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

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1a. Research Topic

The topic of this proposal is the localisation of vibrational energy, electric charge and magnetic flux in nonlinear, spatially discrete systems — Hamiltonian, dissipative and quantum — from theoretical, numerical, and experimental perspectives.

During the present century, physics has been dominated by the linear viewpoint, where any linear combination of solutions is also a solution. Although this is adequate in some contexts, linear models fail to describe many important physical systems where nonlinearity introduces fundamentally different phenomena.

The primary nonlinear phenomenon under investigation in our proposal is localisation of energy in spatially discrete systems. This can be configurational energy (e.g. polarons) or vibrational energy (which we call "discrete breathers"). The combination of nonlinearity with spatial discreteness is natural for many real systems. For example, molecular crystals and biomolecules are not spatial continua but are made up of atoms and show strong anharmonic effects, and many macroscopic systems, such as Josephson junction arrays, have a spatially discrete structure and highly nonlinear characteristics.

Our aims in this proposal are to understand firstly when and how energy localises in nonlinear spatially discrete systems, and secondly the role of localisation in energy transfer.

Let us first discuss vibrational energy. We showed that if the nonlinearity of a network of oscillators or rotors is strong compared with the spatial coupling then "discrete breathers" exist: time-periodic spatially localised vibrations [MA]. Furthermore, under a wide range of circumstances they are stable, meaning that nearby initial conditions remain nearby for a long time [MS]. The phenomenon of discrete breather suggests a reassessment of standard dogma. For example, no longer must one imagine that a molecular crystal remains in thermal equilibrium as the temperature at its surface is reduced: long-lived hot spots may be left behind [TA]. Discrete breathers could open up whole new avenues of understanding, for example in the functions of biomolecules like DNA and myosin, and in the design of oscillators based on the far infrared resonances of Josephson junctions or molecular crystals.

We believe that discrete breathers can also have important technological applications. Josephson junctions have been proposed for the next generation of computers because of their extremely fast timescale (e.g. [Li]), and play a prominent role in a big new USA project on "Petaflop computing". One method of coding (though not that currently envisaged) is to hold a junction in a regime where it has two possible attractors: an equilibrium and a periodic oscillation, and to switch between these by small impulses. If this is implemented in an integrated circuit then the question arises whether the state of one junction might not influence that of its neighbour and render the coding unreliable. Under mild conditions on the coupling we proved that the states consisting of a single excitation are robust [SM], and we have a clear plan how to prove this for general states. Furthermore, two of our groups have recently demonstrated the robustness of the coding experimentally in Josephson ladders [B+, TMO]. This coding is worth promoting. Josephson arrays are also central to plans to realise quantum computing [Nat], and an understanding of quantum breathers may lead to a breakthrough there.

Polarons are objects analogous to breathers except that instead of a phonon packet, it is an electronic wavefunction which self-localises. Bipolarons are bound pairs of polarons in the spin singlet state. Numerical studies of the Holstein-Hubbard model suggest that there is a parameter regime in which a certain type of bipolaron is quite mobile [PA]. This could contribute towards an understanding of the role of polarons in high temperature superconductors.

Related localised excitations are already finding technological applications in light-emitting polymer displays. Cambridge Display Technology is going into production this year, but they are sorely aware that the theoretical foundations of their product are weak, and we propose to collaborate with them on some of the fundamental questions about the size and nature of the excitations.

So, in solid-state physics, molecular biology and high technology, one sees a new class of problems emerging which share a common denominator, namely the concept of energy localisation. Therefore, a fundamental understanding of this concept is timely: it will benefit several scientific disciplines, and will lead to new technological applications.

1b. Project Objectives

The research objectives of this project are to capitalise on recent developments in the theory of breathers and polarons which have opened up a wide range of fascinating fundamental questions and potential applications to solid-state, biomolecular and electronic physics, including three particular classes of system that we shall study experimentally. Our objectives are challenging, but at the same time realistic. All participants are committed to making major contributions in several areas and to collectively making a breakthrough. An outline of our objectives follows (we regret that we could not fit them into the required 2 pages!).

1.1 Classical breathers

Although classical models are not directly applicable to real systems, since quantum or dissipative effects must be included, the classical case is an excellent starting point from which to develop theory and intuition, giving insight that will later be developed in either the quantum or dissipative directions.

We will extend the existence theorems for optic breathers to general anharmonic systems with many degrees of freedom per unit cell including acoustic phonons. We will also prove existence of discrete breathers associated with acoustic phonons, observed by [ST] and Page, and predicted in a wide range of situations via modulational instability.

We shall numerically investigate bifurcations of breathers, to understand the ways they may lose stability or even existence and to stimulate a general theory of such phenomena. Of particular interest are local modes of vibration on top of breathers, and we intend to develop theory to predict the number of such local modes.

A major challenge is to understand numerical results showing mobile breathers. Although there are strong conditions for existence of exact moving breathers, under investigation by the Warwick, Nice and Dresden groups, a tentative explanation for approximate slowly moving breathers has been proposed by a Warwick-Nice collaboration [AMS], and it will be a significant advance to realise this idea. Breather dynamics in the presence of external ac-fields will also be investigated, paying particular attention to the possibility of controlling energy transport and storage in discrete systems, cf. [J+].

1.2 Quantum breathers in Molecular Crystals

Real crystals and biomolecules are quantum mechanical, so it is essential to understand the quantum analogues of classical breathers and their experimental signatures. As a first step, an approximate quantum treatment of breathers can be obtained by applying semiclassical EBK methods (Einstein-Brillouin-Keller) to their linear stability analysis [Au1]. We will apply the quantization of rotobreathers in models of coupled rotors to the interpretation of experiments of the group in Thiais [FC] on 4-methyl pyridine, and similar approximate quantum treatments of anharmonic oscillators to an experiment to be carried out shortly by the Warwick group at Rutherford Lab on PtCl ethyldiamine chlorate. We shall develop new methods of data analysis for neutron scattering, because the standard treatment is based entirely on harmonic models. If the PtCl experiment is successful, we propose to perform further experiments on ^{35}Cl-enriched samples, to separate the localisation effects due to randomness from those due to nonlinearity. More sophisticated treatments of the quantum problem will also be developed, and applied to the experiments.

Experimental works on nonlinear excitations in molecular crystals are very few. The historical case of soliton dynamics in the acetanilide crystal was based on the lack of any satisfactory alternative explanation. One of the ambitious goals of this network is to provide direct evidence for nonlinear excitations, firmly based on experimental data, in order to enhance interaction between theory and experiments. The Thiais group has proposed experimental protocols to distinguish between linear (phonons) and nonlinear (breathers) excitations, which we shall test.

We shall try to resolve a controversy about two alternative interpretations of the experiments, one in terms of quantum sine-Gordon breathers and the other in terms of rotobreathers, by measuring the variation of the band intensity as a function of the orientation of the momentum-transfer vector with respect to the chain direction should be quite different for the two models. Such measurements will be performed on triple-axis spectrometers at the Laboratoire Léon Brillouin (Saclay).

A very important part of our project is to put quantum breathers on a mathematically rigorous footing, which is essential for a true understanding of the phenomenon. We propose to achieve this by proving persistence (from the uncoupled case) of spectral projections for various types of excitation in a network of anharmonic quantum units, and deriving localisation properties of resulting spatial correlation functions. This would constitute a revolution in many body theory, where dubious expansion techniques with cancellation of infinities and unjustified approximations have held reign for 50 years and it is time to put the whole subject on a firm mathematical foundation, which history has demonstrated to be crucial to permit further advances (e.g. Poincaré's proof of non-convergence of perturbation series in Celestial mechanics and his discovery of chaos).

1.3 Vibrational energy distribution and flow

The existence of propagating spatially inhomogeneous but time-periodic waves in classical networks of oscillators has been established, suggesting that energy propagating states of these forms occur even in random systems, where linear models would indicate that Anderson localisation prevents all transport. We shall explore the implications of this result. As well as these exact solutions, we shall study approximate solutions, christened "generalised multi-breathers" [AMS], which are not necessarily exactly periodic, but the relative phases (and possibly amplitudes) of oscillation evolve slowly.

We aim to understand the creation and the annihilation of breathers. Among the possible mechanisms are the nonlinear interaction of breathers with phonons and breather collisions. This theory should help to understand the spontaneous formation and destruction of breathers at non-zero temperature.

The role of breathers has been recognized as essential for generating unexpected glassy behaviour for the energy relaxation in systems without any metastable states [TA]. The energy transport in anharmonic systems could involve either breather mobility or inhomogeneous waves or both. We expect that a better understanding of the statistical mechanics of breathers will result from these studies. We aim to explain spectral hole burning in terms of formation of breathers, in contrast to the traditional 2-level model (e.g. [Sma]) for which no-one has ever given genuine evidence. We will also investigate the possible role of discrete breathers in detonation, cf. [BB], and try to solve the old problem of the microscopic mechanism of Fourier's law of heat conduction in electrical insulators.

Similarly, we will attempt to interpret observations on interstellar carbonated dust in terms of breathers. The observation of IR lines emitted by very cold and dilute carbonated dust (around 20 Kelvin) which exists around many stars, is found to be incompatible with their expected black body radiation: there are intense energy lines around 2000 cm^{-1} which demonstrate that the carbonated aggregate cannot be at thermal equilibrium during the emission of these lines. An explanation suggested by Renaud Papoular, from the department of Astrophysics of Saclay, supposes that these aggregates could capture energy from collision with hydrogen atoms of the interstellar gas, which would remain localised in small regions of the grain and be released as IR radiation before thermalization. We wish to investigate accurately the possibility of existence of discrete breathers in complex carbonated molecules by using our recently developed numerical tools.

1.4 Polarons and Bipolarons

Arrays of bipolarons generate insulating bipolaronic charge density waves for weak electron hopping. In 1D systems, the minimum energy structures are believed to form periodic or quasiperiodic CDWs. We would like to prove this for some models or under some general conditions. In addition, in the incommensurate case, the inverse of a *transition by breaking of analyticity* is observed numerically as the hopping amplitude is increased, by which the system becomes a conducting Peierls-Fröhlich CDW. We wish to prove that this transition belongs to the same universality class as that for Frenkel-Kontorova models [Mac1].

In 2D models, the nesting of the Fermi surface generated by a CDW is generally not perfect, and the questions that are understood in 1D models are unsolved. The most important question that we shall address here concerns the coexistence of a metallic state with bipolarons. Problems with a magnetic field are also of interest. New types of metal-insulator transitions are expected, which we wish to explore.

The Warwick group proved that bipolarons persist to non-zero temperature and in any dimension [BM2], but the proof gives little information about which configuration has the minimum energy. In particular, we wish to understand the behaviour of the 2D bipolaronic CDWs with temperature. The bipolarons in the Holstein-Hubbard model also have puzzling properties because of the competition between the electron-phonon interaction which tends to form bipolarons and the repulsive Hubbard interaction which tends to break them. In some restricted region of the model parameters, the quantum bipolaron could become highly mobile which would open up the possibility of superconductivity at high temperature.

The dynamics of an electron in an anharmonic lattice also exhibit interesting solutions called *polarobreathers*, corresponding to a localised electron bound to a localised lattice vibration. It is connected with the Davydov soliton [Dav] proposed for describing energy transfer in proteins, and we shall explore these connections.

The Hubbard Model, which describes electrons with on-site repulsion treated within the extended Hartree-Fock approximation, also has an anti-integrable limit with a magnetic degree of freedom. We aim to exploit this limit, to obtain chaotic polaronic states, for example. We will seek to prove existence of polarons in the SSH model of polyacetylene [SSH], and to formulate and study models for excitons in polyphenylenevinylene [GF].

1.5 Josephson junction arrays

Using low temperature scanning laser microscopy, we propose to perform detailed experiments on Josephson junction ladders and larger arrays to excite and investigate localised dynamical states in these systems. In particular, our objectives will be to systematically study the stability and parameter range of the existence of the localised modes in ladders, investigate multi-cell localised states and interaction between individual rotobreathers, and attempt to study the effects of rotobreathers on transmission of plasmons and fluxons.

In parallel, we shall develop the dissipative extension of the theory of breathers. In particular, we will have to investigate to what extent breather properties such as resonances, plane wave scattering and mobility, extend from the Hamiltonian case to these dissipative systems. An important step will be a uniform persistence of normally hyperbolic submanifolds result, as proposed by [Mac2], to establish existence of generalised multibreathers in this context. We will also study aggregation of fluxons (cf. [V+]) and flux interactions on stacked Josephson junctions under the influence of external fields, cf. [SP] and [Pe+].

Finally, the recent wave of interest in quantum computing, the potential advantages of Josephson-based devices for new computing concepts and technologies, and our recent demonstrations of rotobreathers in these systems, make it worthwhile to investigate the possibility of observing quantum rotobreathers in the quantum regime of operation of Josephson-based devices.

1.6 Friction and Nonlinear Conductivity

Friction between solids and nonlinear conductivity in charge density wave (CDW) materials are related topics where there is a wide range of models but no overwhelmingly "right" model (despite the popularity of the Fukiyama-Lee-Rice model for the latter, e.g. [Gru]), which share the common feature of "pinning". We shall begin by further developing theory for a class of modulated elastic media (cf. [Fis]), concentrating particularly on tilted Frenkel-Kontorova models. In particular, we shall extend a proof of globally attracting sliding state when there are no equilibria [BM4] to the overdamped inertial case, and answer further questions posed by [FM]. If the damping is weak, however, breathers and waves can form, and this introduces different possibilities which we shall study. Models of friction with contact and non-contact areas will also be studied. Numerical simulations using realistic potentials and geometries for copper-copper friction show that long-lived hot spots are created in the contact area. We intend to see if they can be described and understood in terms of discrete breathers. Finally, we shall carry out a critical examination of the applicability of elastic media models to CDW materials by comparing experimental data and theory, and explore alternative models of the Holstein type.

1.7 Breathers in Biomolecules

While the famous discovery of the double helix structure of DNA has attracted attention to the link between form and function in biological molecules, there is now a growing consensus that *dynamics* is also essential for function. In the case of DNA this is obvious because the genetic code is embedded in the interior of the double helix and could not be read without a local unwinding of the helix. This involves very large motion of the bases, whose interactions are highly nonlinear. Local openings of DNA are observed experimentally and they may have dramatic consequences because when the bases close again they may trap a small molecule, which introduces a defect in the genetic code. This is believed to be one of the mechanisms by which some chemicals can cause cancer. We propose to develop models to the stage where actual biological problems will become solvable (for instance the formation of the open complex between DNA and RNA-polymerase), and to open the way to an understanding of DNA transcription that could allow its control (a crucial question for many genetic diseases).

The role of finite curvature on the charge and energy transport in bent molecules will be investigated. Preliminary results show that there is a spontaneous symmetry breaking in the spectrum of stationary states of nonlinear localised excitations. Because of the genetic code, DNA is highly inhomogeneous, and we propose to study its effects on dynamics (for the effects on statics, see [CD]).

More generally, biological molecules are highly deformable objects where nonlinear dynamics plays a very large role. Nonlinear energy localisation leads to a distribution of fluctuations which may be very unusual, allowing very large events. This could have a profound consequence on the kinetics of biological reactions, which we shall investigate. The active center of an enzyme is part of a nonlinear network and therefore subjected to fluctuations which have nothing to do with the random forces exerted by a fluid on the small molecules involved in standard chemical kinetics. The statistical mechanics of nonlinear lattices may help us understand how biological molecules could play the role of an "intelligent thermal bath" for the active site of an enzyme and control the kinetics of a biological reaction in a very unusual way.

Concerted proton transfer along chains of hydrogen bonds between peptide units is widely regarded as a possible mechanism in protein-mediated proton transfer and polarisation. Recent measurements of the full neutron scattering function on polyglycines have revealed the tunnelling of hydrogen bonding protons between peptide groups. Further experiments are planned to sort out factors determining the proton transfer rate: secondary structure, side chains, environment. The Montpellier group will perform STM studies on α-helices of polyalanine ordered under an electric field. Theoretical modelling will be carried out to represent these nonlinear dynamics (polarons, breathers) and to propose realistic mechanisms.

The fundamental physical mechanisms of the unidirectional translatory and rotatory motions in biomotors such as actomyosin, kinesin, dynesin and others will be studied using nonlinear dynamical models, concentrating particularly on the ATP synthase. Soliton and ratchet mechanisms in hydrogen-bonded chains will be investigated. Finally, we will examine a speculation about how in muscle the energy of hydrolysis of ATP is transferred into mechanical motion of the heads of a myosin molecule along an actin filament, based on the concept of discrete breathers, and which sharply contradicts standard phenomenological models of energy relaxation. Within our interpretation, the ATP energy is supposed to induce the formation of a discrete breather at a specific site of the myosin. Subsequently, a targetted transfer of a specific amount of this focused energy may occur toward another specific site [Au2] with a high rate of efficiency. This process might repeat many times for a well-designed biomolecule so that as a result the energy packet released by ATP travels in a non-random and reproducible manner along a selected sequence of protein sites while remaining well focused for a long time. If one also takes into account that discrete breathers on a macromolecule should induce in general a change of its conformation, this coherent energy transfer along the biomolecule should be associated with a coherent motion of the biomolecule. Such a system would realise a transduction of the breather vibrational energy into mechanical energy. At the present stage, this speculation is supported by a few numerical investigations on highly simplified models using the tools we implemented recently for the study of breathers, but if correct the impact would be dramatic.

2 Scientific Originality

One thread of the historical roots of this work can be traced to the 1920s, when it became evident to physical chemists (both from infrared spectroscopy and from measurements of specific heats) that vibrational energy of small molecules is often localised on a single degree of freedom. Studies of such *local modes* were continued throughout the 1930s by Mecke and his colleagues, and in the 1970s such interest was reawakened with the hope of developing laser catalysis of chemical reactions and also new means for isotope separation (for a recent survey of the work on local modes in physical chemistry, see [Qua]). Meanwhile, the idea of local modes was extended to systems like molecular crystals, under the name of *bi-phonon*, to understand infrared measurements of the late 1960s [Agr].

A second thread of the historical development behind this proposal extends back to the concept of a *polaron* (in which electric charge is localised in a crystal by interaction with a local distortion of the lattice), which was first suggested by Landau in 1933 [Lan]. This idea was extensively studied in the Soviet Union during the 1950s [Pek] (for a careful introduction to and review of the polaron concept, see the classic book by Haken [Hak]).

Yet another thread goes back to the 1960s when it became evident that certain nonlinear partial differential equations (PDE) and difference differential equations (which had arisen in the fields of hydrodynamics, nonlinear optics, and solid state electronics, among others) have exact solutions, comprising *solitons* which represent localised vibrational energy, electric charge or magnetic flux, according to the specific experimental context [SCM]. Of particular interest to this proposal was the discovery in the early 1970s of certain soliton solutions of the sine-Gordon equation (representing magnetic flux propagation on an extended Josephson junction, dislocations in a crystal, and domain walls in ferromagnets), which were then called *breathers.* In the present proposal, the term "breather" is used in a broader sense to mean spatially localised vibrations in any system, which does not necessarily possess the complete integrability properties of the sine-Gordon equation.

A related line of work is on classical (and quantum) field theory models for particles and their more recent applications to continuum approximations for excitations in some solid-state physics contexts. The classical models are mostly PDEs for which the state takes values in a topologically non-trivial manifold and hence minimisers occur in certain homotopy classes, which are often spatially localised (e.g. skyrmions, BPS monopoles, GL vortices, and sine-Gordon kinks). Similarly, there is very interesting current work on localised solutions of dissipative PDEs (reaction-diffusion, CGL...). In both contexts, the interactions of the localised objects are in general highly non-trivial and it is a fascinating field, but we choose to concentrate on problems where spatial discreteness plays a fundamental role.

Another well known source of localisation is spatially random linear systems (Anderson localisation). Our work links with this is an interesting way: although discrete breathers are robust to the addition of some spatial randomness, Anderson modes are very sensitive to the addition of nonlinearity [AMM, KA]. Indeed, extended states propagating energy occur for arbitrarily weak nonlinearity in a large enough system!

In the biological context, a polaron-like mechanism was proposed in 1973 by Davydov for the storage and transport of CO vibrational energy in protein [Dav]. Interestingly, it was also in 1973 that Careri discovered a spectral anomaly in hydrogen bonded crystals of acetanilide (a model protein) [Car], which was later shown to be an example of Davydov's polaronic mechanism [Car1, ELS1, Sco].

Since the mid-1980s, the investigators engaged in this proposal have played leading roles in extending the concept of breather to a wide variety of physical, chemical, and biological systems that localise vibrational energy, electric charge, or magnetic flux, and to extending the polaron concept. In 1985, for example, Eilbeck (a UK subcontractor) and Scott (a member of the Lyngby team) established the relationship between discrete breathers and the local modes of physical chemistry [SLE, SE], extending the local mode concept to a general analytic model (called the discrete self-trapping equation) with a wide range of physical and chemical applications [ELS]. Following further generalizations by Sievers (USA) and Takeno (Japan) [ST] and by Campbell (USA) and Peyrard (a subcontractor of Saclay) [CP]—who introduced the term "discrete breather"—MacKay (coordinator of this proposal and Warwick group leader) and Aubry (Saclay group leader) established the existence of breathers for networks of weakly coupled Hamiltonian oscillators [MA]. Conditions for the stability of discrete breathers have been formulated by three of our nodes [CE, Au1, MS].

On the experimental side, extensive evidence for the existence of breathers in molecular crystals was obtained for the 4-methyl pyridine crystal by Fillaux (Thiais group leader) [FC] and in acetanilide (a model protein) and related hydrogen bonded crystals by Barthes (Montpellier subcontractor) [BAS]. This has been complemented recently by experimental work in the USA: Bishop has encouraged research that has led to experimental evidence for breathers in PtCl ethyldiamine chlorate [S+], and Sievers and his colleagues have advanced experimental evidence for discrete breathers in a spin lattice [SES]. On a larger scale, two of our nodes have recently demonstrated rotobreathers in Josephson junction ladders [B+, TMO]. The existence of breathers and rotobreathers in arrays of Josephson junctions was predicted by the Zaragoza group in collaboration with Saclay, and is a consequence of theory by Warwick-Nice [SM]. Moreover, the Erlangen group succeeded to *directly visualize* [B+] spatially-localized states associated with rotobreathers in ladders.

The concept of polaron has been greatly ramified by Aubry by continuation of various configurations from the tight binding limit ([AAR], see also [BM1]). This has led to the discovery of the quadrisinglet bipolaron in the 2D Holstein-Hubbard model, which appears remarkably mobile in certain parameter regimes [PA] and is a prime candidate for explaining hihg temperature superconductivity in CuO planes.

Concerning the quantum formulation of lattice breathers, the problem is completely solved for the discrete self-trapping equation [SEG], and the corresponding Hartree approximation has been developed for the large quantum numbers needed for the construction of coherent states [Sco1]. For more general models and the polaron problem, exact solutions of the quantum problems are not available [Hak], but the polaron problem can be solved in the discrete limit and extended via perturbation theory, which is adequate for the analysis of local modes of CO oscillation in crystalline acetanilide [Sco1].

A general result of [KT] can be used to prove the persistence of non-degenerate ground states and of a gap to the rest of the spectrum, and a paper of [FaM] provides some results about the ground state of quantum crystals with hardening anharmonicity, but the main problem of the low lying excitations remains open. We believe that our ideas of strategy for proof are original and will have a highly significant effect on developments in mathematical physics and the interpretation of vibrational spectra.

The Lyon group made a pioneering contribution which attracted a great deal of attention [Mad], by showing that nonlinear energy localisation could be responsible for the local openings of DNA that lead to thermal denaturation when temperature is increased. Our proposals on biomolecules are likely to be highly controversial, but we believe they are very promising. Our ideas on spectral hole burning, interstellar carbon and biomotors, are totally original, dare we say, revolutionary.

The originality of our proposals is, we hope, already clear from the preceding section and various remarks made throughout the current section, but we wish to conclude with a few general comments.

Our project represents a major step beyond the current state of the art. Discrete breathers are a new paradigm in physics. It is a vastly more general concept than the breather of integrable systems. It has broad applicability, even to realistic models of real systems, thanks to our accurate numerical tools. It will lead to a totally new mode of interpretation of neutron scattering data, and of other probes of dynamics at the atomic level.

3 Research Method

Our research methods will comprise a combination of mathematical proof, numerical computation, physical insight, experiment and design of data analysis. Some remarks on the methods for specific problems already appear in Section 1b, but we summarise here the major themes of our methods.

Our mathematical approaches to these nonlinear problems differ from the standard expansions in weak nonlinearity which frequently introduce convergence problems and for which the interesting phenomena are often out of reach. Instead we aim to set up the problems as applications of the implicit function theorem, by identifying some nonlinear but tractable limit like tight binding (meaning that interactions between adjacent lattice sites are negligible), and establishing non-degeneracy of the linearised problem at this limit. Similarly, in the quantum mechanical context, the standard tool is cluster expansion, but we propose to avoid this by correct choice of function spaces. Another mathematical tool to be used is the theory of homology index, which enables one to deduce existence of large numbers of critical points of a functional on perturbation from a degenerate case, e.g. [BM3]. For specific forms of perturbation, an effective potential can be computed to leading order to infer more precise information about these critical points, cf. [Au1]. Furthermore, an effective Hamiltonian can be computed, whose dynamics gives a manifold of approximate solutions [AMS]. This will be used to provide rigorous error bounds on the "collective coordinate" approach, which itself will be used to gain qualitative insight into the dynamics of the nonlinear excitations.

We will use extensions of Levinson's theorem, which give relations between the number of local modes and the scattering of phonons, to understand the number of local modes on a breather. A result of [Fl] will be used as a starting point for a proof of existence of acoustic breathers in FPU models. Some partial extensions on breathers in the presence of acoustic phonons have already been obtained independently with different methods by the groups in Warwick, Saclay [Au3] and Dresden [FKT], from which we intend to build a general result.

A first approach to rigorous theory of quantum breathers will be via cluster expansions, on which the Warwick team already has experience in related problems (correlation decay for coupled map lattices), but the long term goal will be to achieve the result by employing a suitable choice of norms on tensor products and the implicit function theorem.

Many of our numerical computations are and will be implementations of the mathematical proofs. Others will be of an exploratory nature. The implementations of the rigorous proofs are mainly based on solving implicit function problems numerically, via a Newton or approximate Newton iteration, and implementing ideas and expertise developed by several of us on curve-following methods.

The proposed experiments are of two types. The first deal with Josephson junction arrays, which we design, fabricate, and then study in the laboratory. The visualisation of localised oscillations in Josephson arrays became possible due to a unique spatially-resolved method of electrical imaging developed in Erlangen, low temperature scanning laser microscopy (LTSLM).

The second deal with probes of the dynamics in molecular crystals using mostly the vibrational spectroscopy techniques. In addition to the more conventional infrared and Raman spectroscopy, the experimental team has great expertise in the neutron scattering technique. This technique is unique for observing the dynamics of hydrogenous species (methyl rotation, hydrogen bonding, proton transfer, mobile protons) because the incoherent scattering cross section of the hydrogen atom is about one order of magnitude greater than for any other atom and totally independent of the chemical bonding. Another great advantage is that intensities can be measured over a range of momentum transfer values Q (this is the vector difference between the incident and scattered neutron wavevectors). Because the interaction of neutrons with matter is very weak, the full scattering function $S(Q,\omega)$, where ω is the energy transfer, can be calculated rigorously in a number of cases, allowing us to distinguish linear and nonlinear excitations. These calculations cannot be performed for the optical techniques, mainly because of the complexity of interaction of photons with matter.

In addition, partial deuteration provides information at two different levels. Firstly, the scattering cross section for the deuterium atom is about 10 times smaller than for the H atom. Therefore, partial deuteration allows us to focus the spectra on the protons undergoing dynamics with large amplitude and anharmonicity. This is of great importance for infinite chains of amides and polypeptides. Secondly, isotopic mixtures of hydrogenated and deuterated molecules allow us to change the effective mass for collective dynamics and to create local impurities under well controlled conditions. The Thiais group has a long expertise in the synthesis of isotopically labelled molecules and in the growth of large single crystals required for neutron scattering experiments. We will use facilities like the ISIS pulsed source at Rutherford Appleton Lab (UK) or LANSCE at Los Alamos and the reactor sources at the Institut Laue-Langevin (Grenoble) or the Laboratoire Léon-Brillouin (Saclay).

In addition to optical and neutron techniques, the Montpellier group brings its own expertise in studies of local order and dynamics with high resolution solid-state NMR and nanophysics techniques (STM and AFM). This group will extend experimental studies of breather dynamics to the quasi-elastic neutron scattering regime.

For the work on biomolecules, we propose to interact closely with molecular biology experimentalists in our teams at Saclay and Lyon and via contacts outside the network like Libchaber (USA). Time-resolved experiments to search for discrete breathers in biological macromolecules will be carried out with new techniques available at ESRF (Grenoble).

For the data analysis, we propose to implement Bayesian inference techniques, cf. [Bri], to distinguish between the fingerprints in reciprocal space of spatially localised and extended states.

To summarise, the aim of the present network is to make breakthroughs in the application of ideas on localised excitations in spatially discrete nonlinear systems. Some of the basic ideas, means and methods have already been developed by this group in the previous HCM collaboration phase. Several conceptual and mathematical breakthroughs as well as experimental investigations have been accomplished in the subsequent two years. In the planned IHP phase, our mature and active collaboration will extend the previously developed ideas and relate them to real physical, chemical and biological systems.

We believe that our network acts collectively as a steady source of new ideas, providing international leadership in understanding the role of nonlinearity in extended systems. In addition to resolving fundamental scientific issues, the proposed research has applications to technology and biotechnology that will be fully addressed by the network.

4 Work Plan

Below we itemise our work plan, divided into tasks for clear management. Several of the tasks involve Subcontractors or Associates (Associates are groups which will be involved in the research but not directly in the training). They are listed here (indicating their parent Participant), and giving the reasons that their contributions are essential.

Our plan is to carry out most of the research and the training in the first three years, leaving the fourth year mainly to assess the impact of the network and to plan the way ahead. A table of the major milestones follows. The section is completed by a table indicating the size of the professional research effort expected.

4.1 Subcontractors

Edinburgh (Warwick): Lattice breathers. High performance computing, computer algebra, and Mathematical skills

Lyon (Saclay): Statistical physics of nonlinear lattices, Nonlinear dynamics of biological molecules, Kinetics of biological reactions

Dresden (Erlangen): Theory for the Josephson junction experiments and numerics and theory on various aspects of breathers

Barcelona (Zaragoza): Stochastic perturbations in extended systems

Madrid (Zaragoza): Massive computation

Athens (Heraklion): Phase transition in biopolymers, thermal solitons. Expertise in soliton statistical mechanics, theory of critical phenomena, and application of nonlinear methods to condensed matter physics.

Montpellier (Thiais): Optical and Neutron scattering experiments on acetanilide and related materials

4.2 Associates

Cambridge (Warwick): Links with Material Physics, e.g. Light-emitting polymers, colossal magnetoresistance oxides, high temperature superconductors, ferroelectrics and ferroelastics, quantum Hall materials

Nice (Saclay): Mathematics on propagating breathers and expertise in centre manifold techniques

Berlin (Erlangen): Travelling breathers

Sevilla (Zaragoza): Numerics on interplay between nonlinearity and randomness

Salerno (Firenze): Open quantum systems, Quantum solitons, and DNA and globular protein dynamics

Milano (Firenze): Rigorous mathematics on the breather life-times and polaron models.

4.3 Tasks

The tasks are broken down into pieces with start and end dates indicated in months from the beginning of the contract. The main teams that will be involved in the task are indicated.

T1. Breather Existence Theorems: Extension of the existence theorems to anharmonic crystals with several degrees of freedom per unit cell and acoustic phonons (0-12), and to acoustic breathers (0-12). Rigorous relation between modulational instability and discrete breathers (12-36). Normally hyperbolic persistence theorems for generalised multibreathers in dissipative systems like Josephson arrays, proof (0-12) and applications (6-18). Number of localised modes on a breather (0-12). Explicit estimates on breather continuation (0-12). Life-time of quasiperiodic breathers (0-24). Saclay-Warwick-Nice-Zaragoza-Milano

T2. Breather Quantization: Semiclassical EBK quantization of breathers (0-12). Breather tunnelling (0-12). Rigorous theory of quantum breathers as spectral projections (0-24). Comparisons with experiments (0-36). Warwick-Saclay-Salerno-Montpellier-Thiais-Dresden-Milano

T3. Rotobreathers: Measurements of the full neutron scattering function on single crystals (0-24). Analysis of experimental results (12-36) and development of semi-classical theory (0-24). Lyon-Thiais-Saclay-Cambridge

T4. Breather Mobility: Analytical approaches (0-24), extensive numerical simulations (0-24), tests of new concept of Peierls-Nabarro barrier (0-6), breather mobility in NLS systems (0-12). Heraklion-Lyngby-Lyon-Warwick-Zaragoza-Saclay-Dresden-Edinburgh -Nice-Berlin-Milano

T5. Phonon-Breather interactions and Self-Localisation of Thermal Energy : Analytical and numerical study of elastic and inelastic scattering of phonons from breathers, in 1,2 and 3D models (0-24). Spontaneous breather growth and decay in systems at finite temperature (0-24), breather collisions (0-24). Spectral hole-burning (12-36). Interstellar carbon (12-36). Detonation (24-26). Lyon-Lyngby-Heraklion-Saclay-Firenze-Warwick-Berlin-Madrid

T6. Spatial randomness and nonlinearity: Interaction between Anderson and nonlinear localisation (0-24). Application to DNA models (12-36). Warwick-Saclay-Sevilla-Firenze-Lyngby

T7. Breather Induced Slow Relaxation: Interpretation of experimental results on methyl pyridine (0-24). Stretched exponential relaxation of breathers (0-24), thermodynamic consequences (12-36), dynamical response functions (12-36). Heraklion-Zaragoza-Saclay-Firenze-Thiais-Lyon

T8. Polarons and Bipolarons: Formation of polarons and bipolarons in the 2D Holstein-Hubbard model (0-24), investigation of conditions favouring superconductivity (12-24). Theory for SSH polarons (12-36), and PPV excitons (24-42). Warwick-Zaragoza-Lyngby-Saclay-Edinburgh-Salerno-Milano-Cambridge

T9. Josephson Junction Arrays: Breather stability and movability in Josephson junction ladders and forced-damped arrays of oscillators (0-24). Interactions with fluxons (in JJ arrays) or discommensurations (oscillator arrays) and linear waves (0-24). Aggregation of breather-breather interactions on arrays and stacked Josephson junctions (0-24). Experiments and their analysis (0-36). Zaragoza-Lyngby-Saclay-Erlangen-Dresden-Salerno

T10. Solid Friction and Nonlinear Conductivity: Theory and numerics for one and two-dimensional generalized Frenkel-Kontorova models with tilt, inertia and damping (0-24). Application to solid friction and nonlinear conductivity (but including an assessment of the applicability of the model to this problem) (12-30). Energy dissipation and coupling with other degrees of freedom (24-36). Extension of proof of globally attracting sliding states from gradient to overdamped inertial case (0-12). Study formation of breathers in underdamped case (24-42). Warwick-Zaragoza-Lyon-Saclay-Edinburgh.

T11. Proton transfer: Experiments using inelastic neutron scattering technique that allows the quantum regime in proton transfer to be observed along pre-existing hydrogen bonds (0-36). Collective proton transfer in infinite networks of hydrogen bonds, tunnelling transitions in polyglycines (0-36). Thiais-Heraklion-Lyon-Montpellier

T12. Discrete polarobreathers: Polarobreathers in hydrogen-bonded networks, Holstein and Fröhlich-type models (0-12). Energy localisation in biological systems due to discreteness and nonlinearity (12-36), collapse studies (12-36). Heraklion-Lyon-Lyngby-Saclay-Zaragoza-Thiais

T13. DNA and globular protein dynamics: Statistical mechanics of models for DNA and their dynamics near the denaturation transition, focussing on the role of discrete breathers (0-24). The DNA model will be extended to include the elastic field associated to the twist and its coupling with DNA openings (12-24). Application of extended DNA model to study bending induced by RNA polymerase, coupling of bending and local unwinding (12-36). Molten globular protein states (12-36). Lyon-Lyngby-Athens-Salerno

T14. Biological Motors: Extension of molecular motor model for motion of proteins in biopolymers to include nonlinear aspects of the biopolymeric substrate (0-12), stochastic simulations and analytical work targeting the role of nonlinear localised modes and collective motor function (12-24). Interpretation of experiments of Bellisent-Funel (Saclay) and Berge (Lyon) (12-42). Heraklion-Zaragoza-Saclay-Lyngby-Firenze-Salerno-Lyon-Barcelona

Major Milestones	
Month	*Milestones*
6	Proofs of existence of acoustic breather in FPU models, optic breathers in general models with acoustic phonons, and globally attracting sliding state for overdamped tilted FK models
12	Development of data analysis techniques for neutron scattering experiments. Understand number of local modes on a breather. Proof and properties of generalised multibreathers in dissipative oscillator networks, and observation in Josephson arrays.
18	In depth assessment of role of breathers in interstellar carbon, spectral hole burning, 4-methyl pyridine, DNA and some biomotors. Rigorous theory of quantum breathers as spectral projections.
24	Theory of breather mobility. Mid-term review
30	Understanding of heat conduction. Proof of existence of SSH bipolarons. Understanding of role of polarobreathers in hyrogen-bonded systems.
36	Understanding of solid friction and CDW conductivity. Understanding of proton transfer problems. Assessment of effect of genetic code on DNA breathers. Theory of relaxation of thermal energy in molecular crystals.
42	Theory for PPV excitons. Conceptual design of breather-based materials and Josephson computing elements. Extension of biomolecule work to other biomotors
48	Assessment of status. Final report.

Table 1: Major milestones for the project.

Professional Research Effort			
Participant	*YVR*	*R*	*N*
1. Warwick, UK	50	134	17
2. Saclay, FR	40	216	12
3. Erlangen, DE	44	163	11
4. Zaragoza, ES	40	360	16
5. Lyngby, DK	36	336	12
6. Heraklion, GR	38	150	10
7. Firenze, IT	60	110	10
8. Thiais, FR	21	150	12
TOTALS	329	1619	100

Table 2: Size of professional research effort by participant (including dependent subcontractors and associates) in person-months, differentiating between young visiting researchers (YVR) financed by the network, and researchers (R) financed from other sources (including the group leaders), and indicating the total number of researchers likely to contribute to the project (N).

5 Collective Expertise

Members of the research teams collected under this proposal are involved in a wide range of scientific expertise and physical insights on the localisation of vibrational energy, electric charge, and magnetic flux in a variety of physical systems. This includes both mathematical analyses and numerical studies, and in addition, several of our groups regularly conduct state-of-the-art experimental investigations involving extended Josephson junctions and junction arrays, infrared spectroscopy and Raman and neutron scattering studies of molecular crystals and chemical molecules. Thus the entire spectrum—theoretical, numerical, and experimental—of modern applied science is covered at the highest levels of current practice.

To suggest the quality of this research, it should be noted that three of the node leaders (Ustinov, Tsironis, and MacKay) are winners of the biennial "Stephanos Pnevmatikos Prize for Research in Nonlinear Science," which is awarded by an international committee of leaders in nonlinear science. Details for each team follow.

5.1 Warwick

Group leader: Robert MacKay, Director of Mathematical Interdisciplinary Research, Mathematics Institute, University of Warwick, Coventry CV4 7AL, UK

Role in the network :
The primary role of Warwick in the network is to provide, and to train young researchers to provide, clean mathematical formulations and mathematical proofs for phenomena of physical interest. Warwick's subcontractor, Heriot-Watt University, provides high performance computing facilities and experience in using them for breather computations. Warwick's Associates in the Cavendish Laboratory, Cambridge, provide expertise in electron-phonon and exciton problems including connecting to materials physics and commercial technology. Warwick will play a central role in tasks T1,T2,T4,T5,T6,T8 and T10, and Edinburgh will contribute to tasks T4, T8 and T10.

Existing research linkages with the network : The Warwick team has published papers with the groups of Saclay, Dresden, Sevilla, Edinburgh, Firenze and Nice. Baesens worked with Aubry at Saclay for 14 months. MacKay and Baesens were active participants in the HCM network coordinated by Tsironis. MacKay and Baesens organized a workshop on Electron-phonon systems at the University of Warwick in Sept 94 in which Aubry, Moudden, Tsironis, Floria and Roncaglia participated. MacKay and Baesens have discussed several research topics with Floria, and Marin's work with Aubry inspired research of MacKay and Baesens with Kim. Christiansen's comments led to applications by MacKay and Aubry to DNLS. Former HCM fellow Sepulchre of MacKay now works in Nice. MacKay and Flach organised a workshop in Dresden.

Existing research linkages with industry :
Cambridge Display Technology: They are designing light-emitting polymer displays, based on recombination of electron-hole excitons, and are very keen for us to supply some theory. Hewlett-Packard Basic Research Institute for Mathematical Sciences, Bristol: Informal discussions with the Director J Gunawardena on applications to computer technology.

Key scientific staff to be involved (with % of full-time employment on the project):
Prof. R.S.MacKay (Director) 40%, Dr. C.Baesens (Lecturer) 40%, Dr. H.H.Rugh (Research Fellow) 15%, Dr V Rothos (current Marie Curie fellow) 80%, Dr. N.d'Ambrumenil (Lecturer in Physics) 5%, Dr. B Mouzykantskii (Physics) 5%, Dr. M Turner (Physics) 5%
Subcontractor (Mathematics, Heriot-Watt University, Edinburgh): Prof JC Eilbeck (leader) 5%, Prof J Carr 5%, Dr J-L Marin (current Marie Curie fellow) 50%
Associates (Cavendish Laboratory, Cambridge): Prof P Littlewood (leader) 5%, Prof R Friend 5%, Dr N Greenham 5%, Dr Cote 5%, Dr A Green 5%; and in Earth Sciences: Prof E Salje 5% and Dr Dove 5%.

Two recent relevant publications :
RS MacKay, S Aubry, Proof of existence of breathers for Hamiltonian or time-reversible networks of oscillators, *Nonlinearity* **7** (1994) 1623-1643.
C Baesens, RS MacKay, Effect of temperature on polaronic and bipolaronic states of the adiabatic Holstein model, *J. Stat. Phys.* **85** (1996) 471-488

5.2 Saclay

Group leader: Serge Aubry, Laboratoire Léon Brillouin, CE Saclay 91191-Gif-sur-Yvette, France

Subcontractor leader: Michel Peyrard, Laboratoire de Physique, ENS-Lyon, France

Role in the network : The main activity of Laboratoire Léon Brillouin, is on neutron scattering spectroscopy techniques in condensed matter. Its theory group has been active for many years in nonlinear physics and has been seminal in major developments in the theory of nonlinear localisation. It has played a leading role in formulating nearly all the tasks of this project, and will be central to their execution. The experimental group headed by M.C.Bellissent-Funel is expert in the dynamics of biological macromolecules studied by NMR, Raman and neutron techniques. For example, they studied photosynthetic proteins and enzymatic systems like Atcase and lyzozyme. They will develop new high tech experiments at the ESRF Grenoble to search for discrete breathers in real proteins (for example, time resolved X-ray experiment associated with femtosecond laser spectroscopy).

The Laboratoire de Physique of ENS-Lyon has a good reputation in statistical physics and nonlinear science. M.Peyrard was elected in 1997 to the Institut Universitaire de France where he holds a chair in "Nonlinear physics and physics of biological systems". Localisation through energy exchange between breathers was discovered in this group. Moreover the Laboratoire de Physique is starting a strong programme on experimental biological physics, which will provide data for our theoretical studies. The CNRS has allocated special funding for it and created a position for a *biologist* to work in the lab, in close interaction with physicists. Under the direction of B.Berge, studies of the motion of RNA polymerase along DNA, by direct observation of a single molecule, will be conducted. They will provide very detailed information for tasks T13 and T14. Lyon will also contribute to tasks T3,T4,T5,T7,T11 and T12.

Existing research linkages with the network : Many papers written in collaboration with R.S.MacKay and C.Baesens from Warwick, T.Cretegny from Lyon, G.Tsironis from Heraklion and PhD students: G.Kalosakas, A.Bikaki, N. Voulgarakis; S.Flach from Dresden, P.Christiansen, Y.Gaididei, M.Johansson and K.Rasmussen from Lyngby. Theodorakopoulos spent 2 months in Lyon, and Lyon hosted a CECAM meeting in July 98 with participants from most of the nodes.

Existing research linkages with industry :
The group of M-C Bellissent has linkage with the company Rhone-Poulenc for problems concerning ultrathin layers of polymers adsorbed on glasses.

Key scientific staff to be involved (with % of full-time employment):
Serge Aubry, Theoretical Physicist (100 %) (ex-Marie Curie fellow)
M-C. Bellissent-Funel, Experimentalist (30 %) (Groupe Diffraction et Dynamique).
G. Kopidakis, frequent visitor in Saclay (50 %) (ex-Marie Curie fellow)
Postdoctoral research fellows: M. Johansson (Swedish, Marie Curie fellow) 50%
PhD students: Anna-Maria Morgante (Italian) (66%)
Subcontractor (ENS, Lyon): M Peyrard (Professor) 40%, T Dauxois (Researcher) 50%, J Farago (agrégé préparateur) 33%
Associate (INLN, Nice): J-A Sepulchre (Maitre de Conférence) 50%, G Iooss (Professeur) 10%

Two recent relevant publications :
S.AUBRY, *Breathers in Nonlinear Lattices:Existence, Linear Stability and Quantization*, Physica **103D** (1997) 201-250
G. KOPIDAKIS and S. AUBRY, *Intraband Discrete Breathers in Disordered Nonlinear Systems I: Delocalization.*, Physica **D** (1999) in press, *II: Localization*, to be submitted

5.3 Erlangen

Group leader: Alexey V. Ustinov, Professor of experimental physics, Physikalisches Institut III, University of Erlangen-Nüremberg, Erwin-Rommel-Str. 1, D-91058 Erlangen, Germany

Role in the network :
The Erlangen group will focus on experiments with Josephson junction ladders. Using these structures, the Erlangen group have very recently for the first time *experimentally observed* localized excitations in the form of roto-breathers. The group has internationally established expertise in the field of experimental fluxon physics, long Josephson junctions and arrays. Both low-noise dc and high frequency measurement techniques are available in Erlangen to investigate localized dynamics states in Josephson ladders, the subject of great theoretical effort of other partners in the proposed network. Moreover, the group recently established a spatially-resolved measurement technique using the low temperature scanning laser microscope. This method is suitable for visualization of roto-breathers. Experiments will be performed at liquid helium temperatures in a well-shielded and electromagnetically isolated environment. Experimental work will be done in close interaction with the theoretical groups of the proposed consortium. Erlangen will play a leading role in task T9.

Subcontractor :
Group leader: Sergej Flach, Privatdozent in theoretical physics, Max Planck Institute for the Physics of Complex Systems, Noethnitzer Str. 38, D-01187 Dresden, Germany

Role in the network :
The Dresden group will focus on two directions of theoretical studies of dynamical localization. The first direction is to study the properties of localized excitations in Josephson junction systems in close collaboration with experimental research performed by the Erlangen group. The second direction is subdivided into the following aspects of localized excitations in nonlinear lattices: the interplay of disorder, noise, finite temperatures and nonlinearity with respect to their properties and quantization of classical localized excitations. The group has recently contributed to the explanation of rotobreather experiments by the Erlangen group, and has an internationally established expertise in the field of localized excitations in nonlinear Hamiltonian, dissipative and quantum lattices. Dresden will be involved in tasks T2,T4,T9.

Existing research linkages with the network : The Dresden group has especially close research linkages (see publications) with the groups in Saclay, Lyon, Warwick and Edinburgh. Close research linkages (through visits and meetings) exist with all other groups in the proposed network. In addition, Dr L Proville, who was a PhD student of Aubry and is currently a postdoc of MacKay, will move to Dresden this September.

Existing research linkages with industry :
On the subject of superconducting BSCCO multi filamentary tapes (not related to the present proposal) the Erlangen group has a cooperation with Siemens.

Key scientific staff to be involved (with % of full-time employment):
Prof. Dr. A.Ustinov (35%)
PhD students: P.Binder (35%), D.Abraimov (35%)
Subcontractor (Dresden): Priv.-Doz. Dr. S.Flach (50%), Dr. Y.Kosevich (50%), Dr. Y.Zolotaryuk (50%), Dr. L.Proville (50%)
Associate (Berlin): D. Hennig (35%)

Two recent relevant publications :
AV Ustinov, Solitons in Josephson junctions, Physica D 123 (1998) 315–329.
S Flach, CR Willis, Discrete breathers, Phys Rpts 295 (1998) 181–264.

5.4 Zaragoza

Group leader: Professor Luis M. Floría.
Depto. de Física de la Materia Condensada. Facultad de Ciencias. Universidad de Zaragoza.
E-50009 Zaragoza (SPAIN).

Role in the network :
The team has a large expertise in numerical studies on dynamics of nonlinear many-body models of condensed matter, and pioneered the applications of intrinsic localisation to Josephson devices. The subcontractor team at Barcelona is expert in stochastic perturbations in extended systems, and that at Madrid in massive computation. Associate team at Sevilla has expertise on the Anderson localisation problem. Our contributions will be centered on tasks T4,T7,T8,T10,T12 and T14:

a) Discrete Breathers (DB) in forced-damped systems: Stability, Bifurcations and Regimes of Mobility of DB's. Localised Chaos. Interactions with discommensurations. DB's in Josephson-junction arrays (Proposals of new experiments and interpretation of existing experimental results). Intrinsic localisation versus Anderson localisation (associate at Sevilla). Noise effects on intrinsic localisation: Noise-induced transitions (subcontractor at Barcelona).

b) Directed transport in periodic potentials: Ratchet effect for fluxons in Josephson devices (Proposals of experiments and applications). Role of internal degrees of freedom in directed transport of biomolecules in microtubules.

c) Gradient Dynamics of Frenkel-Kontorova models under dc and ac fields. Applications to friction modelling.

Existing research linkages with the network :
Extended collaborations with S. Aubry (Saclay) from 1989. Ongoing collaboration with C. Baesens and R.S. MacKay (Warwick), and J.L. Marín (Edinburgh).

Existing research linkages with industry :
Silicon Graphics (Prof. Vázquez) concerning algorithm parallelisation.

Key scientific staff to be involved :
Profs. L.M. Floría (80%), F.Falo (80%), P.J. Martínez (80%).
Postdoctoral researchers: J.J. Mazo (80%), J.C. Ciria (40%).
PhD student: S. Cilla (100%).
Subcontractors: Profs. J.M. Sancho (60%) and J. Garcia-Ojalvo (60%) at Barcelona, Profs. L. Vázquez (30%) and S. Jimenez (30%) at Madrid.
Associates: Profs. J.F.R. Archilla (80%), F. Romero (40%) and F.Palmero (40%) at Sevilla.

Two recent relevant publications :
L.M. Floría *et al.*, Intrinsic localisation in the dynamics of a Josephson-junction ladder. Europhysics Letters **36** (1996) 539-544.
P.J. Martínez *et al.*, Intrinsically localised chaos in discrete nonlinear extended systems. Europhysics Letters **45** (1999) 444-449.

5.5 Lyngby

Group leader: Peter L. Christiansen, Professor, Department of Mathematical Modelling, Technical University of Denmark, DK-2800 Lyngby, Denmark

Role in the network: Over the past 20 years, the Lyngby group has applied modern nonlinear dynamics and wave theory to solid state and optical physics and biomolecular dynamics with the participation of Alwyn Scott, who is one of the pioneers of nonlinear science. At present, we are studying localized excitations in discrete systems with long-range interactions and stochastic environments using analytic as well as computational techniques. With the nodes indicated we have research collaboration on molecular crystals (1-2, 4, 6-7), biomolecules (1, 7-8), and Josephson arrays (3, 6-7). During the past five years, we have awarded 9 PhD degrees, 8 Master's Theses, 1 postdoctoral associate (Swedish Research Academy). Lyngby will play a major role in tasks T4,T5,T6,T8,T9,T12,T13 and T14.

Existing research linkages with the network: Christiansen coordinated and participated in EU networks with Aubry, Peyrard, Tsironis, and Eilbeck since 1989. Visited Heraklion in 1994, 95, 96, and 99 (conferences), Edinburgh 1995 (Soliton Physics), Madrid 1994 and 95 (conferences), Les Houches 1994 (Euroconference).
Gaididei visited Heraklion several times, last in 1997 and 99, and Edinburgh 1995.
Scott and Sørensen visited Heraklion in 1990 (biomolecular dynamics), Heraklion in 1992 (Josephson arrays) and Edinburgh in 1995 and 99 (Soliton Physics).
Bang, Post Doc 1993-95 with Peyrard. Presently Lyngby.
Magnus Johansson, Lyngby 1995-97. Presently Post Doc with Aubry.
Yaroslav Zolotaryk, Lyngby 1997-98. PhD with Eilbeck 1998. Post Doc with Flach.
Leonor Cruzeiro-Hansson, Ph.D. with Christiansen and Scott 1988. Post Doc with Eilbeck.
Several French, Spanish and Greek PhD students have worked for extended periods in Lyngby. Danish PhD students have studied in Greece, Spain, and France.
Over the last 5 years, 6 joint papers annually have been published with members of the network.

Existing research linkages with industry: Research collaboration with the Biostructure Department of Novo Nordisk, a leading international pharmaceutical manufacturer, includes a Ph.D. study of molten globular states in proteins.

Key scientific staff to be involved :
Peter L. Christiansen, professor (25 %),
Alwyn Scott, professor (10 %),
Mads Peter Sørensen, professor (20 %),
Yuri B. Gaididei, visiting professor (25 %),
Ole Bang, research professor (25 %),
Joel Corney, post doc (25 %),
Morten Bache, PhD student (30 %),
Jacob Broe, PhD student (30 %),
Jens Schjoedt-Eriksen, PhD student (30 %)

Two recent relevant publications :
A. Scott, Davydov's Soliton, Phys. Reports 217 (1992) 1-67.
P.L.Christiansen, Yu.B.Gaididei, M.Johansson, K.O.Rasmussen, D.Usero, and L.Vazquez, Stabilization of nonlinear excitations by disorder, Phys. Rev. B 56 (1997) 14407-14413.

5.6 Heraklion

Group leader: G.P.Tsironis, Associate professor, Institute for Electronic Structure and Laser, Foundation for Research and Technology-Hellas, 71003 Heraklion, Crete, Greece

Subcontracting laboratory: Dr. N. Theodorakopoulos, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 11635 Athens

Role in the network :
The team has long expertise in nonlinear physics, statistical mechanics, computations and multimedia. Network work will involve statistical relaxation of breathers, heat transfer in nonlinear lattices, breather induced targeted energy transfer in biomolecules, phase transitions in biopolymers, DNA denaturation, statistical mechanics of helix-coil transitions and modelling. They will contribute to tasks T4, T5, T7, T11, T12 and T14. Subcontractor Athens will play a major role in T13.

Eight PhD degrees, five diploma theses, two postdoctoral associates (one Marie-Curie fellow) constitute the training effort of the group in the last five years.

Existing research linkages with the network :
The team, in addition to coordinating the predecessor of the present network in the HCM program (CHRX-CT93-0331), coordinates an INTAS network (where Saclay and Lyngby also participate), organized several meetings, summer-schools and conferences with wide participation from young EU researchers, postdocs and students. Tsironis visited many times Zaragoza, Barcelona, Lyngby, Warwick, Saclay (two months 1996). Greek graduate students spent one year at Saclay and several months in Lyngby, and a student from Lyngby spent two months in Heraklion. Aubry has spent several months in Crete during the last three years, and during 1997 he came as a Marie-Curie-fellow (category 40). The group has over the last five years on average three joint papers annually with other members in the net (from different countries). N.Theodorakopoulos was a visiting professor at the Ecole Normale Superieure, Lyon (1998) and one publication with Peyrard has been submitted.

Existing research linkages with industry :
There are many contacts with Greek financial firms (eg. National Consulting, subsidiary of National bank of Greece) for the developement of software in multimedia format for use in volatility estimates and professional education.

Key scientific staff to be involved :
Prof. G. P. Tsironis (network member) (50%), Dr. G. Neofotistos (20%), Dr. M. Genius (50%), Dr. G. Kopidakis (ex-Marie-Curie fellow, 25%)
Dr. N. Theodorakopoulos (subcontracting network partner)(50%) Dr. N.C. Bacalis (20%), Dr. V. Constantoudis (20%)
PhD students: P. Maniadis (50%), N. Voulgarakis (50%), M. Eleftheriou (50%).

Two recent relevant publications :
G. Tsironis and S. Aubry, Phys. Rev. Letts. **77** (1996) 5225-5228
V. Constantoudis and N. Theodorakopoulos, Phys. Rev. **E56**, 5189 (1997)

5.7 Firenze

Group leader: Roberto Livi, Associate Professor, Dipartimento di Fisica, Universitá di Firenze, Largo E. Fermi 2, 50125 Firenze, Italia

Role in the network :
The FIRENZE team aims to investigate the role of genuine nonlinear dynamical modes (solitons, breathers and Fourier-like) on transport properties in steady-nonequilibrium regimes in models of molecular crystals, heteropolymeric chains, clusters etc. Experimental studies of weakly chaotic regimes and localization phenomena induced by external modulation in samples of nematic liquid crystals will also be performed.

This research project can benefit from the wide spectrum of competences present in the FIRENZE team. On a theoretical ground they include rigorous methods of Statistical Mechanics and Theory of Dynamical Systems, complex dynamical phenomena emerging from nonlinearity and disorder, equilibrium and nonequilibrium simulation techniques of many-degrees-of-freedom dynamical systems, characterization of complexity and chaoticity indicators in strongly non-linear systems, modelling of polymer dynamics. The experimental expertises mainly rely upon techniques in optics, nonlinear optics and electronics; neutron-scattering facilities are also usually available by the access to European facilities. The Italian groups will contribute to tasks T1,T2,T4,T5,T6,T7,T14.

Existing research linkages with the network :
The FIRENZE team has linkages since many years with most of the other teams in the Network that produced fruitful collaborations and the organization of research meetings.

Existing research linkages with industry :
Existing collaboration with the ENEL (Italian energy agency) research center in Pisa on instabilities in large scale gas-burners.

Key scientific staff to be involved (with % of full-time employment):
R. Livi (Associate Professor, 40%), L. Fronzoni (Associate Professor 30%), S. Ruffo (Associate Professor, 40%), M. Pettini (Researcher, 40%), A. Politi (Researcher, 40%), S. Lepri (Postdoc 60%), A. Torcini (Postdoc 60%)
Associates (Salerno): M Salerno (Associate Professor) 30%
Associates (Milano): D Bambusi 20%

Two recent relevant publications :
S. Lepri, R. Livi, A. Politi: Heat Conduction in Chains of Nonlinear Oscillators, Phys. Rev. Lett. vol. 78, 1896 (1997).
T. Dauxois, S. Ruffo and A. Torcini: Modulational estimate of the Lyapunov exponent for Fermi-Pasta-Ulam chains, Phys. Rev. E Rapid Comm., vol.56, R6229 (1997).

5.8 Thiais

Group leader: François Fillaux, Laboratoire de Dynamique, Intéractions et Réactivité, CNRS, 2 rue Henry-Dunant, 94320 Thiais, France.

Subcontracting laboratory: Dr Mariette Barthès, Groupe de Dynamique des Phases Condensées. Université de Montpellier 2, Place E. Bataillon, 34095 Montpellier Cedex 5, France.

Role in the network :
The groups in Thiais and Montpellier have long expertise in the interpretation of rotational tunnelling and vibrational spectra (infrared, Raman and inelastic neutron scattering) of hydrogen bonded systems. They have both contributed to experimental characterization of nonlinear excitations in infinite chains of coupled rotors (the quantum sine-Gordon breather mode) or NH...O hydrogen bonds (e.g. N-methylacetamide, acetanilide, polyglycines...). The primary role of this team will be to provide neat experimental protocols to assess the existence of nonlinear excitations (polarons, breathers...) in molecular crystals. Measurements of the full neutron scattering function with single crystals are anticipated to provide clean evidence. In addition to vibrational spectroscopy, quasi-elastic neutron scattering, NMR and nanophysics (STM, AFM...) techniques will be used. Major benefits are anticipated from intensive exchanges with the theoretical groups. Thiais and Montpellier will contribute to tasks T2,T3,T7,T11 and T12.

Existing research linkages with the network :
Many discussions with S.Aubry, M.Peyrard, G.Tsironis and A.C.Scott on the nature of nonlinear excitations in chains of coupled rotors. Participant in previous (HCM) network. Seminars given at Saclay, Lyon and Lyngby.

Existing research linkages with industry :
The Thiais group is working on the characterisation of proton dynamics in materials in collaboration with industrial companies. Manganese dioxides for battery electrodes in collaboration with Tekkosha (Japan) and Sedema (Spain) companies. Coals in collaboration with the Centre d'Etude et de Recherche des Charbonages de France (CERCHAR) and carbon blacks in collaboration with Degussa (Germany).

Key scientific staff to be involved :
Dr F.Fillaux (Directeur de Recherche) 100%
Pr M.-H.Baron (Maître de Conférence) 25%
Pr A.Lautié (Maître de Conférence) 25%
Dr Ph.Colomban (Directeur de Recherche) 25%
Dr R.Baddour-Hadjean (Chargé de Recherche) 25%
Dr M.-F.Lautié (Ingénieur de Recherche) 50%.
Subcontractor (Montpellier): Dr. M.Barthès (Directeur de Recherche) 100%
PhD student: A.Spire 100% until 2001

Two recent relevant publications :
F.Fillaux, C.J.Carlile and G.J.Kearley, Phys. Rev. B 58 (1998) 11416
M.Barthès and M.Ribet, Ber.bunsenges. Phys. Chem. 102 (1998) 1-3.

6 Collaboration

We will collaborate on the research by deep interaction between members of different nodes, leading to at least two joint publications per task with authors from nodes in more than one country. This will be facilitated by visits of researchers from one team to another, hiring good PhD students from other teams in the network as part of the postdocs to be funded here, e-mail correspondences, network meetings and contact at other conferences, shared supervision of some PhD students, and secondment of some postdocs to other nodes for specific projects.

We have already established excellent mutually beneficial working relationships in both research and training, as supported by the following record of collaboration.

Members of each node have already published papers with members of one or often more nodes in other countries. Some examples, with numbers, since 1994 are: Zaragoza-Saclay-Edinburgh (4), Sevilla-Warwick-Edinburgh (1), Warwick-Nice (6), Warwick-Firenze (1), Warwick-Dresden (2 + a conference proceedings), Warwick-Saclay (2), Dresden-Heraklion (1), Erlangen-Heraklion (1), Dresden-Saclay (1), Erlangen-Lyngby (1), Edinburgh-Dresden-Lyon (1), Edinburgh-Dresden (1), Saclay-Lyon-Dresden (1), Dresden-Edinburgh (1), Dresden-Lyngby (2), Lyon-Lyngby (1), and this is a very incomplete list.

There has been huge mobility, at the levels of both recruitment of young researchers and visits by senior staff. People who have spent time as a student or postdoc at more than one of the nodes include: Sepulchre (Brussels →Warwick →Cambridge →Nice), Marin (Zaragoza →Saclay →Cambridge →Edinburgh), Proville (Saclay →Lyngby →Saclay →Cambridge →Dresden), Lorenzo (Saclay →Lyngby), Spicci (Firenze →Dresden →Cambridge), Lepri (Firenze →Dresden →Firenze), Zolotaryuk (Kiev →Lyngby →Edinburgh →Dresden), Usero (Madrid →Lyngby), Kalosakas (Heraklion →Lyngby), Panagiotis (Heraklion →Lyngby).

Some of the senior visits since 1994 were: Warwick →Zaragoza, Heraklion →Zaragoza, Saclay →Zaragoza, Lyngby →Madrid, Zaragoza →Warwick and Cambridge, Zaragoza →Saclay, Zaragoza →Heraklion, Edinburgh →Saclay, Sevilla →Cambridge, Madrid →Lyngby, Saclay →Heraklion, Edinburgh →Lyngby, Salerno →Lyngby, Saclay →Lyngby, Firenze →Lyngby.

At least five previous EU networks have involved people from more than one of the present nodes, especially:

- HCM network on "Nonlinear approach to coherent and fluctuating phenomena in condensed matter and optical physics": Heraklion (coordinator), Saclay, Warwick, Lyngby, Zaragoza, Barcelona, Madrid, Thiais
- EEC Science Programme network on "Transport properties in nonlinear condensed matter physics", Lyngby (coordinator), Rome, Heraklion, Saclay, Edinburgh, and München.

We have a strong record in organising training schools and workshops. We highlight briefly some of the activities organised primarily by people in the current network (in bold) and in which others from the network have played an active role:

Nonlinear Excitations in Biomolecules Les Houches, France, May 30 - June 4, 1994. Euroconference, organized by **M. Peyrard** with additional members **M. Barthes**, G. Careri, **P. Christiansen**, J.Krumhansl, **A.C.Scott** and **G.P.Tsironis**.

Advanced School of Physics Heraklion, Crete, 15 June - 30 July, 1994, sponsored by the Transatlantic Interuniversity Cooperation Program between the European Community and USA. Organized by **G.P.Tsironis** with lectures given by **S.Aubry**, **P.Christiansen**, D.K.Campbell, V.Konotop and K.Lindenberg. More than twenty-five graduate students and young researchers participated.

Electron-Phonon Workshop University of Warwick, 5-16 September 1994. Organized by **R. S. MacKay** with participation of several people from the network and several EU young researchers.

Fluctuation Phenomena: Disorder and Nonlinearity San Lorenzo de El Escorial, Madrid, Spain, 26-30 September 1994. Organized by **L.Vazquez**, S.Jimenez and A.R.Bishop, and included network members and many young researchers.

Nonlinear Klein-Gordon and Schrödinger systems: Theory and Applications : Euroconference, San Lorenzo de El Escorial, Madrid, Spain, 25-30 September 1995. Organized by **L.Vazquez**, L.Streit and V.M.Perez-Garcia.

International Conference on Fluctuations, Nonlinearity and Disorder Heraklion, Crete, 30 September - 4 October 1996, organized by **G.P.Tsironis**, A.R.Bishop and E.N.Economou. More than thirty young EU researchers participated in addition to many of the network members.

Nonlinear localization in lattices Dresden, **Flach** and **MacKay**, 7-11 April 1997. Participants included Aubry, Ustinov, Eilbeck, Sepulchre, Salerno, Bambusi, Baesens.

Solitons and Coherent Structures in Physics and Biology (SOLPHYS), Lyngby, **Christiansen, Scott, Sørensen, Eilbeck, Flytzanis, Peyrard, Salerno, Tsironis**, 30 May - 3 June 1997, 75 participants half of them young EU researchers.

Nonlinear localized excitations in condensed matter and molecular physics Lyon, **M Peyrard**, 7-10 July 1998. Members from most teams of this proposal participated.

Nonlinearity '99 Heraklion, 10-14 May 1999, T Geisel and **G Tsironis**, including Aubry, MacKay, Christiansen, Hennig, Baesens

Less experienced teams will be integrated into the network project via individual contacts and participation in network workshops. In particular, the leaders of the Associate nodes at Nice, Berlin and Sevilla are relatively junior, and care will be taken to involve them appropriately, specifically in the following tasks: Nice (T1,T4), Berlin (T4), Sevilla (T6). We anticipate no problems, however, because we have already established good working relationships with them and indeed already have joint publications with each of them.

7 Organisation and Management

The network will be managed hierarchically as indicated in the attached chart. There are four levels of unit: Coordinator, Members, Subcontractors and Associates. We shall refer to them collectively as Nodes. The first three levels are official Research Training Network categories, the Coordinator and Members together forming the Participants. The Associates are groups with whom one or more of us have an active research collaboration on the theme of the project and whose participation in the research will be beneficial to the project though they will not play a direct role in the training. They will be invited to join in relevant network meetings, and their expenses paid via their parent participant.

The tasks will be carried out by the nodes indicated in section 4.3. For each task, one person will be elected from these nodes to coordinate the work.

The contributions of each node to research and training will be monitored by the coordinator and assessed more formally on the basis of annual reports. Reporting will be hierarchical with strict deadlines for collation of information. We will seek to resolve any perceived problems by discussion together. In case of inability of a node to carry out its commitments, a redistribution of the budget will be drafted for approval at the mid-term review.

Communication will be primarily by e-mail. There will also be a network of webpages to display the function, activities and work of the network, with a central website at Warwick.

The coordinator has extensive experience in managing research projects of a range of sizes. He set up and ran a Nonlinear Systems Laboratory at Warwick from 1986-94 together with Rand, which hosted a total of 12 postdoctoral fellows and organised 10 international meetings, workshops and symposia of durations from 2 days to 8 months. He set up a Nonlinear Centre at Cambridge in 1995, which has hosted 7 postdocs and many visitors (20 for more than 2 weeks), and is one of the scientific directors of a current 4-year project on Spatially Extended Dynamics at King's College Cambridge. He is running the Nonlinear Centre until the end of this year, when he returns to Warwick to take over the Directorship of Mathematical Interdisciplinary Research at Warwick. He has organised or co-organised 11 other meetings, in Germany, USA, Italy and the UK. He has been scientific officer in charge of Warwick's participation in 3 different EU networks (Nonlinear Phenomena and Complex Systems, Nonlinear approach to coherent and fluctuating phenomena in condensed matter and optical physics, Stability and Universality in classical mechanics). He also wrote Warwick's part of the proposal for a current EU network on "Nonlinear dynamics and statistical physics of spatially extended systems", and is the scientific officer in charge of a subcontract at Cambridge on that network. He has raised over 2.75M Euro in research grants since 1984. He has produced 7 PhDs, with a further 4 in the pipeline. Although now in a Mathematics department and concentrating on rigorous results, the coordinator also has extensive experience of computation and theoretical physics. He is also no stranger to experimental physics: as a PhD student in the Plasma Physics Lab, Princeton, he carried out experiments on destabilisation of drift waves and dispersion of whistler waves, and built electronic demonstrations of bifurcations and chaos; he is also about to conduct a neutron scattering experiment at Rutherford, 4-8 June. Thus he is able to appreciate the wide range of approaches that will be taken here.

The results of the project will be disseminated by publication in standard refereed journals and by presentations at international conferences. Many papers will also be made available on web servers. As was explained in section 6, we have established a culture of collaborative publication which will continue during and after the end of the contract, ensuring complete dissemination of the results into the public literature. In addition, it is likely that we will produce conference proceedings from some of our network meetings, cf. the special issue of Physica D **119** edited by Flach and MacKay, from their conference on Localization in Nonlinear Lattices.

Coordinator	Members	Subcontractors	Associates
1. Warwick, UK		Edinburgh	Cambridge
	2. Saclay, FR	Lyon	Nice
	3. Erlangen, DE	Dresden	Berlin
	4. Zaragoza, ES	Barcelona, Madrid	Sevilla
	5. Lyngby, DK		
	6. Heraklion, GR	Athens	
	7. Firenze, IT		Salerno, Milano
	8. Thiais, FR	Montpellier	

Table 3: Organisational Chart for the Nodes of the network. The Coordinator and Members form the Participants. The Subcontractors will subcontract from the indicated Participants. The Associates will report to the indicated Participants.

8 Training Need

The mathematical techniques used in the project (implicit function theorem, function spaces, homology index...), although basic in mathematics, are not standard in the physics community. The network will play a unique role in training young researchers in these techniques. Similarly, the network will provide an opportunity for young mathematicians to learn about fascinating problems in physics and molecular biology which rarely appear on the standard mathematics curriculum. Again, the computational expertise which the network has developed, although elementary in some respects, is not standard, and it is important for young researchers to be trained in these techniques.

Finally, there is a need to train young researchers in how to confront real experiments as opposed to numerical computations. Our network has experimental work at four of the nodes, and they are keen to involve interested and intelligent but not necessarily experimentally trained young researchers in the experiments.

The results of our research and our way of thinking are unfamiliar to mainstream physics. We believe they are vital to the future development of physics, particularly solid-state and biomolecular physics. To bring the concepts into the mainstream of physics, training of significant numbers of bright young researchers is crucial. There is also a need to expose young researchers to the intellectual riches that can be gained by combining the insights of a variety of disciplines and transferring skills between them.

The skills which the young researchers will gain will place them in a unique position in the job market, both for academia and company research. We already have great success in placing young researchers into stable careers. For example, former PhD students and postdocs of just one of us now occupy the following positions, and similar lists could be compiled by each participant: Maitre de conference in Physics (Nice), Research scientist (Sainsbury's Innovation Centre, London), Professor of Nonlinear Dynamics (University College, London), Professor of Mathematics (U Southern California), Charge de Recherche CNRS in Theoretical Physics (Marseille), Reader in Mathematics (Univ Surrey, UK), Lecturer in Mathematics (UMIST, Manchester), Lecturer in Mathematics (Exeter, UK), Reader in Mathematics (Queen Mary and Westfield College, London), Lecturer in Mathematics (Warwick), Research Scientist (Brookhaven Nat Lab, USA), Maitre de conference in Mathematics (Toulouse).

The students and young postdocs of the network will find a truly integrated circuit of well known scientists with whom to interact, exchange ideas, do collaborative work, and plan their European future as scientists. The theorists among them will be able to get first hand feedback and information on their work from world-leading experimentalists that have done pioneering work in many areas of physics and chemistry. The experimentalists among them, on the other hand, will have some of the world's leading theorists to discuss with, collaborate with, acquire ideas from, sharpen their acumen and thus deepen their knowledge and improve their research work. From the past network (HCM) experience, as well as the other multitude programs that link various of our groups together, we experienced that our network acts as a truly *Delocalized European University* spread all over Europe. The frequent visits, the successful meetings, the close Internet interaction, the abundance of joint work, the challenging intellectual atmosphere and the excellent personal relations among the members of the network, create a great knowledge atmosphere for the young European students and postdocs.

9 Justification of the Appointment of Young Researchers

Each participant and subcontractor has personnel who are expert in hosting pre- and postdoctoral researchers, good facilities (e.g. computing or experimental equipment where appropriate), and a record of successful training. Some information about the training roles of the participants and subcontractors already appears in Section 5. A detailed justification by participant for the above requests follows, explaining which staff will carry out the training and their previous training experience.

Note that the initial requests for young-researcher-months by our nodes exceeded by about 25% the maximum amount that such a network contract could normally support. So

Young Researchers to be financed by the contract				
Participant	*Predocs*	*Postdocs*	*Total*	*Specialities*
1. Warwick, UK	0	50	50	M-05, M-14, P-16
2. Saclay, FR	0	40	40	P-16, P-09, P-10, L-01, P-07, P-15
3. Erlangen, DE	20	24	44	P-10, P-16
4. Zaragoza, ES	0	40	40	P-09, P-16
5. Lyngby, DK	0	36	36	M-05, P-09, P-10, P-16, L-01
6. Heraklion, GR	0	38	38	P-09, P-16
7. Firenze, IT	0	60	60	P-09, P-16
8. Thiais, FR	0	21	21	P-10, P-11, P-14, P-16, C-05
TOTALS	20	309	329	

Table 4: Numbers of young researchers to be financed by the network (in person-months) and the scientific specialities of the training to be provided. Appointments will be made just at these participant institutions but some of the postdocs will be seconded to subcontractors, as indicated below.

we had to restrict the requests to those judged by a small group of the participant leaders to be of the highest priority. Furthermore, a late request for 12 postdoc-months was received which was judged to be very important but regretfully it could not be included. Thus our requests have already gone through a rigorous preselection procedure.

1. **Warwick** MacKay has a range of suitable (challenging but realistic) mathematical research problems for postdocs to work on, and wishes to provide 35 months postdoc training for this network. He has provided training for 8 postdocs on previous EU network grants for a total of 65 person-months (in addition to hosting 4 EU individual fellows). The Mathematical Interdisciplinary Research programme at Warwick provides a superb environment for postdoctoral research in terms of facilities, expertise, lively supportive atmosphere, and an afternoon workshop nearly every week on a huge range of subjects in the use of mathematics in science and stimulation of mathematics by science (for example, the next two are 7 June: Spatially extended dynamics, 18 June: Turing patterns and their symmetries). Eilbeck (subcontractor) will provide 15 months postdoc training in high performance computing, and is currently hosting a Marie Curie fellow.

2. **Saclay** Since 1995, the theory group at Saclay hosted 3 postdocs (two of them with EU individual fellowship) for a total of 50 postdoc-months, and will provide training for 20 postdoc-months for this network. 3 PhD students from LLB and 4 other students from outside institutions were trained since 1995. 4 of them already obtained their PhD. The experimental group in Saclay hosted 5 postdocs, 3 PhD students from LLB and 5 PhD students from outside institutions. The group in Lyon hosted 1 postdoc with EU individual fellowship and 4 PhD students (2 of them already obtained their PhD). It will also provide training for 20 postdoc-months for this network. The Ecole Normale Supérieure de Lyon (ENS-Lyon) is one of the most prestigious higher education and research institutions in France. ENS-Lyon offers high level courses in Physics, Chemistry and Biology, that the visiting researchers will be able to attend, in addition to their training in a laboratory which is open to various areas of physics. The ENS-Lyon is initiating a strong European exchange program, which will include special help for visiting students, including facilities to learn French with special courses, in order to facilitate the exchange between visitors and French students and staff.

3. Erlangen The Erlangen group, in spite of its relatively young age (Alexey Ustinov became professor there in 1996) is already experienced in training PhD students (N.Thyssen - stacked Josephson junctions, A.Wallraff - experiments with fluxons in long junctions, P.Binder - Josephson ladders, A.Abraimov - low temperature scanning laser microscopy) and young postdocs (P.Caputo - array oscillators, Yu.Koval - ultra-narrow junctions, M.Fistul - analysis of Josephson array dynamics, G.Logvenov - experiments at millikelvin temperatures) in the field of the proposal. Young members of the Erlangen group benefit from frequent visits of experienced scientists such as B.Malomed (Tel Aviv), V.Ryazanov (Chernogolovka), V.Kurin (Nizhnii Novgorod), S.Sakai (Tsukuba) and others. Ustinov will host 20 predoc and 16 postdoc months. In Dresden, Flach has experience with training of PhD students (Kladko: moving breathers, electron+breather, breathers in 3D, quantum breathers) and young postdocs (Spicci: Josephson ladders, Zolotaryuk: moving pulses, Josephson ladders, spin systems) in the field of the proposal. Visits of experienced scientists (up to 6 months, e.g. Fleurov (Tel Aviv), Ovchinnikov (Moscow)) will support the training aspect. The MPIPKS has a dense seminar program and a large number of experienced visitors. This surrounding will help in general to broaden the scientific horizons of collaborators. Flach will host 8 postdoc months.

4. Zaragoza Since January 94, the node at Zaragoza has provided 48 months of postdoc hosting and training. The recently created Department of Theory and Simulation at the joint Institute of CSIC-UZAR will offer a good environment for 16 months of training in stochastic and deterministic approaches to localisation in nonlinear lattice systems, that Floria will provide. Vazquez (42 postdoc-months in the last four years) will provide 12 months of postdoc training in large scale computations of dynamical lattice systems, and Sancho will provide 12 months of postdoc training in stochastic techniques in spatially extended discrete systems.

5. Lyngby Christiansen is Head of the **Graduate School in Nonlinear Science** (GSNS), a 5-year project starting in 1997, sponsored by the Danish Research Academy. It is a collaboration between the DTU Nonlinear Centre, MIDIT, Lyngby, Risø National Laboratory, The Niels Bohr Institute, and Danish Industry. It provides a PhD training program at the highest international level with the aim of preparing students to apply recent advances in Nonlinear Science to outstanding problems of science and technology and to strengthen international exchange of PhD students, via PhD courses, lectures, and workshops. In 1998 35 Danish PhD students, and 29 PhD students, 15 Postdocs and various guest professors from other countries attended. Similar numbers are expected in the coming years. Every year the GSNS organizes a thematic workshop. The most recent was the **Nonlinear Science Festival**, held December 7-12, 1998 at the Niels Bohr Institute, coordinated by P.Cvitanovic and P.L.Christiansen with 120 participants. In 1999 a similar **Nonlinear Science Workshop** will be held in December at Risø National Laboratory. The GSNS has raised funds for 15 PhD grants for studies in Nonlinear Science and its applications. There is a great need for postdoc funding, however, hence the request here for 36 months.

6. Heraklion The Greek group will provide 38 man-month of postdoctoral training in the context of the network. The group has graduated eight PhD's over the last five years as well as hosted two Marie Curie fellows during the last three years. An ex-Marie Curie fellow is currently working in the group.

7. Firenze The FIRENZE team has provided training in the last years for 4 postdocs for a total amount of 60 person-months, and aims to provide 60 person-months training for this network. Moreover, since 1994 the team has been training 8 PhD students and 11 undergraduates producing their thesis for the "Laurea" degree in Physics. Training activities are coordinated inside the team that is organized in a local research group named DOCS (Dynamics Of Complex Systems), operating in various University Departments and Research Institutions in Florence, while all of its members share the association to INFM and the participation in INFM research projects. DOCS activities include organization of research seminars and periodic research meetings, that provide a stimulating background for postdocs and PhDs. Frequently, the associates from Milano and Salerno also take part in these research meetings.

8. Thiais The Thiais group is unique in providing multidisciplinary training at the frontier between Chemistry and Physics, with important prospects for biophysics and theory. Measurements carried out at the most advanced neutron sources complement optical measurements (infrared and Raman) performed at the laboratory. Data analysis requires good physics and computing knowledge. The chemistry facility is unique to master the synthesis of isotopically labelled molecules specially designed to study specific dynamics. The Laboratory of about 40 staff members (CNRS and university) offers a rich multidisciplinary environment. F.Fillaux has provided training to 4 PhD students and 2 postdocs since 1994 and will provide 13 months of experimental and theoretical training. The Montpellier group is quite complementary. M.Barthes has provided training for two PhD students since 1994 and will provide experimental and theoretical training for 8 months. This group offers a unique opportunity to gain experience in solid state NMR, STM and AFM techniques.

We are requesting funds mainly to train postdoctoral researchers, rather than predoctoral researchers. This is not because we consider the latter unimportant: on the contrary, each of us trains a large number of PhD students. Rather it is because there are already quite good mechanisms in place for funding PhD students in most of our countries whereas it is very hard work against intense competition to obtain funds for postdoctoral researchers from our national research councils. A slight downside to this choice is that the national mechanisms for funding PhD students do not always give equal opportunities to candidates from other EU countries (e.g. UK grants for non-UK EU PhD students pay fees only), so less mobility will be achieved at this level. Nevertheless, the record shows good mobility, e.g. Aubry (Saclay) currently has a student from Italy, MacKay (Warwick) has a student from Portugal, Peyrard (Lyon) has one from Italy, and so on. Special care will be taken in recruiting pre-doctoral researchers to make sure that their funding is complemented if necessary to make up the full duration of the period of study required to obtain their PhD.

The vacancies will be advertised via the CORDIS vacancies webpages, a central webpage for this network at Warwick, the host laboratory's webpage, electronic newsletters such as UK Nonlinear News, advertisements sent to laboratories likely to have appropriate candidates, advertisements in newspapers or magazines if appropriate, and e-mail to all group leaders in the network. We expect that a significant fraction of the appointments will be made via exchange between the participants. The duration of the appointments will vary from 2-36 months. Although positions of less than one year may not sound attractive, our experience with previous network grants is that there are many PhD students for whom this provides an excellent first employment prior to obtaining a more stable position somewhere. We anticipate no problems in recruiting young researchers. The salaries will be the standard ones for appointments at the given level in the given institution (see section 13). Although some of these differ significantly from the Marie Curie rates, we feel that the latter are unnecessarily high in Germany and Denmark, and too low in Greece. The salary we are proposing for appointments in Firenze is significantly lower than the others, but this is compensated for by extremely low tax and social deductions which INFM has negotiated, so the take-home pay is more or less equivalent to that in the other countries. Even though industry can offer them more, postdoctoral positions are quite attractive to people who are just completing a PhD and wish to retain the freedom to pursue curiosity-driven research. In the event that some participant has difficulty in attracting candidates of sufficient calibre and promise, we would at the end of the second year seek permission to redeploy the funds to hire additional young researchers at some of the nodes in the other countries.

All 8 participant institutions are committed to equal opportunity (within the constraints of age, nationality etc. imposed by the IHP programme, and the necessity to train at least the given number of person-months within the budget), in particular with regards to sex. Although there is a long way to go to achieve a representative gender balance, our network does have one female node leader and several of the teams contain women as well as men. Male and female researchers are treated on an equal basis; it is the science that counts.

10 Training Programme

The training objectives of the project are to give experience to promising young researchers in first-rate research in interesting areas in other EU countries than their own, and often introducing them to problems and methods that are new to them.

The network has a tremendous range of expertise, from Mathematics, Theoretical Physics and Scientific computing to Experimental Physics on Josephson junction arrays, Raman and Neutron scattering. We intend that the young researchers benefit from this breadth of approaches. For each country in the network there are aspects of training that can not be provided there but are available in nodes in other countries of this network. Appointees will be given a copy of this proposal as an introduction to the area of research.

Although we are requesting little money on this grant to train pre-doctoral students, we intend to provide a significant number of training schools, to which all our PhD students shall be invited, and indeed interested PhD students from outside the network.

We shall also organise a series of workshops to share results and ideas, which will have a significant training aspect, because the young researchers will learn how to present results, how to benefit from informal discussions, and will pick up invaluable advice, feedback and second opinions about their research projects.

Some of our network postdocs will be seconded by the Thiais team and their subcontractor at Montpellier for periods of a few months to gain experience in Raman and neutron scattering experiments, in addition to postdocs employed at Thiais. In case of projects using dangerous equipment or materials, young researchers will be thoroughly briefed in safety procedures. Similarly, some network postdocs will be seconded to Edinburgh or Madrid to train in the use of high performance computing. Others may spend some of their time visiting another network node in order gain training in some specific area and to collaborate on research. There will be some training involvement with industry, as indicated in Section 12.

To enhance its teaching and training possibilities, the network will experiment with *virtual training mobility* for the interaction between partners and in particular the trainees. We plan to use public domain software, such as CUSEEME (Cornell University See Me) in order to have real-time audio-video exchanges among the partners. This means of intercommunciation and interaction will be developed by the Multimedia Lab at Heraklion.

The ratio between individual and group training is difficult to quantify, but in terms of recipient contact hours we would expect a roughly even split.

The nodes of the network already have great experience in training at both the PhD and postdoctoral levels, as has been listed in Sections 5 and 9.

Schools and workshops planned

Dresden Flach and Bishop (USA) are planning a large scale seminar at MPIPKS in 2001 with both a school and a workshop, to be part-funded locally. Flach has considerable experience of organising such events and the infrastructure of MPIKPS for hosting them is excellent.

Risø/Lyngby Annual Thematic Workshop on Nonlinear Science, organized by the Graduate School in Nonlinear Science, to be held December 1999 at Risø National Laboratory, organizers: J. Juul Rasmussen and P. L. Christiansen.

Firenze Livi proposes to host a meeting in June or Autumn of 2001 or 2003. He has experience of organising research workshops, e.g. three in Torino.

Heraklion Tsironis proposes to hold a school and workshop. He has great experience in this (e.g. his latest workshop was just two weeks ago: 10-14 May 1999). and the facilities at FORTH are excellent.

Les Houches Aubry (Saclay) and Peyrard (Lyon) will apply to organise a Les Houches meeting (cf. the successful school Peyrard organised there 30 May - 4 June 1994 on "Nonlinear excitation in Biomolecules ").

Spain The Spanish group propose to host a meeting in Spain.

Trieste It is possible that we may submit an application to ICTP to run a school and workshop. They have good infrastructure.

Relevant Master's Level courses run by the nodes

Lyon The Diplome d'Etudes Approfondies on Statistical physics and nonlinear phenomena at ENS Lyon provides education at the Master's level in many of the topics of this proposal. It was attended by two Danish students recently for 6 months, and young researchers conncted with this network are welcome.

Warwick The 1-year MSc degree in Mathematical Interdisciplinary Research will include a component on the topics of this proposal from Oct 2000, in addition to a range of courses in mathematics, physics, engineering, computer science and other domains.

11 Multidisciplinarity in the Training Programme

The project incorporates a wide range of disciplines: Mathematics, Physics (both theoretical and experimental), Scientific computation, Data Analysis, Chemistry and Molecular Biology. Indeed it touches on the following discipline codes: M-05, M-14, P-07, P-08, P-09, P-10, P-11, P-12, P-13, P-15, P-16, C-03, C-05, C-08, L-01, L-05, I-05, I-10, though we bring new views to many of these areas that are not yet universally accepted. This multidisciplinarity will be exploited in the training programme by encouraging applications by young researchers to work in a new area for them and by providing the opportunity for young researchers to be involved part-time in another discipline. For example, MacKay hosted a young researcher on a previous network who had worked mainly on computation but wished to develop skill in mathematical proof; he learnt very rapidly and by the end of his time was producing high quality mathematical work. Similarly, MacKay has a postdoc on another EU network at present who was expert at computation but is assisting him with the interpretation of a neutron scattering experiment to observe breathers June 99 at Rutherford Lab. With the significant experimental component of our network, we intend that opportunities such as this will be frequent.

12 Connections with Industry in the Training Programme

Some industrial companies will be involved in the training, as follows:

Cambridge Display Technology, Cambridge, UK There will be an opportunity for young researchers to interact with this company which is linked to Warwick's Associate in Cambridge, and who are designing light emitting polymer displays based on creating excitons in PPV chains which decay via radiation.

Hewlett-Packard, Bristol, UK Interaction with Hewlett-Packard's Basic Research Institute in the Mathematical Sciences will be arranged; they are interested in potential applications of breathers to computing.

Novo Nordisk, DK Via the Graduate School in Nonlinear Science Lyngby collaborates with several Danish industrial companies about training of PhDs in industrial applications of Nonlinear Science. One project is with the biotechnology company Novo Nordisk and deals with molten globular states in proteins.

Spanish Army, ES The Spanish army will provide laboratory facilities for further experiments on Josephson junction arrays.

Rhône-Poulenc, FR This company is likely to be willing to interact with network postdocs on problems in polymers, via M-C Bellisent-Funel of the Saclay team.

13 Financial Information

13.1 Summary of requested funding

Network Budget in Euro				
Participant	*A*	*B*	*C*	*Totals*
1. Warwick, UK	160,000	58,000	42,000	260,000
2. Saclay, FR	150,000	62,600	37,400	250,000
3. Erlangen, DE	132,000	48,000	20,000	200,000
4. Zaragoza, ES	96,000	42,667	21,333	160,000
5. Lyngby, DK	108,400	25,000	26,600	160,000
6. Heraklion, GR	114,000	45,600	30,400	190,000
7. Firenze, IT	100,000	20,000	20,000	140,000
8. Thiais, FR	84,000	34,500	21,500	140,000
TOTALS	944,400	336,367	219,233	**1,500,000**

Table 5: Network budget in Euro. Abbreviations stand for A: Costs of appointment of young researchers, B: Networking costs, C: Overheads

13.2 Explanation of requested funding

The initial total budget requested by our nodes came to 1944 KE. Thus we had to prune the requests quite seriously to fit within the normal allowed budget of this scheme (1500 KE). Because of the preselection procedure we have had to implement, we consider all the requested funding presented here to be essential. Furthermore, an excellent late request was received but could not be included, so if the panel is able to allocate an additional 43 KE, we would make excellent use of it.

Note that most of the participant institutions insist on the full 20% of overheads allowed. For many of them, this is insufficient to cover the full costs of hosting the young researchers (including contributions to the infrastructure necessary to maintain a suitable research environment), but all the institutions accept that the educational and social benefits are worth the additional cost to them. Details of the financial calculation by participant follow.

1. Warwick :
A: 50 Postdoc-months at £1,676 per month (assuming average age 30) plus 7.5% national insurance and 14% pension contributions at 1.52 Euro/£ plus 2% allowance for inflation or exchange rate movement = 3156 Euro/month $\times$ 50 months = 157,800 Euro. 15 of these months are to be seconded to Edinburgh. Travel expenses for the postdocs = 2,200 Euro.
B: Travel expenses, consumables, use of computing: 30 KE; subcontract to Heriot-Watt for the same purposes: 8 KE. Fund to help finance network meetings and training schools: 20 KE.
C: 20% of A+B−subcontract = 42 KE

2. Saclay :
A: 40 postdoc-months at CEA rates of 3,750 Euro per month = 150 KE, of which 20 months will be seconded to Lyon

B: 37 KE networking costs and a subcontract of 25.6 KE to Lyon = 62.6 KE
C: 20% of A+B−subcontract = 37.4 KE

3. Erlangen :
A: 24 postdoc months (of which 8 will be seconded to Dresden) at 2,695 E/mo, and 20 predoc months at 1,750 E/mo: 132 KE
B: networking, conferences, consumables: 48 KE
C: overheads: 20 KE

4. Zaragoza :
A: 40 postdoc-months (of which 12 to each of Barcelona and Madrid) at 27 KE plus 1.8 KE social charges per year, making 2,400 E/mo = 96 KE
B: Networking costs: 10,667 Euro, Subcontracts to Madrid and Barcelona: 16 KE each
C: Overhead: 20% of (A+B−subcontracts) = 21,333 Euro.

5. Lyngby :
A: 36 postdoc months including travel and insurance, at 3,011 E/mo: 108,400 E
B: Staff exchanges, external experts, conference and publication fees: 25,000 E
C: Overhead: 20% of (A+B) = 26,600 E

6. Heraklion :
A: 38 postdoc-months (of which 10 to be seconded to Athens) at 3,167 E/mo = 114 KE
B: 38KE networking costs plus 7.6KE subcontract to Athens = 45.6 KE
C: 20% of (A+B−subcontract) = 30.4 KE

7. Firenze :
A: 60 postdoc-months at INFM rates of 1,667 E/mo (which allow for a special dispension on tax and social charges): 100 KE
B: 20 KE
C: 20 KE
By a cofinancing agreement, INFM is expected to provide an additional 30 KE for category A and 10 KE for category B.

8. Thiais :
A: 21 postdoc-months at the CNRS rate of 4,000 Euro per month = 84 KE (8 of these months are to be seconded to Montpellier).
B: Travel expenses, chemicals, sample preparation, optical and neutron scattering experiments 23.5 KE. Subcontract to Montpellier: 11 KE.
C: 20% of (A+B−subcontract) = 21.5 KE.

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