# Solitons in anharmonic chains with power-law long-range interactions

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(Received 20 February 1998)

We study the influence of long-range interactions with distance dependence $r^{-s}$ of the elastic coupling constant on the properties of pulse solitons in a one-dimensional anharmonic chain. Introducing the approximations of small amplitude and long wavelength, we have arrived at the Boussinesq equation for $s>5$ and the Benjamin-Ono equation for $s=4$. For $s>5$ the soliton tails are exponential while for $3<s\leqslant 5$ they are algebraic. For $s\leqslant 3.5$ there is an energy gap between the spectra of plane waves and the soliton states.
[S1063-651X(98)00108-1]

PACS number(s): 03.40.Kf, 62.30.+d, 63.20.Ry

## I. INTRODUCTION

The dynamics of nonlinear lattices and related solitonlike excitations have been intensively studied since the advent of solitons (for reviews, see, e.g., [1–5]). It has been found that anharmonic molecular chains with nearest-neighbor interaction (NNI) or next-NNI [6] can bear solitonlike compressive and supersonic (for realistic interatomic potentials) excitations which are solutions, in the long-wavelength approximation, of the Boussinesq or Korteweg–de Vries (KdV) equations. The soliton excitations are very robust and propagate without energy loss. Moreover, their collisions are almost elastic even beyond the range of validity of the continuum approximation. The foregoing renders the soliton excitations important for the coherent energy transfer [2] and recently they have been invoked in order to explain the energy transport in DNA [7].

But the DNA molecule is known to contain charged groups with long-range Coulomb interactions between them. For a general lattice consisting of uncharged molecular units one can have a situation where the dipole moment is very small while the quadrupole moment is significant. Thus the dominant interaction between neighbors will be a quadrupole-quadrupole interaction, but one must also take into account dipole-dipole interactions due to their much longer range.

The objective of the paper is to elucidate the effects of power-law long-range interactions (LRI) on the properties of soliton excitations in anharmonic chains. The pioneering paper of Ishimori [8] on this subject already indicated an interesting feature of the power-law LRI system: namely, a crossover takes place from sech-shaped solitons (which are solutions to the Boussinesq or KdV equations), prototype for rapidly decreasing LRI, to algebraic solitons (solutions to the Benjamin-Ono equation and related ones), typical for systems with slowly decaying LRI's. To be specific, Ishimori studied nonlinear waves in a one-dimensional lattice with the Lennard-Jones $(2n,n)$ intermolecular potential and showed that the dynamics is governed by the Benjamin-Ono equation in the case $n=2$ or by the Korteweg–de Vries equation for $n>4$. Quite recently Gaididei, Mingaleev, Christiansen, and Rasmussen [9] have shown that the introduction of power-law LRI into the nonlinear Schrödinger model produces very similar effects. It was also stated [10] that, although having very much in common, the power-law LRI system bears features essentially different from those of the exponential law (called also Kac-Baker [11,12]) one. One-dimensional anharmonic systems, in their turn, should be expected to have an analogous behavior.

The solitary excitations in anharmonic chains with harmonic Kac-Baker LRI's have already been much studied [13–17]. Remoissenet and Flytzanis [13] studied a renormalization of the solitonic parameters due to the effect of LRI's and they also investigated the effect of LRI's on the stability of long-wavelength plane waves. Tchawona, Kofane, and Bokosah [14] studied the influence of the LRI on solitons in diatomic chains and investigated both pulse and envelope solitons. Neuper, Gaididei, Flytzanis, and Mertens [15–17] investigated pulse solitons in anharmonic chains with cubic or Toda NNI and exponentially decaying harmonic LRI's. They have demonstrated that the interplay of short- and long-range interactions leads to the existence of two branches of solitons: low-velocity and high-velocity ones, separated by a gap. The low-velocity solitons exist at supersonic velocities below some critical velocity. At the critical velocity the shape of the soliton changes drastically: instead of the usual sech shape a crest soliton appears. This soliton is very similar to the peak solitons which were discussed earlier in different contexts [18–22]. The high-velocity solitons are made up of two components: short- and long-range ones. The interplay of these components leads to an unusual behavior of soliton amplitude and energy as a function of velocity. Bonart [23] investigated intrinsically localized modes, their stability and optical absorption in a linear chain with long-range Coulomb interaction.

We demonstrate in this paper that power law LRI leads to a drastic change of the soliton properties, compared to Kac-Baker LRI's. Namely, there is only one type of solitons and their tails can become algebraic. In a particular case the dynamics is governed by the Benjamin-Ono equation which is well known to possess algebraic soliton solutions. Unlike NNI or Kac-Baker LRI's, it is possible to have a situation

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when the energy of the solitons does not vanish for velocities close to the speed of sound. On the contrary, in this case there is an energy gap between the spectra of plane waves and soliton states. The remainder of the paper is outlined as follows. In Sec. II we derive the equation of motion for the strain in the anharmonic lattice with power-law LRI using a quasicontinuum approach which is necessary in the case of LRI [16,17]. We show that the dynamics of the system is governed by the Boussinesq equation only for $s>5$. In the particular case $s=4$ it is described by the Benjamin-Ono equation. In Sec. III we investigate the long-distance behavior of the nonlinear excitations and show that the high-velocity solitons have algebraic tails if the LRI's decay slower than $1/r^5$. In Sec. IV we develop a variational approach exploiting an exp-like function as trial function and show that for $s\leqslant 3.5$ there is an energy gap between the spectra of plane waves and the soliton states. In Sec. V we describe the numerical method by which we obtained the soliton solutions in the previous sections. In Sec. VI we summarize our conclusions.

## II. SYSTEM AND EQUATIONS OF MOTION

We consider a chain of equally spaced particles of unit mass whose displacements from equilibrium are $u_n(t)$ when the equilibrium spacings are unity. The Hamiltonian of our system is given by

$$H=T+U_{NN}+U_{LR}, \tag{1}$$

where

$$T=\frac{1}{2}\sum_n \left(\frac{du_n}{dt}\right)^2 \tag{2}$$

is the kinetic energy and

$$U_{NN}=\sum_n V(u_{n+1}-u_n) \tag{3}$$

is the short-range part of the potential energy, with the potential between first neighbors

$$V(w)=\frac{1}{2}w^2-\frac{1}{3}w^3. \tag{4}$$

The long-range interaction is of the harmonic form

$$U_{LR}=\frac{1}{2}\sum_n \sum_{m>n} J_{m-n}(u_n-u_m)^2, \tag{5}$$

with a power dependence of the elastic coupling constant

$$J_{m-n}=J\ |m-n|^{-s} \tag{6}$$

on the distance between particles. Here $s$ is a parameter introduced to cover different physical situations including the nearest-neighbor approximation ($s=\infty$), dipole-dipole interaction ($s=5$), and the Coulomb interaction between charged particles of a chain ($s=3$).

The equations of motion for the relative displacements $w_n=u_{n+1}-u_n$ are

$$\frac{d^2}{dt^2}w_n+2F(w_n)-F(w_{n+1})-F(w_{n-1}) + \sum_{m\neq n} J_{m-n}(w_n-w_m)=0, \tag{7}$$

where

$$F(w)\equiv\frac{d}{dw}V(w)=w-w^2. \tag{8}$$

To obtain analytical solutions of Eq. (7) we pass to the continuum limit treating $n$ as a continuous variable [$n\to x$, $w_n(t)\to w(x,t)$] and keeping formally all terms in the Taylor expansion in Eq. (7). Then the equation can be cast in the operator form

$$\partial_t^2 w(x,t)-4\sinh^2\left(\frac{\partial_x}{2}\right)F(w(x,t))+JQ(s,\partial_x)w(x,t)=0, \tag{9}$$

where $\partial_x$ and $\partial_t$ are the derivatives with respect to $x$ and $t$, respectively, and the operator

$$Q(s,\partial_x)=2\sum_{m=1}^{\infty}\frac{1-\cosh(m\partial_x)}{m^s} \tag{10}$$

can be expressed in the long wave limit (that is for $k\ll 1$) as follows (see, e.g., [8]):

$$Q(s,ik)\approx\zeta(s-2)k^2-\frac{1}{12}\zeta(s-4)k^4 \quad \text{for } s>5, \tag{11}$$

$$Q(5,ik)\approx\zeta(3)k^2+\frac{1}{12}k^4\ \ln|k|, \tag{12}$$

$$Q(s,ik)\approx\zeta(s-2)k^2-\nu_s|k|^{s-1} + \frac{s-3}{24(5-s)}k^4 \quad \text{for } 3<s<5, \tag{13}$$

$$Q(4,ik)\equiv\frac{\pi^2}{6}k^2-\frac{\pi}{6}|k|^3+\frac{1}{24}k^4, \tag{14}$$

$$Q(3,ik)\approx -k^2\ln|k|+\frac{3}{2}k^2+\frac{1}{144}k^4, \tag{15}$$

where

$$\nu_s=\frac{2^{1-s}\pi^{3/2}}{\Gamma(s/2)\Gamma((s+1)/2)\cos(\pi s/2)}, \tag{16}$$

and $\zeta(s)$ is Riemann's zeta function

$$\zeta(s)=\sum_{n=1}^{\infty} n^{-s} . \tag{17}$$

From the dispersion relation for linear waves

$$\Omega^2(k)=4\sin^2\left(\frac{k}{2}\right)+JQ(s,ik), \tag{18}$$

one gets the sound velocity

$$c=\sqrt{1+J\zeta(s-2)}. \tag{19}$$

It should be remarked that $c$ increases with decreasing the range parameter $s$, and becomes infinite at $s=3$ (i.e., in the chains with charged particles). On the other hand, it is well known that in the chains with NNI [1,2] and Kac-Baker LRI [15–17] there are only supersonic solitons. Thus, since for $s=3$ every velocity is subsonic, the question for the existence of soliton solutions must be raised in this case. In this paper we restrict ourselves to the case $s>3$. The nonlinear dynamics of a chain with long-range Coulomb interaction is considered in [24].

There are two cases when one can write down Eq. (9) in a more convenient form, namely, $s>5$ and $s=4$. First, consider the case $s>5$ for which the operator

$$Q(s,\partial_x)\approx-\zeta(s-2)\partial_x^2-\frac{1}{12}\zeta(s-4)\partial_x^4 \tag{20}$$

has the same form as in the NNI approximation. In this case the equation of motion (9) becomes the Boussinesq equation

$$\left(\partial_t^2-c^2\partial_x^2-\frac{\mu_s}{12}\partial_x^4\right)w(x,t)+\partial_x^2 w^2(x,t)=0, \tag{21}$$

where

$$\mu_s=1+J\zeta(s-4) \quad \text{for } s>5 \tag{22}$$

is the dispersion parameter. It is well known that the Boussinesq equation is integrable with a sech-shaped soliton solution

$$w(x,t)=\frac{w_0}{\cosh^2[\sigma(x-vt)]}, \tag{23}$$

where $v$ is the soliton velocity,

$$w_0=-\frac{3}{2}(v^2-c^2) \tag{24}$$

is the strain amplitude, and

$$\sigma=\sqrt{\frac{3}{\mu_s}(v^2-c^2)} \tag{25}$$

is the inverse width of the soliton. The kink amplitude

$$A=\int_{-\infty}^{\infty}w(z,t)dz=-\sqrt{3\mu_s(v^2-c^2)} \tag{26}$$

vanishes when the soliton velocity nears the speed of sound. Since the Hamiltonian (1) of the system takes the form

$$H=\frac{1}{2}\int_{-\infty}^{\infty}dx\left\{(\partial_t u)^2+c^2(\partial_x u)^2-\frac{\mu_s}{12}(\partial_x^2 u)^2-\frac{2}{3}(\partial_x u)^3\right\}, \tag{27}$$

the energy of the soliton (23) near the speed of sound is

$$H_{\rm sol}\approx\sqrt{3\mu_s}\left(c^2-\frac{\mu_s}{30}\right)(v^2-c^2)^{3/2}. \tag{28}$$

For $s=4$, using the Hilbert transform

$$\mathcal{H}\{f(x)\}=\frac{1}{\pi}\mathrm{P}\int_{-\infty}^{\infty}\frac{f(y)dy}{y-x}, \tag{29}$$

where P denotes the Cauchy principal value, we can rewrite Eq. (14) in the form

$$Q(4,\partial_x)\equiv-\frac{\pi^2}{6}\partial_x^2-\frac{\pi}{6}\mathcal{H}\partial_x^3+\frac{1}{24}\partial_x^4. \tag{30}$$

Thus the equation of motion (9) becomes the Hilbert-Boussinesq equation

$$\left(\partial_t^2-c^2\partial_x^2-\frac{J\pi}{6}\mathcal{H}\partial_x^3\right)w(x,t)+\partial_x^2 w^2(x,t)=0, \tag{31}$$

which can be reduced to the integrable Benjamin-Ono form. Contrary to the former case ($s>5$) this equation is well known to have algebraic soliton solutions

$$w(x,t)=\frac{w_0}{1+\sigma^2(x-vt)^2}, \tag{32}$$

with the soliton velocity $v$, the strain amplitude

$$w_0=-2(v^2-c^2), \tag{33}$$

and the inverse width of the soliton

$$\sigma=\frac{6}{\pi J}(v^2-c^2). \tag{34}$$

In contrast to Eq. (26) for the case $s>5$, the kink amplitude for $s=4$,

$$A=-\frac{\pi^2}{3}J, \tag{35}$$

does not depend on the velocity $v$. Since the Hamiltonian (1) of the system takes the form

$$H=\frac{1}{2}\int_{-\infty}^{\infty}dx\left\{(\partial_t u)^2+c^2(\partial_x u)^2-\frac{J\pi}{6}(\partial_x^2 u)(\mathcal{H}\partial_x u)-\frac{2}{3}(\partial_x u)^3\right\}, \tag{36}$$

the energy of the soliton (32) near the speed of sound is

$$H_{\rm sol}\approx\frac{\pi^2c^2J}{3}(v^2-c^2). \tag{37}$$

In the next section we extend these results and show that the solitonlike solutions have algebraic tails in the entire interval $3<s\leqslant5$.

### III. NONLINEAR EXCITATIONS AT HIGH VELOCITIES

Seeking solutions with a stationary profile $w(z)=w(x-vt)$ ($v$ being the soliton velocity) we can write the equation of motion (7) as follows:

$$v^2\frac{d^2}{dz^2}w(z)+2F(w(z))-F(w(z+1))-F(w(z-1))+\sum_{m\neq z}J_{m-z}(w(z)-w(m))=0. \tag{38}$$

To investigate the asymptotic behavior of solitonlike solutions it is convenient to rewrite Eq. (38) in the form

$$w(z)=\sum_m G(s,v,z-m)\ w^2(m)\equiv\hat{G}\ w^2, \tag{39}$$

where

$$G(s,v,z)=\frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{2[1-\cos(k)]e^{-ikz}dk}{2[1-\cos(k)]+JQ(s,ik)-v^2k^2} \tag{40}$$

is the Green function. For large $|z|$ the main contribution to the integral of Eq. (40) is given by small values of $k$. Hence we can extend the integration over the whole axis and, applying Jordan's lemma and taking into account Eqs. (11)–(15), we can write the Green function (40) for $|z|\gg1$ and $s>5$ as

$$G(s,v,z)=-\frac{1}{2\,(v^2-c^2)\ell_s}e^{-|z|/\ell_s}, \tag{41}$$

where

$$\ell_s=\sqrt{\frac{\mu_s}{12(v^2-c^2)}} \tag{42}$$

is the length scale of the Boussinesq soliton with $\mu_s$ determined by Eq. (22). We are interested in the case when the intensity of the long-range part of the dispersion interaction is small: $J\ll1$ and/or the velocity of the soliton is high: $v\gg c$. In this case the Green function (40) for $3<s\leqslant5$ can be approximately represented in the form (see the Appendix for details)

$$G(s,v,z)=G_S(s,v,z)+G_L(s,v,z), \tag{43}$$

where the short-range part $G_S(s,v,z)$ of the Green function coincides with the Green function (41)–(42) but with

$$\mu_s=1-\frac{J}{2}\frac{s-3}{5-s}\quad\text{for}\ \ 3<s<5, \tag{44}$$

and the long-range part of the Green function has the form

$$G_L(s,v,z)=-\frac{\Gamma(s-2)\ 2^{1-s}\sqrt{\pi}}{\Gamma(s/2)\Gamma((1+s)/2)(v^2-c^2)^2}\times\frac{J}{|z|^{s-2}}\left(1-\frac{\Gamma(s-2,\alpha|z|/\ell_s)}{\Gamma(s-2)}\right), \tag{45}$$

where $\Gamma(s,x)$ is the incomplete gamma function [25].

So, only for $s>5$ does the Green function (40) decay exponentially for $|z|\to\infty$. When $3<s\leqslant5$ only for intermediate distances $|z|$ does the Green function behave in the same way as in the system with short-range dispersion. But for $|z|\to\infty$ the exponential decay is replaced by a power law. This suggests that in the systems with the dispersive parameter $s$ in the interval $3<s\leqslant5$ there are two characteristic length scales: the usual length scale of the Boussinesq soliton $\ell_s$ and the length scale coupled with the existence of the long-range dispersion interaction. Therefore we will seek a solution of Eq. (39) as the sum

$$w(z)=w_S(z)+w_L(z), \tag{46}$$

where $w_S(z)$ is the short-range component of the strain and $w_L(z)$ is the long-range one. Here $w_S(z)$ will dominate the strain in the center, while $w_L(z)$ will dominate in the tails. Inserting Eq. (46) into Eq. (39) yields

$$w_S+w_L=(\hat{G}_S+\hat{G}_L)\ (w_S^2+2\,w_S\,w_L+w_L^2). \tag{47}$$

Assuming that the function $w_S(z)$ satisfies the equation

$$w_S=\hat{G}_S\ (w_S^2+2\,w_S\,w_L) \tag{48}$$

we obtain from Eq. (47) an equation for $w_L(z)$ in the form

$$w_L=\hat{G}_S\ w_L^2\ +\ \hat{G}_L\ (w_S^2+2\,w_S\,w_L+w_L^2). \tag{49}$$

It is seen from Eqs. (41) and (48) that the equation for the short-range component may be represented in an equivalent form

$$-\frac{\mu_s}{12}\partial_z^2w_S(z)+[v^2-c^2+2w_L(z)]w_s(z)+w_S^2(z)=0. \tag{50}$$

We solve Eq. (50) using the multiple-scale method [26] (see [17] for details), and obtain for the short-range component $w_S(z)$ the expression

$$w_S(z)=-\frac{3}{2}[v^2-c^2+2w_L(z)]\times\text{sech}^2\left(\frac{1}{2\ell_s}\int_0^z d\overline{z}\sqrt{1+2\frac{w_L(\overline{z})}{v^2-c^2}}\right). \tag{51}$$

The long-range part of the Green function (45) is proportional to the small parameter $J$. Therefore neglecting terms of the order of $J^n(n>1)$ one can linearize Eq. (49) and write approximately

$$w_L(z)\approx\hat{G}_Lw_S^2\approx\frac{9}{4}(v^2-c^2)^2G_L(s,v,z), \tag{52}$$

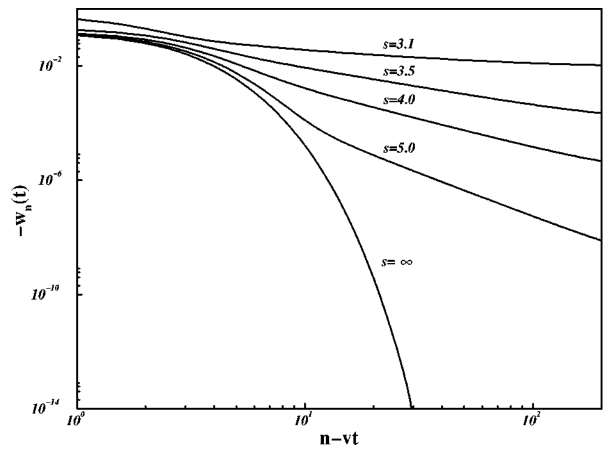


FIG. 1. Plot of minus strain at $J=0.1$ and $v^2-c^2=0.1$ for different $s$ obtained from numerical calculations. The soliton tails have a power dependence vs lattice site for $s\leqslant 5$.

where we also took into account the big difference in the short-range scale $\ell_s$ and the length scale of the long-range part of the Green function $G_L(s,v,z)$. Substituting Eq. (45) into Eq. (52) we see that the asymptotics ($|z|\to\infty$) of the solitons at high velocities and $3<s\leqslant 5$ is given by the expression

$$w(z)\approx-\frac{9\sqrt{\pi}\Gamma(s-2)}{2^{1+s}\Gamma(s/2)\Gamma((s+1)/2)}\frac{J}{|z|^{s-2}}. \tag{53}$$

Thus we can conclude here that only in the case $s>5$ do the tails of the solitons have the usual exponential form. In the systems with long-range harmonic interactions with $3<s\leqslant 5$ the solitons have algebraic tails. Figure 1 shows the long-distance behavior of soliton tails for different values of the range parameter $s$. It is seen that the form of the tails predicted by Eq. (53) is in good agreement with the results of numerical simulations described in Sec. V. Moreover, Fig. 2 shows a good fit of Eq. (53) to the numerically calculated

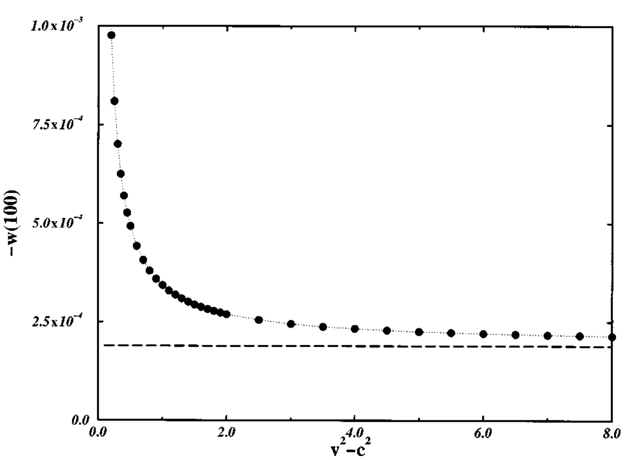


FIG. 2. Amplitude in the soliton tail at a range of 100 lattice sites for $J=0.1$ and $s=3.3$ obtained from numerical calculations (circles) and its analytical high-velocity limit (dashed line) from Eq. (53).

amplitudes of the soliton tails. It is worth remarking that for $3<s\leqslant 5$ the amplitude of the soliton tails tends to a nonzero value at high velocities.

## IV. VARIATIONAL APPROACH

In what follows we shall develop a variational approach to the investigation of the qualitative characteristics of the solitons under consideration. It was shown in the preceding section that the long-distance behavior of $u(z)$ depends on the value of the dispersive parameter $s$. Only for $s>5$ are the tails of $u(z)$ exponential while for $s<5$ the tails are algebraic. But the behavior for intermediate distances is described by the sech-like function (51) which smoothly depends on the dispersive parameter $s$. This suggests looking for an approximate description of the system in the framework of variational approach with the trial function in the form

$$u_n(t)=\frac{1}{2}A(1-e^{-2\sigma|n-x(t)|})\,\theta(n-x(t)), \tag{54}$$

where

$$\theta(x)=\begin{cases}1 & \text{for } x>0\\ -1 & \text{for } x<0.\end{cases} \tag{55}$$

In other words, we suppose here that the main contribution is due to the short-range exponential-like part $u_s(z)$ of the solution. This assumption is confirmed by the good agreement between the results of variational approach and the numerical calculations.

Substituting Eq. (54) into the Lagrangian

$$L=T-U_{NN}-U_{LR}, \tag{56}$$

we arrive at some effective Lagrangian $L(x,\dot{x})$. In principle, such Lagrangians demonstrate two qualitatively different types of motion, namely, a pinning of the excitation at some particle and a moving of the excitation along the chain. But in our case, considering the supersonic solitons, we may restrict ourselves to the second case only. To be specific, let us consider a soliton moving with an average velocity $v>c$. Thus the time dependent parameter $x(t)$ allows the form $x(t)=vt+\eta(t)$ where an average value of $\eta$ $[0\leqslant\eta(t)<1]$ equals $\frac{1}{2}$. We are interested now only in the average parameters of the soliton motion, which can be obtained from minimizing the action

$$S=\frac{1}{T}\int_0^T dt L(x,\dot{x})=\frac{1}{T}\int_{x(0)}^{x(T)}\frac{dx}{\dot{x}}L(x,\dot{x})$$
$$\simeq\frac{1}{vT}\int_{x(0)}^{x(T)}dx L(x,v)=\frac{1}{v}\langle L\rangle, \tag{57}$$

where the angle brackets denote the average value

$$\langle f(t)\rangle=\int_0^1 d\eta f(\eta). \tag{58}$$

The kink amplitude $A$ and the inverse width of the soliton, $\sigma$, are the variational parameters to be determined as func tions of the soliton velocity $v$. Substituting Eq. (54) into Eqs. (2) and (3) we get

$$T=\frac{1}{2}A^2\sigma^2\frac{\cosh[2\sigma(1-2\eta)]}{\sinh(2\sigma)}\left(\frac{dx}{dt}\right)^2 \tag{59}$$

and

$$U_{NN}=\frac{1}{2}A^2\left(e^{-2\sigma}\frac{\sinh^2(\sigma)}{\sinh(2\sigma)}\cosh[2\sigma(1-2\eta)] + \{1-e^{-\sigma}\cosh[\sigma(1-2\eta)]\}^2\right) - \frac{1}{3}A^3\left(e^{-3\sigma}\frac{\sinh^3(\sigma)}{\sinh(3\sigma)}\cosh[3\sigma(1-2\eta)] + \{1-e^{-\sigma}\cosh[\sigma(1-2\eta)]\}^3\right). \tag{60}$$

To calculate the long-range part of the potential energy (5) we use the discrete Fourier transform

$$\tilde{u}(k)=\sum_n e^{ikn}u_n, \quad u_n=\frac{1}{2\pi}\int_{-\pi}^{\pi}e^{-ikn}\tilde{u}(k)dk, \tag{61}$$

which allows us to rewrite Eq. (5) in the form

$$U_{LR}=\frac{J}{4\pi}\int_{-\pi}^{\pi}dk|\tilde{u}(k)|^2Q(s,ik), \tag{62}$$

where the spectrum function $Q(s,ik)$ is defined by Eq. (10). Using

$$|\tilde{u}(k)|^2=\frac{1}{4}A^2\left(\frac{2}{1-\cos(k)}-\frac{4\cosh(\sigma)\cosh[\sigma(1-2\eta)]}{\cosh(2\sigma)-\cos(k)} + \frac{1+\cosh(2\sigma)\cosh[2\sigma(1-2\eta)]-\{\cosh(2\sigma)+\cosh[2\sigma(1-2\eta)]\}\cos(k)}{[\cosh(2\sigma)-\cos(k)]^2}\right), \tag{63}$$

we obtain for the long-range part of the potential energy

$$U_{LR}=\frac{1}{4}JA^2\left(2\zeta(s-1)+F(e^{-2\sigma},s-1) - \frac{4\cosh(\sigma)\cosh[\sigma(1-2\eta)]-\cosh[2\sigma(1-2\eta)]}{\sinh(2\sigma)} \times[\zeta(s)-F(e^{-2\sigma},s)]\right), \tag{64}$$

with $F(z,s)$ being Jonqière's function

$$F(z,s)=\sum_{n=1}^{\infty}\frac{z^n}{n^s}. \tag{65}$$

To find out an extremum of the action we need only the time-average values of the kinetic and potential energies. They have much simpler forms

$$\langle T\rangle=\frac{1}{4}A^2\sigma v^2, \tag{66}$$

$$\langle U_{NN}\rangle=\frac{1}{2}A^2\left(1+\frac{1}{2}e^{-2\sigma}-\frac{3}{4\sigma}(1-e^{-2\sigma})\right) - \frac{1}{3}A^3\left(1+\frac{3}{2}e^{-2\sigma}-\frac{1}{8\sigma}(9-8e^{-2\sigma}-e^{-4\sigma})\right), \tag{67}$$

and

$$\langle U_{LR}\rangle=\frac{1}{4}JA^2\left(2\zeta(s-1)-\frac{3}{2\sigma}[\zeta(s)-F(e^{-2\sigma},s)] + F(e^{-2\sigma},s-1)\right). \tag{68}$$

Finally, their derivatives with respect to $\sigma$ are

$$\frac{d}{d\sigma}\langle U_{NN}\rangle=\frac{1}{8\sigma^2}A^2[3-(3+6\sigma+4\sigma^2)e^{-2\sigma}] - \frac{1}{24\sigma^2}A^3[9-8(1+2\sigma+3\sigma^2)e^{-2\sigma} - (1+4\sigma)e^{-4\sigma}] \tag{69}$$

and

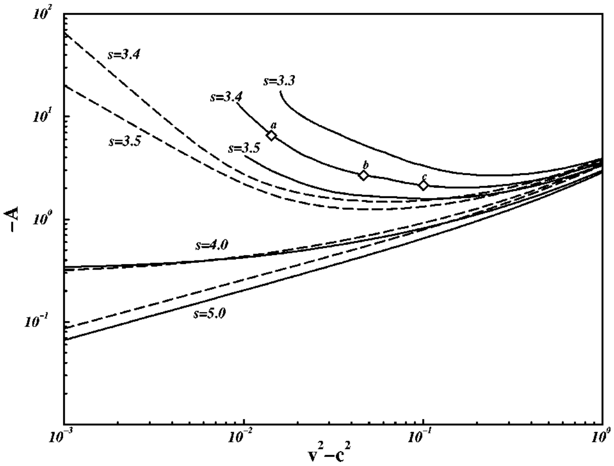


FIG. 3. Kink amplitude $A$ vs velocity $v$ for $J=0.1$ and different $s$ obtained from the variational approach with exponential trial function (dashed lines) and from numerical calculations (full lines).

$$\frac{d}{d\sigma}\langle U_{LR}\rangle=\frac{3}{8\sigma^2}JA^2\bigg(\zeta(s)-F(e^{-2\sigma},s)-2\sigma F(e^{-2\sigma},s-1)-\frac{4}{3}\sigma^2F(e^{-2\sigma},s-2)\bigg). \tag{70}$$

Thus one can now find the parameters $A$ and $\sigma$ solving the following equations minimizing the action:

$$\frac{\partial}{\partial\sigma}\langle L\rangle=0 \quad \text{and} \quad \frac{\partial}{\partial A}\langle L\rangle=0, \tag{71}$$

where $\langle L\rangle=\langle T\rangle-\langle U_{NN}\rangle-\langle U_{LR}\rangle$. In Figs. 3 and 4 we plot the dependences of the kink amplitude and energy vs soliton velocity $v$ for solutions of Eqs. (71) at different values of the long-range parameter $s$. The results of numerical calculations described in Sec. V are sketched along with it. One can see the good (for $s\geq 3.3$) qualitative agreement between the results of the variational approach and numerical calculations.

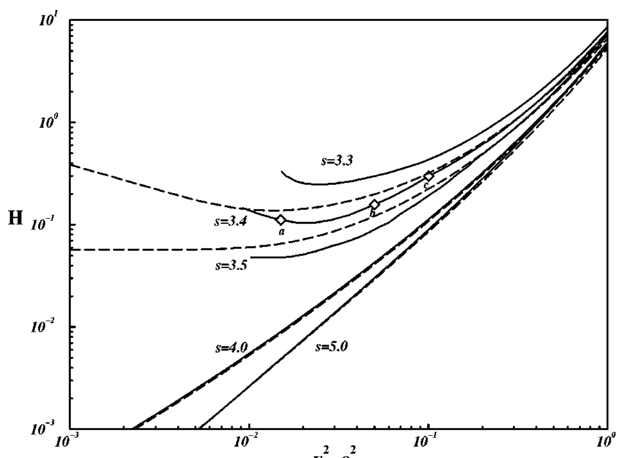


FIG. 4. Soliton energy $H$ vs velocity $v$ for $J=0.1$ and different $s$ obtained from the variational approach with exponential trial function (dashed lines) and from numerical calculations (full lines).

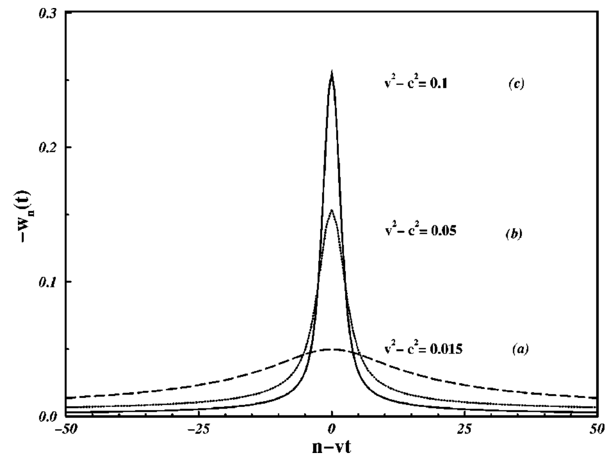


FIG. 5. Soliton forms for $J=0.1$, $s=3.4$ and three different velocities obtained from the numerical calculations: (a) $v^2-c^2=0.015$, (b) $v^2-c^2=0.05$, and (c) $v^2-c^2=0.1$. These solitons are indicated in Figs. 3 and 4 as diamonds.

Using the following form of Jonqière's function:

$$F(e^{-\alpha},s)=\Gamma(1-s)\alpha^{s-1}+\sum_{l=0}^{\infty}\zeta(s-l)\frac{(-\alpha)^l}{l!} \tag{72}$$

we can find that in the limit of wide solitons (that is, small $\sigma$) the dependence of variational parameters versus velocity takes on the form

$$\sigma=\left(\frac{3}{5\mu_s}(v^2-c^2)\right)^{1/2}$$

and

$$A=-\left(\frac{27\mu_s}{5}(v^2-c^2)\right)^{1/2} \quad \text{for } s>5, \tag{73}$$

$$\sigma=\left(\frac{v^2-c^2}{2^{s-2}\Gamma(1-s)(s-4)(3s-10)J}\right)^{1/(s-3)} \quad \text{and}$$
$$A=-\frac{9(s-3)}{2(3s-10)}\frac{(v^2-c^2)}{\sigma} \quad \text{for } 3<s<5, \tag{74}$$

where $\mu_s=1+J\zeta(s-4)$. It is important that at $s<3.5$ the soliton energy grows,

$$H_{\text{sol}}\sim A^2\sigma\sim(v^2-c^2)^{(2s-7)/(s-3)}, \tag{75}$$

when the soliton velocity approaches that of sound. One can see from Fig. 4 that in this case the soliton energy does not vanish at any velocity and there is an energy gap between the spectra of plane waves and solitons.

In Fig. 5 we plot the shapes of the solitons at three different velocities indicated as diamonds in Figs. 3 and 4. The characteristic property of these solitons is a slow decay of the soliton tails discussed in detail in Sec. III.

## V. NUMERICAL METHOD

In this section we develop a numerical scheme for seeking solitary solutions of Eq. (38). There are several effective methods for this purpose; among those which have enjoyed the widest application are spectral [27–29] and discrete functional minimization [30,31] methods. For our system dealing with dispersive long-range interactions the most effective method must be a spectral one.

To be specific, the method we use is a combination of the methods [27,28]. Let us look for solutions of Eq. (38) with period $2M$: in the large $M$ limit we expect to get good approximations to solitary waves which have infinite period. The equation of motion (38) is symmetric with respect to the transformation $z\to -z$. Hence, the solution $w(z)$ can be chosen to be symmetric about the point $z=0$ and may be represented by an infinite cosine series. But to obtain the approximate solution numerically, we must cut off the series. It is known from the harmonic approximation theory that the best approximation of $w(z)$ is given by the function

$$W(z)=\frac{1}{2}\widetilde{W}(0)+\sum_{j=1}^{N}\widetilde{W}(k_j)\cos(k_j z), \tag{76}$$

where

$$\widetilde{W}(k_j)=\frac{2}{2N+1}\sum_{r=-N}^{N}W(z_r)\cos(k_j z_r), \tag{77}$$

and

$$k_j=\frac{2\pi p}{2N+1}j,\quad z_r=\frac{r}{p},\quad N=Mp-\frac{1}{2}. \tag{78}$$

The parameter $p$ may be arbitrary, but $Mp$ must be half integer to get integer $N$. Applying the Fourier transform (76) to the equation of motion (38) leads to

$$[v^2k_j^2-JQ(s,ik_j)]\widetilde{W}(k_j)-2[1-\cos(k_j)]\widetilde{F}(k_j)=0 \quad \text{for } j=1,\,2,\,\ldots,N, \tag{79}$$

where

$$\widetilde{F}(k_j)=\widetilde{W}(k_j)-\frac{2}{2N+1}\sum_{r=-N}^{N}W^2(z_r)\cos(k_j z_r). \tag{80}$$

To complete the set of equations we need another equation. For $s>3$, multiplying both sides of Eq. (38) by $z^2$ and integrating by parts, we get

$$[v^2-J\zeta(s-2)]\widetilde{W}(0)-\widetilde{F}(0)=0. \tag{81}$$

Equations (79)–(81) are nonlinear in the unknowns $\widetilde{W}(k_j)$ and are solved by a quadratically convergent Newton-Raphson iteration. Usually convergence to the solutions of Eqs. (79)–(81) up to machine round-off at each step is reached during 8–12 iterations. The size of the system $N$ varied between 75 and 500 and the parameter $p$ varied between 3 and 0.1, correspondingly.

In order to check the stability of the solutions found we have used them as initial conditions to the equations of motion (7), which were integrated by an eighth order Runge-Kutta scheme with the step size control [32].

## VI. SUMMARY AND CONCLUSIONS

We investigated the effect of harmonic power-law long-range interactions in a chain with anharmonic nearest-neighbor interactions. We have demonstrated that the power-law LRI's lead to a drastic change of the soliton properties. Namely, we arrive at the Boussinesq equation only for $s>5$ but, for example, for $s=4$ the dynamics of nonlinear excitations is governed by the Benjamin-Ono equation which is well known to possess algebraic soliton solutions. Generally, for $s>5$ the soliton tails are exponential while for $3<s\leqslant 5$ they are algebraic. Unlike NNI or Kac-Baker LRI the energy of the soliton excitations for $s\leqslant 3.5$ does not vanish at velocities close to that of sound. On the contrary, there is an energy gap between spectra of plane waves and soliton states.

## ACKNOWLEDGMENTS

Two of the authors (Yu.G. and S.M.) are grateful for the hospitality of the University of Bayreuth where the major part of this work was done. Partial support was provided by Project No. X 271.5 of scientific and technological cooperation between Germany and Ukraine, and from the Ukrainian Fundamental Research Foundation (Grant No. 2.4/355).

## APPENDIX

The long-distance behavior of nonlinear excitations is determined by the Green function

$$G(s,v,z)=\frac{1}{2\pi}\int_{-\pi}^{\pi}\frac{2[1-\cos(k)]e^{ikz}dk}{2[1-\cos(k)]+JQ(s,ik)-v^2k^2}, \tag{A1}$$

where the dispersion function $Q(s,ik)$ is given by Eq. (10). For large $|z|$ the main contribution to the integral in the left-hand side of Eq. (A1) is due to small $k$. Hence we can extend the integration over the whole axis and taking into account that in the $k\to 0$ limit the dispersion function $Q(s,ik)$ for $s>3$ has the form given by Eq. (13), write the Green function as

$$G(s,v,z)=-\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{e^{ikz}dk}{v^2-c^2+J\nu_s|k|^{s-3}+\frac{1}{12}\mu_s k^2}, \tag{A2}$$

where

$$\mu_s=\begin{cases}1+J\zeta(s-4) & \text{for } s>5\\ 1-\dfrac{J}{2}\dfrac{s-3}{5-s} & \text{for } 3<s<5\end{cases} \tag{A3}$$

is the dispersion parameter. We consider the cases (i) when $3<s<5$ and $\mu_s>0$, and (ii) when $s\simeq 5$ and $\mu_s<0$ separately.

(i) It is useful to represent the Green function (A2) in the form

$$G(s,v,z)=-\sqrt{\frac{12}{\mu_s(v^2-c^2)}}\,I_s,$$

$$I_s=\frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{e^{iqx}dq}{1+\epsilon\ \sec(\pi s/2)|q|^{s-3}+q^2},\tag{A4}$$

where

$$\epsilon=\frac{J}{\ell_s^{s-3}(v^2-c^2)}\frac{2^{1-s}\pi^{3/2}}{\Gamma(s/2)\Gamma((s+1)/2)},$$

$$x=z/\ell_s,\quad q=\ell_s k\tag{A5}$$

wheretheabbreviation

$$\ell_s=\sqrt{\frac{\mu_s}{12(v^2-c^2)}}\tag{A6}$$

was used. To evaluate the integral $I_s$ we use Jordan's lemma with the contour in the upper right quarter of the complex $q$ plane. Thus taking into account that inside the contour the function $1/[1+\epsilon\ \sec(\pi s/2)q^{s-3}+q^2]$ for $s<5$ has no poles, we obtain

$$I_s=\frac{1}{\pi}\ \mathrm{Re}\int_0^{\infty}\frac{e^{iqx}dq}{1+\epsilon\ \sec(\pi s/2)q^{s-3}+q^2}$$
$$=\frac{1}{\pi}\ \mathrm{Im}\int_0^{\infty}\frac{e^{-q|x|}dq}{1-q^2+\epsilon\ \sec(\pi s/2)q^{s-3}\ \exp\{-i(\pi/2)(s-3)\}}=\frac{1}{\pi}\int_0^{\infty}e^{-q|x|}f_s(q)dq,\tag{A7}$$

where the notation

$$f_s(q)=\frac{\epsilon q^{s-3}}{\{1-q^2-\epsilon q^{s-3}\ \tan[(\pi/2)\,s]\}^2+\epsilon^2q^{2(s-3)}}\tag{A8}$$

was used. We are interested in the case when the intensity of the long-range part of the dispersion interaction is small: $J\ll 1$ and/or the velocity of the soliton is high: $v\gg c$. In this case the parameter $\epsilon$ is small and the function $f_s(q)$ has a sharp maximum at $q\simeq 1$. In its turn the function $e^{-q|x|}f_s(q)$ has two maxima at $q\sim 1/|x|$, and $q\simeq 1$ and a minimum at $q=\alpha\leqslant 1$ whose position in the limit of small $\epsilon$ is almost independent of $x$. This suggests representing the integral $I_s$ as the sum

$$I_s=I_s^{(1)}+I_s^{(2)},$$

$$I_s^{(1)}=\frac{1}{\pi}\int_0^{\alpha}e^{-q|x|}f_s(q)dq,\tag{A9}$$

$$I_s^{(2)}=\frac{1}{\pi}\int_{\alpha}^{\infty}e^{-q|x|}f_s(q)dq.$$

When $q\in(0,\alpha)$ the function $f_s(q)$ can be expanded into a power series and the integral $I_s^{(1)}$ can be represented in the form

$$I_s^{(1)}\approx\frac{1}{\pi}\epsilon\int_0^{\alpha}e^{-q|x|}q^{(s-3)}dq$$
$$=\frac{\epsilon\Gamma(s-2)}{\pi|x|^{(s-2)}}\left(1-\frac{\Gamma(s-2,\alpha|x|)}{\Gamma(s-2)}\right),\tag{A10}$$

where $\Gamma(s,x)$ is the incomplete gamma function [25]. In the interval $q\in(\alpha,\infty)$ the function $f_s(q)$ has a $\delta$-function-like form and the integral $I_s^{(2)}$ can be approximated as

$$I_s^{(2)}\approx\int_{\alpha}^{\infty}e^{-q|x|}\delta(q^2-1)dq=\frac{1}{2}e^{-|x|}+O(e^{-(1+\alpha)|x|}).\tag{A11}$$

From Eqs. (A2), (A5), (A10), and (A11) we obtain that the Green function (A1) for $3<s<5$ can be approximately represented as the sum

$$G(s,v,z)=G_S(s,v,z)+G_L(s,v,z),\tag{A12}$$

where

$$G_S(s,v,z)=-\frac{1}{2(v^2-c^2)\ell_s}e^{-|z|/\ell_s},\tag{A13}$$

$$G_L(s,v,z)=-J\sqrt{\pi}\frac{\Gamma(s-2)2^{1-s}}{\Gamma(s/2)\Gamma((1+s)/2)}\frac{1}{(v^2-c^2)^2}$$
$$\times\frac{1}{|z|^{s-2}}\left(1-\frac{\Gamma(s-2,\alpha|z|/\ell_s)}{\Gamma(s-2)}\right)\tag{A14}$$

are the short-range part and the long-range part of the Green function, respectively.

(ii) Let us consider now the case $s=5$. In accordance with Eq. (10) the Green function (A2) has the form

$$G(5,v,z) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} \frac{e^{ikz}dk}{v^2 - c^2 - (J/12)k^2 \ln(|k|) + \frac{1}{12}k^2}. \tag{A15}$$

Applying Jordan's lemma we get

$$G(5,v,z) = -\frac{1}{\pi}\,\mathrm{Im}\int_0^{\infty} \frac{e^{-k|z|}dk}{v^2 - c^2 + (J/12)k^2[\ln(k) + i\pi/2] - \frac{1}{12}k^2}. \tag{A16}$$

In the limit of small $J$ we again can split the integral in the left-hand side of Eq. (A16) in the same way as was done-above and obtain that the Green function (A15) can be written as the sum (A12) with the short-range component $G_S(5,v,z)$ in the form

$$G_S(5,v,z) = -\sqrt{\frac{3}{v^2 - c^2}}\exp[-|z|\sqrt{12(v^2 - c^2)}]. \tag{A17}$$

The long-range component $G_L(5,v,z)$ is determined by Eq. (A14) with $s=5$.


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