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Statistical approach of the modulational instability of the discrete self-trapping equation

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Abstract. The discrete self-trapping equation (DST) represents an useful model for several properties of one-dimensional nonlinear molecular crystals. The modulational instability of DST equation is discussed from a statistical point of view, considering the oscillator amplitude as a random variable. A kinetic equation for the two-point correlation function is written down, and its linear stability is studied. Both a Gaussian and a Lorentzian form for the initial unperturbed wave spectrum are discussed. Comparison with the continuum limit (NLS equation) is carried out.

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1 Introduction

The discrete self-trapping (DST) equation

$$i\frac{\mathrm{d}a_n}{\mathrm{d}t} - \omega_0 a_n + \lambda(a_{n+1} + a_{n-1}) + \mu|a_n|^2 a_n = 0 \qquad (1)$$

is a typical equation for a system of harmonically coupled nonlinear oscillations [1,2] relevant for several physical problems. We mention here only Davydov's model of energy transport in α-helix structures in proteins [2–4], where (1) appears as a certain approximation of the model. In (1) a_n is the complex classical dimensionless amplitude of the oscillator of frequency ω_0 in the nth molecule, and λ, μ (of dimension of frequency) are the coupling constants between nearest neighbor oscillators and the one-site nonlinearity respectively. It is well known that depending upon of the parameters and the chosen initial condition the equation (1) can lead either to self-trapping (*i.e.* local modes or solitons), or to chaos, or to a mixture of the above two behaviors [1,2,5]. Instead of (1) we shall consider the equation

$$i\frac{\mathrm{d}a_n}{\mathrm{d}t} + \lambda(a_{n+1} + a_{n-1}) + \mu|a_n|^2 a_n = 0 \qquad (2)$$

which is obtained if $a_n \to a_n \mathrm{e}^{-i\omega_0 t}$. This equation admits plane wave solutions with constant amplitude

$$a_n = a\mathrm{e}^{i(kn-\omega t)}$$

(the lattice constant is taken equal with unity) but with an amplitude depending dispersion relation

$$\omega(k) = -2\lambda\cos k - \mu|a|^2.$$

This is a Stokes wave solution and it is well known to be unstable at small modulation of the amplitude (Benjamin-Feir or modulational instability) [6]. This can be discussed by two distinct approaches. The first one is a deterministic approach [6–16] and is very used in different physical situations. Applied to our equation (2) it gives

$$\mathrm{Im}\Omega = 4\lambda\cos k \sin\frac{K}{2}\sqrt{\frac{\mu}{2\lambda}|a|^2\frac{1}{\cos k} - \sin^2\frac{K}{2}}.$$

This instability appears if $\mathrm{Im}\Omega > 0$ and from the previous expression this takes place if μ, λ have the same sign and $\sin\frac{K}{2} < (\frac{\mu}{2\lambda\cos k}|a|^2)^{\frac{1}{2}}$.

The second approach takes into consideration the statistical properties of the medium where the instability develops. This is less used although there are notable results, especially in hydrodynamics [17,18] and in plasma physics [13].

In this approach $\dot{a}_n$ is considered a random variable and the statistical properties are introduced through two-point correlation functions. Such a discussion for a discrete system is still missing and the present paper wants to fill this gap.

In the next section a kinetic equation for a two-point correlation function is obtained. Using a Wigner-Moyal transform the equation is written in a mixed

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configuration-wave vector space. The linear stability around a homogeneous basic solution is discussed in Section 3. An integral stability equation is derived, very similar with the dispersion relation of the linearized Vlasov equation in ionized plasmas. Different forms for the spectrum of the initial unperturbed condition will be considered, namely a δ-spectrum, a Gaussian and a Lorentzian form and the increment of the modulational instability is calculated. Comparison with the continuum limit, when (1) transforms into the nonlinear Schrödinger equation is done. Few concluding remarks are also presented.

2 Kinetic equation for two-point correlation function

Introducing the displacement operator by $a_{n\pm1} = \mathrm{e}^{\frac{\partial}{\partial n}} a_n$ the equation (2) becomes

$$i\frac{\partial a_n}{\partial t} + 2\lambda \cosh\frac{\partial}{\partial n} a_n + \mu|a_n|^2 a_n = 0. \tag{3}$$

In order to find a kinetic equation we write (3) for $n = n_1$, multiply it by $a^*_{n_2}$, add it to the complex conjugated of (3) for $n = n_2$ multiplied by a_{n_1} and finally take an ensemble average. One obtains

$$i\frac{\partial}{\partial t}\langle a_{n_1} a^*_{n_2}\rangle + 2\lambda\left(\cosh\frac{\partial}{\partial n_1} - \cosh\frac{\partial}{\partial n_2}\right)\langle a_{n_1} a^*_{n_2}\rangle + \mu(\langle a_{n_1} a^*_{n_1} a_{n_1} a^*_{n_2}\rangle - \langle a_{n_2} a^*_{n_2} a_{n_1} a^*_{n_2}\rangle) = 0 \tag{4}$$

which besides the two point correlation function $\rho(n_1, n_2, t) = \langle a_{n_1}(t) a^*_{n_2}(t)\rangle$ contains also four-point correlation functions. If a_n corresponds to a Gaussian process, and this property is retained during the evolution, a four-point correlation function factorizes exactly in products of two-point correlation functions [19]

$$\langle a_{n_1} a^*_{n_1} a_{n_1} a^*_{n_2}\rangle = 2\langle a_{n_1} a^*_{n_2}\rangle\langle a_{n_1} a^*_{n_1}\rangle = 2\rho(n_1, n_2)\bar{a^2}(n_1) \tag{5}$$

where $\bar{a^2}(n) = \langle a_n a^*_n\rangle$ is the ensemble average of the mean square amplitude. Although the factorization (5) is true only for a Gaussian process we shall assume to be at least approximately valid also for processes slightly different from a Gaussian one, and this represents the main approximation of the present analysis.

It is convenient to use a Wigner-Moyal transform [20]. One introduce the new variables

$$M = \frac{n_1 + n_2}{2}, \qquad m = n_1 - n_2. \tag{6}$$

Then the equation (4) becomes

$$i\frac{\partial\rho}{\partial t} + 4\lambda \sinh\frac{1}{2}\frac{\partial}{\partial M} \sinh\frac{\partial\rho}{\partial m} + 2\mu\left(\bar{a^2}\left(M + \frac{m}{2}\right) - \bar{a^2}\left(M - \frac{m}{2}\right)\right)\rho = 0. \tag{7}$$

We consider a chain of N molecules and impose cyclic boundary conditions. The Fourier transform of the two-point correlation function is defined by

$$F(k, M, t) = \sum_m \mathrm{e}^{-ikm}\rho\left(M + \frac{m}{2}, M - \frac{m}{2}, t\right) \tag{8}$$

where k takes values in the first Brillouin zone (BZ), $k \in (-\pi, \pi)$. The inverse formula is

$$\rho\left(M + \frac{m}{2}, M - \frac{m}{2}, t\right) = \frac{1}{N}\sum_k^{BZ} \mathrm{e}^{ikm} F(k, M, t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} \mathrm{e}^{ikm} F(k, M, t) dk. \tag{9}$$

For $m = 0$ one obtains

$$\bar{a^2}(M, t) = \frac{1}{N}\sum_k^{BZ} F(k, M, t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} F(k, M, t) dk. \tag{10}$$

Now Fourier transforming equation (7) we get

$$\frac{\partial F}{\partial t} + 4\lambda \sin k \sinh\frac{1}{2}\frac{\partial}{\partial M} F + 4\mu\sum_{j=1}^{\infty}\frac{(-1)^{j\pm1}}{(2j-1)!2^{2j-1}} \times\left(\frac{\partial^{2j-1}}{\partial M^{2j-1}}\bar{a^2}(M)\right)\left(\frac{\partial^{2j-1}}{\partial k^{2j-1}} F(k, M)\right) = 0 \tag{11}$$

which is the expected nonlinear evolution equation for $F(k, M, t)$ in a mixed configuration-wave number space (M, k). Using the definition (8) we see that $F(k, M, t)$ is a periodic function in the reciprocal space, $F(k + 2\pi) = F(k)$.

3 Stability analysis

As the unperturbed problem we shall consider a basic solution $F_0(k)$ independent of M and t. This is the random counterpart of the Stokes wave in a deterministic approach. A small perturbation around this homogeneous background is considered, namely

$$F(k, M, t) = F_0(k) + \epsilon F_1(k, M, t). \tag{12}$$

According to (10) we have also

$$\bar{a^2}(M, t) = \bar{a_0^2} + \epsilon\bar{a_1^2}(M, t) \tag{13}$$

where

$$\bar{a_0^2} = \frac{1}{2\pi}\int_{-\pi}^{\pi} F_0(k) dk$$

$$\bar{a_1^2}(M, t) = \frac{1}{2\pi}\int_{-\pi}^{\pi} F_1(k, M, t) dk. \tag{14}$$

When (12) is introduced into (11), neglecting terms of order ϵ^2, the following linear evolution equation for F_1 is obtained

$$\frac{\partial F_1}{\partial t} + 4\lambda \sin k \sinh \frac{1}{2}\frac{\partial}{\partial M} F_1 + 4\mu \sum_{j=1}^{\infty} \frac{(-1)^{j+1}}{(2j-1)!2^{2j-1}} \frac{\partial^{2j-1} F_0}{\partial k^{2j-1}} \frac{\partial^{2j-1} \bar{a}_1^2(M)}{\partial M^{2j-1}} = 0. \tag{15}$$

Looking for a plane wave solution

$$F_1(k, M, t) = f_1(k) \mathrm{e}^{i(KM - \Omega t)}$$

after little algebra the following stability integral equation is found

$$1+\frac{\mu}{4\pi\lambda \sin \frac{K}{2}} \int_{-\pi}^{\pi} \frac{F_0\left(k+\frac{K}{2}\right) - F_0\left(k-\frac{K}{2}\right)}{\sin k - \frac{\Omega}{4\lambda \sin \frac{K}{2}}} dk = 0. \tag{16}$$

The modulational instability is related to Ω complex with a positive imaginary part, $\Omega_i = \mathrm{Im}\Omega > 0$. It is convenient to compare (16) with the similar result for the continuum case of the nonlinear Schrödinger equation [16]

$$1 + \frac{\mu}{2\pi K \lambda} \int_{-\infty}^{\infty} \frac{F_0\left(k+\frac{K}{2}\right) - F_0\left(k-\frac{K}{2}\right)}{k - \frac{\Omega}{2K\lambda}} dk = 0. \tag{17}$$

The two expressions look very similarly and consequently the final results will differ only quantitatively, although the differences can be quite significant.

As a first example let us consider a δ-spectrum for $F_0(k)$

$$F_0(k) = 2\pi \bar{a}_0^2 \delta(k). \tag{18}$$

This corresponds to an uniform unperturbed $\rho_0(x)$, which is a very unphysical assumption, but the final result becomes very simple, to which other more realistic situations can be compared

$$\Omega_i = 4\lambda \sin \frac{K}{2} \sqrt{\frac{\mu}{\lambda} \bar{a}_0^2 - \sin^2 \frac{K}{2}}. \tag{19}$$

It represents a limiting situation, the most favorable for the development of the instability. From (19) the instability exists if λ, μ are positive quantities (focusing case) and if $\sin^2 \frac{K}{2} < \frac{\mu}{\lambda} \bar{a}_0^2$.

3.1 Gaussian spectrum

In the next example let us assume $F_0(k)$ to be a Gaussian function

$$F_0(k) = \frac{\sqrt{2\pi}}{\sigma} \bar{a}_0^2 \mathrm{e}^{-\frac{k^2}{2\sigma^2}}. \tag{20}$$

This expression doesn't satisfy the periodicity condition but for σ vanishingly small the errors introduced are negligible. Also the relation (14) is satisfied up to exponentially small terms.

It is convenient to introduce the new integration variable $t = \frac{1}{\sqrt{2}\sigma}(k \pm \frac{K}{2})$ and the notations

$$z_{\pm} = \frac{1}{\sqrt{2}\sigma} \left(\frac{\Omega}{2\lambda \sin K} \pm \tan \frac{K}{2} \right) \tag{21}$$

$$f_{\pm}(t) = \frac{1}{\sqrt{2}\sigma} \left(\sin \sqrt{2}\sigma t \pm \tan \frac{K}{2} \left(1 - \cos \sqrt{2}\sigma t\right) \right).$$

Then (16) becomes

$$\frac{\bar{a}_0^2}{\sqrt{2\pi}\sigma} \frac{\mu}{\lambda \sin K} \int_{-\frac{\pi}{\sqrt{2}\sigma}}^{\frac{\pi}{\sqrt{2}\sigma}} \mathrm{e}^{-t^2} \left(\frac{1}{z_+ - f_+} - \frac{1}{z_- - f_-} \right) \mathrm{d}t = 1. \tag{22}$$

In leading order in σ the integral (22) can be evaluated using the steepest descent method [21]. Denoting $G_{\pm}(t) = t^2 + \ln(z_{\pm} - f_{\pm}(t))$, $t_{\pm}$ the zeros of the first derivatives $\frac{\mathrm{d}G_{\pm}(t)}{\mathrm{d}t} = 0$, $A_{\pm} = \frac{1}{2}\frac{\mathrm{d}^2 G_{\pm}}{\mathrm{d}t^2}$ for $t = t_{\pm}$, and extending the integration limits to infinity the integral is given by

$$\sqrt{\pi} \left(\frac{1}{\sqrt{A_+}} \mathrm{e}^{-G_+(t_+)} - \frac{1}{\sqrt{A_-}} \mathrm{e}^{-G_-(t_-)} \right). \tag{23}$$

In the limit $\sigma \ll 1$ we have approximatively $t_{\pm} \simeq \frac{1}{2z_{\pm}} = \sqrt{\frac{\sigma}{2}} \frac{1}{\frac{\Omega}{2\lambda \sin K} \pm \tan \frac{K}{2}}$, $\mathrm{e}^{-G_{\pm}(t_{\pm})} \simeq \frac{1}{z_{\pm}}$ and $A_{\pm} \simeq 1$ and the integral becomes $\frac{-2\sqrt{2\pi}\sigma \tan \frac{K}{2}}{(\frac{\Omega}{2\lambda \sin K})^2 - (\tan \frac{K}{2})^2}$. Considering Ω purely imaginary, $\Omega = i\Omega_i$, we re obtain the result (19) of the δ-spectrum case.

3.2 Lorentzian spectrum

A simpler example is a Lorentzian form for $F_0(k)$

$$F_0(k) = \bar{a}_0^2 \frac{p\sqrt{1+p^2}}{\sin^2 \frac{k}{2} + p^2}. \tag{24}$$

It satisfies the periodicity condition and relation (14). The unperturbed two-point correlation function is easily calculated using (24) in the definition relation (9). Straightforward calculations give

$$\rho_0(m) = \frac{\bar{a}_0^2}{[1 + 2p(\sqrt{1+p^2} + p)]^m} \tag{25}$$

representing an exponentially decreasing law. For $p \ll 1$ we have $\rho_0(m) \simeq \bar{a}_0^2 \mathrm{e}^{-2pm}$.

In order to calculate the integral (16) it is convenient to introduce the new integration variable $t = \tan \frac{k}{2}$. Then the integral is over the whole real axis and can be done in the t-complex plane. In the new variable $F_0(k\pm\frac{K}{2})$ writes

$$F_0\left(k\pm\frac{K}{2}\right)\to \frac{\bar{a}_0^2 2p\sqrt{1+p^2}(1+t^2)}{\left(1+\cos\frac{K}{2}+2p^2\right)t^2\pm 2\left(\sin\frac{K}{2}\right)t+\left(1-\cos\frac{K}{2}+2p^2\right)} \tag{26}$$

having poles at

$$t_{1,2}^{+}=-a\pm ib \qquad t_{1,2}^{-}=a\pm ib$$

where

$$a=\frac{\sin\frac{K}{2}}{1+\cos\frac{K}{2}+2p^2},\qquad b=\frac{2p\sqrt{1+p^2}}{1+\cos\frac{K}{2}+2p^2}. \tag{27}$$

Considering Ω purely imaginary, $\Omega=i\Omega_i$ and denoting $z=\frac{\Omega_i}{4\lambda\sin\frac{K}{2}}$ we have also

$$\frac{1}{\frac{\Omega}{4\lambda\sin\frac{K}{2}}-\sin k}\to -i\frac{1+t^2}{zt^2+2it+z}$$

having poles at

$$t_3=i\frac{\sqrt{1+z^2}-1}{z}\qquad t_4=-i\frac{\sqrt{1+z^2}+1}{z}.$$

We shall consider z as a small quantity and consequently $t_4\gg 1$. Closing the contour in the lower complex half-plane t its contribution can be neglected in the first order. Therefore we shall take into account only the poles $t_2^{(\pm)}$ and after straightforward calculations the relation (16) becomes

$$1=\frac{\mu\bar{a}_0^2}{\lambda\sin\frac{K}{2}}\frac{MA+MX}{X^2+M^2} \tag{28}$$

where

$$\begin{aligned} A&=1+a^2-b^2, & B&=2ab\\ X&=zA+2b, & M&=2a-zB. \end{aligned} \tag{29}$$

When $p\ll 1$ we approximate

$$a\simeq\frac{\sin\frac{K}{2}}{1+\cos\frac{K}{2}},\qquad b\simeq\frac{2p}{1+\cos\frac{K}{2}} \tag{30}$$

terms of order p^2 being neglected. Then (28) can be considerably simplified and finally we get

$$\Omega_i=4\lambda\sin\frac{K}{2}\left(\sqrt{\frac{\mu}{\lambda}\bar{a}_0^2-\sin^2\frac{K}{2}}-2p\frac{1+\cos\frac{K}{2}+\cos k}{1+\cos\frac{K}{2}}\right). \tag{31}$$

Modulational instability occurs for λ and $\mu>0$, $\sin^2\frac{K}{2}<\frac{\mu}{\lambda\bar{a}_0^2}$ and if p is smaller than a critical value. Both results (19) and (31) can be compared with the similar results obtained in the NLS case [16]

$$\Omega_i^{(L)}=2K\lambda\left(\sqrt{\frac{\mu}{\lambda}\bar{a}_0^2-\frac{K^2}{4}}-p\right) \tag{32}$$

where the superscript L refers to Lorentzian form of $F_0(k)$. It is easily seen that (32) is obtained in a long wave limit ($K\ll 1$). In the Lorentzian case both relations (31) and (32) show a behavior similar to the well known phenomena of Landau damping in plasma physics [22,23] namely with increasing p the imaginary part Ω_i can become negative and no instability develops.

In other words any disturbance in the initial state is evolving into an instability only if a certain long range correlation between the amplitudes in two different points exists. If the correlation is shorter than a certain limit (depending on the wave vector of the disturbance and the amplitude of the initial correlation function) the instability is suppressed. This was several times emphasized in hydrodynamics [17,18], and remains valid also for discrete systems (like nonlinear molecular chains) in which case the randomness can be attributed to the temperature and to the interactions with the surrounding media.

In conclusion, in this paper the influence of statistical properties of a discrete medium where the modulational instability takes place was discussed through the simplest possible model. The techniques used in the continuum case were adapted for the discrete situation. No qualitative differences between these two situations can appear, although quantitatively the differences can be quite notable. In the statistical approach the instability is strongly dependent on the parameters characterizing the initial conditions and it would be very interesting to consider other forms for $F_0(k)$, both for continuum and discrete case. The interplay between nonlinearity (even for more complicated models), discreteness and randomness represents a still open problem for the phenomenon of modulational instability.

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