Department of Theoretical Condensed Matter Physics wishes you a Merry Christmas And Happy New Year 2018!

Best Theoretical Doctoral Thesis in Condensed Matter Physics 2017
Carlos Sánchez Muñoz has been awarded by GEFES with the prize for the Best Theoretical Doctoral Thesis in Condensed Matter Physics 2017. Carlos made his doctoral thesis “Generation of Non-classical States of Light” in the Department of Theoretical Condensed Matter Physics, Universidad Autónoma de Madrid and IFIMAC under the supervision of Carlos Tejedor and Fabrice P. Laussy. He currently has a contract as Post-Doc at the Center for Emergent Matter Science (CEMS), in Riken, Tokyo. [Read more]

Peltier Cooling in Molecular Junctions
Thermoelectric cooling is based on the Peltier effect that consists in the generation of a reversible heat flow in response to the passage of an electrical current. Thus, depending on the direction of the electrical current in a junction, one can cool down an electrode at the expense of heating up the other one. Thermoelectric or Peltier coolers have many applications, especially in electronics, and they possess several advantages over conventional vapor-compression refrigeration systems, although they are typically less efficient than these latter ones. In the context of nanoscale systems, a lot of attention has been devoted to the study of thermoelectricity in molecular junctions with the hope, in particular, to increase the efficiency of Peltier cooling. However, in spite of the fact that a lot of progress has been made in probing related phenomena such as the Seebeck effect (the conversion of a temperature difference into an electrical current), the observation of Peltier cooling in molecular junctions has remained inaccessible thus far.

This fundamental problem has now been resolved in a work published in Nature Nanotechnology by a collaboration between the groups of Pramod Reddy and Edgar Meyhofer (University of Michigan) and the members of our department Linda Angela Zotti and Juan Carlos Cuevas. In this work, these researchers report for the first time the direct observation of Peltier cooling in molecular junctions. This observation was possible due to the use of a novel experimental platform that combines conducting-probe atomic force microscopy with home-built calorimetric micro-devices with picowatt resolution. This platform enables the simultaneous measurement of electrical,
thermoelectric and energy dissipation characteristics of molecular junctions. Using this platform, molecular junctions formed with gold electrodes and a variety of organic molecules were investigated. Such studies revealed not only the possibility to achieve molecular-based refrigeration, but they also showed the close relationship between heating or cooling and the transmission characteristics of these junctions. In particular, it was shown that the Peltier cooling can be tuned and optimized by an appropriate choice of the molecular architecture, and all this in exquisite agreement with density-functional-theory-based calculations performed in the framework of the Landauer approach for quantum coherent transport.

The advances reported in this work are expected to stimulate the exploration of atomic-and molecular-scale thermal transport and the quantification of the thermoelectric figure of merit in a variety of interesting molecules, nanostructures and materials. [Full article]

Reference


![Diagram of Weakly Trapped, Charged, and Free Excitons in Single-Layer MoS2 in the Presence of Defects, Strain, and Charged Impurities]

Article: published in ACS Nano by César González, IFIMAC researcher and member of the Department of Theoretical Condensed Matter Physics.
Few- and single-layer MoS2 host substantial densities of defects. They are thought to influence the doping level, the crystal structure, and the binding of electron–hole pairs. We disentangle the concomitant spectroscopic expression of all three effects and identify to what extent they are intrinsic to the material or extrinsic to it, i.e., related to its local environment. We do so by using different sources of MoS2 -a natural one and one prepared at high pressure and high temperature- and different substrates bringing varying amounts of charged impurities and by separating the contributions of internal strain and doping in Raman spectra. Photoluminescence unveils various optically active excitonic complexes. We discover a defect-bound state having a low binding energy of 20 meV that does not appear sensitive to strain and doping, unlike charged excitons. Conversely, the defect does not significantly dope or strain MoS2. Scanning tunneling microscopy and density functional theory simulations point to substitutional atoms, presumably individual nitrogen atoms at the sulfur site. Our work shows the way to a systematic understanding of the effect of external and internal fields on the optical properties of two-dimensional materials. [Full article]

Title: Geometry-invariant Phenomena in Near-zero-index Media

When: Friday, December 15, (2017), 12:00.
Place: Department of Theoretical Condensed Matter Physics, Faculty of Science, Module 5, Seminar Room (5th Floor).
Speaker: Iñigo Liberal, Department of Electrical and Electronic Engineering, Public
Continuous media and metamaterials with a near-zero refractive index (NZI media) provide alternative pathways for the control and manipulation of light-matter interactions. The exotic behavior of NZI media is rooted in the fact that the wavelength gets effectively stretched as the refractive index vanishes. This allows for pathological solutions to the wave equation, including spatially static fields distributions which nevertheless dynamically oscillate in time. This paradoxical behavior gives access to a regime of qualitatively different wave dynamics, where the importance of the geometry is lessened, and certain observables are invariant with respect to geometrical deformations, even including changes in the topology of the system.

In this talk, I’ll review and discuss some of the geometry-invariant phenomena related to near-zero-index media. Examples will include: (i) transmission (tunneling) of waves through deformed waveguides. (ii) Unconventional resonators supporting modes whose eigenfrequency is independent of the geometry of their external boundary. (iii) Violation of effective medium theory geometrical restrictions, enabling, for example, single unit-cell metamaterials. (iv) Existence of bound states in open 3D compact resonators with arbitrarily shaped boundaries.

Different technological applications and implementations of these concepts will be discussed.

Polariton Lattices: A Novel Platform for Analogue Simulation
A large variety of computationally intractable systems can be mapped into certain universal classical spin models such as an Ising, XY or Heisenberg models that are characterised by given degrees of freedom, “spins”, their interactions, “couplings” and their associated cost function, “Hamiltonian”. Various physical platforms have been proposed to simulate such models using superconducting qubits, optical lattices, coupled lasers etc.

We introduce polariton lattices as a new platform for analogue simulation; based on well-established semiconductor and optical control technologies polariton simulators allow for rapid scalability, ease of tunability and effortless readability. Polariton condensates can be imprinted into any twodimensional lattices either by spatial modulation of the pumping laser or by lithographic techniques during the growth process, offering straightforward scalability. In the case of optically imprinted polariton lattices with freely propagating polariton condensates, we recently demonstrated that the phasecon configuration acquired in a polariton dyad or triad is chosen so as to maximise polariton occupancy [1], while by expanding to square, and rhombic lattices as well as to arbitrary polariton graphs we simulated annealing of the XY Hamiltonian through bosonic stimulation [2]. The bottom-up approach of bosonic stimulation is achieved here by gradually increasing the excitation density to condensation threshold. This is an advantage over classical or quantum annealing techniques, where the global ground state is reached through transitions over metastable excited states with an increase of the cost of the search with the size of the system.

By controlling the separation distance, in-plane wavevector, and spin of the injected condensates in polariton graphs, we acquire several degrees of freedom in the tunability of inter-site interactions, whilst the continuous coupling of polaritons to free photons offers effortless readability of all the characteristics of the polariton condensates such as energy, momentum, spin, and most critically their phase. The above constitute a unique toolbox for realising intriguing discrete giant vortices, controllable next nearest neighbour interactions, dynamic phase transitions and simulating artificial solids.

References
The time-dependent driving of nanoscale conductors allows for the controlled creation of single-electron excitations. This effect has been demonstrated experimentally both by application of time-dependent driving to gates coupled to confined systems, such as quantum dots [1], and by specifically shaped ac-driving of two-dimensional conductors [2,3]. However, the spectral properties of the injected signal are in general not known; moreover, the particle emission goes along with the excitation of electron-hole pairs with some unknown energy distribution. These issues can be addressed by studying...
fluctuations in the detected currents: not only do such fluctuations provide more insight into how to increase the precision of the single-particle emission, but also they allow for obtaining more information about the character of the emitted signal. Here, I will present a theoretical study of charge and energy currents and their fluctuations in coherent conductors driven by different types of time-periodic bias voltages, based on a scattering matrix approach [4,5]. Specifically, we investigate the role of electron-like and hole-like excitations created by the driving in the charge current noise, where they only contribute separately. In contrast, additional features due to electron-hole correlations appear in the energy noise. We then compare two different types of driving schemes [6], that is for a driven mesoscopic capacitor [1] as well as for a Lorentzian-shaped bias voltage [3], which do not differ in the number of injected particles, but only in their energetic properties. Finally, I will discuss proposals for the detection of charge and energy noise, either through power fluctuations [4], or via frequency-dependent temperature and electrochemical-potential fluctuations in a probe reservoir [7].

References