Dynamics of breathers in discrete nonlinear Schrodinger models

We review some recent results concerning the existence and stability of spatially localized and temporally quasiperiodic (non-stationary) excitations in discrete nonlinear Schrodinger (DNLS) models. In two dimensions, we show the existence of linearly stable, stationary and non-stationary localized vortex-like solutions. We also show that stationary on-site localized excitations can have internal 'breathing' modes which are spatially localized and symmetric. The excitation of these modes leads to slowly decaying, quasiperiodic oscillations. Finally, we show that for some generalizations of the DNLS equation where bistability occurs, a controlled switching between stable states is possible by exciting an internal breathing mode above a threshold value. (C) 1998 Elsevier Science B.V.

Dynamics of breathers in discrete nonlinear Schrodinger models

We review some recent results concerning the existence and stability of spatially localized and temporally quasiperiodic (non-stationary) excitations in discrete nonlinear Schrodinger (DNLS) models. In two dimensions, we show the existence of linearly stable, stationary and non-stationary localized vortex-like solutions. We also show that stationary on-site localized excitations can have internal 'breathing' modes which are spatially localized and symmetric. The excitation of these modes leads to slowly decaying, quasiperiodic oscillations. Finally, we show that for some generalizations of the DNLS equation where bistability occurs, a controlled switching between stable states is possible by exciting an internal breathing mode above a threshold value. (C) 1998 Elsevier Science B.V.
Localized excitations in discrete nonlinear Schrödinger systems: Effects of nonlocal dispersive interactions and noise

A one-dimensional discrete nonlinear Schrödinger (DNLS) model with the power dependence, \( r^{-s} \) on the distance \( r \), of dispersive interactions is proposed. The stationary states of the system are studied both analytically and numerically. Two kinds of trial functions, exp-like and sech-like are exploited and the results of both approaches are compared. Both on-site and inter-site stationary states are investigated. It is shown that for \( s \) sufficiently large air features of the model me qualitatively the same as in the DNLS model with nearest-neighbor interaction. For \( s \) less than some critical value, \( s(\text{cr}) \), there is an interval of bistability where two stable stationary states exist at each excitation number. The bistability of on-site solitons may occur for dipole-dipole dispersive interaction \( (s = 3) \), while \( s(\text{cr}) \) for inter-site solitons is close to 2.1.
In the framework of the DNLS equation with nearest-neighbor coupling we discuss the stability of highly localized, "breather-like", excitations under the influence of thermal fluctuations. Numerical analysis shows that the lifetime of the breather is finite and in a large parameter region inversely proportional to the noise variance for fixed damping and nonlinearity. We also find that the decay rate of the breather decreases with increasing nonlinearity and with increasing damping. Copyright (C) 1998 Elsevier Science B.V.
Solitary excitations in discrete two-dimensional nonlinear Schrödinger models with dispersive dipole-dipole interactions

The dynamics of discrete two-dimensional nonlinear Schrödinger models with long-range dispersive interactions is investigated. In particular, we focus on the cases where the dispersion arises from a dipole-dipole interaction, assuming the dipole moments at each lattice site to be aligned either in the lattice plane (anisotropic case) or perpendicular to the lattice plane (isotropic case). We investigate the nature of the linear dispersion relation for these two cases, and derive a criterion for the modulational instability of a plane wave with respect to long-wavelength perturbations. Furthermore, we study the on-site localized stationary states of the system numerically and analytically using a variational approach. In general, the narrow, intrinsically localized states are found to be stable, while broad, "continuumlike" excitations are unstable and may either collapse into intrinsically localized modes or disperse when a small perturbation is applied.
Stabilization of nonlinear excitations by disorder

Using analytical and numerical techniques we analyze the static and dynamical properties of solitonlike excitations in the presence of parametric disorder in the one-dimensional nonlinear Schrodinger equation with a homogeneous power nonlinearity. Both the continuum and the discrete problem are investigated. We find that otherwise unstable excitations can be stabilized by the presence of disorder in the continuum problem. For the very narrow excitations of the discrete problem we find that the disorder has no effect on the averaged behavior. Finally, we show that the disorder can be applied to induce a high degree of controllability of the spatial extent of the stable excitations in the continuum system.
General information
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Organisations: Department of Informatics and Mathematical Modeling, Department of Mathematics, Universidad Complutense de Madrid, Technical University of Denmark
Authors: Christiansen, P. L. (Intern), Gaididei, Y. B. (Intern), Johansson, M. (Ekstern), Rasmussen, K. (Intern), Usero, D. (Ekstern), Vazquez, L. (Ekstern)
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ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 3.206 SNIP 1.394 CiteScore 3.57
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ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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Scopus rating (2009): SJR 3.109 SNIP 1.474
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 2.982 SNIP 1.524
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Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.763 SNIP 1.607
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.742 SNIP 1.606
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.75 SNIP 1.536
Stationary states of the two-dimensional nonlinear Schrödinger model with disorder

Solitonlike excitations in the presence of disorder in the two-dimensional cubic nonlinear Schrodinger equation are analyzed. The continuum as well as the discrete problem are analyzed. In the continuum model, otherwise unstable excitations are stabilized in the presence of disorder. In the discrete model, the disorder is found to leave the narrow excitations unaffected. Our results suggest that the disorder provides a possibility to control the spatial extent of the stable excitations in the continuum system.
Switching between bistable states in a discrete nonlinear model with long-range dispersion

In the framework of a discrete nonlinear Schrödinger equation with long-range dispersion, we propose a general mechanism for obtaining a controlled switching between bistable localized excitations. We show that the application of a spatially symmetric kick leads to the excitation of an internal breathing mode and that switching between narrow, pinned states and broad, mobile states with only small radiative losses occurs when the kick strength exceeds a threshold value. This mechanism could be important for controlling energy storage and transport in molecular systems.
General information
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Organisations: Department of Informatics and Mathematical Modeling, Technical University of Denmark, Bogolyubov Institute for Theoretical Physics
Authors: Johansson, M. (Ekstern), Gaididei, Y. B. (Ekstern), Christiansen, P. L. (Intern), Rasmussen, K. (Intern)
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BFI (2011): BFI-level 1
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ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.69 SNIP 1.215
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.694 SNIP 1.259
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BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.96 SNIP 1.314
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.926 SNIP 1.332
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.787 SNIP 1.324
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.71 SNIP 1.302
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.672 SNIP 1.214
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.371 SNIP 1.166
Web of Science (2003): Indexed yes
Amalgamation of interacting light beamlets in Kerr-type media

The interaction of optical filaments in bulk self-focusing media is investigated theoretically and numerically. The nature of this interaction is shown to vary with the incident individual powers and relative phases of the beamlets. By means of virial arguments supported by numerical results it is found that three distinct evolution regimes characterize two in-phase interacting filaments: (i) When each filament has a power below $N_c/4$, where $N_c$ is the critical self-focusing threshold for a single wave, both filaments disperse along their propagation axis. (ii) When their respective powers lie between $N_c/4$ and $N_c$, they fuse into a single central lobe that may self-focus until collapse, depending on their initial separation distance. The critical distance below which a central lobe forms and collapses is estimated analytically. (iii) When their incident powers both exceed $N_c$, initially separated filaments individually self-focus without mutual interaction. In contrast to in-phase beamlets, two light cells with opposite phase are shown to never coalesce. The extension of the self-focusing dynamics to optical filaments in bulk media with anomalous group-velocity dispersion is discussed. (C) 1997 Optical Society of America.
Breatherlike excitations in discrete lattices with noise and nonlinear damping

We discuss the stability of highly localized, "breatherlike," excitations in discrete nonlinear lattices under the influence of thermal fluctuations. The particular model considered is the discrete nonlinear Schrödinger equation in the regime of high nonlinearity, where temperature effects are included as multiplicative white noise and nonlinear damping. Numerical analysis shows that the lifetime of the breather is always finite and, in a large parameter regime, inversely proportional to the noise variance for fixed damping and nonlinearity. We also find that the decay rate of the breather decreases with increasing nonlinearity and with increasing damping. Using a collective-coordinate approximation, we show how the qualitative features of the numerical results can be analytically understood. Finally, in the dimer case we show that the multiplicative noise can be transformed into additive noise, and an exact stationary solution to the Fokker-Planck equation is obtained. From this solution, the dimer system is found to exhibit a noise (temperature) induced phase transition.
Effects of noise on localized excitations in the discrete Nonlinear Schrodinger system.: Proceedings of the Estonian Academy of Sciences

General information
State: Published
Organisations: Department of Informatics and Mathematical Modeling
Authors: Christiansen, P. L. (Intern), Rasmussen, K. (Intern), Johansson, M. (Ekstern), Gaididei, Y. (Ekstern)
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Main Research Area: Technical/natural sciences
Source: orbit
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Publication: Research › Article in proceedings – Annual report year: 1997

Effects of nonlocal dispersive interactions on self-trapping excitations
A one-dimensional discrete nonlinear Schrodinger (NLS) model with the power dependence r(-s) on the distance r of the dispersive interactions is proposed. The stationary states psi(n) of the system are studied both analytically and numerically. Two types of stationary states are investigated: on-site and intersite states. It is shown that for s sufficiently large all features of the model are qualitatively the same as in the NLS model with a nearest-neighbor interaction. For s less than some critical value s(cr), there is an interval of bistability where two stable stationary states exist at each excitation number N = Sigma(n)
 psi(n) (2). For cubic nonlinearity the bistability of on-site solitons may occur for dipole-dipole dispersive interaction (s = 3), while s(cr) for intersite solitons is close to 2.1. For increasing degree of nonlinearity sigma, s(cr) increases. The long-distance behavior of the intrinsically localized states depends on s. For s > 3 their tails are exponential, while for 2 < s < 3 they are algebraic. In the continuum limit the model is described by a nonlocal MLS equation for which the stability criterion for the ground state is shown to be s < sigma + 1.

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Organisations: Department of Informatics and Mathematical Modeling, Bogolyubov Institute for Theoretical Physics
Authors: Gaididei, Y. (Ekstern), Mingaleev, S. (Ekstern), Christiansen, P. L. (Intern), Rasmussen, K. (Intern)
Pages: 6141-6149
Publication date: 1997
Main Research Area: Technical/natural sciences

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SYSTEMS, BREATHERS, INTRINSIC LOCALIZED MODES, POLYACETYLENE, STABILITY, RANGE INTERPARTICLE INTERACTIONS, 2-DIMENSIONAL ANHARMONIC LATTICES, SOLITON, DYNAMICS, NONLINEAR SCHRODINGER-EQUATION
Nonlinear and stochastic dynamics of coherent structures
This Thesis deals with nonlinear and stochastic dynamics in systems which can be described by nonlinear Schrödinger models. Basically three different models are investigated. The first is the continuum nonlinear Schrödinger model in one and two dimensions generalized by a tunable degree of nonlinearity. Various perturbations such as fluctuating forces, localized impurities, and dissipation are considered. The second kind of model is the discrete nonlinear Schrödinger model, which also is investigated in one and two dimensions. External perturbations similar to the continuum case are also considered in the discrete model. Finally, nonlinear Schrödinger continuum and discrete models with nonlocal dispersion are investigated. In the introductory chapter the physical situation of energy transport on molecular aggregates in which the results apply is discussed in detail. This chapter also introduces the nonlinear Schrödinger model in one and two dimensions, discussing soliton solutions in one dimension and the collapse phenomenon in two dimensions. Also various analytical methods are described. Then a derivation of the nonlinear Schrödinger equation is given, based on a Davydov like system described by a tight-binding Hamiltonian and a harmonic lattice coupled by a deformation-type potential. This derivation results in a two-dimensional nonlinear Schrödinger model, and considering the harmonic lattice to be in thermal contact with a heat bath we show that the nonlinear Schrödinger equation must be augmented by a multiplicative noise term. The resulting stochastic model is investigated in the continuum limit and the behavior of the coherent excitations under the influence of the noise is studied. Similarly, we study the fluctuation effects on the two-dimensional collapse phenomenon. We find numerically and analytically that the collapse can be delayed and ultimately arrested by the fluctuations. Allowing the system to reach thermal equilibrium we further augment the model by a nonlinear damping term and find that this prohibits collapse in the strict mathematical sense. However a collapse like behavior still persists in the presence of the nonlinear damping. Apart from the absence of the collapse in the strict mathematical sense we find that the nonlinear damping term has rather weak influence on the interplay between fluctuations and self-focusing. The study of the continuum model is concluded by an investigation of the dynamics of localized states in the vicinity of an impurity. Studying the discrete nonlinear Schrödinger model, we first analyze the intrinsically localized excitations supported by this model in one dimension. This analysis is accomplished using analytical methods developed for nonlinear maps. It is demonstrated how the nonanalyticity of the map through homoclinic and heteroclinic connections permits the existence of localized states on the lattice. The pinnning effect of the discrete lattice is also investigated, constructing a Melnikov function describing quantitatively the difference between on-site and inter-site states. Since the intrinsically localized excitations are rather robust we further study the implications of fluctuations and nonlinear damping in this discrete model. The fluctuations are found always to destroy the localized states. Existence and dynamics of the intrinsically localized excitations in the two-dimensional discrete model are also studied. It is found that in two dimensions a bistability phenomenon of the localized states appears. The bistability expresses itself by allowing localized states of various width to have equal norms. We find in the two-dimensional discrete model that the interplay of the collapse effect and the discrete pinning allows dynamical creation of a spatially distributed set of localized states from a broad initial excitation. The last kind of models studied in the Thesis is nonlinear Schrödinger models with nonlocal dispersive interaction. First a continuum model with an exponential dependence of dispersive interaction is studied. This model shows in contrast to the ordinary continuum nonlinear Schrödinger models that the nonlocality imposes an upper bound on the norm of a possible localized excitation. The model is also shown to support a cusp soliton. A similar discrete nonlocal model is discussed. This model has an algebraic dependence of the dispersive interaction. There exists no upper limit of the norm in the discrete model, but the possibility of a bistability phenomenon similar to that of the two-dimensional model is shown to occur. Finally, we show that a two-dimensional Kronig-Penney model describing for example propagation of electromagnetic waves in photonic bandgap materials can be reduced to a one-dimensional nonlocal nonline Schrödinger model, which is similar to the nonlocal models considered previously.

General information
State: Published
Organisations: Department of Informatics and Mathematical Modeling
Authors: Rasmussen, K. (Intern), Christiansen, P. L. (Intern)
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Original language: English
Two-dimensional effects in nonlinear Kronig-Penney models.
An analysis of two-dimensional (2D) effects in the nonlinear Kronig-Penney model is presented. We establish an effective one-dimensional description of the 2D effects, resulting in a set of pseudodifferential equations. The stationary states of the 2D system and their stability is studied in the framework of these equations. In particular it is shown that localized stationary states exist only in a finite interval of the excitation Dower.

General information
State: Published
Organisations: Department of Mathematics, Department of Informatics and Mathematical Modeling, Technical University of Denmark
Authors: Gaididei, Y. B. (Intern), Christiansen, P. L. (Intern), Rasmussen, K. (Intern), Johansson, M. (Ekstern)
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Web of Science (2015): Indexed yes
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ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.206 SNIP 1.394 CiteScore 3.57
ISI indexed (2012): ISI indexed yes
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ISI indexed (2011): ISI indexed yes
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Scopus rating (2010): SJR 3.417 SNIP 1.451
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.109 SNIP 1.474
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
We study the effect of adding noise and nonlinear damping in the two-dimensional nonlinear Schrödinger equation (NLS). Using a collective approach, we find that for initial conditions where total collapse occurs in the unperturbed NLS, the presence of the damping term will instead in an exponentially decreasing width of the solution in the long-time limit. We also find that a sufficiently large noise variance may cause an initially localized distribution to spread instead of contracting, and that the critical variance necessary to cause dispersion will for small damping be the same as for the undamped system.
Discrete Localized States and Localization Dynamics in Discrete Nonlinear Schrödinger Equations

Dynamics of two-dimensional discrete structures is studied in the framework of the generalized two-dimensional discrete nonlinear Schrödinger equation. The nonlinear coupling in the form of the Ablowitz-Ladik nonlinearity is taken into account. Stability properties of the stationary solutions are examined. The importance of the existence of stable immobile solitons in the two-dimensional dynamics of the travelling pulses is demonstrated. The process of forming narrow states from initially broad standing or moving excitations through the quasi-collapse mechanism is analyzed. The typical scenario of the two-dimensional quasi-collapse of a moving intense pulse is the formation of pinned narrow spikes.

General information
State: Published
Organisations: Department of Informatics and Mathematical Modeling, Bogolyubov Institute for Theoretical Physics, Risø National Laboratory, Institute of Automation and Electrometry, Institut fuer Theoretische Physik
Authors: Christiansen, P. L. (Intern), Gaididei, Y. (Ekstern), Mezentsev, V. (Ekstern), Musher, S. (Ekstern), Rasmussen, K. (Intern), Rasmussen, J. J. (Ekstern), Ryzhenkova, I. (Ekstern), Turitsyn, S. (Ekstern)
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BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.61
Dynamics in discrete two-dimensional nonlinear Schrödinger equations in the presence of point defects

The dynamics of two-dimensional discrete structures is studied in the framework of the generalized two-dimensional discrete nonlinear Schrödinger equation. The nonlinear coupling in the form of the Ablowitz-Ladik nonlinearity and point impurities is taken into account. The stability properties of the stationary solutions are examined. The essential importance of the existence of stable immobile solitons in the two-dimensional dynamics of the traveling pulses is demonstrated. The typical scenario of the two-dimensional quasicollapse of a moving intense pulse represents the formation of standing trapped narrow spikes. The influence of the point impurities on this dynamics is also investigated.

General information

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Organisations: Department of Informatics and Mathematical Modeling, Department of Mathematics, Risø National Laboratory for Sustainable Energy, Plasma Physics and Technology Programme
Authors: Christiansen, P. L. (Intern), Gaididei, Y. B. (Intern), Rasmussen, K. (Intern), Mezentsev, V. (Intern), Juul Rasmussen, J. (Intern)
Pages: 900-912
Publication date: 1996
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.667 SNIP 1.262 CiteScore 3.3

Dynamics in discrete two-dimensional nonlinear Schrödinger equations in the presence of point defects

The dynamics of two-dimensional discrete structures is studied in the framework of the generalized two-dimensional discrete nonlinear Schrödinger equation. The nonlinear coupling in the form of the Ablowitz-Ladik nonlinearity and point impurities is taken into account. The stability properties of the stationary solutions are examined. The essential importance of the existence of stable immobile solitons in the two-dimensional dynamics of the traveling pulses is demonstrated. The typical scenario of the two-dimensional quasicollapse of a moving intense pulse represents the formation of standing trapped narrow spikes. The influence of the point impurities on this dynamics is also investigated.
Effect of nonlocal dispersion on self-interacting excitations.
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.
Nonlinear and stochastic modelling of energy transfer in Scheibe aggregates.

The oxacyanine Scheibe aggregate is modelled by a two-dimensional cubic nonlinear Schrödinger equation with multiplicative noise, accounting for thermal fluctuations. For a possible choice of the physical parameters collapse of the initial state.

General information
State: Published
Organisations: Department of Informatics and Mathematical Modeling, Bogolyubov Institute for Theoretical Physics, Ecole Normale Superieure de Lyon
Authors: Christiansen, P. L. (Intern), Rasmussen, K. (Intern), Gaididei, Y. B. (Ekstern), Bang, O. (Ekstern)
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Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 0.643 SNIP 1.096 CiteScore 1.29
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Scopus rating (2014): SJR 0.579 SNIP 1.147 CiteScore 1.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.581 SNIP 1.067 CiteScore 1.16
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.61 SNIP 1.029 CiteScore 1.11
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.591 SNIP 1.098 CiteScore 1.21
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
On some NLS systems and their applications.

General information
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Organisations: Department of Informatics and Mathematical Modeling, Technical University of Denmark, National Academy of Sciences of Ukraine, Australian National University
Authors: Christiansen, P. L. (Intern), Rasmussen, K. (Intern), Johansson, M. (Ekstern), Gaididei, Y. (Ekstern), Bang, O. (Ekstern)
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Solitonlike solutions of the generalized discrete nonlinear Schrödinger equation
We investigate the solution properties of a generalized discrete nonlinear Schrödinger equation describing a nonlinear lattice chain. The generalized equation interpolates between the integrable discrete Ablowitz-Ladik equation and the nonintegrable discrete Schrödinger equation. Special interest is paid to the creation of stationary localized solutions called breathers. To tackle this problem we apply a map approach and illuminate the linkage of homoclinic and heteroclinic map orbits with localized lattice solutions. The homoclinic and heteroclinic orbits correspond to exact nonlinear solitonlike eigenstates of the lattice. Normal forms and the Melnikov method are used for analytical determinations of homoclinic orbits. Nonintegrability of the map leads to soliton pinning on the lattice. The soliton pinning energy is calculated and it is shown that it can be tuned by varying the ratio of the nonintegrability parameter versus the integrability parameter. The heteroclinic map orbit is derived on the basis of a variational principle. Finally, we use homoclinic and heteroclinic orbits as initial conditions to excite designed stationary localized solutions of desired width in the dynamics of the discrete nonlinear Schrodinger equation. In this way we are able to construct coherent solitonlike structures of profile determined by the map parameters.
Breatherlike impurity modes in discrete nonlinear lattices

We investigate the properties of a disordered generalized discrete nonlinear Schrödinger equation, containing both diagonal and nondiagonal nonlinear terms. The equation models a linear host lattice doped with nonlinear impurities. We find different types of impurity states that form itinerant breather states in the vicinity of the impurities. We analyze the properties of these breathers analytically and numerically.

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Breatherlike impurity modes in discrete nonlinear lattices

We investigate the properties of a disordered generalized discrete nonlinear Schrödinger equation, containing both diagonal and nondiagonal nonlinear terms. The equation models a linear host lattice doped with nonlinear impurities. We find different types of impurity states that form itinerant breather states in the vicinity of the impurities. We analyze the properties of these breathers analytically and numerically.

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Organisations: Department of Informatics and Mathematical Modeling
Authors: Hennig, D. (Ekstern), Rasmussen, K. (Intern), Tsironis, G. P. (Ekstern), Gabriel, H. (Ekstern)
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The Nonlinear Schrödinger System: Collapse, Nonlinear damping, Noise, Impurities and Nonlocal dispersion. [PLC12]

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Organisations: Department of Informatics and Mathematical Modeling, Bogolyubov Institute for Theoretical Physics, Technical University of Denmark
Authors: Christiansen, P. L. (Intern), Gaididei, Y. (Ekstern), Mingaleev, S. (Ekstern), Yakimenko, I. (Ekstern), Johansson, M. (Ekstern), Rasmussen, K. (Intern)
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Breatherlike impurity modes in discrete nonlinear lattices

We investigate the properties of a disordered generalized discrete nonlinear Schrödinger equation, containing both diagonal and nondiagonal nonlinear terms. The equation models a linear host lattice doped with nonlinear impurities. We find different types of impurity states that form itinerant breather states in the vicinity of the impurities. We analyze the properties of these breathers analytically and numerically.

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Nonlinear excitations in two-dimensional molecular structures with impurities

We study the nonlinear dynamics of electronic excitations interacting with acoustic phonons in two-dimensional molecular structures with impurities. We show that the problem is reduced to the nonlinear Schrödinger equation with a varying coefficient. The latter represents the influence of the impurity. Transforming the equation to the noninertial frame of reference coupled with the center of mass we investigate the soliton behavior in the close vicinity of the impurity. With the help of the lens transformation we show that the soliton width is governed by an Ermakov-Pinney equation. We also investigate bound state of the soliton with impurity and show that in addition to the radially symmetric bound state a dipolelike state can exist if the number of excitations in the soliton does not exceed some threshold value. We study both the equilibrium states and the dynamics of the dipolelike excitations. Analytical results are in good agreement with numerical simulations of the nonlinear Schrödinger equation.
Temperature effects in a nonlinear model of monolayer Scheibe aggregates

A nonlinear dynamical model of molecular monolayers arranged in Scheibe aggregates is derived from a proper Hamiltonian. Thermal fluctuations of the phonons are included. The resulting equation for the excitons is the two-dimensional nonlinear Schrodinger equation with noise. Two limits of the complicated spectrum of the noise are considered: time independent, spatially white noise, simply corresponding to disorder in the arrangement of the molecules, and pure white noise. Parameter values are found by comparison with experiments by Mobius and Kuhn [Isr. J. Chem. 18, 375 (1979)] and order of magnitude estimates given where experiments are not available. The temperature dependent coherence time is found from numerical simulations. Experiments show that the excitons stay coherent during their lifetime. This is in correspondence with the model at temperatures lower than 3 K. To increase this limiting temperature it is found that the dipole-dipole coupling and the exciton-phonon coupling must be decreased significantly.

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Molecular and biomolecular dynamics

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Ikke-lineær dynamik og termiske fluktuationer i kohærente strukturer

Technical University of Denmark
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