Session XI - Friday, September 4 - morning

PL10

LATTICE DYNAMICS IN THE APPROXIMANT-CRYSTAL o-Al$_{13}$Co$_4$

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Complex metallic alloys are long range ordered materials which often have characteristic clusters and are characterized by large unit cells [1]. Numerous complex phases can thus be described as periodic or quasiperiodic packing of atomic clusters [2]. The lattice dynamics of CMAs have been the subject of both theoretical and experimental investigations [3], the main objective being to undertsand their low thermal conductivity.

In this context, we present a combined experimental and atomistic simulation study of the lattice dynamics of the complex metallic alloy Al$_{13}$Co$_4$ phase [4], which is a periodic approximant to the decagonal phase. Inelastic neutron and X-rays scattering measurements carried out on a single grain are compared to simulations, both in terms of dispersion relations and mode intensity of $S(Q,)$. These simulations use DFT methods and empirical oscillating pair potentials extracted from DFT results [5].

Our investigations reveal the structure-dynamics relation. Coupling of acoustic and localised, optic modes in the cluster structure is observed along high symmetry directions and gives rise to phonon broadening. Limited phonon lifetimes are also observed near Brillouin zone boundaries in low symmetry directions.

Empirical potentials allow large scale molecular dynamics simulations to be performed and therefore the effects of atomic disorder and the temperature dependence of anharmonicity, giving additional insight into experimental data. Additionally thermal conductivity can be determined from the Green-Kubo relations, revealing a weak anisotropy [6].

Our investigations show that the low thermal conductivity of the approximant o-Al$_{13}$Co$_4$ is due mainly to the cluster-based structure and the atomic disorder.

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S11-L1

ANOMALOUS MOTION AND FREE FLIGHT LENGTH DISTRIBUTION IN QUASIPERIODIC LORENTZ GASES

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For scatterers arranged on a quasiperiodic lattice that can be embedded into a higher-dimensional periodic hyperlattice, a simple and efficient algorithm for numerical simulation of the dynamics of particles moving through such quasiperiodic structures has been constructed [1]. Employing this algorithm, we have performed simulations in a two-dimensional quasicrystal and observed three different cases of motion, namely diffusion, weak super-diffusion in the presence of channels with infinite horizon, and motion with extended regimes of subdiffusion at intermediate times. This last case does not occur for periodic arrangements of scatters [1]. The directions along which such subdiffusion occurs are called channels with locally finite horizon.

We explore what type of channels exist in such systems. For motion within the channels, we determine the free path length distribution, numerically and analytically. In the case of channels with infinite horizon, we find that the distribution of path lengths is a power law with exponent -3, as expected from periodic Sinai billiard [2]. For the channels with locally finite horizon that occur only in quasicrystals, we find an unexpected power law with exponent -5, which, as far as we know, has not previously been found either in periodic or random environments.

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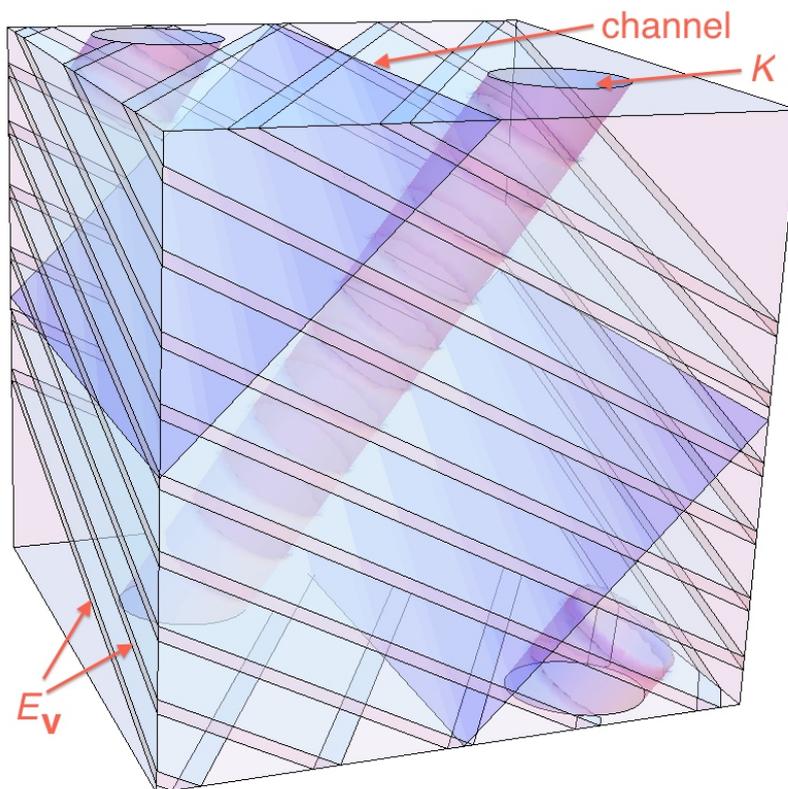
Figure 1. 2D quasiperiodic Lorentz Gas embedded in a 3D cube.

S11-L2

FRACTAL EXPONENTS FOR THE ELECTONIC PROPERTIES OF THE FIBONACCI CHAIN

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The unique structural properties of quasicrystals result in unusual electronic properties. Tight binding models on the Fibonacci chain have been extensively studied since understanding the properties of this one dimensional quasicrystal is an important first step towards understanding the physics of more complex quasicrystals in higher dimensions.

We consider a pure hopping Hamiltonian with nearest-neighbor hopping amplitudes t_1 and t_2 arranged according to the Fibonacci sequence. The resulting Fibonacci chain can be partitioned into *atomic* and *molecular* sites.
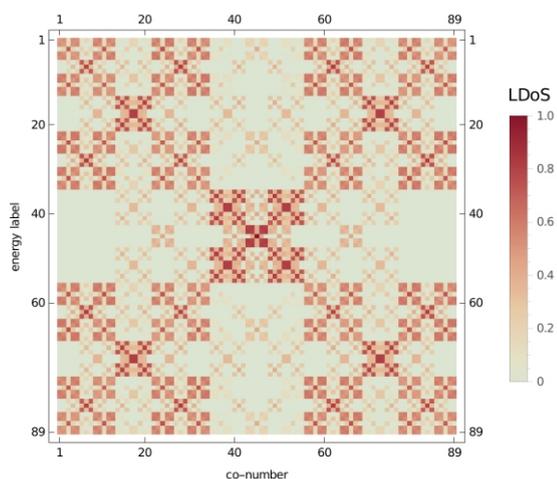
Figure 1. Local density of states as function of the energy label and of the reordered position along the chain (co-number label). The fractal structure of the local density of states is made evident by the reordering.

The chain of atoms and the chain of molecules are again Fibonacci chains, of smaller length. This geometric property allows one to build a renormalization group for the Fibonacci Hamiltonians. In the limit of small t_1/t_2, this renormalization group can be used to construct the spectrum [1, 2]. Interestingly, each energy level can be labelled by its *renormalization path* [2,3], the path it has followed through the renormalization procedure. In the present work we extend this relabelling procedure to the sites of Fibonacci chains. We exhibit a natural correspondance between the renormalization path of a site and its labelling in perpendicular space, or co-numbering [4].

As an illustration, we plot (Fig. 1) the local density of states. Its fractal structure is made evident by the relabelling.

Using the relabelling, we obtain explicit expressions for the fractal dimensions of the spectrum and the wavefunctions. We also obtain a simple relation between the fractal dimensions of the wavefunctions, and of the local and global spectral measures. Extensions of this result to other quasiperiodic models such as the Harper model will be discussed.

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S11-L3

INTERPLAY BETWEEN 3D CLUSTER SUBSTRUCTURE AND 2D SURFACES IN Al$_5$Co$_2$

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Recent advances in heterogeneous hydrogenation catalysis have identified few Al-Co complex intermetallic compounds as promising candidates for the development of efficient cheap catalytic materials [1]. The performances of these catalysts have been ascribed to their specific surface structure, made of small, stable, and well-separated atomic ensembles containing generally a unique active transition-metal element.

To elucidate the reactivity of the Al-Co complex intermetallic catalysts, an investigation at the atomic scale is mandatory. Here, we focus on the low-index surfaces of Al$_5$Co$_2$ (P6$_3$/*mmc*, $a = b = 7.67$ Å, $c = 7.61$ Å). The intermetallic compound Al$_5$Co$_2$ plays an important role in the understanding of the electronic structure and the atomic interactions in Complex Metallic Alloys (CMAs), i.e., intermetallic phases with complex crystal structures. It was shown that it is an approximant of the quasicrystalline decagonal phase with the shortest periodic stacking sequence along the tenfold axis [2].

In the present work, three low-index surfaces are investigated -(001), (100) and (2$\bar{1}$10) – by an approach combining both surface science techniques under ultra-high vacuum and calculations based on the density functional theory. In all cases, the surface terminates at specific bulk layers where various fractions of specific sets of Al atoms are missing, leading to different surface reconstructions, also depending on the surface preparation conditions [3]. Such reconstructions are non usual in the case of metallic surfaces. The preservation of the cluster substructure up to the surface, along with the specific chemical bonding network present in Al$_5$Co$_2$ [4], are identified as key factors at the origin of the observed reconstructions. Finally, the surface electronic density of states has been calculated for the three low-index surfaces investigated so far. The results are discussed in light of the catalytic behaviour of Al$_5$Co$_2$.

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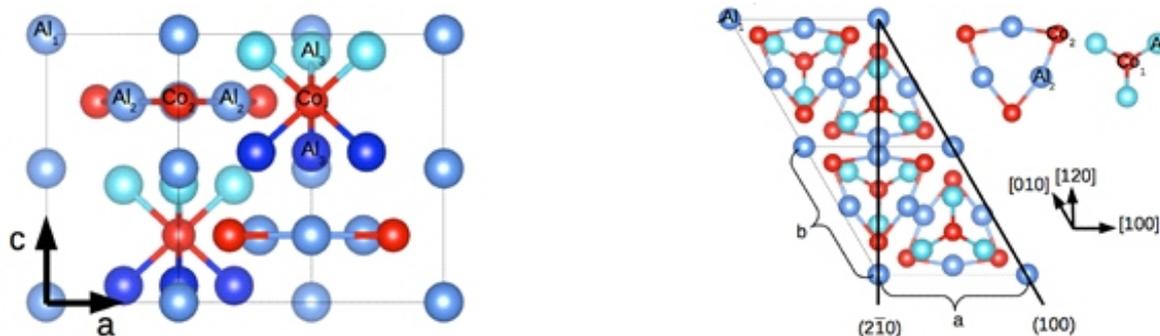
Figure 1. Al$_5$Co$_2$ crystal structure.