CENTRE NATIONAL
DE LA RECHERCHE
SCIENTIFIQUE

Laboratoire
Léon Brillouin

THEORY

LABORATOIRE LÉON BRILLOUIN

THEORY

The theoretical activity at LLB for the last few years can be divided into three parts.

One activity is concerned with fundamental developments in the field of non linear physics [*C1,* **S. Aubry**] with application to different fields.

One example is the suggestion of a possible implication of polarons in the transmission of a long distance electromechanical signal in regulatory enzymes (in collaboration with enzymologist G.Hervé).

Another example is the suggestion of a new mechanism concerning the origin of sonoluminescence (in collaboration with B. Dey). In this scenario sonoluminescence is produced by the tremendously large adiabatic pressure pulse (shock wave) generated by the close to supersonic impact of the fluid on the hardcore bubble and the light fhash is emitted by the fluid surrounding the bubble.

The second one is concerned with the field of strongly correlated electron systems and mainly with the fundamental development of a theory of high Tc superconductors [*C2,* **F.Onufrieva**].

The asymmetry between hole-doped and electron-doped cuprates has been explained on the basis of the existence of two different topological quantum critical points monitoring the change of Fermi surface when doping is varied. In particular one consequence is the very small q width of the antiferromagnetic dynamical spin response in electron-doped cuprates oberved by neutron scattering.

For the mechanism of superconductivity the role of spin fluctuations is enphasized and quantitative calculations have been achieved which are based on the spin fluctuation spectrum obtained by neutron scattering with the presence in the superconducting state of a spin exciton mode close to the antiferromagnetic wave vector. The most interesting results obtained recently in 2006 are the rather high value of the maximum superconducting gap close to that observed experimentally and the symmetry of the order parameter which is of the d-wave type but with large deviations from the pure d-wave symmetry with an antinodal part gap quite different from the nodal part gap as seen experimentally by photoemission and Raman scattering.

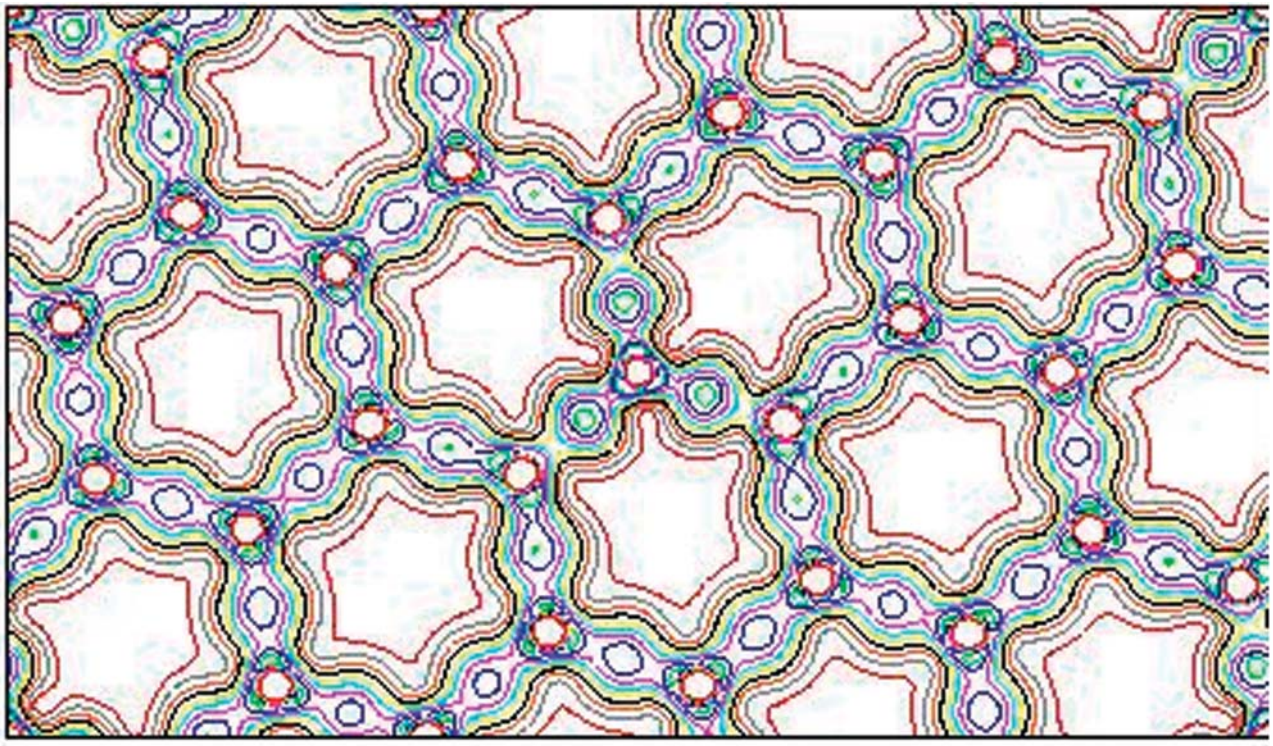
Another development by H.Moudden [*C3,* **H. Moudden**] concerns the physics of the novel superconductor MgB2 with the study of the effects of carbon substitution on the superconducting properties from realistic ab initio calculations.

The third one by G.Kneller and K.Hinsen [*C4,* **G. Kneller**] is concerned with simulation studies of brownian and fractional brownian dynamics with application to the study of the dynamics of proteins in relation to quasielastic neutron scattering developped at LLB.

A new approach has been developped to descibe the relaxation dynamics of proteins. A theoretical model such as the fractional brownian dynamics has been used to study the dynamics of proteins and to connect the dynamical events seen on the pico-nanosecond time scale, accessible to quasielastic neutron scattering, to the functional dynamics of proteins on much longer time scales of the order of the milisecond.

The combined simulation and neutron scattering studies of proteins in solution under hydrostatic pressure, have been started in collaboration with M.C. Bellissent in the framework of the thesis of V. Hamon and currently continued as part of the thesis work of P. Calligari

THEORY



[*C1.* **S. Aubry**] About the Origin of Sonoluminescence

[*C2.* **F. Onufrieva**] Magnetic and Electronic properties of the High-Tc Cuprates: from electron- to hole- doping.

[*C3.* **H. Moudden**] Effects of Carbon Substitution on Magnesium Diboride : Ab Initio Study

[*C4.* **G. Kneller**] Relaxation dynamics and quasielastic neutron scattering in proteins from the model of fractional brownian dynamics

[*C1*. S. Aubry] About the Origin of Sonoluminescence

Some liquids (typically water), submitted to intense ultrasounds (at typically 40 kHz), may emit broadband light (sonoluminescence) over frequencies ranging from IR to UV. It has been proven experimentally that sonoluminescence is generated by stable spherical microbubbles (of the order of μm) of some insoluble gas (typically rare gas). The radius of those bubbles oscillates at the frequency of the driving ultrasound. When the pressure amplitude of the ultrasound field becomes larger than a certain threshold (typically 1B), the gas in the bubble reaches its minimum Van der Waals volume and there is a radial impact of the fluid onto the core of the bubble. This situation occurs at radial bubble velocities comparable to the sound velocity in the liquid. During this sharp impact which lasts few 100 ps, the flash of light which produces sonoluminescence, is emitted. The most frequent interpretation of this phenomena is that the energy of the shock wave generated at the impact focuses and diverges at the bubble center (in quasilinear theories) which should generate a plasma at a very high temperature emitting the light flash. It was even argued that nuclear fusion could be generated in that way. However, this interpretation is ruled out by some crucial experiments for example by the fact that near threshold, sonoluminsecence becomes dim with a spectrum shifted toward IR which moreover is much more pronounced with deuterated water. Up to now the physical origin of this pheneomena remains an enigm.
We suggest a new interpretation for this phenomena. Shockwaves which are generated by quasisupersonic impacts becomes tremendously nonlinear. We prove in that conditions with rigourous arguments only based on mass conservation and the existence of a Van der Waals minimum volume that energy focusing cannot occur at the bubble center. A compacted sphere appears right after the impact which includes the compacted gas of the bubble but also and mostly a part of the surrounding liquid. The pressure and temperature inside becomes very high but remains spatially rather uniform. The radius of this compacted sphere expands up to few minimum bubble radius while its pressure and temperature simultaneously drops very fast. Next the pressure profile in the liquid continues to evolve but as a standard quasi linear pressure pulse which radially propagates and decays. It is also proven that the sound velocity in the liquid of that highly compacted sphere, is enhenced by a factor λ near unity at weak impacts but which suddenly increases as soon the impact becomes close to supersonic. It may easily reach one or several order of magnitudes in the experimental conditions. Thus beyond a certain threshold, this Grüneisen coefficient λ becomes large, so that the frequency spectrum of the thermal radiation of the compacted liquid and gas is strongly dilated from IR toward UV while its temperature is (adiabatically) increased by the same factor λ (which correspond to a power of the thermal radiation increased by λ^4). The sonoluminescent light flash is thus due to the intense thermal radiation of this compacted sphere (which is mostly composed of the liquid surrounding the bubble) during the short time of its existence.

[B. Dey and S.Aubry Physica D 216 (2006) 136-156]

[*C2*. F. Onufrieva] Magnetic and Electronic properties of the High-Tc Cuprates: from electron- to hole- doping.

We have shown that a basic difference between electron- and hole- doped cuprates is their proximity to two different topological quantum critical points (QCP's), one related to saddle point electrons and relevant for hole-doped Cuprates and the other related to nodal electrons and relevant for electron-doped cuprates. This has consequences for both magnetic and electronic properties.

1. Spin dynamics
We have shown [1] that the striking features observed recently in the electron-doped cuprates (neutrons), the extremely narrow q width and very low spin gap, are consequences of the proximity to the "nodal" quantum critical point while the resonance peak that is a remarkable property of the hole-doped cuprates (also observed by neutrons) is a consequence of the proximity to the "saddle point" quantum critical point.

2. Electronic properties:
We have shown [2] that the presence of these QCP's imposes srtong constraints on electronic properties in the cuprates. One of the consequences is the existence of the electron pseudogap of density wave origin, large pseudogap, that increases towards low doping from both sides, electron- and hole- doping. The qualitative behaviour and even absolute values of the pseudogap are in a good agreement with experiment (ARPES, optical conductivity etc.). Another effect is the existence at low doping of a second pseudogap, one order of magnitude smaller (at T=0 it becomes a true gap). This small gap also increases towards zero doping and could explain the recent ARPES observation of the small gap observed for both electron and hole doping in the whole Brillouin zone. The most interesting feature is the existence at low doping of a specific insulating state different from the Mott-Hubbard (MH) insulator. It is characterized by a small chemical potential jump (much smaller than in the MH insulator), this feature is close to that observed experimentally.

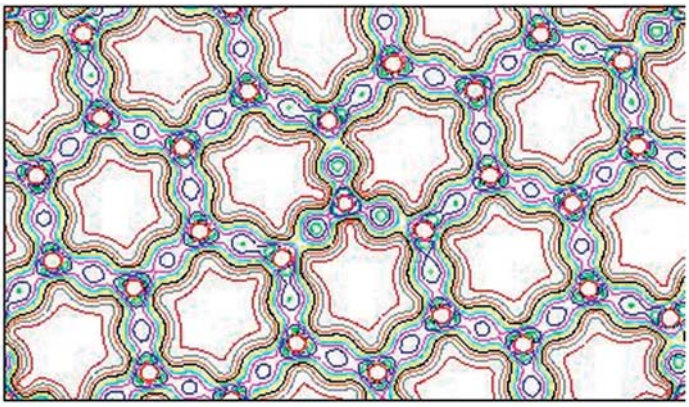
[Collaboration: F.Onufrieva et P.Pfeuty, LLB]

[1] F.Onufrieva and P.Pfeuty Phys.Rev.Lett. 92 247003 (2004).
[2]F.Onufrieva and P.Pfeuty Phys.Rev.Lett. 95 207003 (2005).

[*C3.* H. Moudden] Effects of Carbon Substitution on Magnesium Diboride : Ab Initio Study

MgB_2 is now widely considered as a non-cuprate high T_c superconductor for which the electron-phonon coupling is unambiguously determined as the main ingredient in the mechanism of its high T_c. But many aspects such as the presence of multi-bands, low concentration of holes and two-dimensionality could be important as well. The C-substitution revealed many new features including the presence of two regimes of T_c depression, and strong enhancement of the critical field. These features are currently under intense research. I made numerical simulations of the C-doping effects [A.H. Moudden, J. Phys. Chem. of Solids 67(2006)115], using super-cells method for high doping, larger than 7% (figure), and recently using the virtual crystal approximation VCA, for doping smaller than 5%. The electronic structure, the Fermi surface, the density of states and the lattice dynamics have been determined carefully within the density functional theory with all electrons and full potentials. Strong electron-phonon coupling could be determined by pseudo-potential codes only. These quantities were then used in the Eliashberg strong coupling approach of superconductivity [G.A. Ummarino et al. Phys. Rev. B.71, 134511(2005)] with some success in describing the C dependence of T_c. The role of inter band scattering and Coulomb screening remain under active investigation.

[Collaboration: A.H. Moudden , LLB,G.A.Ummarino et al. Politecnico di Torino]



Valence electron redistribution near the doped C at the centre:
Hexagonal Super-cell √7x√7

[*C4.* G. Kneller] Relaxation dynamics and quasielastic neutron scattering in proteins from the model of fractional brownian dynamics

The non exponential relaxation in a complex system like a protein can be described by the **fractional brownian dynamics** of a single particle. Such a model describes a protein on a coarse grained scale and localised motions cannot be described within such a model. The fractional brownian dynamics which has absolutely no characteristic time scale is certainly an idealized mathematical model of a physical system which has a very broad but limited distribution of relaxation times. The simulation study that we performed for **lysosyme** revealed a signature of fractional Brownian dynamics in the collective dynamics of the protein. The concept of fractional brownian dynamics leads to the introduction of generalized lorentzians which describe empirically the very broad quasielastic neutron scattering spectrum obtained from internal protein dynamics. The study of the average mean square displacement of the atoms in **lysosyme** has shown that fractional brownian dynamics models may be used to extrapolate the dynamics in a certain way to very long time scales. In this respect these models describe the slow relaxation processes. Thus the extrapolation of the properties of these models in combination with computer simulations can help to study the slow relaxation processes in proteins in particular to establish a signature of protein function.

These type of models we have introduced help to connect the **rapid** dynamics seen by **Quasielastic Neutron Scattering** to the **slow** dynamics more characteristic of the of the protein

[G.Kneller, Phys. Chem. Chem. Phys., 2005, 7, 2641-2655]