



# PhDay Físicas 2021



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## 1. Relajación rotacional del CO<sub>2</sub>: rotura del equilibrio rotación-traslación

Carlos Alvarez Nicolas

Los jets supersónicos de gases enrarecidos son un medio ideal para estudiar procesos elementales entre moléculas como la relajación de los diferentes grados de libertad mediante choques inelásticos. Combinados con la espectroscopía Raman, que nos permite medir poblaciones individuales podemos analizar la evolución rotacional, vibracional y traslacional de las moléculas. El CO<sub>2</sub> en particular presenta un problema interesante de estudiar ya que sus modos vibracionales pueden ser excitados de una manera sencilla lo que permite medir la relajación vibracional y rotacional partiendo de diferentes temperaturas. La rapidez de los procesos que ocurren dentro del jet supersónico lleva a una ruptura del equilibrio entre los grados de libertad internos de las moléculas. Desde el principio de la expansión se produce una ruptura entre la vibración y la rotación-traslación. Sin embargo, estos últimos tardan más en salir del equilibrio ya que la separación energética de los niveles rotacionales es lo suficientemente pequeña como para que se mantengan en equilibrio, aunque cada vez haya menos colisiones. Experimentalmente se pueden medir las poblaciones rotacionales y vibracionales lo que nos permite obtener temperaturas rotacionales, vibracionales, sus respectivas derivadas y las number density. A partir de estas y del estudio de las roturas de equilibrio se pueden empezar a obtener diferentes magnitudes termodinámicas como tiempos de relajación, la entropía o la viscosidad de volumen.



## 2. One-Dimensional Moiré Superlattices and Flat Bands in Collapsed Chiral Carbon Nanotubes

Olga Arroyo Gascón

We demonstrate that one-dimensional moiré patterns, analogous to those found in well-known twisted bilayer graphene (TBG), can arise in collapsed chiral carbon nanotubes (CNTs). Resorting to a combination of approaches, namely, molecular dynamics to obtain the relaxed geometries and tight-binding calculations validated against ab initio modeling, we find that magic angle physics occur in collapsed carbon nanotubes. Chiral collapsed carbon nanotubes stand out as promising candidates to explore many-body effects, topology and superconductivity in low dimensions, emerging as the one-dimensional analogues of twisted bilayer graphene.



## 3. Spin control in topological semimetals

Yuriko Baba

Topological materials have attracted great interest since they exhibit new fundamental phenomena and hold great promise for far-reaching technological applications. Their hallmark is quantized response functions and the existence of protected gapless surface states named Fermi arcs. The gapped case was the first under study, starting the fruitful field of topological insulators. On the other hand, gapless systems assemble the family of topological semimetals. In particular, in Dirac and Weyl semimetals the phenomenology is enriched by the chirality as a new degree of freedom of the topological states. The objective of this thesis is to study the robustness of the protected topological states as well as to propose mechanisms to control the spin-chiral degree of freedom. In particular, we study the effect of electric fields in the direction of decay of the states, Rashba spin-orbit coupling induced by local fields in the substrate, electric and magnetic fields in Hall bars and the robustness of the states against disorder.



## 4. Lumped element on-chip resonators for molecular spin qubits control and read-out

Marina Calero de Ory

Artificial magnetic molecules, with electronic (VO-Porphyrin, PTM or Mn(Me6Tren)) and nuclear (Yb-trensal) spins, coherently coupled to the electromagnetic field of a superconducting resonator, are promising building blocks to test basic operations of a hybrid quantum processor. These molecules are the smallest object that is tunable and fully reproducible by nature, they can be designed to show quite long coherence times and they often possess multiple low-lying spin states that can provide the basis to encode qubits or even to implement simple algorithms. In the strong coupling regime, the collective coupling enables using the superconducting circuit to coherently manipulate and dispersively read-out the qubit spin state, and to establish communication channels between different molecular spins. The resonators design is of paramount importance as it defines the amplitude of the electromagnetic field and its orientation with respect to the crystal axes. In this sense, we tailor high quality factor superconducting lumped element resonators (LERs), which consist of LC circuits coupled to a transmission line, for their performance in magnetic and electric coupling to molecular spin qubits. Tailoring the resonator impedance, its inductor and capacitor, and quality factor allows engineering each resonator for a specific spin system. Additionally, LERs are intrinsically multiplexable on-chip, this permits the simultaneous readout of several qubits at different drive frequencies.



## 5. Hyperdoped germanium photodetectors by ion implantation and pulsed laser recrystallization

Daniel Caudevilla Gutiérrez

Infrared photodetection has aroused a great deal of interest due to the wide range of applications, including free-space communication, surveillance and biomedical imaging. Nowadays, this market is dominated by binary or ternary compounds (InGaAs, PbSe or HgCdTe which are not abundant in the earth's crust, they are expensive and some of them are toxic. Moreover, these semiconductors are not compatible with silicon-based CMOS technology. In contrast, Ge does exhibit this compatibility.

Ge bandgap energy is 0.67 eV, so it already responds up to 2  $\mu\text{m}$  (SWIR), but hyperdoping Ge with deep centres within the semiconductor gap could extend the photoresponse at room temperature to longer wavelengths (MWIR), where there are the most interesting applications. For hyperdoping, we need to surpass the Solid Solubility Limit (SSL) of a deep impurity and recover the crystallinity of the material. For that we propose Te as a deep-donor and two out of the equilibrium techniques: Ion implantation followed by Pulsed Laser Melting (PLM) recrystallization.

Ion implantation of heavy ions, at high energies or with high doses produces porosity in the surface of the semiconductor which cannot be suppressed after any conventional annealing process. In order to avoid that porosity we have designed and assembled a modification to the ion implanter for implanting at liquid nitrogen temperatures (77K). We overcome the SSL of Te in Ge by several orders of magnitude, and we recover the crystallinity of the implanted layers after the PLM process. In this work I present the main results of my thesis and the technological challenges of hyperdoping Ge.



## 6. Electrodeposited nanowires for composite bonded magnets: scaling-up the synthesis process

Claudia Fernández González

In the last years, nanowires (NWs) appear to be materials with a key role in the development of new nanodevices in many fields of technology. The quantity of nanowires produced in a lab-scale is enough to design and test prototypes devices. However, to go from the lab to real industry production, the development of new synthesis processes is needed. One of the most common technique to growth nanowires is template assisted electrodeposition. It is a versatile and non-expensive technique that allows the synthesis of a wide range of metallic and oxide materials. However, to use this technique in industrial application two main issues should be addressed: to increase the mass of produced nanowires and to reduce the synthesis cost. In this work we have modified and optimized the NWs synthesis process to scale -up the production. The main part of the work was focused on the production of the alumina templates because it was the most time limiting process. Changing the purity of the initial Al and modifying the anodization and growth conditions we have reduced the price and the synthesis time, increasing the nanowire's production in our laboratory and we have established the conditions to implement this process in industry. We have synthesized a prototype of composite based permanent magnet combining NWs with strontium ferrite. The magnetic properties of this prototype are improved with respect to the strontium ferrite magnets, filling the gap between ferrites and rare-earth magnets.



## 7. Seismic Phase Picking with Deep Learning

Luis Fernández Prieto

The popularisation of the use of large-N arrays of seismometers has resulted in a significant increase of the size of the datasets recorded during these experiments. Therefore, new challenges have arisen on how to process all these data efficiently, and in an automated fashion. This is particularly true in the case of induced seismicity monitoring, where often a large number of number of events are recorded at high frequency sampling rates. Several methods of automatic picking have been developed during recent years, from triggering algorithms to higher order statistics or waveform similarity. Latest development in computational power and the popularization of GPUs have made possible to apply machine learning methods to several problems, from arrival picking and phase detection to earthquake location. We have developed a deep neural network to detect the arrivals of seismic body waves, using an architecture based on convolutional layers. This type of models is widely used in computer vision applications, which is the most similar case to the phase picking by an operator. Trained with the data of the Southern California Seismic Network, this network is able to differentiate P and S waves from background noise with a precision higher than 98%. Also, we have analyzed the performance of some Deep Learning pickers recently published, using datasets with different seismic sources.





## 8. Keplerian disks and outflows around binary post-AGB stars

Iván Gallardo Cava

There is a class of binary post-AGB stars that are surrounded by Keplerian disks and that often present outflows resulting from gas escaping from the disk. To date there are seven sources that have been studied in detail through interferometric millimeter-wave maps of CO lines. For the cases of the Red Rectangle, IW Carinae, IRAS 08544-4431, and AC Herculis, it is found that 90% of the total nebular mass is located in the disk: these are the disk-dominated sources. On the contrary, our maps and modeling of 89 Herculis, IRAS 19125+0343, and R Scuti, which allowed us to study their morphology, kinematics, and mass distribution, suggest that in these sources the outflow is the dominant component of the nebula, resulting in a new subclass nebulae around binary post-AGB stars: the outflow-dominated ones. Besides CO, the molecular content of this kind of sources was barely known. We also present a very deep single-dish radio molecular survey in the 1.3, 2, 3, 7, and 13 mm bands. Our results allow us to classify our sources as O- or /C-rich. We also conclude that these sources present in general a low molecular richness, especially those that are disk-dominated, compared to circumstellar envelopes around AGB stars and other post-AGB stars.



## 9. NMC Core-Shell: characterizing the future of Li-ion battery cathodes

Javier García Alonso

Li-ion batteries have suffered an enormous increase in their demand due to the popularization of technologies like electric vehicles and renewable energies. These and the fact that almost all of the present consumer devices depend on this type of batteries makes the improvement of their characteristics a necessary step in technological development. Inside of the needed improvements, the in depth study of the problems faced by the cathodes presents in this batteries and solutions to them is one of the main ones. Different approaches have been taken for the cathodes, being the use of microparticles of Ni-Mn-Co oxides one of the most popular. Here an study of the morphology and crystal structure of Ni-Mn-Co oxides based cathodes (NMC) with core-shell structure is presented, it is expected that the use of this NMC crystal structures, due to their layered nature, and the core-shell morphology of the particles will lead to big improvements in the cyclability and capacity of future Li-ion batteries.



## 10. Subsurface thermal structure: a climate science perspective

Félix García Pereira

Land-atmosphere interaction occurs at a wide range of time scales in the form of mass, momentum, and energy exchange (Melo-Aguilar et al., 2018). Further, subsurface holds a water and mostly energy storehouse for the climate system, accounting for around a 6 % of the terrestrial energy storage (Cuesta-Valero et al., 2021). Therefore, determining the subsurface thermal structure is key to understanding its influence on the global energy balance and hydrological cycle. This work explores the nature of the subsurface thermal regime both in models and in observations. The Max Planck Institute Earth System Model (MPI-ESM) is considered and the sensitivity of its subsurface thermal regime analyzed in changes of the model depth, this being a limitation in the current generation of climate models. It is found that such changes have important implications for the evolution of subsurface temperatures and energy storage in climate change simulations. Additionally, monitoring of subsurface temperatures at some sites allows for estimating thermal diffusivity and seeking causes for its variability in time and space. Results indicate that changes in soil moisture are responsible for the bulk of spatial and temporal variability in apparent thermal diffusivity. The approach developed herein shows a large potential compared to standard approximations focused on the annual cycle.



## 11. Studying the phase transition of the four dimensional Ising spin glass in magnetic field: a replica-symmetric Hamiltonian works

Isidoro González-Adalid Pemartín

Which is the field-theory for the spin-glass phase transition in a magnetic field? This is an open question in less than six dimensions. So far, perturbative computations have not found a stable fixed-point for the renormalization group flow. We tackle this problem through a numerical analysis of the Ising spin glass in four spatial dimensions (data obtained from the Janus collaboration) and in the Bethe lattice. We find strong numerical evidence supporting that the phase transition of the four dimensional Ising spin glass in a field is described by a replica-symmetric Hamiltonian.



## 12. Cat states in a kinetically-driven superfluid

Jesús Mateos Maroto

We investigate the behavior of a one-dimensional Bose-Hubbard model whose kinetic energy is made to oscillate with zero time-average. The effective dynamics is governed by an atypical many-body Hamiltonian where only even-order hopping processes are allowed. At a critical value of the driving, the system passes from a Mott insulator to a superfluid formed by a cat-like superposition of two quasi-condensates with opposite non-zero momenta. We analyze the robustness of this unconventional ground state against variations of a number of system parameters. In particular we study the effect of the waveform and the switching protocol of the driving signal. Knowledge of the sensitivity of the system to these parameter variations allows us to gauge the robustness of the exotic physical behavior.



## 13. Can ice sheets internally oscillate?

Daniel Moreno Parada

The North Atlantic sediment cores contain quasi-periodic layers with extremely high percentages of lithic fragments during glacial periods. These sediments were captured by the ice, transported from the Northern Hemisphere ice sheets and eventually unloaded onto the seafloor when the enclosing ice melted. A non-homogenous sediment distribution suggests that ice flow might fluctuate in time. Several mechanisms have been proposed, among which internal-free oscillations rest on the assumption that there exists a transition between two potential states of basal lubrication. The current work presents a more realistic formulation to estimate the period of such oscillations and further determines under what conditions (if any) these events may occur in 3-dimensional numerical simulations.



## 14. Rapid synthesis of 2D materials by resistive heating

Beatriz Rodríguez Fernández

Transition metal oxides nano- and microstructured are considered promising candidates for multiple applications in electrochromic devices, catalysers, gas sensors, and so forth, because of their attractive properties. One of these metal oxides is  $\text{WO}_3$ , a wide-bandgap n-type semiconductor representative of the electrochromic group materials. Study of the rapid synthesis of semiconductor oxide nano- and microstructures from assisted electromigration processes through an external electric field in a metallic W wire. This method has already been demonstrated as an effective route to obtain metallic oxides, such as  $\text{MoO}_3$  [1]. The growth mechanism is discussed in terms of diffusion processes associated with the flow of an intense electric current and local oxidation processes on the surface of the wire [2]. By applying an external electric field oriented parallel to the electric current flow, i.e. to the wire, growth of structures on the electrodes is achieved. The structural analysis by means of Raman spectroscopy and X-ray diffraction shows that the structures grown on the wire are  $\text{WO}_3$  in monoclinic, triclinic and orthorhombic phase, as well as monoclinic and with oxygen deficiency for the structures grown in the electrodes. The results obtained show that it is a simple and effective method to synthesize tungsten oxide in a fast and low-cost way with promising applications.



## 15. Measurement of the associated production of a W boson and a charm quark at $\sqrt{s} = 13$ TeV at the CMS detector of the LHC.

Sergio Sánchez Navas

A measurement of the associated production of a W boson and a charm (c) quark in proton-proton collisions at a centre-of-mass energy of 13 TeV is reported. The analysis uses a data sample corresponding to a total integrated luminosity of  $137 \text{ fb}^{-1}$  collected by the CMS detector at the LHC. W bosons are identified through their leptonic decays to an electron or a muon, and a neutrino. Charm jets are tagged by the presence of a muon or a secondary vertex inside the jet. The W + c production cross section and the cross section ratio  $\sigma(W+ + c)/\sigma(W- + c)$  are measured inclusively in a fiducial region of phase space, and differentially as a function of the transverse momentum and the absolute value of the pseudorapidity of the lepton from the W boson decay. Measurements are performed at the particle and parton levels and are compared to Monte Carlo generators that implement calculations up to next-to-leading order in perturbative quantum chromodynamics interfaced with parton showering.