COMET 2024 : COrrelated Materials & Electrons in Toulouse

October, 23rd-24th 2024

Program

- Wednesday, october 23rd : FERMI seminar room, 3r4 building

14:45 **15:00**	**Cyril MARTINS,** LCPQ, Toulouse University	***Welcoming talk***
15:00 **15:60**	**Jan TOMCZAK & Harry TOMLINS** King's College London	***Transport simulations in narrow-gap semiconductors and across the 2D Lifshitz metal-insulator transition***
16:00	*Coffee break*	
16:15 **17:15**	**Markus AICHHORN,** ITPCP, University of Technology, Graz	***Strong correlations and spin-orbit coupling in heavy and light elements***

- Thursday, october 24th : FERMI seminar room, 3r1 building 3rd floor

10:00 **11:00**	**Emmanuel FROMAGER,** LCQ – Strasbourg University	***Density matrix embedding theory: A density (matrix) functional perspective***
11:00 **12:00**	**Anna KAUCH,** Institute of Solid State Physics, TU Wien	***Two-particle response with parquet equations***

- Thursday, october 24th : FERMI seminar room, 3r4 building

14:00 **16:00**	**Léo GASPARD,** **LCPQ, Toulouse University**	***Towards an accurate description of spin-orbit correlated materials (PhD defense)***

Transport simulations in narrow-gap semiconductors and across the 2D Lifshitz metal-insulator transition
Jan TOMCZAK & Harry TOMLINS :

We present an efficient methodology for computing the transport of charge, heat, and entropy in solids. In the first part, we establish a comprehensive phenomenology for the transport properties of narrow-gap semiconductors. Their resistivity typically saturates below a characteristic temperature T*. In our scenario, finite lifetimes of intrinsic carriers cause residual conduction, impose the existence of a crossover temperature T*, and control – on par with the charge gap – the quantum regime emerging below. We showcase this mechanism for the Kondo insulator $Ce_3Bi_4Pt_3$ before extending the discussion to signatures of finite electronic lifetimes in the coefficients of Hall, Seebeck and Nernst in other narrow-gap semiconductors.

In the second part, we study the charge transport across a band-tuned metal-insulator transition in two dimensions. For high temperatures T and chemical potentials μ far from the transition point, conduction is ballistic and the resistivity R(T) verifies a simple one-parameter scaling relation. Here, we explore the limits of this semi-classical behaviour and study the quantum regime beyond. We derive an analytical formula for the simplest Feynman diagram of the linear-response conductivity $\sigma = 1/R$ of a parabolic band endowed with a finite lifetime. Finding excellent agreement for experiments for a field-tuned $MoTe_2/WSe_2$ moiré bilayer, we quantify the breakdown of scaling observed for low T and small μ, thus critically assessing the phenomenological Mott-Ioffe-Regel criterion. We go on to discuss a fascinating prediction of our model: The conductance at the quantum-critical Lifshitz point (μ = 0 ; T = 0) has the universal value, \$$\sigma_L = e^2/(2\pi h)$, per band and valley. Analysing experiments for a variety of 2D materials (transition-metal dichalcogenides, metal-oxide-semiconductor field-effect transistors (MOSFETs), heterostructure quantum wells) we contextualize our findings for the Lifshitz transition with respect to the Wigner-Mott and the Anderson transition.

Strong correlations and spin-orbit coupling in heavy and light elements
Markus AICHHORN

I will present some recent results on the effect of spin-orbit coupling in strongly-correlated systems. As we have learned in the past two decades, spin-orbit coupling can change the multiplet structure of materials drastically, leading to unexpected results. For instance, so-called Dirac-Mott, or spin-orbit assisted Mott insulators are prime examples.

We will focus here first on the intriguing behaviour of spin-orbit coupled double perovskite systems, and look for an explanation of the magnetic ground states of Ba2YIrO6. With the help of dynamical mean-field theory (DMFT) and new developments in the solver technology, we can study the fate of the magnetic state down to zero Kelvin. We find that the small moments that are found in DFT studies are actually dynamically screened, such that the magnetic suszeptibility does not depend on temperature.

The second example is a hypothetical phase of FeS, which exists as single layers with honeycomb geometry. It has been argued that this phase could exhibit large topologically non-trivial gaps, although only light elements are present in this system. We investigate whether this picture still holds when dynamical correlations, which are known to be important in the iron chalcogenide systems, are included.

Density matrix embedding theory: A density (matrix) functional perspective
Emmanuel FROMAGER
(abstract not yet available)

Two-particle response with parquet equations
Anna KAUCH
(abstract not yet available)