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Effect of nonlocal dispersion on self-interacting excitations

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Abstract

The dynamics of self-interacting quasiparticles in 1D systems with long-range dispersive interactions is expressed in terms of a nonlocal nonlinear Schrödinger equation. Two branches of stationary solutions are found. The new branch which contains a cusp soliton is shown to be unstable and blowup is observed. Moving solitons radiate with a wavelength proportional to the velocity.

The basic dynamics of deep water and plasma waves, light pulses in nonlinear optics and charge and energy transport in condensed matter and biophysics [1] is described by the fundamental nonlinear Schrödinger (NLS) equation

$$\mathrm{i}\psi_t + \psi_{xx} + |\psi|^2\psi = 0. \tag{1}$$

In the continuum theory of charge (energy) transfer, $\psi(x, t)$ is the wave function of the carriers. The nonlinear term, $|\psi|^2\psi$, represents a self-interaction of the quasiparticle and the second space derivative, ψ_{xx}, describes its dispersion in the effective mass approximation. Thus the characteristic width of the excitation [1,2] is assumed larger than the distance between the atoms (molecules) when the nearest-neighbor approximation for the quasi-particle transfer is used. However, realistic transfer mechanisms are not short range. The excitation transfer in molecular crystals [2] and the vibron energy transport in biopolymers [3] are due to transition dipole–dipole interactions, which have a relatively slow dependence on the distance. In systems where the dispersion curves of two elementary excitations are close or intersect, effective long-range transfer occurs at the cost of the coupling between the excitations. Such a situation arises for excitons and photons in semiconductors and molecular crystals. In vibrational molecular spectra where Fermi resonance occurs important nonlocal effects are caused by the Coulomb interactions between charged regions of molecules. Only recently, effects of long-range interactions were studied in nonlinear lattice dynamics [4–6] and static, dynamic and thermodynamic nonlinear Klein–Gordon models [7–13].

In order to investigate the dynamics of self-interacting quasiparticles in 1D-systems with long-range

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dispersive interactions we consider the Hamiltonian

$$H = -\int_{-\infty}^{\infty}\left\{\tfrac{1}{2}|\psi(x,t)|^4 + \int_{-\infty}^{\infty} J(x-y)\left[\psi^*(x,t)\psi(y,t) - |\psi(x,t)|^2\right] \mathrm{d}y\right\} \mathrm{d}x \tag{2}$$

and the corresponding Lagrangian

$$L = \frac{\mathrm{i}}{2}\int_{-\infty}^{\infty}\left[\psi^*(x,t)\partial_t\psi(x,t) - \text{c.c.}\right] \mathrm{d}x - H. \tag{3}$$

The double integral in Eq. (2) describes the excitation transfer in the system. The matrix element of transfer, $J(x)$, is chosen to be of the Kac–Baker form $J(x) = J\exp(-\alpha|x|)$ with α being the inverse radius of interaction, and J its intensity. The equation of motion for the excitation wave function then becomes the nonlocal nonlinear Schrödinger equation

$$\mathrm{i}\partial_t\psi + \int_{-\infty}^{\infty} J(x-y)\left[\psi(y,t) - \psi(x,t)\right] \mathrm{d}y + |\psi|^2\psi = 0. \tag{4}$$

The kernel $J(x)$ in this integro-differential equation is the Green function given by the equation $(\partial_x^2 - \alpha^2)J(x) = -2J\alpha\delta(x)$. As a consequence Eq. (4) may be rewritten as

$$\mathrm{i}\partial_t\psi + \frac{2J}{\alpha}\frac{\partial_x^2}{\alpha^2 - \partial_x^2}\psi + |\psi|^2\psi = 0. \tag{5}$$

The linear part of Eq. (5) corresponds to the dispersion law $\omega(k) = (2J/\alpha)k^2/(\alpha^2 + k^2)$. For $\alpha = 1.58$ and $J = 2.06$ this dispersion law agrees, in the interval $k \in [0, \pi]$ (within 5%) with the discrete model excitation dispersion law, $\omega_d(k) = \Sigma_{n=1}(1/n^3)[1 - \cos(kn)]$, corresponding to dipole–dipole interaction. Thus Eq. (5) can be considered as an improved continuum approximation for self-trapping excitations with a dipole–dipole dispersive interaction. When the characteristic length scale of the excitations is large compared with the radius of the dispersive interaction (i.e. $\alpha \to \infty$, $J \to \infty$, $J\alpha^{-3} \to \text{const}$) Eq. (5) reduces to the NLS equation (1). However, if the width of the excitations and the radius of interaction, α^{-1}, are of the same order, the nonlocal effects represented by the pseudo-differential operator in Eq. (5) become important.

Rescaling variables $z = \alpha x$, $\tau = (2J/\alpha)t$, $\phi(z,\tau) = \sqrt{\alpha/2J}\,\psi(x,t)$ we obtain instead of Eq. (5)

$$\mathrm{i}\partial_\tau\phi + \frac{\partial_z^2}{1 - \partial_z^2}\phi + |\phi|^2\phi = 0, \tag{6}$$

and

$$\int_{-\infty}^{\infty} |\phi(z,\tau)|^2 \,\mathrm{d}z = \frac{\alpha^2}{2J}N \equiv \mathcal{N}, \tag{7}$$

where N, the excitation number, like the Hamiltonian, H, is an integral of motion. Stationary solutions to Eq. (6) in the form

$$\phi = \frac{b}{\sqrt{b^2 - 1}}F(z, b)\exp(\mathrm{i}\lambda^2\tau), \tag{8}$$

where λ is a spectral parameter and with $b = \lambda^{-1}\sqrt{\lambda^2 + 1}$ being the width of the solution. Here F must satisfy $(\mathrm{d}^2/\mathrm{d}z^2)(F - F^3) - Fb^{-2} + F^3 = 0$. Under the boundary conditions $F(\xi) \to 0$ for $\xi \to \pm\infty$ this equation has the solution

$$\exp\left(\frac{2z}{b}\right) = \frac{F_1 + F_2\mu}{F_1 - F_2\mu}\left(\frac{1-\mu}{1+\mu}\right)^{3/b}, \tag{9}$$

where

$$F_{\frac{1}{2}}^2 = \frac{1}{b^2}\left[\frac{b^2+3}{4} \mp \sqrt{\left(\frac{b^2+3}{4}\right)^2 - b^2}\right]$$

and $\mu = (F_1^2 - F^2)^{1/2}(F_2^2 - F^2)^{-1/2}$. The solution given by Eq. (9) exists only at $b \geqslant 3$ $(\lambda^2 \leqslant \frac{1}{8})$. Introducing Eq. (9) into Eq. (7) we get

$$\mathcal{N} = \frac{1}{b^2 - 1}\left[3b + \frac{b^2 - 9}{8}\ln\left(\frac{b^2 + 4b + 3}{b^2 - 4b + 3}\right)\right]. \tag{10}$$

Fig. 1 shows that the stationary solution exists only for $\mathcal{N} \leqslant \mathcal{N}_{\max} \simeq 1.128$, or $N \leqslant N_{\max} \simeq 2.255J\alpha^{-2}$. Thus in contrast to the usual NLS equation which has stationary solutions for any excitation numbers the nonlocal NLS equation has stationary solutions only in a finite interval of $\mathcal{N} \in [0, \mathcal{N}_{\max}]$. $\mathcal{N}_{\max}$

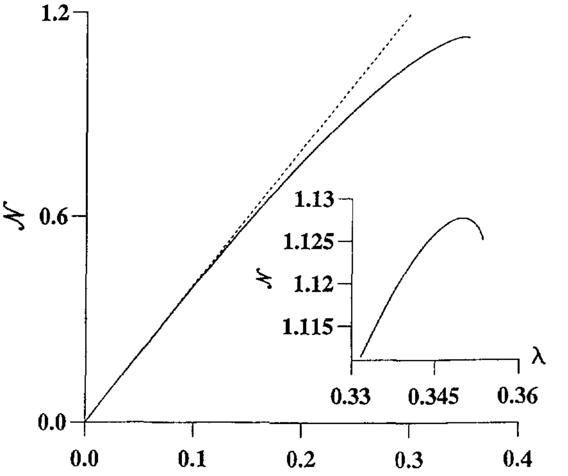

Fig. 1. Excitation number, $\mathcal{N}$, versus spectral parameter, λ, for the stationary solutions. Dashed line: NLS equation (1). Solid line: nonlocal NLS, equation (6). The inset shows the two branches at the maximal excitation number. The endpoint corresponds to the cusp soliton.

tends to infinity in the limit of the usual NLS. Fig. 1 shows that when the excitation number $\mathcal{N}$ varies in the interval $[1.125, \mathcal{N}_{max}]$ there are two values of λ, for a given $\mathcal{N}$, i.e. two branches of stationary solutions exist in that interval. The first branch corresponds to the part of the $\mathcal{N}(\lambda)$ for which $d\mathcal{N}/d\lambda > 0$ and it exists for any $\mathcal{N} \leqslant \mathcal{N}_{max}$. For $\mathcal{N} \ll \mathcal{N}_{max}$ ($\lambda \ll 1/\sqrt{8}$) the solution reduces to $F = \sqrt{2}b^{-1}\,\mathrm{sech}(z/b)$ such that it coincides with the stationary solution of the usual NLS equation. The second branch with $d\mathcal{N}/d\lambda < 0$ exists only in the interval $[1.125, \mathcal{N}_{max}]$. Fig. 1 shows that the effect of nonlocal dispersion starts to be important for $\mathcal{N} > 0.5\mathcal{N}_{max}$ or $N > (J/\alpha^2)\mathcal{N}_{max}$. For dipole–dipole coupling we get the condition $N > 2.06/1.58^2\mathcal{N}_{max} \simeq 0.93$, which may be fulfilled in physical systems. For example for nonlinear excitations of Scheibe aggregates, where our estimations give an excitation number of more than 10 [14]. At $\mathcal{N} = \mathcal{N}_{cusp} = 1.125$ we obtain from Eq. (9) a cusp soliton of the form $\phi(z, \tau) = (3/8)^{1/2}\exp(i\tau/8 - \frac{1}{3}|z|)$. A similar solution was first found in the theory of shallow water waves [15]. Recently it was obtained in Ref. [12] as a static solution of the nonlocal Klein–Gordon equation. However, an investigation of the stability of the solution is needed.

For this purpose we use the trial function

$$\phi(z, \tau) = \exp\left[i\lambda^2\tau + i\sigma(\tau)z^2\right]\frac{\beta}{\sqrt{\beta^2 - 1}} \times\sqrt{\frac{\mathcal{N}(b)}{\mathcal{N}(\beta)}}\,F(z, \beta), \tag{11}$$

where $\sigma(\tau)$ and $\beta(\tau)$ are time dependent variational parameters. The functions $F(z, \beta)$ and $\mathcal{N}(\beta)$ are defined by Eqs. (9) and (10), respectively. For $\sigma = 0$, $\beta = b$ our test function reduces to the stationary solution. Introducing Eq. (11) into the Lagrangian Eq. (3) we obtain an effective action for the variational parameters σ and β. Using the Euler–Lagrange equations a lengthly but straightforward calculation shows that $\ln|\beta - b| \propto -(d\mathcal{N}/d\lambda)t$. Thus the stationary point $\sigma = 0$, $\beta = b$ is unstable for $d\mathcal{N}/d\lambda < 0$, i.e. the solitons of the second branch, and in particular, the cusp soliton are unstable. Using a slightly perturbed stationary solution of the two branches as initial condition the numerical integration of Eq. (6) shown in Figs. 2a and 2b exhibits oscillatory and blowup behavior, respectively, as indicated by our analysis. The oscillatory

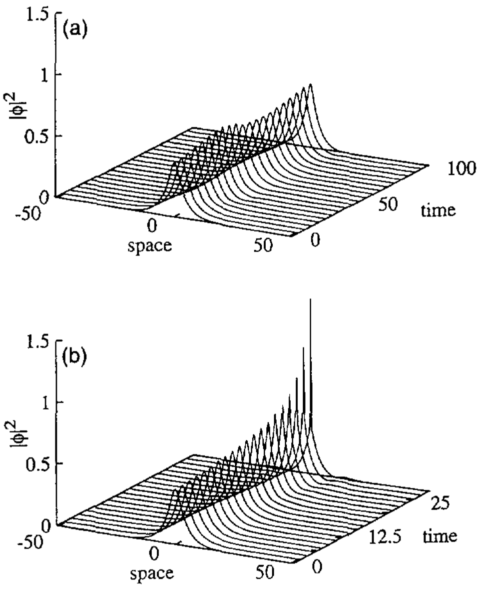

Fig. 2. Dynamical behavior of solutions to nonlocal NLS. Eq. (6) for initial conditions given by Eq. (9) with slightly perturbed amplitude. (a) Stable branch, $\lambda = 0.279$; (b) unstable branch, $\lambda = 0.352$.

behavior indicates stability of the soliton of the first branch.

Since the usual NLS equation is Galilean invariant the solitons can move without changing their shape and velocity. This is not the case for the nonlocal NLS equation. To investigate propagating solutions we introduce the moving frame of reference in which the center of mass of the excitation is at rest: $\xi = z - v\tau$, $\bar{\tau} = \tau$

$$\phi(z, \tau) = \varphi(\xi, \bar{\tau}) \exp\left(\tfrac{1}{2}\mathrm{i}v\xi + \mathrm{i}\lambda^2\bar{\tau} + \tfrac{1}{4}\mathrm{i}v^2\bar{\tau}\right), \tag{12}$$

where v is the velocity. Applying this set of transformations to Eq. (6) we obtain for small velocities v

$$\mathrm{i}\partial_{\bar{\tau}}\varphi - \frac{\lambda^2\left(1 - \partial_\xi^2\right) - \left(1 + \mathrm{i}v\partial_\xi\right)\partial_\xi^2}{1 - \mathrm{i}v\partial_\xi - \partial_\xi^2}\varphi + |\varphi|^2\varphi = 0. \tag{13}$$

Following Kuehl and Zhang [16] we use the Fourier transform $\varphi^{\mathrm{F}}(k, \tau) = \int_{-\infty}^{\infty} \exp(\mathrm{i}k\xi)\varphi(\xi, \tau)\,\mathrm{d}\xi$, and convert Eq. (13) into

$$\mathrm{i}\partial_\tau\varphi^{\mathrm{F}}(k, \tau) - \omega_v(k)\varphi^{\mathrm{F}}(k, \tau) + NL(k, \tau) = 0, \tag{14}$$

where $\omega_v(k) = [\lambda^2(1 + k^2) + (1 + vk)/k^2]/(1 - vk + vk^2)$, the dispersion law in the moving frame of reference, and $NL(k, \tau) \equiv \int_{-\infty}^{\infty} \exp(\mathrm{i}k\xi)|\varphi(\xi, \tau)|^2\varphi(\xi, \tau)\,\mathrm{d}\xi$ is introduced.

The equation $\omega_v(k) = 0$ has the real root $k = k_{\mathrm{r}} \simeq -(\lambda^2 + 1)/v$ for small v. The existence of the root $k = k_{\mathrm{r}}$ means [16,17] that a wave with wavenumber k_{r} will be resonantly excited by a soliton, forming an oscillatory tail.

We introduce $\varphi(\xi, \tau) = \phi_0(\xi) + f(\xi, \tau)$ where $\phi_0(\xi)\exp(\mathrm{i}\lambda^2\tau)$ is the stationary solution given by Eq. (8) and the function $f(\xi, \tau)$ describes the change of the shape of the soliton and the radiation. We obtain for the Fourier transform of $f(\xi, \tau)$

$$\begin{aligned}
&\mathrm{i}\partial_\tau f^{\mathrm{F}} - \omega_v(k) f^{\mathrm{F}} \\
&\quad= \left[\omega_v(k) - \omega_{v=0}(k)\right]\phi_0^{\mathrm{F}}(k) \\
&\qquad - \int_{-\infty}^{\infty} \exp(\mathrm{i}k\xi)\Big[\phi_0^2(2f + f^*) \\
&\qquad + \phi_0\left(f^2 + 2|f|^2\right) + |f|^2 f\Big]\,\mathrm{d}\xi.
\end{aligned} \tag{15}$$

In the resonant region $k \simeq k_{\mathrm{r}}$, we neglect nonlinear terms in Eq. (15) as was done in Refs. [16–19] and use $\omega_v(k) \simeq v(k - k_{\mathrm{r}})$, $[\omega_v(k) - \omega_{v=0}(k)]\phi_0^{\mathrm{F}}(k_{\mathrm{r}}) \simeq -(\lambda^2 + 1)\phi_0^{\mathrm{F}}(k)$. Thus, returning to the real space (ξ, τ), we obtain

$$\begin{aligned}
&\mathrm{i}\partial_\tau f - \mathrm{i}v\partial_\xi f + \left(vk_{\mathrm{r}} + 2\phi_0^2\right)f + \phi_0^2 f^* \\
&\quad = -(\lambda^2 + 1)\phi_0^{\mathrm{F}}(k_{\mathrm{r}})\delta(\xi).
\end{aligned} \tag{16}$$

With the initial condition $f(\xi, \tau = 0) = 0$, the solution of Eq. (16) for $k_{\mathrm{r}} \gg 1$ becomes

$$\begin{aligned}
f(\xi, \tau) &= -\mathrm{i}k_{\mathrm{r}}\phi_0^{\mathrm{F}}(k_{\mathrm{r}}) \exp(-\mathrm{i}\kappa_{\mathrm{r}}\xi) \\
&\quad \times \left[\theta(\xi + v\tau) - \theta(\xi)\right],
\end{aligned} \tag{17}$$

where $\theta(z)$ is the Heaviside function and

$$\kappa_{\mathrm{r}} = k_{\mathrm{r}} + \frac{1}{v\xi}\int_0^\xi \phi_0^2(\xi')\,\mathrm{d}\xi' \tag{18}$$

is the effective resonant wavenumber. Thus, a moving soliton stimulates radiation in the rear with a wavelength proportional to the velocity v. The amplitude of the radiation is proportional to $\phi_0^{\mathrm{F}}(k_{\mathrm{r}})$ and for small values of λ (i.e. for small values of the excitation number, $\mathcal{N}$) it decreases as $\exp(-\pi/2\lambda v)$. In Fig. 3 the Fourier spectrum of the propagating soliton is shown. The numerical simulations of the dependence of the resonant wavenumber on the soliton velocity are in reasonable agreement with our analytical prediction. To calculate the radiation reaction force we use conservation of energy arguments.

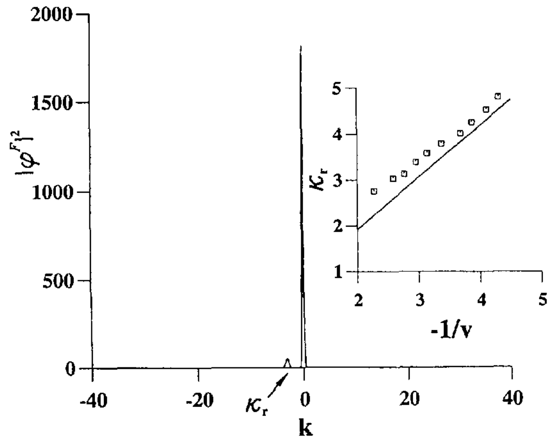

Fig. 3. Fourier spectrum of the moving soliton. Peak at $k = 0$ (soliton), $k = \kappa_{\mathrm{r}}$ (radiation). Inset shows the resonant radiation wave number, κ_{r}, versus $-1/v$, v being the soliton velocity: Solid curve Eq. (18); Squares, from numerical simulations of Eq. (6).

From Eqs. (2) and (6) one obtains that $\partial_\tau \epsilon + \partial_\tau P = 0$, where $\epsilon = -\frac{1}{2}|\varphi|^4 - \{\frac{1}{2}\varphi^*[\partial_z^2/(1-\partial_z^2)]\varphi + \text{c.c.}\}$ is the energy density and

$$P = -\frac{1}{2}\left[\left(\frac{\partial_\tau}{1-\partial_z^2}\varphi\right)\frac{\partial_z}{1-\partial_z^2}\varphi^* - \left(\frac{\partial_z\partial_\tau}{1-\partial_z^2}\varphi\right)\frac{1}{1-\partial_z^2}\varphi^* + \text{c.c.}\right] \tag{19}$$

is the energy flux. Inserting Eq. (17) for large τ and z we obtain the power radiated by the soliton

$$P_r \simeq 2v\left[\phi_0^F(k_r)\right]^2 \tag{20}$$

for small v. Thus the damping force, F_d, given by $F_d v = P_r$, is $F_d = 2[\phi_0^F(k_r)]^2 \simeq 16\pi^2 \exp(-\pi/\lambda v)$ for small excitation numbers.

In conclusion, we propose a nonlocal NLS equation for systems with long range dispersion effects. In contrast to the usual NLS equation stationary solutions only exist for a finite interval of the excitation number, N. In the upper part of this interval two stationary solutions appear. The branch corresponding to the bigger values of the spectral parameter is shown to be unstable and blowup occurs. A cusp soliton occurs at the maximal spectral parameter value.

The moving soliton radiates energy with wavelength proportional to the velocity of the soliton. The intensity of the radiation decreases exponentially with the soliton velocity and the excitation. As a result the soliton slows down and eventually stops.

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