# Perturbation analysis of weakly discrete kinks

S. Flach* and K. Kladko
*Max-Planck-Institut für Physik komplexer Systeme, Bayreuther Strasse 40 H.16, D-01187 Dresden, Germany*
(Received 22 December 1995)

We present a perturbation theory of static kink solutions of discrete Klein-Gordon chains. The unperturbed solutions correspond to the kinks of the adjoint partial differential equation. The perturbation theory is based on a reformulation of the discrete chain problem into a partial differential equation with spatially modulated mass density. The first-order corrections to the kink solutions are obtained analytically and are shown to agree with exact numerical results. We use these findings to reconsider the problem of calculating the Peierls-Nabarro barrier. [S1063-651X(96)08308-0]

PACS number(s): 03.20.+i, 03.40.−t, 63.20.Ry

## I. INTRODUCTION

In recent years there has been considerable effort in understanding the effects of discreteness on solitonlike solutions [1–9]. In this work we will restrict ourselves to kink solutions. Kinks connect two ground states of a chosen system. Let us consider a nonlinear Klein-Gordon equation

$$\frac{\partial^2\Phi}{\partial t^2} - C\frac{\partial^2\Phi}{\partial x^2} + \frac{\partial V}{\partial \Phi} = 0 . \tag{1.1}$$

To allow for kink solutions the potential $V(z)$ has to have at least two degenerate minima. Throughout this paper we will consider only static solutions, i.e., the field $\Phi$ will not be time dependent. Then Eq. (1.1) is reduced to an ordinary differential equation

$$-C\frac{\partial^2\Phi}{\partial x^2} + \frac{\partial V}{\partial \Phi} = 0 . \tag{1.2}$$

The phase space of (1.2) is two dimensional. A kink solution corresponds to a heteroclinic orbit. This orbit connects the two hyperbolic fixed points (the ground states) in phase space. The invariant manifolds of these fixed points overlap, according to the continuous translational symmetry of (1.1), or due to the existence of an integral of motion of (1.2).

There exist different possibilities to modify the spatial differentials in (1.2) into differences. The most common way is to represent the differences in terms of interaction forces between neighboring particles $X_l$ and $X_{l-1}$

$$-C(X_{l+1}+X_{l-1}-2X_l) + \left.\frac{\partial V}{\partial \Phi}\right|_{\Phi=X_l} = 0 . \tag{1.3}$$

Here $X_l=\Phi(x=l)$, and $l$ is an integer (without loss of generality the periodicity of the discrete chain is assumed to be equal to one). Equation (1.3) is a two-dimensional symplectic map, similar to the standard map. In general the invariant manifolds of different fixed points do not overlap anymore. Instead they generally intersect in heteroclinic points at nonzero angles. The iteration of a heteroclinic point is again a heteroclinic point. One can then consider different sequences of heteroclinic points (let us call them heteroclinic orbits). All of these orbits will be exponentially attracted to the two fixed points for sufficiently large absolute values of $l$. Exactly two of these orbits correspond to kink solutions, and are thus related to their counterparts of the differential equation (1.2). However these two orbits have different energies (in contrast to the differential equation case). The energy difference is called a Peierls-Nabarro barrier.

Let us note that there exist also choices of the difference operator such that the invariant manifolds still overlap [11]. In that nongeneric case static kink solutions exist, which can be positioned at any place on the lattice. However, the difference operators are rather unphysical, and we will not consider these nongeneric cases here.

So far different methods have been developed in order to understand the effect of discreteness in principle. A recent approach is due to T. Munakata who used the method of constraint [10]. Up to now all these methods have not yielded analytical solutions. To obtain say a kink profile numerical tools are used. In this paper we will demonstrate that a simple method known as the time-averaging method is capable of finding analytical expressions for kink shapes in a well-defined perturbation approach.

In the limit $C\to\infty$ the two kink-type heteroclinic orbits of (1.3) approach their counterparts of (1.2). This is due to the fact, that large values of $C$ imply slow variations of these solutions as compared to the lattice spacing. Consequently it is tempting to use a perturbation approach, which links the kink solutions of (1.2) with the adjoint solutions of (1.3). In this paper we will present a first-order perturbation calculation for the heteroclinic orbits of (1.3). In Sec. II the difference equation (1.3) is transformed into a differential equation with spatially modulated densities. This differential equation is analyzed in Sec. III with the help of separation into slow and fast variables, such that analytical expressions for the kink solutions of (1.3) (in the first-order perturbation theory) are obtained. In Sec. IV we apply our method to two model cases and derive explicit expressions for the kink solutions. Section V is devoted to a discussion of the calculation of the Peierls-Nabarro energy.

## II. REFORMULATION OF THE PROBLEM

Let us consider the following differential equation:

$$C\Phi_{,xx} - \rho(x)V'(\Phi) = 0 . \tag{2.1}$$

*Electronic address: flach@idefix.mpipks-dresden.mpg.de

 

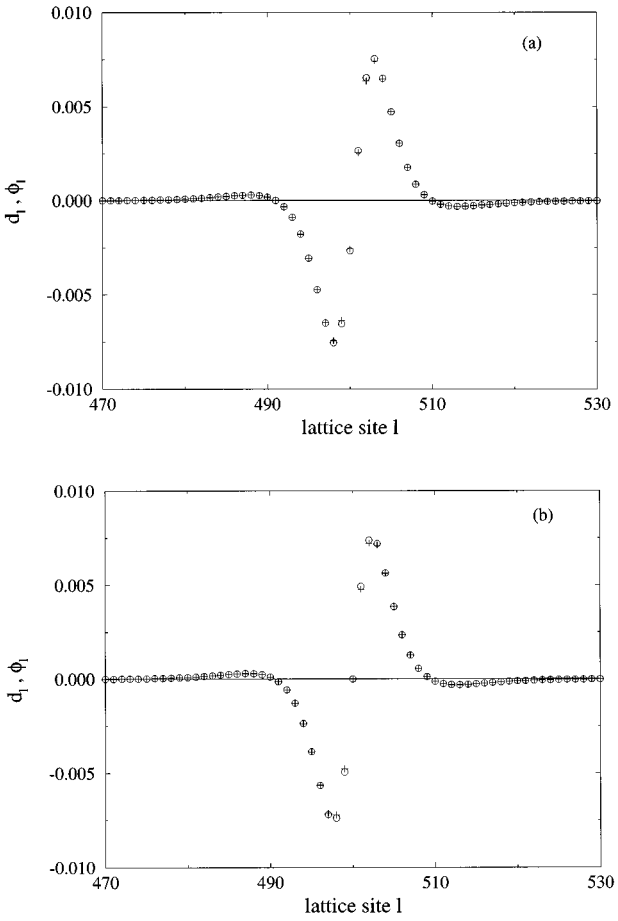


FIG. 1. Discrete kink shape deviations from the kink solution of the adjoint differential equation versus lattice site $l$ for the sine Gordon chain with $C=10$. Circles—exact result $d_l$; crosses—first-order perturbation result $\phi_l$. (a) $\alpha=0.5$; (b) $\alpha=0$.

Here $A_{,x}$ means (partial) derivative of $A$ with respect to $x$, and $V'$ is the derivative of the potential $V(z)$.

If we choose $\rho(x)=1$, we obtain (1.2). If we choose

$$\rho(x)=\sum_{l=-\infty}^{+\infty}\delta(x-l) \tag{2.2}$$

we obtain (1.3) [12]. This is easy to see by the following reasons. First we note that $\Phi_{,xx}[l<x<(l+1)]=0$ or $\Phi_{,x}[l<x<(l+1)]=\text{const}$. Thus it follows

$$\Phi(l+1)-\Phi(l)=\Phi_{,x}(l+0.5). \tag{2.3}$$

By integrating (2.1) from $x=l-0.5$ to $x=l+0.5$ and using (2.2) we obtain

$$C[\Phi_{,x}(l+0.5)-\Phi_{,x}(l-0.5)-V'(\Phi(l)]=0. \tag{2.4}$$

Combining (2.3) and (2.4) we arrive at Eq. (1.3), where $\Phi(l)=X_l$. In other words, the field $\Phi(x)$ is given by straight lines connecting its values at integer $x=l$, the field $\Phi_{,x}$ is given by a function with finite steps at integer $x=l$ and constant elsewhere, and $\Phi_{,xx}$ is a sum over $\delta$ functions, with weights given by (2.1) using (2.2).

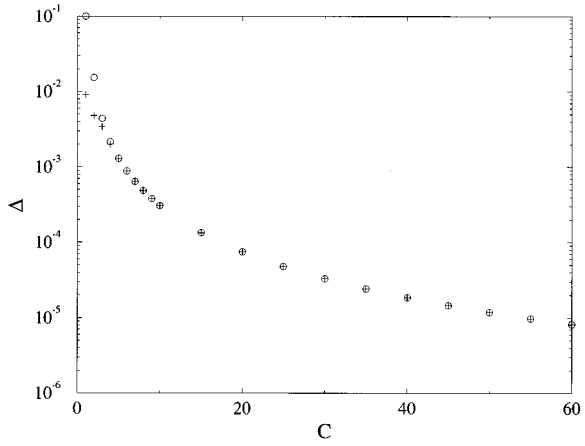


FIG. 2. The normalized deviation $\Delta$ of the first-order perturbation result $\phi_l$ from the exact $d_l$ versus $C$. Circles—$\alpha=0.5$, crosses—$\alpha=0.5$.

It is clear that one can make a continuous transition from (2.2) to (2.3) by varying $\rho(x)$ from $\rho(x)=1$ to (2.2).

We rewrite (2.2) into

$$\rho(x)=\sum_{l=-\infty}^{+\infty}\delta(x-l)=1+2\sum_{k=1}^{\infty}\cos(2\pi kx). \tag{2.5}$$

Thus we finally arrive at the following equation:

$$C\Phi_{,xx}-\left[1+2\sum_{k=1}^{\infty}\cos(2\pi kx)\right]V'(\Phi)=0. \tag{2.6}$$

Note that (2.6) is still an exact reformulation of (1.3).

## III. PERTURBATION APPROACH

Let us introduce new coordinates $x=\sqrt{C}T$ and $\Omega=2\pi\sqrt{C}$. Then (2.6) becomes

$$\Phi_{,TT}-\left[1+2\sum_{k=1}^{\infty}\cos(k\Omega T)\right]V'(\Phi)=0. \tag{3.1}$$

In the limit of large values of $C$ the cosine terms in (3.1) rapidly oscillate due to the increase in $\Omega$. Thus we can apply standard perturbation treatments using the separation of the field $\Phi$ into slow $\Phi^{(s)}$ and fast $\xi_k$ parts [13]

$$\Phi=\Phi^{(s)}+\sum_{k=1}^{\infty}\xi_k. \tag{3.2}$$

Inserting (3.2) into (3.1) and linearizing with respect to the variables $\xi_k$ we obtain

$$\Phi^{(s)}_{,TT}+\sum_{k=1}^{\infty}\xi_{k,TT}=\left[1+2\sum_{k=1}^{\infty}\cos(k\Omega T)\right]\times\left[V'(\Phi^{(s)})+V''(\Phi^{(s)})\sum_{k=1}^{\infty}\xi_k\right]. \tag{3.3}$$

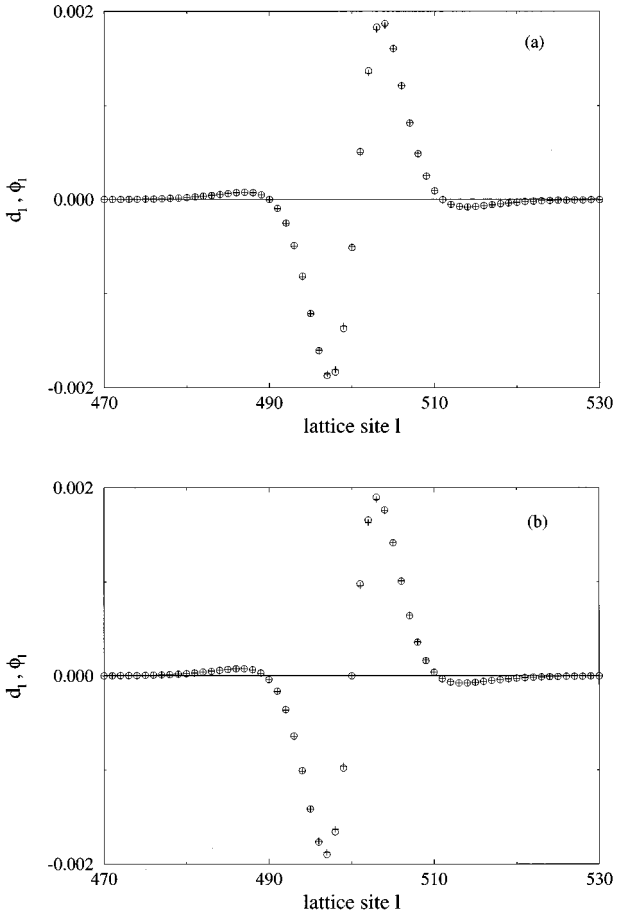


FIG. 3. Same as in Fig. 1 but for the $\Phi^4$ chain and $C=15$.

For the fast variables the leading order contribution yields

$$\xi_{k,TT}=2\cos(k\Omega T)V'(\Phi^{(s)}), \tag{3.4}$$

$$\xi_k=-\frac{2}{k^2\Omega^2}\cos(k\Omega T)V'(\Phi^{(s)}). \tag{3.5}$$

Averaging (3.3) over the periods of oscillation of the fast variables and using (3.5) and $\Sigma_{k=1}^{\infty}1/k^2=\pi^2/6$ it follows

$$\Phi^{(s)}_{,TT}=V'_{\rm eff}(\Phi^{(s)}), \tag{3.6}$$

$$V_{\rm eff}(z)=V(z)-\frac{1}{24C}[V'(z)]^2. \tag{3.7}$$

Note that Eq. (3.6) is a simple differential equation, which will be integrated for two examples in the following section.

Since we are interested in the solution of (3.1) at integer points, the arguments $k\Omega T=2\pi n$ with $n$ being an integer in (3.5). The final solution of (3.1) to first order in $1/C$ is then given by

$$\Phi(l)=\Phi^{(s)}(l)-\frac{1}{12C}V'(\Phi^{(s)}). \tag{3.8}$$

Actually (3.8) contains also (incomplete) terms of order $1/C^2$. One can expand the solution in powers of $1/C$ and extract the first-order term after solving along the given path.

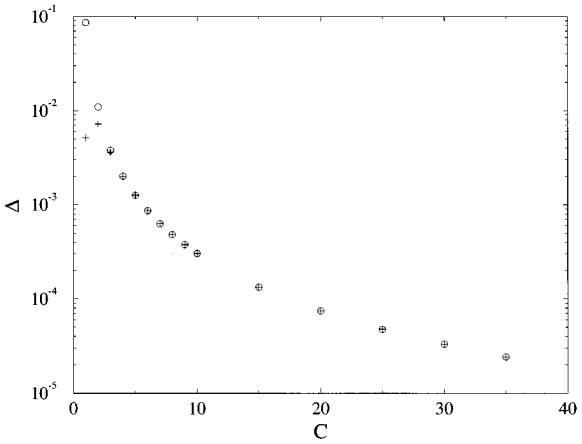


FIG. 4. Same as in Fig. 2 but for the $\Phi^4$ chain.

## IV. TWO EXAMPLES

### A. Sine Gordon case

Let us consider

$$V(z)=1-\cos(z). \tag{4.1}$$

The kink solution of (1.2) is given by

$$\Phi^{(c)}(x+\alpha)=4\arctan(e^{x\sqrt{C}}). \tag{4.2}$$

Let us consider the slow part $\Phi^{(s)}$ of the first-order perturbation. The effective potential (3.7) is given by

$$V'_{\rm eff}(z)=\sin(z)-\frac{1}{24C}\sin(2z). \tag{4.3}$$

Consequently $\Phi^{(s)}$ is the solution of the double sine Gordon equation and can be found in [14] (note that there is an error in Eq. (3.7) of [14]—the sign of the power $-1/2$ has to be changed to $+1/2$) or can be simply calculated by integration:

$$\Phi^{(s)}(x+\alpha)=2\pi-2\arctan\left\{\left(1-\frac{1}{12C}\right)^{1/2}\times\operatorname{cosech}\left[\left(1-\frac{1}{12C}\right)^{1/2}\frac{x}{\sqrt{C}}\right]\right\},\quad x\geqslant 0, \tag{4.4}$$

$$\Phi^{(s)}(x+\alpha)=-2\arctan\left\{\left(1-\frac{1}{12C}\right)^{1/2}\times\operatorname{cosech}\left[\left(1-\frac{1}{12C}\right)^{1/2}\frac{x}{\sqrt{C}}\right]\right\},\quad x\leqslant 0. \tag{4.5}$$

Here $\alpha$ is an integration constant. Using Eq. (3.8) and expanding in $1/C$ we finally obtain the following first-order perturbation correction for the discrete sine Gordon chain:

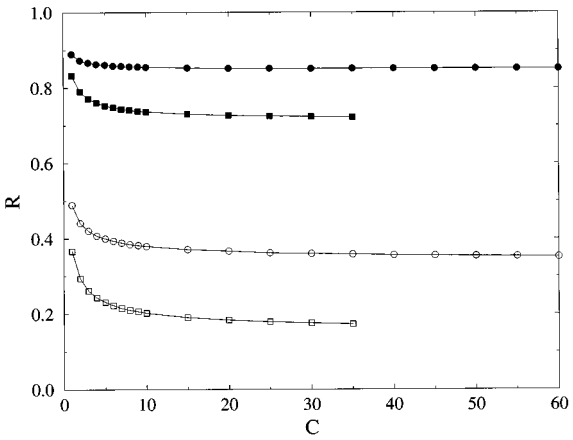


FIG. 5. The ratio $R$ of the approximated $E_{PN}$ over the exact one as a function of $C$. Open circles—zero order result for sine Gordon chain; filled circles—first order perturbation result for sine Gordon chain; open squares—zero order result for $\Phi^4$ chain; filled squares—first-order perturbation result for $\Phi^4$ chain. Lines are guides to the eye.

$$\Phi(l)=\Phi^c(x+\alpha)+\frac{1}{6C}\mathrm{sech}\left(\frac{x+\alpha}{\sqrt{C}}\right)\times\left[2\tanh\left(\frac{x+\alpha}{\sqrt{C}}\right)-\frac{x+\alpha}{\sqrt{C}}\right]. \tag{4.6}$$

Since the invariant manifolds of the two relevant fixed points of (1.3) do not overlap, but only intersect at finite angles, we have to choose the right values of $\alpha$. Clearly they are $\alpha=0$ and $\alpha=0.5$, which correspond to a kink centered on a lattice site and between two lattice sites respectively. These two possible kink solutions are known to exist for the map (1.3) [1–10].

In order to test our result we compute the exact kink solutions of (1.3) with (4.1) for different values of $C$. We use the steepest gradient method (minimization of the potential energy) and work in quadruple precision. The result will be denoted as $X_l$. The deviations $d_l$ from its adjoint solution (4.2) of (1.2) is then given by $d_l=X_l-\Phi^c(l)$. The perturbation approach yields $\phi(l)=\Phi(l)-\Phi^c(l)$ and is defined by the second term on the right-hand side of (4.6). In Fig. 1 we plot $d_l$ and $\phi_l$ for $C=10$ for both kink solutions ($\alpha=0$ and $\alpha=0.5$). Clearly the perturbation result fits well to the exact one. In order to be more precise, we calculate the normalized squared deviation $\Delta$ of the perturbation result from the exact one

$$\Delta=\frac{\Sigma_{l=-\infty}^{+\infty}(d_l-\phi_l)^2}{\Sigma_{l=-\infty}^{+\infty}d_l^2}. \tag{4.7}$$

Now we can evaluate $\Delta$ for different values of $C$ and see, whether it is monotonously decreasing with increasing $C$. The results for both kink solutions are shown in Fig. 2. No doubt the perturbation theory gives the correct first-order result.

### B. $\Phi^4$ case

The second example is given by

$$V(z)=\tfrac{1}{4}(z^2-1)^2. \tag{4.8}$$

The kink solution of (1.2) is given by

$$\Phi^c(x+\alpha)=\tanh\left(\frac{x}{\sqrt{2C}}\right). \tag{4.9}$$

The effective potential (3.7) reads

$$V_{\mathrm{eff}}(z)=\frac{1}{4}(z^2-1)^2\left[1-\frac{z^2}{6C}\right]. \tag{4.10}$$

Thus the slow part $\Phi^{(s)}$ is the solution of the $\Phi^6$ differential equation. It can be easily integrated using [15]

$$\Phi^{(s)}(x+\alpha)=\frac{\tanh\left(\left[1-\frac{1}{6C}\right]^{1/2}\frac{x}{\sqrt{2C}}\right)}{\left[1-\frac{1}{6C}\mathrm{sech}^2\left(\sqrt{1-\frac{1}{6C}}\frac{x}{\sqrt{2C}}\right)\right]^{1/2}}. \tag{4.11}$$

Using (3.8) we finally obtain the first-order perturbation result

$$\Phi(l)=\Phi^{(s)}(x+\alpha)-\frac{1}{12C}\Phi^{(s)}(x+\alpha)\times[\Phi^{(s)}(x+\alpha)\Phi^{(s)}(x+\alpha)-1]. \tag{4.12}$$

As in the sine Gordon case we calculate $d_l$ and $\phi_l$ and plot the results for $C=15$ in Fig. 3. The normalized deviation $\Delta(C)$ is plotted in Fig. 4. Clearly the perturbation theory gives the correct result.

## V. THE PEIERLS-NABARRO BARRIER PROBLEM REVISITED

Considering the success of the presented perturbation approach with respect to the kink solutions, it is tempting to use this result for calculating the Peierls-Nabarro barrier $E_{PN}$ which is given by the energy difference of the two different kink solutions. However, as it was shown in [16], one has to expect that the leading order asymptotics of $E_{PN}$ contains contributions from all orders of the perturbation series for the kink solutions for large values of $C$. This is already clear by noting that the zero-order result (i.e., replacing the exact kink solution of the lattice by its counterpart of the adjoint differential equation) yields a nonzero $E_{PN}^{(0)}$. As shown in [16], these contributions are not enough to fit the exact numbers. Clearly at least the first-order perturbation result for the discrete kink has to be taken into account (yielding $E_{PN}^{(1)}$). But then it follows that contributions have to be expected throughout all higher orders of perturbation theory [16]. Since we have calculated the first-order corrections to the kink shape, we can test these predictions.

Let us introduce $R^{(1)}=E_{PN}^{(1)}/E_{PN}$ and $R^{(0)}=E_{PN}^{(0)}/E_{PN}$, which measure the ratio of the first-order energy difference

(zero order, respectively) over the exact one. In Fig. 5 these results are plotted for the two examples considered in the preceding section. Clearly $R^{(1)}$ is much closer to unity than $R^{(0)}$, but still there exist discrepancies, which even grow with increasing $C$. This circumstance implies that the contributions from higher orders of the presented perturbation theory in $E_{PN}$ gain more weight with increasing $C$.

## VI. CONCLUDING REMARKS

We have derived first-order corrections to the kink shape of a discrete chain. We used the methods of slow and fast variables. The resulting differential equations can be integrated explicitly, as demonstrated for two examples. Note that the presented method can be generalized to the case of anharmonic interactions as well as to time-dependent solutions. The generalization of (2.1) gives

$$\sum_l \delta(x-l)\Phi_{,tt} - \left.\frac{\partial^2 W}{\partial y^2}\right|_{y=\Phi_{,x}} \Phi_{,xx} + \sum_l \delta(x-l)V'(\Phi) = 0. \tag{6.1}$$

Here $W(y)$ denotes the nearest neighbor interaction on the discrete chain ($y = X_l - X_{l-1}$), which could well be anharmonic. In the examples considered above we used only harmonic interactions

$$W(y) = \frac{1}{2} C y^2$$

so that the second derivative in (6.1) simply yields $C$.

Using our results we have tested predictions from [16] on the Peierls-Nabarro barrier dependence on $C$. It is worthwhile to note that for the sine Gordon chain there exists an alternative splitting angle approach for the barrier problem [17]. Those results confirm our findings on the problems of conventional perturbation approach for the barrier value cited.

We thank S. Aubry, P. Fulde, R. S. MacKay, C. Simo, O. Usatenko, and C. R. Willis for valuable discussions, and C. Simo for providing us with numerical details on the splitting angle approach.

[1] M. Peyrard and M. Remoissenet, Phys. Rev. B **26**, 2886 (1982).
[2] Y. Ishimori and T. Munakata, J. Phys. Soc. Jpn. **51**, 3367 (1982).
[3] J. A. Combs and S. Yip, Phys. Rev. B **28**, 6873 (1983).
[4] V. L. Pokrovsky, J. Phys. **42**, 761 (1981).
[5] N. Theodorakopoulos, W. Wünderlich, and R. Klein, Solid State Commun. **33**, 213 (1980).
[6] M. Remoissenet, Phys. Rev. B **33**, 2386 (1986).
[7] C. R. Willis, M. El-Batanouny, and P. Stancioff, Phys. Rev. B **33**, 1904 (1986).
[8] P. Stancioff, C. R. Willis, M. El-Batanouny, and S. Burdick, Phys. Rev. B **33**, 1912 (1986).
[9] C. R. Willis and R. Boesch, Phys. Rev. B **41**, 4570 (1990).
[10] T. Munakata, Phys. Rev. A **45**, 1230 (1992).
[11] J. M. Speight and R. S. Ward, Nonlinearity **7**, 475 (1994).
[12] R. S. Sagdeev, D. A. Usikov, and G. M. Zaslavski, *Nonlinear Physics: from the Pendulum to Turbulence and Chaos* (Harwood Academic, Chur, Switzerland, 1988).
[13] L. D. Landau and E. M. Lifshitz, *Theoretische Mechanik, Lehrbuch der Theoretischen Physik I* (Akademie, Berlin, 1991).
[14] C. A. Condat, R. A. Guyer, and M. D. Miller, Phys. Rev. B **27**, 474 (1983).
[15] I. S. Gradshtein and I. M. Ryzhik, *Table of Integrals, Series, and Products* (Academic, New York, 1994).
[16] S. Flach and C. R. Willis, Phys. Rev. E **47**, 4447 (1993).
[17] V. F. Lazutkin, I. G. Schachmannski, and M. B. Tabanov, Physica D **40**, 235 (1989).