SYIM 1 Intrinsic Modes I

Time: Thursday 14:30–16:30 Room: HSZ 04

Invited Talk SYIM 1.1 Thu 14:30 HSZ 04

Energy Transport and Vibrational Self-Trapping in Peptide Models and Peptide Helices — •Peter Hamm — Physikalisch-Chemisches Institut, Universität Zürich, Winterthurerstr. 190, CH-8057 Zürich, Switzerland

Based on femtosecond IR-pump-probe spectroscopy, we have recently provided compelling experimental evidence that vibrationally self-trapped states in the amide I band of hydrogen-bonded model peptides and peptide models does indeed exist [1-3]. We have furthermore shown that polaron theory can explain the anomalous temperature dependence of the amide I spectrum of crystalline ACN only if taking into account the 3D nature of the system [4]. I will briefly review this work.
As an alternative approach to study energy flow in peptide helices, we have constructed a rigid helix with a dye molecule (azobenzene) attached to one side. The dye is electronically excited and dissipates the energy on an ultrafast 200 fs timescale through internal conversion, thereby locally heating the helix on one side. Vibrational labels attached at various distances from the dye molecule act as local thermometers and directly report on the energy flow through the helix. We hope to be able to distinguish diffusive from ballistic energy transport. I will report on the results of ongoing experiments.
[1] J. Edler, P.Hamm, A. C. Scott, Phys. Rev. Lett. 88 (2002) 067403
[2] J. Edler, P. Hamm, J. Chem. Phys. 117 (2002) 2415.
[3] J. Edler, R. Pfister, V. Pouthier, C. Falvo and P. Hamm, Phys. Rev. Lett. 93, (2004) 106405
[4] P. Hamm, J. Edler, Phys. Rev. B, submitted

Invited Talk SYIM 1.2 Thu 15:00 HSZ 04

Can we predict DNA biological activity from the study of its local fluctuations? — •Michel Peyrard[1], T.S. van Erp[1], S. Cuesta-Lopez[2], and J.-G. Hagmann[1] — [1]Laboratoire de Physique, Ecole Normale Supérieure de Lyon, 46 allée d'Italie, 69364 Lyon Cedex 07, France — [2]University of Zaragoza, Dept. Física de la Materia Condensada, c/ Pedro Cerbuna s/n, 50009 Zaragoza, Spain

DNA dynamics is essential for its biological function. The genetic code could not be read without a local unwinding of the double helix, and large openings, the so-called "DNA bubbles", are supposed to allow the formation of some specific DNA structures, such as the T-loop that stabilizes the end of the chromosomes.
Mesoscopic DNA models give a fairly accurate description of the thermal denaturation of DNA, i.e. the separation of the two strands by heating, and they predict the existence of localized fluctuations which are reminiscent of the "breathing" of the double helix observed by biologists.
Thus it is tempting to try to use these models to predict the biological activity of DNA. It has been speculated that the formation of bubbles of several base-pairs, due to thermal fluctuations, are indicators of biologically active sites. Comparison between molecular dynamics simulations of the PBD DNA model and experiments suggest that it could be the case, but this observation is however difficult because large bubbles appear only seldom so that the statistical significance of the results can be questioned. We introduce a new method, that is orders-of-magnitude faster than molecular dynamics to analyze these bubbles and show that presently the PDB model is not yet able to detect biologically active sites.
This does not imply that DNA fluctuations are not signs of the biological meaning of some sections of the genetic code, but could mean that the model is not yet able to properly relate the local opening and the base-pair sequence. In order to improve it, a comparison with experiments measuring the local fluctuations of DNA as a function of its sequence is necessary. We discuss such experiments and introduce some improvements of the model to bring it closer to the goal of predicting biological activity of DNA from physical studies of a highly simplified model.

Invited Talk SYIM 1.3 Thu 15:30 HSZ 04

Generating and shepherding intrinsic localized modes in macroscopic and microscopic lattices — •Albert J. Sievers — Laboratory of Atomic and Solid State Physics, Cornell University, Ithaca, NY 14853-2501, USA

It had been known for some time that nonlinearity and discreteness play important roles in many branches of condensed matter physics as evidenced by the appearance of domain walls, kinks and solitons. A recent discovery is that localized dynamical energy in a perfect nonlinear lattice can be stabilized by the lattice discreteness. Intrinsic localized modes (ILMs) are the resulting feature. Their energy profiles resemble those of localized modes at defects in a harmonic lattice but, like solitons, they can propagate; however, in contrast with solitons, collisions between such excitations result in energy transfer between them with the more localized excitations stealing energy from the less localized ones. Our recent experimental studies involve near steady state locking of ILMs. We demonstrate both the manipulation of localized energy along micromechanical arrays [1] and also the generation of countable ILMs [2] and their controlled switching [3] in an atomic lattice. Such steady-state ILM locking techniques should be useful for producing other kinds of dynamical energy localization.
This work is supported by NSF-DMR. Work in collaboration with L. English, B. Hubbard, M. Sato, U. Schwarz and J. Wrubel.
[1] M. Sato, B. E. Hubbard, A. J. Sievers, Rev. Mod. Phys., in press (2005).
[2] M. Sato & A. J. Sievers, Nature 432, 486 (2004).
[3] J. Wrubel, M. Sato, A. J. Sievers, Phys. Rev. Lett., accepted (2005).

Invited Talk SYIM 1.4 Thu 16:00 HSZ 04

Discrete Breathers: dynamical localization in nonlinear lattices — •Andrey Gorbach — Max-Planck-Institut für Physik komplexer Systeme Nöthnitzer Strasse 38 01187 Dresden

Classical nonlinear lattice models support time-periodic and spatially localized solutions - discrete breathers, equally coined intrinsically localized modes in solid state physics and discrete solitons in nonlinear optics. Being exact solutions of the underlying nonlinear coupled differential equations, discrete breathers persist in a quite general class of models, independent on the actual size of the lattice, spatial dimensionality, actual choice of nonlinear forces acting on the lattice, etc. I will introduce the concept of discrete breathers and review basic properties of these objects including spatial localization rate, dynamical and structural stability. In the second part of my talk I will focus on recent advances in the theory of discrete breathers, in particular in the direction of wave scattering by discrete breathers. The effect of resonant reflection of waves by discrete breathers and its possible application for frequency filtering and spectral hole burning will be discussed.