflections for a case where these conditions are violated, and we discussed how to generalize the results to other graph topologies. The results can be directly applied to several important problems such as Josephson junction network and DNA double helix. In Josephson junction network the parameter $1/\beta$ describes the Josephson penetration depth for each bond of the network. In such an approach our model corresponds to continuous version of the system considered in [19, 20]. Finally, a very important application can be DNA double helix models where the energy transport is described in terms of sine-Gordon equations [29, 30]. Base pairs of the DNA double helix can be considered as a branched system and modeled by a star graph [30]. Then the H-bond energy between two base pairs in such system can be characterized by the parameter, β. In summary, the sine-Gordon model considered in this paper can be useful for the problem of tunable soliton transport in various networks, and thus for engineering branched structures, providing reflectionless transport of energy, charge, and information in the form of solitons.

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