Midterm Progress Report

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Network title: Localisation by Nonlinearity and Spatial Discreteness, and Energy Transfer, in Crystals, Biomolecules and Josephson Arrays

Network short title: LOCNET

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Part A - RESEARCH RESULTS

A.1 Scientific Highlights

A huge range of results has been obtained. The main ones are summarised below under the tasks headings of the work programme. In addition, a new idea emerged once the project started - Targeted energy transfer between DBs - which merits its own section, T16.

We would invite the assessors to contrast the breadth of our achievements with the statement of the evaluators of the proposal that "The proposal is ... perhaps too focussed, resulting in a subject matter that is narrow."

Throughout the report, "DB" stands for "discrete breather", one of the central concepts in the project. A discrete breather is a spatially localised time-periodic excitation in a dynamical network of units.

T1 Breather existence An existence proof of hard DBs in FPU lattices was constructed by reduction to a centre manifold [J1, J2], and is being extended to more general situations (James) and applied to existence of breathers in diatomic chains with arbitrary mass ratio (James & Noble). In parallel, a variational proof of existence of discrete breathers has been developed, which applies to a range of systems including many which were inaccessible to previous proofs, like hardening FPU lattices and models with acoustic phonons in any dimension [AKK]. A general framework was formulated for existence of optic DB in Euclidean-invariant systems with an optic band [M0a]. Explicit estimates for continuation of discrete breathers were obtained for some models [K]. A thorough study was made of spatial decay properties of breathers in lattices with zero linear dispersion [DEFT]. An algebraic method has been proposed to construct analytically DBs in 1D chains [Ts] and numerical methods are being investigated for finding DB in 1D nearest neighbour chains as homoclinic orbits of a 2nd order recurrence relation on a loop space (Bergamin, Kadelburg & MacKay). Existence of DB in spin lattices has been proved [ZFF, FZ]. Evidence for existence of DB was found numerically in realistic models for hydrocarbons [KA2] and in dipole-dipole chains with long-range interactions and curvature [ACMG, ACG, CGMM]. Stability of FPU solitons was proved [FrP], as well existence of solitary waves in some 2D lattices [FrM1], and atomic-scale localization of high-energy solitary waves on lattices [FrM2]. Nonlinear phonons were viewed as multibreathers [MJKA0a, MJKA0b, MJKA, MJKA1]. Quasiperiodic breathers have been studied in (dissipative) Josephson junction systems with external DC bias [FMFSU]. In Hamiltonian systems their existence was proved when there is an integral of motion independent of the Hamiltonian [BV].

T2 Breather Quantisation This divides into three parts.

1. Exact treatment

1.1. Existence proofs.

RS MacKay studied the persistence of spectral projections of eigenstates for networks of quantum units [M1]. One problem solved is the proper choice of the norm in order to avoid orthogonality catastrophes. Localization of energy is associated with the presence of anticorrelations in density matrices of projected states. These anticorrelations are shown to persist for a range of weak coupling independent of the system size. Litvak-Hinenzon and MacKay are working on completing the details of MacKay's proposed proof of persistence of spectral projections.

Oliver Penrose, with Chris Eilbeck (both Heriot-Watt), have developed a new theory of two-quanta breathers in the DNLS and other models, which is valid in any finite number of dimensions. In particular, threshold effects occur for dimension 3 and higher.

1.2. Analytical computation of spectra

E. D. Belokolos et al [BEES] considered special cases of Schrödinger equations in 2D and 3D with periodic and quasiperiodic potentials based on elliptic and hyper-elliptic functions, for which spectra and Fermi surfaces may be computed analytically. Applications include electron spectra in quantum dot arrays.

1.3. Breather tunneling and numerical methods

A model for a two-bond molecule is used to study tunneling of energy between bonds [FFO]. The presence of a third partially excited bond (acting as an energy reservoir) is shown to increase the tunneling probability by several orders of magnitude. Wavefunction analysis yields the order of tunneling, while semiclassical calculations confirm the tunneling probability results. In addition avoided level crossings are found to resonantly increase or decrease the tunneling probability.

Dorignac and Flach prepared a work on aspects of rotobreather tunneling [DF02]. The fine structure of the weakly splitted states is related to two different tunneling effects - tunneling from site to site and tunneling of total momentum. In addition this work provides with an exhaustive treatment of different (semiclassical) approximations and their comparison when related to the properties of quantum rotobreathers. Another work is in progress where the influence of external magnetic fields on that fine structure is discussed and applied to such different physical situations as rotational excitations in molecules or molecular crystals, spin tunneling and possibly also to the very interesting case of rotobreathers in Josephson junction systems.

Eilbeck (Heriot-Watt) and Salerno (Salerno) have now improved their computer programs to give an order of magnitude speedup in the calculations for many boson bound states. This puts a number of new possibilities within reach, and several papers are in preparation.

2. Mixed treatment

A class of one-dimensional acoustic polaron problems has been found with analytical solutions [ZE]. While the electron degree of freedom is treated quantum mechanically, the lattice vibrations are classical. Contrary to an isolated molecular chain the polaron state exists only in certain parameter ranges, while the delocalized exciton exists in the whole parameter space. If the polaron state exists, it may be either the ground state or not. If not, the delocalized exciton turns to be the proper ground state. Notably the polaron, while usually pinned to the lattice, may depinn resulting in a transparent regime of uniform propagation of a soliton with small size.

In a similar approximation discrete breathers are obtained for realistic hydrocarbon clusters, e.g. $C_{22}H_{24}$, C_6H_6 (Benzene) and $C_{26}H_{30}$ [KA2]. In addition to the mixed treatment only the carbon-hydrogen stretch vibrations are taken into account. Results suggest that pure classical localized vibrations due to anharmonicity persist with very large lifetimes in realistic models.

3. Classical treatment

Moving breathers have been obtained in classical models of two-dimensional lattices similar to the copper oxygen planes in High Tc superconductors [MRE]. The results are used to formulate expectations that such moving breathers may interact strongly with free charges moving in nearby located C2 chains. Some correlations have been observed between the existence and number of such chains and the transition temperature Tc.

T3 Coupled quantum rotors or spins Analysis of the neutron scattering function $S(\mathbf{Q},\omega)$ measured with single crystal of 4-methylpyridine in terms of the extended sine-Gordon theory is in progress in Thiais. MacKay wrote a speculative review mainly on quantum discrete breathers, which in particular discusses the interpretation of Fillaux and Carlile's experiments on 4-methyl pyridine and proposes a tentative alternative [M2]. The angular probability densities for the methyl deuterated lithium acetate dihydrate have been measured with the single crystal neutron diffraction techniques. A new dynamical model is proposed to account for the interplay of methyl dynamics and crystal structure, with special attention focussed on the deuterium induced phase transition [NCF]. A theoretical study of energy and momentum tunneling in a system of two coupled quantum rotors has been completed in Dresden. This is both an abstract model for rotational degrees of freedom in molecules and a paradigmatic model for quantum rotobreathers in extended systems [DF02].

T4 Breather mobility An abstract framework has been proposed for the description of approximate travelling discrete breathers (DB) in Hamiltonian chains of oscillators. The method is based on the construction of an effective Hamiltonian, enabling a more accurate description of the dynamics of moving breathers and the associated Peierls-Nabarro barrier [AMS01, MS02].

Analytical conditions for breather mobility between two sites were determined [AKMT], showing the DB energy oscillates between the two sites. This effect was detected and tested numerically in some complex models, including a biological model for photo-synthesis [KAT01].

The existence and properties of static and moving breathers in a DNA model with both nearest-neighbour and long-range interactions has been studied [CAGR, HAA, CPAR-I].

A study of the integrable massive Thirring model, a field theory model, has been completed [eeh02]. In addition our understanding of how generalized Weierstrass Elliptic functions of higher genera can be used to solve nonlinear wave equations has increased [aee02a, eep02].

A normal form technique has been developed to obtain the nonlinear Schrödinger equation as a modulation equation for moving quasiperiodic breathers in FPU–type systems [bcp02].

An investigation of DB mobility in curved chains has been carried out [RSIT, TIS, IST, AGCC, SAPR]. This work demonstrates that the DBs change but do not lose their mobility properties while in curved parts of a chain. These results were extended to curved polymer chains with first and second neighbor interactions as well as with local on site potentials. These are the simplest models for biomolecules and demonstrate that breathers are very robust and survive even dramatic geometric shape changes.

T5 Phonon-breather interactions and self-localisation Localisation of energy in the N-H stretch of methylacetamide was studied by Raman and infrared (Barthes). Femtosecond IR spectroscopy of delocalized NH excitations of crystalline acetanilide confirms that self-trapping in hydrogen-bonded peptide units exists and does stabilize the excitation [EHS]. Shock waves were found to form in a dissipative nonlinear Schrödinger lattice [SMK]. Localisation of energy from pattern states was studied in a weakly forced and damped anharmonic chain [KLR01]. A shell model of turbulence involving creation, interaction and decay of breathers was studied [PD02]. Clustering was found in a model of coupled rotors [DHR00, BDR01]. These non equilibrium structures correspond to statistical equilibria of an effective dynamics, derived using averaging techniques [BBDR02, BBDR02b]. Under some conditions, breathers were found to grow at the expense of phonons [JA, Jo]. Discreteness effects on phase separation were studied (Carr & Chmaj). Interactions between breathers and phonons were studied in discrete nonlinear Schrodinger systems [RABT]. Standing phonons has been constructed in Klein Gordon chains as multibreathers and numerically analyzed [MJKA1]. It was shown that any small nonlinearity is sufficient to make the standing wave unstable which might be strong or weak for some incommensurate standing waves [MJKA]. The thermalization of the system following the instability has also been analysed and involves sometimes transient DBs [JMAK]. The origin of puzzling solutions called Phantom DBs found only in relatively small finite system has been elucidated [MJAK02]. The energy relaxation process produced by thermal baths at zero temperature acting on the boundary atoms of chains of classical anharmonic oscillators [PLL] has been investigated. Relaxation phenomenon in the 2D FPU emphasizes the role of the threshold for the creation of breathers [PLLa]. The role of breathers' modes in a phenomenological model dedicated to the study of polymers aging properties has been studied [GCD02]. Consequences on their presence to the so-called alpha and beta relaxations characteristics of real polymers are investigated.

T6 Randomness and nonlinearity 1) Spatial disorder in strict sense: Breather in disordered

systems can be continued in some cases inside the linearised spectrum, and arbitrary weak nonlinearity was shown to allow energy transport [KA0a, KA0b]. The relation between breathers and Anderson modes is studied in a 2–dimensional model [CAPR].
2) Spatial inhomogeneities due to impurities, shape or other causes: Properties of nonlinear impurity modes and their stability are studied in the generalized Schrödinger equation [SKBRC], and their effect on trapping in a Klein–Gordon model [CPAR-II]. Characteristic frequencies of breathers at bending points in curved alpha–helix proteins are found [AGCC]. Properties of moving breathers in FPU systems with segments of different masses are analyzed [BSS].
3) Temporal randomness, i.e., temperature: The survival of breather mobility across bending points in polymers with temperature is observed in [RSIT, IST, TIS]. The thermalization of standing phonons leading to transient DB is studied in [JMAK]. Work is still in progress on nonlinear conductivity of CDW materials by thermal nucleation of pairs of discommensurations (Baesens, MacKay, Floria & Sancho).
4) Application to DNA: Mobility of polarobreathers is observed to survive to weak diagonal and structural off-diagonal disorder in a 3D DNA model [HAA].

T7 Slow Relaxation Considerable progress has been made in the understanding of the mechanism for spontaneous formation of breathers by cooling the lattice from the boundaries and the role played by boundary conditions. In 1d models we have explained the relaxation to standing breather solutions by relying on the linear response and on the modulational instability mechanism [PLL]. In particular, we have shown that while approaching the breather state, the energy decays first exponentially and afetrwards by following a power-law behaviour that emerges as a collective effect of all the decay rates of Fourier modes. This scenario is particular to lattices with nearest-neighbour interactions, while the presence of a local (substrate) potential changes the first regime to a stretched exponential one. This study has been extended to the 2d case, where the same scenario is observed with two main additional features: the existence of an activation threshold in the breather energy demands that the initial energy stored in the lattice exceeds a sufficiently large value to observe a final breather state; and such a state is obtained after a complex transient dynamics where large breathers incorporate small breathers until a "closely packed" configuration of breathers is attained. Such a configuration may survive over a time scale that is some orders of magnitude larger than the typical period of breather solutions [PLLa].

T8 Polarons The stability and dynamics of magnetic polarons were studied [CBP]. An electron-vibron-breather interaction was studied [Ha, Hb].
A theorem of existence of the many polaron structures in the Holstein-Hubbard model has been published [PA02].
Electron transfer, an essential phenomena in chemical and biochemical reactions, involves a reorganisation of the molecule and its environment (Marcus theory) and thus has to be viewed as a polaron transfer. Considering the interaction of the electron with the phonons and the electrostatic field, we derive an extended nonlinear Shroedinger equation with a retarded damping term and a colored multiplicative noise. This model allows one to recover in one limit the adiabatic Marcus theory and in the other limit the so called diabatic approximation of chemists [AK02b]. Our model has to be used for understanding ultrafast Electron Transfer where neither limit is valid. Polaron transfer is a nonlinear problem similar to those of DB transfer where the concept of targeted transfer has to play an essential role (see task [T13]).

T9 Josephson arrays Discrete breather states have been generated in Josephson junction ladders with open boundaries and imaged in Erlangen using the low temperature scanning laser microscope. Interaction of discrete breathers with linear cavity modes of Josephson junction ladders have been studied theoretically in detail by Dresden group [MFFZP]. These interactions have been experimentally observed in Erlangen, as resonant steps in the I-V characteristic of Josephson junctions ladders [SBU]. Incommensurate resonant breather states in Josephson junction ladders have been also observed in experiment and studied theoretically [FMFSU]. A detailed theoretical study of the existence, stability and resonance behavior of breather-like states in small Josephson system (3-junction cell) has been done by Dresden group [BFF], [FFB]. Such a cell of Josephson junctions has been prepared and is currently under investigation by the Erlangen group. In recent experiments in Erlangen, broken-symmetry states in the small Josephson system were observed and the region of existence of these states was found to be in good agreement with the theoretical expectations. The predicted resonant states in the cell were also observed (Pignatelli & Ustinov).

T10 Friction and nonlinear conductivity Existence of globally attracting sliding solutions in some classes of configuration was proved for overdamped inertial dynamics of tilted Frenkel-Kontorova chains (Baesens & MacKay). Existence of some types of travelling discommensuration was deduced from work of Mallet-Paret (Baesens & MacKay). An idea for noise-induced nonlinear conductivity in charge density wave materials was proposed (Baesens, MacKay & Floria) and is under investigation (Floria & Sancho).

Topological defects and dislocations in strongly anisotropic crystals are shown to propagate freely with stationary profile and velocity [SKCZ]. The problem of heat conduction in 1-D nonlinear chains was addressed; we showed that, acting on the parameter which controls the strength of the on site potential inside a segment of the chain, we induce a transition from conducting to insulating behavior in the whole system. Quite remarkably, the same transition can be observed by increasing the temperatures of the thermal baths at both ends of the chain by the same amount. The control of heat conduction by nonlinearity opens the possibility to propose new devices such as a thermal rectifier [TPC].

T11 Proton transfer A model of two-dimensional water has been studied in order to analyze dielectric measurements on protein hydration water: the frustration induces a glass transition [P1, P2, CP]. A mechanism is suggested to describe fast proton transfer in hydrogen-bonded chains with weak proton-proton interactions, and admits an exact soliton solution [ZPS]. The dynamical behavior of the proton transfer in the hydrogen bonds in the base-pairs of the double helices of the DNA type shows an interplay between the tunneling of protons and the symmetry of double helix [GKP].

Potential functions for proton transfer in crystals of benzoic acid have been determined from analysis of optical spectra. The tunneling transition has been observed by INS. A stepwise mechanism for the transfer of uncorrelated protons is presented in 2D. New evidence for localized modes in $KHCO_3$ crystals is obtained [FLR, IKSYBF, F1, FP, F2]. The INS spectra of various isotopes of polypyrrole give evidences for the existence of free protons [FPY].

Breathers (or vibrational polarons) have been sought in crystals containing networks of H-bonded molecules (as models for proteins):

In Acetanilide, the polaron theory describes the anomalous spectra (now confirmed by time-resolved measurements [EHS]), but no breather proper frequency could be found in the far-infrared [SBKN].

- Our neutron diffraction structural data show that the anomalous Amide spectra in N-methylacetamide are not due to proton transfer [EBKAAK].

- Precise infrared and Raman investigations on L-Alanine - the most frequent amino-acid in proteins - shows for the first time an anomalous peak near the NH_3 torsional mode, with a temperature dependent intensity and an intense overtone. While these properties are explained by the polaron theory, a subtle symmetry breaking with a random proton exchange on the ammonium group is also detected [BVSBE, VYBS].

T12 Discrete Polarobreathers has been incorporated into T8 and T13.

T13 DNA and Proteins Progress in the statistical mechanics of DNA melting included (i) the

systematic study of static correlations and scaling [TDP], and (ii) understanding the role of soliton-like excitations in the more general category of one-dimensional thermodynamic instabilities [DTP]. The frequency spectra of a lattice model of DNA denaturation near the critical point has been investigated numerically and analysed in terms of a relaxational / oscillational memory kernel (N. Theodorakopoulos).
Molecular dynamics simulations of the critical dynamics of DNA melting and melting transition of DNA has been studied by a simple mechanical model which includes the double helix geometry [BLP]. The signature of the transition on the dynamical structure factor has been analyzed.
The role of DNA curvature and rigidity on the existence, stability and mobility of breathers have been investigated [GMC0, GMC1, TIS, ACMG, AK02b, ACG, RSIT, TIS, IST, CAGR]. Bending points can be places that act as energy traps in DNA. If the curvature is small, however, they do not hinder breather propagation [CPAR-I].
Work has been initiated on prediction of fracture location for proteins in cyclotron mass spectrometer (MacKay & Derrick). Static and moving breathers in curved alpha-helix proteins have been studied [AGCC]. Breathers, with a characterist frequency which depends on the curvature but only slighty on the energy for high-enough curvature, appear. A model for the diffusion of RNA polymerase along DNA has been proposed [BPPS].
The role of dynamics in protein folding was studied [TLP]. Breathers were found in models of chains with strong hydrogen bonding [ZMT]. Nonlinearity-induced conformational instability has been found in the dynamics of biopolymers [MGCK]. A dynamical approach to protein folding has been studied [TLP]. Further progress has been made in the understanding of the unfolding process in the protein energy landscape in terms of the thermal activation mechanism [BLPT2].
A model of ultrafast electron transfer between a dimer of bacteriochlorophyll and a bacteriopheophytin with an ancilliary bacteriochlorophyll molecule has been introduced [AK02b], based on the results of T8. Studies of electron transfer (ET) in regular and random protein models have shown that the coupling of the electron to the vibrational dynamics of the protein matrix is vital for the initiation of coherent ET, and allows efficient transfer in the presence of randomness [VHGT, H01, H01b, H02b]. Nonlinear charge transport mechanism in periodic and disordered DNA has been analysed [HAA].
A minimal model of polymers has been studied (Kastner & Lazaro). They have identified breather solutions, under specific topological conditions. In non-homogeneous chains localized chaotic excitations are also expected.
It appears more and more clearly that the dynamics of DNA and proteins is affected (and probably stimulated) by the dynamics of the surrounding solvant. It is therefore important to get accurate data on hydration water dynamics. Experimental studies have been initiated with a Young Researcher appointed by LOCNET in Lyon (A. Spanoudaki) and a theoretical analysis has been performed [P1, P2] (also relevant for task T11).

T14 Biomotors A simple rotator model has been proposed to explain the mechanism of the F_1-ATPase [ZCNSZ, ZECNZ]. The emergence of directional motion by time-space symmetry breaking [FYZ, YFZO] was systematized. The rectification effect via breaking of the friction symmetry [NZCZ-I, NZCZ-II], and through an internal degree of freedom [CFF] was demonstrated. The origin of current reversal in ratchets has been also clarified [BS00, CFF] to some extent. Stabilization of ratchets by weak subharmonic signals was investigated [BS]. The possibility of targeted energy transfer by breathers was proposed [KA1a] and analytical conditions for it were derived [AKMT]. Theory and experiments on fluxon ratchet motion in Josephson junction arrays have been reviewed [FMMOST]. Soliton ratchet motion via locking of internal mode and the external force was studied [SQ, SZ]. The collective ratchet effect in "flashing" Frenkel-Kontorova models was rigorously characterized [FFMM, FMFF] in certain limits of the dynamics. Rectification of particle currents [YFZO, DF01, DKUF], energy currents [FZMF] and spin magnetizations

[FMO] due to nonadiabatic nonlinear response to ac fields has been studied in detail. The underlying approach of study and consequent systematic violation of time-space entangled symmetries is of principal importance for the understanding of directed work conducted by biological motors. Generalizations of broken symmetry arguments for interacting many-particle systems were developed [FZMF].

T15 Materials We investigated the presence of breathers in true materials through the use of molecular dynamics simulation utilizing large scale simulation programs with effective force fields. We have tested the case of long chain hydrocarbons and observed breathers associated with the hydrogen motion.
A theory of photoinduced deformation of molecular films was developed [GCR].

T16 Targeted Energy Transfer A highly significant and unanticipated development, issuing from the theory of multibreathers, is an extension to a theory of how DB can exchange energy with very little loss to the rest of the network if they are close to resonant. Ways in which this theory may be relevant to molecular biology are proposed. A quantum version for targeted electron transfer has also been developed, which is suggested to play a crucial role in photosynthesis.
Analytical conditions for the breather mobility between two sites were determined in [AKMT] and called Targeted Energy Transfer (TET). It is shown the DB periodically oscillate between the two sites as well as its frequency. Using the analytical conditions, TET was detected and tested numerically in some complex models [KAT01].
Targeted Energy Transfer of Quantum Breathers (see task T4) persists when the corresponding classical system exhibits the effect (Maniadis*, Kopidakis & Aubry). However, decoherence of the wave packet systematically appears after a certain number of oscillations which becomes large when approaching the classical limit. Actually, it can be checked that Targeted Transfer essentially occurs because of the existence of a discrete pathway of almost degenerate quantum states.

A.2 Joint Publications and Patents

The network has produced 64 joint publications (i.e. with authors from more than one network node) in the period Mar 00 to Jul 02. Table 1 indicates the distribution of the collaborations between countries. Details of the publications are listed below.

Throughout the publication list, and indeed the whole report, young researchers employed on this contract during the period (often abbreviated to "YR") are indicated by an asterisk after their name. LOCNET authors' locations are indicated in parentheses.

Some abstracts and an example of acknowledgement are given in an Appendix.

Joint Publication Numbers							
	UK	*FR*	*DE*	*ES*	*DK*	*GR*	*IT*
UK		$2\frac{1}{3}$		2	3	$\frac{1}{3}$	7
FR	$2\frac{1}{3}$				$1\frac{1}{3}$	$16\frac{2}{3}$	8
DE				2	8	2	
ES	2		2		3	3	1
DK	3	$1\frac{1}{3}$	8	3		$\frac{1}{3}$	1
GR	$\frac{1}{3}$	$16\frac{2}{3}$	2	3	$\frac{1}{3}$		
IT	7	8		1	1		
TOTALS	$14\frac{2}{3}$	$27\frac{4}{3}$	12	11	$16\frac{2}{3}$	$21\frac{4}{3}$	17

Table 1: Numbers of joint publications with authors from network nodes in two countries in the period Mar 00 - Jul 02 (3-way publications are counted as 1/3 for each pair).

[AMS01] T Ahn, RS MacKay (Warwick), J-A Sepulchre (Nice), *Dynamics of relative phases and generalised multibreathers*, Nonlinear Dynamics, *Nonlinear Dynamics* **25** (2001) 157-182

[ACG] JFR Archilla (Sevilla), PL Christiansen (Lyngby), Yu B Gaididei (Lyngby), *Interplay of nonlinearity and geometry in a DNA-related, Klein–Gordon model with long-range dipole-dipole interaction,* Phys Rev E 65 (2001) 016609(1-6).

[ACMG] JFR Archilla (Sevilla), PL Christiansen, SF Mingaleev, Yu B Gaididei (all 3 Lyngby). *Numerical study of breathers in a bent chain of oscillators with long range interaction,* J Phys A **34** (2001) 6363-6373.

[AGCC] JFR Archilla (Sevilla), Yu B Gaididei (Lyngby), PL Christiansen (Lyngby), J Cuevas (Sevilla), *Stationary and moving breathers in curved alpha–helix proteins,* Subm to J Phys A, 2002.

[aee02a] Chris Athorne, JC Eilbeck (Edinburgh), VZ Enolskii (Salerno), *A SL(2) covariant theory of genus 2 hyperelliptic functions*, subm to Trans. Camb. Phil Soc., 2002.

[AK02b] S Aubry (Saclay), G Kopidakis (Heraklion), *A Nonlinear Dynamical Model for Ultrafast Electron Transfer at zero degree K,* subm to Physica A.

[AK] S Aubry (Saclay), G Kopidakis (Heraklion), *Aspects of DISCRETE BREATHERS and New Directions*, in: *Nonlinearity and Disorder: Theory and Applications* (Editors: F.Kh. Abdullaev, O. Bang and M.P. Sørensen), Proceedings of the NATO ARW, Tashkent, Uzbekistan, October 2-6, 2000, NATO Science Series, Kluwer Academic Publishers, Dordrecht, The Netherlands, (2002), 81–98

[AKK] S Aubry (Saclay), G Kopidakis (Heraklion), V Kadelburg (Cambridge), Variational Proof for Hard Discrete Breathers in some classes of Hamiltonian Dynamical Systems, Discrete and Continuous Dynamical Systems B **1** (2001) 271-298

[AKMT] Aubry S (Saclay), Kopidakis G (Heraklion), Morgante AM (Saclay), Tsironis GP (Heraklion), *Analytic conditions for Targeted Energy Transfer between nonlinear oscillators or discrete breathers*, Physica B **296** (2001) 222.

[BLP] M Barbi (Lyon), S Lepri (Florence), M Peyrard (Lyon): Denaturation of a DNA helicoidal model; ENS-Lyon internal report, 2001.

[BPPS] M Barbi (Lyon), C Place (Lyon), V Popkov, M Salerno (Salerno), *Sequence dependent RNA-Polymerase diffusion along DNA*, Biophysical J, submitted

[BS] Barbi M (Lyon), Salerno M (Salerno), *Stabilization of ratchet dynamics by weak periodic signals*, Phys.Rev. E **63** (2001) 066212.

[BS00] M Barbi (Lyon), M Salerno (Salerno), *Phase locking effect and current reversals in deterministic underdamped ratchets*, Phys. Rev. E **62** (2000) 1988.

[BDR01] Barré J (Lyon), Dauxois T (Lyon), Ruffo S (Firenze), *Clustering in a model with repulsive long-range interactions*, Physica A **295**, 254 (2001)

[BBDR02] Barré J (Lyon), Bouchet F (Firenze), Dauxois T (Lyon), Ruffo S (Firenze), *Birth and long-time stabilization of out-of-equilibrium coherent structures*, submitted to Europhysical Journal B (2002); condmat/0203013.

[BBDR02b] Barré J (Lyon), Bouchet F (Firenze), Dauxois T (Lyon), Ruffo S (Firenze), *Out-of-equilibrium states as statistical equilibria of an effective dynamics*, Physical Review Letters, to appear (2002); condmat/0204407.

[BEES] ED Belokolos, JC Eilbeck (Edinburgh), VZ Enolskii, M Salerno (both Salerno), Exact Energy Bands and Fermi Surfaces of Separable Abelian Potentials, J Phys A 34 (2001) 943-959.

[BCS] A.Benabdallah* (Dresden), J.G.Caputo, A.C.Scott (Lyngby), Laminar phase flow for an exponentially tapered Josephson oscillator, J. Appl. Phys. (in press, 2001).

[BES] S.Binczak, J.C.Eilbeck (Edinburgh), A.C.Scott (Lyngby), *Ephaptic Coupling of Myelinated Nerve Fibers*, Physica D **148** (2001) 159-174.

[BEELS] V.M.Buchstaber, J.C.Eilbeck (Edinburgh), V.Z.Enolskii, D.V.Leykin, M.Salerno (Salerno), *Multidimensional Schrödinger equations with Abelian potentials*, submitted to J. Math. Phys., 2001.

[CEMR] L Cruzeiro-Hansson, JC Eilbeck (Edinburgh), JL Marín (Zaragoza), FM Russell, *Pair formation in the Hubbard-Davydov model*, preprint, 2002.

[CAGR] J Cuevas (Sevilla), JFR Archilla (Sevilla), Yu B Gaididei (Lyngby), FR Romero (Sevilla). *Moving breathers in a DNA model with competing short and long range dispersive interactions.* Physica D 163 (2002) 106-126

[DHR00] Dauxois T (Lyon), Holdsworth P (Lyon), Ruffo S (Firenze), *Violation of ensemble equivalence in the antiferromagnetic mean-field XY model*, Europhys J. B 16 (2000) 659

[DTP] T Dauxois (Lyon), N Theodorakopoulos (Athens), M Peyrard (Lyon), *Thermodynamic instabilities in one dimension: correlations, scaling and solitons*, J Stat Phys **107** (2002) 869-891

[DFOYZ] Denisov S, Flach S (Dresden), Ovchinnikov AA (Dresden), Yevtushenko O, Zolotaryuk Y* (Lyngby), Broken space-time symmetries and mechanisms of rectification of ac fields by nonlinear (non)adiabatic response, to appear in Phys Rev E.

[DEFT] B Dey, M Eleftheriou (Heraklion), S Flach (Dresden), GP Tsironis (Heraklion), Shape Profile of Compact-like Discrete Breathers in Nonlinear Dispersive Lattice Systems, Phys Rev E 65 (2001) 017601.

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Part B - COMPARISON WITH THE PROJECT PROGRAMME

B.1 Research objectives

The research objectives set down in Annex I of the contract are still relevant and achievable. Indeed, we have made good progress on all seven objectives: Classical discrete breathers, Quantum discrete breathers in molecular crystals, Vibrational energy distribution and flow, Polarons and bipolarons, Josephson junction arrays, Friction and nonlinear conductivity, and Breathers in biomolecules.

B.2 Methodological Approach and Work Plan

We have followed the research methods specified in the contract, namely, Mathematical proof, Numerical computation, Physical insight, Experiment, and Data analysis.

As a result of discussion at the initial network node leaders' meeting in March 2000, we made a few rationalisations to the distribution of the subject matter between the tasks and to their titles, as follows:

T12 We incorporated the protein part of T12 into T13 and the polarobreather part of T12 into T8, and so eliminated T12 as an itemised task.

T3 We added spin systems to T3 and changed the name to "Coupled quantum rotors or spins".

T5 We moved interstellar carbon from T5 to T7, and spectral hole-burning from T5 to T6.

T6 We enlarged the scope of T6 to include temporal randomness as well as spatial.

The tasks and task coordinators are recalled in Table 2. The table also indicates the nodes assigned to carry out each task.

Tasks			
Task	*Title*	*Coordinator*	*Nodes*
T1	Breather existence	Sepulchre (N)	Sy,W,Z,N,Mi,D
T2	Breather quantisation	Flach (D)	W,Sy,T,So,Mp,D,Mi
T3	Coupled quantum rotors or spins	Fillaux (T)	T,Sy,Ln,C
T4	Breather mobility	Eilbeck (Ed)	H,Lb,W,Z,Sy,Er,Ln,D,Ed,N,Be,Mi,Se
T5	Phonon-DB interactions & self-localisation	Dauxois (Ln)	Lb,H,Sy,F,W,Er,Ln,Be,Ma,D
T6	Randomness and nonlinearity	Archilla (Se)	W,Sy,F,Lb,Se
T7	Slow relaxation	Livi (F)	H,Z,Sy,F,T,Ln,D
T8	Polarons	Aubry (Sy)	W,Z,Lb,Sy,Ed,So,Mi,C,H
T9	Josephson arrays	Ustinov (Er)	Z,Lb,Sy,Er,D,So,Se
T10	Friction and nonlinear conductivity	Baesens (W)	W,Z,Sy,Ln,Ed
T11	Proton transfer	Barthes (Mp)	T,H,Ln,Mp
T12	Polarobreathers (incorp. into T8 & T13)		
T13	DNA and Proteins	Peyrard (Ln)	Lb,Ln,A,So,C,Z,Mp
T14	Biomotors	Floría (Z)	H,Z,Sy,Lb,F,So,Ln,Ba,C
T15	Breather-based materials	Tsironis (H)	H,Er,T,Sy,Z,Lb,F,Mp,Ln

Table 2: List of tasks and task coordinators and nodes assigned to each task, using the following code: A: Athens, Ba: Barcelona, Be: Berlin, C: Cambridge, D: Dresden, Ed: Edinburgh, Er: Erlangen, F: Florence, H: Heraklion, Lb: Lyngby, Ln: Lyon, Ma: Madrid, Mi: Milano, Mp: Montpellier, N: Nice, Sy: Saclay, So: Salerno, Se: Sevilla, T: Thiais, W: Warwick, Z: Zaragoza.

During the first year, an unanticipated significant new idea arose, which merits its own task heading: Targeted Energy Transfer. The emergence of this new direction is a sign of the genuine reseach creativity of the network. Although not required by the contract, it is proposed to organise work and reporting on the topic under a new task T16.

B.3 Schedule and Milestones

Most of the tasks are on schedule. The only deviations are as follows:

T1 Delay on theory of number of localised modes on a breather. Work not complete on normally hyperbolic persistence theorems and applications. Relation between modulational instability and DB established ahead of time.

T2 Rigorous theory of spectral projections not yet totally complete.

T13 36-month goals already attained.

T14 Delay in the role of nonlinear localized modes in biomotors.

T15 Some ideas already developed

Although we are behind schedule on some of the milestones, we are ahead on others, so overall the situation looks good.

6-month milestones: All done, except for finishing touches to a paper on existence of globally attracting sliding state for overdamped tilted FK models (Baesens & MacKay).

12-month milestones: We have not yet developed the proposed data analysis techniques for extracting spatial correlation lengths of vibrations from neutron scattering experiments, but have prepared a plan, and it is a question of finding a suitable postdoc. For the number of local modes on a breather, the DNLS case is clear, and work of Kim suggests how to tackle the general case but we have not yet exploited it. The groundwork for understanding generalised multibreathers in dissipative oscillator networks has been done already by Bates in a different context, so we will adapt this, but conceptually there is little more to do.

18-month milestones: We have assessed the role of breathers in interstellar carbon [KA2] and spectral hole-burning, and are making progress on their role in 4-methyl pyridine, DNA and some biomotors. We have formulated a theory of quantum breathers as spectral projections [M2]: just the finishing touches remain to make it rigorous.

24-month milestones: We have already made some progress on the theory of breather mobility in 1D [MS02], but interesting new observations of Eilbeck in 2D present challenges on this topic which we aim to address shortly.

30-month milestones: We already made some progress on the role of DB in heat conduction (T10) and Hydrogen-bonded systems (T11).

36-month milestones: We already made progress in CDW conductivity (Baesens, Floria, MacKay & Sancho), proton transfer (see T11 report), and thermal relaxation (see T7 report).

B.4 Research effort of the participants

The research effort during the period is summarised in Table 3.

B.5 Cohesion with Less Favoured Regions

The Heraklion node and its subcontractor are the nodes in less favoured regions. Far from requiring efforts to integrate them into the project, the Heraklion node is playing a leading role in the network, initiating highly productive collaborations with Saclay, Barcelona and Berlin, hosting one of the network conferences, and initiating formal links with the USA. The Athens node has been integrated by strong collaboration with Lyon.

Participant	Subcontractor	Associate	YRM	ORM	NR
Professional Research Effort Spent on the Network Project					
Participant	*Subcontractor*	*Associate*	*YRM*	*ORM*	*NR*
1. Warwick			26.7 (35)	57	9
	Edinburgh		0 (15)	20	4
		Cambridge	0 (0)	35	4
Subtotal			26.7 (50)	112 (134)	17 (17)
2. Saclay			17.5 (22)	90	5
	Lyon		8.5 (20)	50	7
		Nice	0 (0)	8	1
Subtotal			26 (42)	148 (216)	8 (12)
3. Erlangen			23.5 (36)	81.5	4
	Dresden		18 (8)	143	7
		Berlin	0 (0)	17	1
Subtotal			41.5 (44)	241.5 (163)	12 (11)
4. Zaragoza			10 (16)	80	6
	Barcelona		6.3 (12)	15	2
	Madrid		0 (12)	8	2
		Sevilla	0 (0)	25	4
Subtotal			16.3 (40)	128 (360)	15 (16)
5. Lyngby			21.4 (35)	200 (300)	12 (11)
6. Heraklion			17 (28)	113	6
	Athens		3 (10)	27	2
Subtotal			20 (38)	140 (150)	8 (10)
7. Firenze			19 (58)	30	5
		Salerno	0 (0)	20	2
		Milano	0 (0)	5	1
Subtotal			19 (58)	55 (110)	12 (10)
8. Thiais			0 (14)	29	4
		Montpellier	8 (8)	21	4
Subtotal			8 (22)	50 (150)	8(12)
TOTALS			178.9(329)	1074.5(1583)	92(99)

Table 3: Number of person-months of professional research effort by participant spent on the project during the reporting period (29 months), including the indicated dependent subcontractors and associates, differentiating between young researcher months (YRM) financed by the network and other researcher months (ORM) financed from other sources (including the group leaders), and indicating the total number of researchers who contributed to the project (NR). Subtotals are given for the nodes attached to each Participant, and the numbers proposed in the contract for the full 48-month period are given in parentheses for comparison.

B.6 Network Organisation and Management

As proposed in the contract, the network is being coordinated by a combination of hierarchical connections for the administration (via the tree in Table 3 of the contract) and horizontal connections (via task coordinators) for the research. Virtually all communication is via e-mail. Information is disseminated via the webpage www.maths.warwick.ac.uk/~mackay/locnet.html for the network. This includes links to webpages for most of the nodes, network meetings, network vacancies, the network's publication archive www.ma.hw.ac.uk/LOCNET/publications.html and the Cordis database.

Network decisions are made at business meetings (20-24 March 00, 13 June 01, 19 June 02). Apart from the first extended planning session, these are held when many members are already present at a network event.

A notable development is the establishment of formal links between the network and the USA. Sievers (Cornell) and Tsironis (Heraklion) obtained an NSF grant to enable USA researchers to participate in a joint meeting with LOCNET in Crete in June 01; it seems we were chosen by the NSF as a test case for the possibility of more extensive NSF funding of collaboration with EC networks, and the initiation of American networks. Sievers also obtained NSF money to send 4 graduate students at USA universities to LOCNET nodes for summer projects in 2002. Furthermore, the network organised a minisymposium on "Localisation and energy transfer in spatially discrete systems" at the SIAM conference on Applications of Dynamical Systems in Snowbird USA in May 01, Flach (Dresden) and Bishop (Los Alamos) organised a month-long session in Dresden in Sept 01 with several USA participants (despite September 11), several LOCNET members participated in a meeting at Los Alamos in July 02 on "Intrinsic localized modes", and Sievers has obtained NATO funding for an Advanced Research Workshop on DB in Erice in July 2003, which will involve many LOCNET members.

Also worth mentioning is that LOCNET has combined forces with a Mathematics EC RT-Network called MASIE to propose a series of PhD Euroconferences on Dynamics, Mechanics and Symmetry (coordinator: Claudia Wulff).

B.6.1 Main Network Meetings

Node Leaders' Meeting, Les Houches, 20-24 March 2000 Nodes represented: Warwick, Saclay, Thiais, Lyon, Dresden, Sevilla, Erlangen, Nice, Edinburgh, Heraklion, Montpellier, Barcelona, Florence, Athens, Zaragoza. 18 participants. We planned the tasks, elected task coordinators, and planned future meetings.

Excitations in Josephson junction ladders, Dresden, 19-21 Nov 00 To exchange theoretical and experimental results on rotobreathers in Josephson systems and plan future works and collaborations between the groups. Nodes represented: Erlangen, Dresden, Zaragoza. 11 Participants: S. Flach, M. V. Fistul, A. Benabdallah*, Y. Zolotaryuk*, A. V. Ustinov, P. Binder, F. Pignatelli*, M. Schuster, L. M. Floria, J. J. Mazo, F. Falo.

EU-US meeting on Discrete Breathers, 13-16 June 2001, Heraklion This meeting, organized by A Sievers and G Tsironis, brought basically all the world experts on breathers to Crete for exchange and discussions. The American scientists were funded directly by NSF who provided a grant especially for this meeting. LOCNET speakers: Archilla, Aubry, Barthes, Benabdallah*, Dorignac, Eilbeck, Eleftheriou, Fillaux, Fistul, Flach, Floria, Gaididei, Hennig, James*, Kadelburg, Kopidakis, MacKay, Maniadis*, Miroschnichenko, Pignatelli*, Sancho, Schuster, Tsironis, Y.Zolotaryuk*; additional LOCNET participants: Catarino, Litvak-Hinenzon*, Mazo, Morgante, Piazza, Ustinov, Voulgarakis. 50 participants.

Nonlinear Lattice Structure and Dynamics, Dresden, 3-28 Sept 2001 organisers: Flach (Dresden), Bishop (Los Alamos). The event was divided into 4 weeks, consisting of 3 focus weeks on the following topics: nonlinear deformation waves, computational approaches to nonlinear phenomena in discrete systems, quantization of localized excitations on lattices, and concluding with a workshop on localized excitations on lattices. LOCNET participants: Aubry, Bambusi, Benabdallah*, Dorignac, Eilbeck, Eleftheriou, Fillaux, Fistul, Flach, Floria, Gaididei, Henning, Kadelburg, Kopidakis, Leon, Lepri, Mingaleev, Miroshnichenko, Morgante, Pignatelli*, Salerno, Sepulchre, Theodorakopoulos, Tsironis, Ustinov, Vik*, Voulgarakis, Y.Zolotaryuk*, Sanchez-Rey, Cuevas, Palmero, including talks by YRs Benadbdallah*, Pignatelli* and Zolotaryuk*. Nodes represented: Warwick, Edinburgh, Cambridge, Saclay, Lyon, Erlangen, Dresden, Berlin, Zaragoza, Sevilla, Lyngby, Heraklion, Athens, Firenze, Milano, Montpellier.

Localisation and energy transfer in Nonlinear systems, 17-21 June 2002, El Escorial A conference to exchange new results and to share results with some researchers from outside the network. Organised by Luis Vazquez (Madrid). Participating nodes: Warwick, Edinburgh, Madrid, Barcelona, Sevilla, Zaragoza, Saclay, Thiais, Montpellier, Lyon, Heraklion, Athens, Firenze, Lyngby, Erlangen, Dresden. Participants: 55.

In addition, though not official network events, the following meetings on research themes of the network had at least one organiser from the network and network speakers from at least two countries:

NATO ARW, 2-6 Oct 00, Tashkent, Uzbekistan Nonlinearity and Disorder, Co-organised by Christiansen. LOCNET speakers: Aubry, Ustinov, Johansson, Soerensen.

SIAM Minisymposium on Energy localisation & Transfer, Snowbird USA, 22 May 01 Organiser: MacKay. LOCNET speakers: MacKay, Dauxois. Other speakers: Sievers, M Weinstein. Audience of about 40.

Nonlinear Science Festival III, 12-15 June 2001, Lyngby Co-organised by Bang (Lyngby). LOCNET speakers: Scott, Aubry, Stirling*

Special session on DB in 4th discussion meeting on relaxation in complex systems 17-19 June 01, Hersonisos, Crete. LOCNET speakers: Aubry, Flach, Tsironis.

Math Interdisciplinary Research day on DB, Warwick, 29 Nov 01 Organised by Litvak-Hinenzon* (Warwick). LOCNET speakers: Fillaux, Sepulchre, James*, Flach, Floria. Number attending: about 20.

B.7 Connections to Industry

The method of low temperature scanning laser microscopy that is being used in experiments on detection of discrete breathers in Erlangen recently turned out to be of potential interest for the company Carl Zeiss in Jena, Germany. The Erlangen group (AV Ustinov, M Schuster, D Abraimov) visited Zeiss in November 2000 and discussed possible use of the Zeiss Pascal laser scanning module for low temperature measurements. Currently, a collaboration proposal between the Erlangen group and Zeiss is in preparation. The possible goal here would be development of a market-oriented instrument that combines laser scanning with a low temperature stage.

Part C - TRAINING

C.1 Employment of Young Researchers

Young Researcher months financed by the contract								
	YR months used so far			*Comm.*	*Contract deliverable*			*Diff.*
Participant	*Pre*	*Post*	*Total*		*Pre*	*Post*	*Total*	
1. Warwick, UK	0	26.7	26.7	22.4	0	50	50	0.9
2. Saclay, FR	0	26	26	16	0	42	42	0
3. Erlangen, DE	23.5	18	41.5	12.5	36	8	44	-10
4. Zaragoza, ES	0	16.3	16.3	23.7	0	40	40	0
5. Lyngby, DK	0	21.4	21.4	13.6	0	35	35	0
6. Heraklion, GR	0	20	20	8	0	38	38	10
7. Firenze, IT	0	19	19	35	0	58	58	4
8. Thiais, FR	0	8	8	14	0	22	22	0
TOTALS	23.5	155.4	178.9	145.2	36	293	329	4.9

Table 4: Numbers of young researcher months financed by the contract up to 31 July 2002, Comm. = committed from 1 Aug 2002, Contract deliverable, and Diff. = shortfall in recruitment (i.e. deliverable - used - committed). Pre and Post denote predoctoral and postdoctoral.

C.2 Training Programme

The underlying principle on which the training of the YRs has been based is "learning by doing". Thus we have involved each YR in one or more tasks of the network, working alongside other researchers in their institute, and in some cases collaborating with researchers from other nodes. We have also given many opportunities to listen to and ask questions of other researchers in the network at our network meetings. In particular, the first three weeks of the session at Dresden were of a pedagogical nature and were attended by several of our YRs.

In addition, YRs have had access to various training courses, such as MSc modules at Warwick, DEA lectures at Lyon, a school in Florence on biological problems for physicists, the many workshops in Dresden, and PhD schools and Nonlinear Science Festivals at Lyngby, and YRs have been financed to attend other relevant workshops, like Dynamical Systems 2000 (Edinburgh), Mechanics and Symmetry (Peyresq, 2001). Many of these are of a multidisciplinary nature.

In the work programme, it was planned to hold some further training events, which have not materialised. These were to have been: (i) an introductory school on localised excitations for a Warwick Symposium Sept 02 - Aug 03, but the Warwick team ended up with so much to organise (not just coordinating this network, but also running a major UK Mathematics conference and serving in a major UK research assessment exercise) that plans for the Symposium had to be dropped; (ii) a school and workshop at Heraklion: it turned out more appropriate to capitalise on the NSF collaboration to hold a more substantial research workshop; (iii) a Les Houches school: it turned out that forward planning at Les Houches is such that this would have been possible only at the end of the project; (iv) a school at ICTP, Trieste: the onus for this lay with the coordinator, who as explained above had too many other commitments. Enthusiasm was expressed at the network meeting in El Escorial by the YRs, however, for some form of training school, and one of them has volunteered to look into the feasibility of arranging one in the summer of 2003.

The evaluators of the proposal expressed scepticism about the need for training of researchers in this area. We propose that the fact that 6 out of our 20 YRs (Benabdallah, Comte, James, Lazaro, Stirling and Vik) have already gone on to further academic jobs, using the skills gained in the network, testifies to the value that employers see resulting from the training. Our YRs are in heavy demand (3 were taken away from us before the end of their YR appointments).

C.3 Factual Information on the Young Researchers

Factual Information on the Young Researchers							
Name	*Nat.*	*Age*	*Dates of Appt*	*Cat.*	*SS*	*Place*	*PN*
Ioana Bena	BE	34	21/1/02-20/1/03	post	P-07	Ba, ES	no
Abdelhadi Benabdallah	MO	33	1/9/00-28/2/02	post	P-16	D, DE	yes
Jerome Benoit	FR	33	1/5/02-28/2/03	post	P-10	H, GR	no
Arno Berger	AS	34	15/9/02-28/2/03	post	M-05	W, UK	no
Jean-Christophe Comte	FR	29	1/9/01-31/8/02	post	P-16	H, GR	no
Jerome Dorignac	FR	30	1/11/02-29/2/04	post	P-10	W/Ed, UK	yes
Carlos Gorria Corres	ES	30	1/4/03-30/9/03	post	P-16	Lb, DK	yes
Guillaume James	FR	27	1/9/00-19/1/01	post	M-04	W, UK	yes
Michael Kastner	DE	29	1/11/01-31/10/03	post	P-16	F, IT	no
Tomas Lazaro	ES	31	1/10/01-30/9/02	post	M-05	F, IT	no
Anna Litvak-Hinenzon	IL	31	29/9/00-28/8/02	post	M-05	W, UK	no
Panagiotis Maniadis	GR	28	15/2/01-14/12/02	post	P-09	Sy, FR	yes
Matthias Meister	DE	29	8/10/01-7/2/04	post	P-16	Z/Ma, ES	no
Marcus Neumann	DE	32	7/10/02-7/12/03	post	C-08	T, FR	no
Francesca Pignatelli	IT	30	15/8/00-14/8/03	PhD	P-13	Er, DE	no
Oliver Rudzick	DE	34	1/9/02-29/2/04	post	P-16	F, IT	no
Anna Spanoudaki	GR	28	15/11/01-14/7/03	post	P-11	Ln, FR	no
James Stirling	UK	28	1/4/00-30/9/00	post	P-16	H, GR	yes
Aasmund Fahre Vik	NO	28	1/4/01-1/12/01	post	P-14	Mp, FR	no
Yaroslav Zolotaryuk	UE	27	19/12/00-18/5/03	post	P-16	Lb, DK	yes

Table 5: Factual information on the YRs (past, present and future). Nat. = Nationality (MO=Morocco but he spent 4 yrs 1mo in FR, 4mos in DK and 7mos in DE before); AS=Austria; NO=Norway; UE=Ukraine but he spent 3 yrs 4mos in UK, 6mos in DK and 2yrs 3mos in DE before). Age means on appointment. Dates of Appt = Dates of employment on LOCNET funds (actual appointment may start earlier or later using other funds). Cat. = postdoc or predoc studying for PhD. SS = Scientific Speciality using EC discipline codes. Place = place and country of work, using node codes from Table 2. PN = previous work or study at a network partner.

Part D - SKETCHES OF THE YOUNG RESEARCHERS

Ioana Carla Bena Position in the LOCNET: Young researcher, University of Barcelona (Professor José-Maria Sancho).
Scientific background:

- 1986 - 91 : Faculty of Physics, Alexandru Ioan Cuza University, Iaşi, Romania :
  - Licenciate in Physics (equivalent of the Master's Degree in Physics)
  - Master's dissertation: The Ferromagnetism of Metals in the Energy-Band Model
  - Graduated with the "highest distinction", I-st Rank.
- 1991 - 92: University Paris XI - Orsay (France): following the courses of D.E.A. ("Diplome d'Etudes Approfondis") in Theoretical Solid State Physics. Exempted of final examinations.
- 1992 - 93: Scientific Researcher, Theoretical Physics Department, University Alexandru Ioan Cuza, Iaşi, Romania
- 1993 - 96: Professor's Assistant, Theoretical Physics Department, University Alexandru Ioan Cuza, Iaşi, Romania. My responsabilities included teaching for about 20 hours per week of courses for the 3-rd, 4-th and 5-th year students in the Master's program in Physics. I was involved in courses on Thermodynamics and Statistical Physics, Quantum Mechanics, Quantum Field Theory, Electrodynamics and Theory of Relativity, Analytical Mechanics, Magneto-hydrodynamics and Plasma Theory, Elementary Particle Theory, and Mathematical Physics.
- For my Ph.D. research, I moved to Belgium. My doctoral work is in two parts:
  - 1996 - 97: at Université Libre de Bruxelles. Advisor, Prof. Mamad Malek Mansour. Topic: Hydrodynamic Fluctuations in Kolmogorov Flow.
  - 1998 - 2001: at Limburgs Universitair Centrum, Belgium. Advisor, Prof. Christian Van den Broeck. Topic: Collective Behavior of Coupled Parametric Oscillators
  - Title of Ph.D. thesis: Topics in Nonequilibrium Statistical Mechanics: I. Collective Behavior of Coupled Parametric Oscillators. II. Hydrodynamic Fluctuations in Kolmogorov Flow
  - Thesis defence on 3 May 2001 at Limburgs Universitair Centrum. Degree received: "Doctoral Degree in Science: Physics".

Jérôme Benoit In the first half of my thesis, I studied Heisenberg spins in the continuum limit (*i.e.* the nonlinear σ-model) on elastic surfaces. The corresponding rigid model exhibits topological soliton configurations with geometrical frustration due to curvature. Assuming small and smooth deformation allows one to find shapes of the elastic support by relaxing the rigidity constraint and introducing the bending energy: novel geometric effects were exhibited. In the second half, I analysed Heisenberg spins on a triangular lattice in the continuum limit. The group representation theory allows one to introduce a novel order parameter defined up to an abelian gauge which should be explicitly considered during the continuum limit computation. This analysis based on the real division algebras applies to low dimensional lattices as well.

Afterwards I was working on problems that involve topology, curved geometry, elasticity and soft/biological matter. My main motivation was to derive fine local descriptions from global behaviours. A novel approach based on the Bogomol'nyi technique was shown to clearly reveal the topological nature of bending phenomena. Recently I showed that projecting this topological approach on spherical vesicles of revolution is equivalent to investigate frustrated sine-Gordon kinks.

Now, as new postdoc within the LOCNET network, I am focusing on the *Helix-Coil* structural phase transition, which may be driven by a breather, through a biological lattice model.

Jérôme DORIGNAC [1]

My scientific background is in condensed matter physics. I have done my Ph.D. in the Centre de Physique Théorique (Ecole Polytechnique, Palaiseau, France) on interchain electronic transfer in nonlinear media (Thesis defended in June 2000). I have done an analytical and numerical study of the Holstein model of electron-phonon interaction in conjugated polymers in the presence of strong external DC electric field. I have studied polaronic states and their motion or, more specifically, soliton formation and propagation in DNLS-like equations. I have also studied the profile and the effect of Peierls-Nabarro barriers present both along a polymer chain and between weakly coupled chains.

Since November 2000, I have studied discrete breathers in collaboration with Sergej Flach. We have mainly focused on the quantum properties of these excitations in small-size systems and particularly in a system of two coupled pendulums. We have analysed the persistence of certain quadruplets in the quantum spectrum over the coupling strength and have shown that they allow for the construction of quantum states very similar to classical rotobreathers [DF02]. Effects of an applied magnetic field on physical systems that are mathematically equivalent to coupled pendulums (large spins, molecular rotors, Josephson junctions, etc.) are currently under investigation.

In addition, I am currently studying properties of isochronous potentials. The purpose of this work is to find whether chains of coupled isochronous oscillators can support classical breathers and how this property depends on the coupling. In perspective is also the study of the corresponding quantum problem dealing with a chain of oscillators whose onsite potential possesses an equispaced spectrum.

Guillaume James I graduated from the University of Nice (France), where I did a PhD thesis in Mathematics under the supervision of professor G. Iooss (1996-1999). My research concerned internal travelling water-waves (e.g solitons) in the presence of gravity and density-stratification. I have provided a mathematical justification of the two-layer approximation (result published in Arch. Rational Mech. Anal. 160, 2001). During 1999-2000 I have been a teaching assistant at the Ecole Polytechnique (Palaiseau, France).

During September 2000-January 2001 I have been appointed as a LOCNET "young researcher" at the University of Warwick, in the group of professor R.S. MacKay. I worked on energy localization in FPU lattices, as a starting point for understanding protein fragmentation in experiments of Derrick and Giannacopoulos (Chemistry department at Warwick). I have proved the existence of discrete breathers in FPU lattices when the interaction potential satisfies a hardening condition, which had been an open problem since their formal prediction by Sievers and Takeno in 1988.

Since February 2001 I am appointed as a lecturer at the Institut National des Sciences Appliquées in Toulouse (France). My research activities have been frequently supported by LOCNET : I have been a visitor at the Mathematics Institute at Warwick (May and November 2001) and have attended several LOCNET conferences (Crete 2001, El Escorial 2002). I have proved a mathematical result which ensures (under quite general assumptions) that ill-posed recurrence relations in Hilbert spaces can be locally reduced to finite-dimensional mappings. This result allows studying small amplitude time-periodic oscillations (including breathers) in a large class of one-dimensional lattices. It has been applied to the existence of breather in diatomic FPU lattices having arbitrary mass ratios,

[1] Although I am currently not a member of LOCNET, my employment as young researcher in the group will start in Warwick (November 2002) and will continue in Edinburgh (January 2003).

in collaboration with P. Noble (Mathematics department at Toulouse). Moreover, we shall study the existence of breathers in polymer models with secondary structure (collaboration with R.S. MacKay).

From a personal point of view, my participation to LOCNET as a "young researcher" has been a totally positive experience. I have been introduced to fascinating topics in lattice dynamics and have been able to make fruitful scientific contacts at different nodes of the network. In addition, the atmosphere at the Warwick mathematics institute was very pleasant and the scientific life of exceptional quality.

Michael Kastner I have studied physics at Friedrich-Alexander Universität Erlangen-Nürnberg in Germany from 1992 to 1997. I obtained my PhD, again in Erlangen with Professor Alfred Hüller, in March 2000 for my thesis on finite-size scaling in the microcanonical ensemble. So the for years before joining the LOCNET I have been working in the field of statistical mechanics, in particular on the theory of phase transitions. The methods used were mainly analytic, but to a certain amount also computer simulations were performed.

In November 2001 I started working with Professor Livi in Florence as a post-doc in the LOCNET project. After some time to familiarize with the topic of Hamiltonian dynamical systems, I started, in collaboration with Tomas Lazaro and Roberto Livi (both members of the LOCNET), to work on the dynamics of a model of a polymer with a secondary structure, investigating in particular the existence and the stability properties of breather solutions. This was done mainly by making use of numerical methods.

The recent LOCNET meeting offered excellent opportunities to make contact with people from the network other than those from Florence. We'll see if future collaborations will arise from this...

J. Tomás Lázaro Ochoa I studied mathematics at the Universitat de Barcelona (Spain). I belong to the Dynamical Systems group formed by people of this university and the Universitat Politècnica de Catalunya (where I have been working as lecturer or assistant professor), leaded by C. Simó, A. Delshams, À. Jorba and G. Gómez. During these years, I have been specially interested on the following subjects: (a) the splitting of separatrices in time-reversible systems (non necessarily Hamiltonian), that is systems exhibiting an invariance under the action of a spatial symmetry and a reversion in time's arrow; (b) the study and development of (pseudo-normal) forms, close to the well known Birkhoff normal forms, with the property of being an extension of the latter and becoming (analytically) convergent in some interesting situations where they are not. The approach to these subjects has been not only theoretical but also numerical. In particular we built our own algebraic manipulator to deal with these (pseudo-normal) forms in a case closely related to the celebrated Center-focus problem (a local version of the the 16th Hilbert's problem).

Concerning LOCNET, I was introduced to Roberto Livi thanks to Dario Bambusi, with whom my group in Barcelona has a very close scientifical and personal relation. Roberto suggested us (Michael Kastner and me) the problem of investigating the existence and stability of breathers in simple chains of polymers. Following ideas from papers by MacKay and Aubry (1994), Zolotaryuk, Christiansen and Savin (1996), Marín and Aubry (1996) and Livi, Spicci and MacKay (1997) we have arrived to a bimolecular zig-zag chain model exhibiting this kind of solutions, from an anticontinuous limit consisting in some particles with infinit mass up to a final situation with mass ratio of order 1. In this moment we are still working on it.

Nevertheless my experience in the network has been quite short (just one year, because of laboral and family reasons), I have found it very attractive and interesting. I have learnt a lot during this period, not only from a scientific point of view but also from a human one (this has been my first collaboration with people not from my home group). In this sense

I am very grateful to Roberto Livi, Michael Kastner and the rest of the group in Firenze for providing me a perfect ambient to develop this work.

Some further information about me could be found at www-ma1.upc.es/personal/lazaro.html

Anna Litvak-Hinenzon I am a LOCNET postdoc (in the period 29.9.00 - 28.8.02), working at the University of Warwick, with Prof. R.S. MacKay.

Scientific background: 1993 - B.A. in Theoretical Mathematics (University of Haifa, Haifa, Israel); 1996 - M.Sc. in Mathematics, 2001 - Ph.D. in Applied Mathematics (Weizmann Institute of Science, Rehovot, Israel).

My research background is in nonlinear dynamical systems; my M.Sc. research included the study of homoclinic tangles of two dimensional systems - Hamiltonian and slightly dissipative, a-symmetry perturbations and strange attractors; my Ph.D. research was on bifurcations, resonances and instabilities in three and more d.o.f. near integrable Hamiltonian systems; numerical and analytical tools were used.

In LOCNET I am involved in a research project which is concerned with quantum discrete breathers and their applications to molecular crystals; in particular, as part of this project it is intended to provide mathematical interpretation to experimental data, obtained for crystals at low temperatures, in terms of tunnelling quantum breathers. I was awarded a Marie Curie Fellowship to continue this research for additional 24 months.

During the time I have spent in LOCNET, I have learnt a great deal about localized modes, discrete breathers, molecular crystals and related subjects. The training I was provided with included: attending courses given at Warwick: "Coherent Structures" (a M.Sc. course, given by Prof. R.S. MacKay), "Quantum Mechanics of Atoms & Molecules" (a 3rd year undergraduate course, given by Prof. Gero Friesecke); reading papers written by members of LOCNET and others, on discrete breathers and their applications, so as papers describing experimental data; attending LOCNET meetings: in Crete (June 2001) and in El Escorial (June 2002), and having discussions with other LOCNET members.

Additional responsibilities: organization of a Discrete Breathers Group seminar (in the academic year 2000/2001) and of a one day workshop on discrete breathers (November 2001) at Warwick.

Matthias Meister Scientific Background: I studied physics at the university of Regensburg, finishing with a diploma. The diploma thesis was about gauge fields and prepared in the group of Prof. Dr. Ernst Werner. After that I went to Bayreuth as a PhD student of Prof. Dr. Franz Georg Mertens. The subject was the diffusion of solitons in (classical) Heisenberg chains. The project involved both analytical and numerical approaches to stochastic differential equations.
Responsibilities in the network: Spokesperson of the Young Researchers at the mid-term review.
Experiences in LOCNET: Accepting the position in LOCNET meant yet another change of my field of research. As I had hoped for, this has offered the possibility to acquire experience with methods I have never before used, like Floquet-analysis or numerical Fourier-transforms. Also, it gives me the opportunity to work with a discrete system in a regime where continuum-approximations are not possible (contrary to my work in Bayreuth). Speaking more generally, the problem I'm working on now requires a type of approach very different from anything I have done before, and I consider this a valuable experience. A further valuable experience simply is living abroad, as it changes the way one sees both the host and the home country. I am also very content with the first workshop of LOCNET I attended (in San Lorenzo de El Escorial). There I could really discuss and interact with other participants in a helpful way.
The only problems I encountered were of bureaucratic nature, following my arrival in

Spain. Some of these problems could have been worse had not Mario Floría offered a lot of support. The problems were, I think, due to the fact that local administration lacked experience with the employment of academic staff from abroad.

Francesca Pignatelli I graduated in Physics at the University of Florence (Italy) the 14th December, 1999 with a thesis on "Macroscopic quantum tunneling in Josephson junctions" with Prof. A. Ranfagni, from Institute for Applied Physics "Nello Carrara" in Florence. During my thesis work I get familiar with physics and macroscopic quantum effects on small Josephson junctions. Besides I learned some experimental techniques on low temperatures dc measurements.

I came to Erlangen on 15 August 2000 for a Ph.D. in the LocNet network on rotobreathers in small Josephson systems. The aim of this investigation is to provide an insight on breather states in more complex Josephson system as Josephson ladders and two dimensional Josephson array. We start investigating broken-symmetry states in a single Josephson cell composed of three Josephson junctions. First results on this system, not yet published, are in good agreement with the theoretical expectations previously obtained by Dresden group.

In the lively laboratories in Erlangen I enjoy the possibility to learn all the fundamental techniques to perform experiments with Josephson systems. These include Cad-design of the single Josephson cells to be investigated, preparation of the sample on the sample holder and making contacts, measurements in liquid helium and in a ^{4}He cryostat. Furthermore the fruitful collaboration with Dresden group helps me to deepen my knowledge in the theoretical aspects of the problem and is a source of many inspiring advices.

Furthermore the possibility to participate to the network conferences gave me the possibility to broaden my knowledge on nonlinear physics, discrete breathers in different experimental systems and to enjoy of fruitful discussions with other groups working in the field.

Anna Spanoudaki Before joining the network, I completed my PhD in Experimental Physics. My research concentrated on the dielectric properties of composite materials and in particular magnetic fluids. The aim of the work was to find out how the dielectric (permittivity) and conduction (dc-conductivity, hopping related polarisation) properties of such materials depend on their microstructure. The experimental method employed was dielectric relaxation spectroscopy in the frequency range 5 Hz–2 GHz, in the temperature range 100–300 K and in a variable magnetic field.

During the same period I had the chance to participate in or conduct dielectric studies on other materials, inorganic (ceramics) or organic (glass-forming liquids in bulk or in confinement, proteins in solution, alcohols).

My project is the realisation of a dielectric measurement set-up in order to measure the dynamics of hydrated biological molecules: We are interested in the role played by the solvent concerning the dynamics of proteins. Dielectric measurements are perfectly suitable for this purpose, because they allow us to follow simultaneously the dynamics of the protein chain, the dynamics of the hydration water and the conductivity. A correlation between these mechanisms can be detected by studying the temperature dependence of the dielectric response (non-Arrhenius behaviour, parallel development of the activation energy as a function of temperature) over a broad temperature range. Apart from helping to understand the dynamics of DNA and proteins, we believe that the dielectric study will also provide insight of the connection between proton transfer and local dynamics at different levels of hydration.

The dielectric measurements will be carried out in a parallel capacitor geometry. Since we are interested in the slow dynamics at low temperatures, a Novocontrol Alpha dielectric analyser in the frequency range 10^{-6}–$2{\cdot}10^{6}$ Hz has been selected. A suitable cell has been designed and tested and preliminary measurements on hydrated starch have been carried out. The temperature can be varied from ca. 170 K to 320 K with an accuracy of 0.1 K. For this an automated system has been constructed. The measurement is fully automated guided through a specially developed computer program that coordinates temperature control and frequency scans. In order to solve some problems connected with low-frequency measurements and improve the temperature control a new version of the cell has been designed and expected to be ready in September.

In the next phase of the project, dielectric measurements on bio-polymers (e.g. starch) and proteins will be conducted as a function of temperature and hydration.

Part of my activity during this time has been devoted to publications presentations at meetings which are related to my phD work.

Yaroslav Zolotaryuk In 1994 I have graduated from Kiev University (Ukraine) with an undergraduate degree (Diploma) in theoretical physics. From 1994 till 1998 I worked on my PhD at the Department of Mathematics in the Heriot-Watt University (Edinburgh, UK). My studies there were devoted to nonlinear lattice dynamics, more precisely - nonlinear coherent structures (solitary waves) on lattices. As a postdoc at the Max-Planck-Institute for Physics of Complex Systems in Dresden (Germany) I continued my research in the field of nonlinear lattice dynamics, focusing on the particular type on nonlinear coherent structures - discrete breathers. Within the LOCNET project I work in the following three main directions: nonlinear localised structures in Josephson junctions, discrete breathers in magnetic systems and mechanisms of nonlinear transport and their applications to functioning of molecular motors. So far my experience from working within LOCNET has been positive. I benefited a lot from finding new collaborations (Salerno) and keeping links with old colleagues (Dresden).

Part E - NETWORK FINANCING

Expenditure and Allocation								
	Estimated Expenditure so far				*Allocated funds*			
Participant	*YRs*	*NW*	*OHs*	*Total*	*YRs*	*NW*	*OHs*	*Total*
1. Warwick, UK	80168	16803	19393	116364	160000	58000	42000	260000
2. Saclay, FR	85824	24540	22072	132436	150000	62600	37400	250000
3. Erlangen, DE	84402	58132	7710	150244	121814	53000	25186	200000
4. Zaragoza, ES	27348	27441	6465	61254	96000	42667	21333	160000
5. Lyngby, DK	78157	3904	16411	98472	129430	3904	26666	160000
6. Heraklion, GR	36264	24782	12208	73254	114000	45600	30400	190000
7. Firenze, IT	23168	4737	5582	33487	104600	12067	23333	140000
8. Thiais, FR	29814	12785	2770	45369	85755	30912	23333	140000
TOTALS	445145	173124	92611	710880	961599	308750	229651	1500000

Table 6: Estimated expenditure up to 31 July 2002, compared with Allocated Funds, in Euros, by categories: YRs = YR personnel costs, NW = networking (including subcontracting), OHs = Overheads.

Part F - PROPOSED REVISION TO THE CONTRACT

The network would to know about the possibility of making the following changes to the contract.

4-month extension The purpose is to complete the appointment of one YR to the end of March 2004 and another to the end of June 2004, which have currently been made to only 29 February 2004, the termination date of the contract.

Secondments to subcontractors Regarding YR months allocated for secondment to subcontractors, we request permission optionally to appoint at the subcontractor with corresponding transfer of funds from the participant node, instead of by secondment from the participant node. This would simplify the lives of our administrators enormously, and hence our lives too.

Toulouse To add Toulouse, FR (node leader: former YR Guillaume James, team: Noble, Terraneo) as an Associate node to Saclay. The Toulouse team is producing excellent work on LOCNET tasks and it would be very useful to have them formally included in the network and for them to be able to use network funds to participate in network activity.

APPENDIX: Selected joint publication abstracts and example of acknowledgement

[AKMT] It is well-known that any amount of energy injected in a harmonic oscillator which is resonant and weakly coupled with a second harmonic oscillator, tunnels back and forth between these two oscillators. When the two oscillators are anharmonic, the amplitude dependence of their frequencies breaks, in general, any eventual initial resonance so that no substantialenergy transfer occurs unless, exceptionally, an almost perfect resonance persists. This paper considers this interesting situation more generally between two discrete breathers belonging to two weakly coupled nonlinear systems, finite or infinite. A specific amount of energy injected as a discrete breather in a nonlinear system (donor) which is weakly coupled to another nonlinear system (acceptor) sustaining another discrete breather, might be totally transferred and oscillate back and forth between these donor and acceptor breathers. The condition is that a certain well defined detuning function is bounded from above and below by two coupling functions. This targeted energy transfer is selective, i.e. it only occurs for an initial energy close to a specific value. The explicit calculation of these functions in complex models with numkerical techniques developed earlier for discrete breathers, allows one to detect the existence of possible targeted energy transfer, between which breathers, and at which energy. It should also help for designing models having desired targeted energy transfer properties at will. We also show how extra linear resonances could make the energy transfer incpomlete and irreversible. Future developments of the theory will be able to describe more spectacular effects, such as targeted energy transfer cascades and avalanches, and energy funnels. Besides rather short term applications for artificially built devices, this theory might provide an essential clue for understanding puzzling problems of energy kinetics in real materials, chmistry, and bioenergetics.

[MS02] Hamiltonian chains of oscillators in general probably do not sustain exact travelling discrete breathers. However solutions which look like moving discrete breathers for some time are not difficult to observe in numerics. in this paper we propose an abstract framework for the description of approximate traveling discrete breathers in Hamiltonian chains of oscillators. The method is based on the construction of an effective Hamiltonian enabling one to describe the dynamics of the translation degree of freedom of moving breathers. Error estimate on the approximate dynamics is also studied. The concept of Peierls-Nabbaro barrier can be made clear in this framework. We illustrate the method on two simple examples, namely the Salerno model which interpolates between the Ablowitz-Ladik lattice and the discrete nonlinear Schrödinger system, and the Fermi-Past-Ulam chain.

[ZFF] Discrete breathers (nonlinear localised modes) have been shown to exist in various nonlinear Hamiltonian lattice systems. In the present paper we study the dynamics of classical spins interacting via Heisenberg exchange on spatial d-dimensional lattices (with and without the presence of single-ion anisotropy). We show that discrete breathers exist for cases when the continuum theory does not allow for their presence (easy-axis ferromagnets with anisotropic exchange and easy-plane ferromagnets). We prove the existence of localised excitations using the implicit function theorem and obtain necessary conditions for their existence. The most interesting case is the easy-plane one which yields excitations with locally tilted magnetisation. There is no continuum analogue for such a solution and there exists an energy threshold for it, which we have estimated analyticially. We support our analytical results with numerical high-precision computations, including also a stability analysis for the excitations.

[ACMG] Most of the studies of breathers in networks of oscillators are limited to next-neighbour interaction. However, long-range interaction becomes critical when the geometry of the chain is taken into account, as the distance between oscillators and, therefore, the coupling, depends on the shape of the system. In this paper we analyse the existence and stability of breathers, i.e. localised oscillations in a simple model for a bent chain of oscillators with long-range interaction.

[TIS] We address energy localisation and transport in discrete curvilinear chains that model biopolymers. We derive a one-dimensional modified Fermi-Past-Ulam model that describes dynamics in curved rigid polymers and investigate the existence of localized energy in the form of discrete breathers. We show that breathers propagate freely in low curvature regions of the chain while there is a critical curvature above which breathers rebounce elastically without however losing their integrity. Furthermore, breathers traverse hairpin geometries that model β-sheet connections, adapting to the local curvature while modifying their propagation speed in the curved segment. These features are stable against small local polymer angle deformations.

Sample acknowledgement (from [AKMT]): This work has been supported by EC under contract HPRN-CT-1999-00163.