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Report on the PhD thesis
„Charge Order in $Ir_{1-x}Pt_xTe_2$ and High-Energy Magnetic Excitations in $La_{2-x}Sr_xCuO_4$"
by Oleh Ivashko

Unconventional superconductivity is typically found in quasi two-dimensional correlated electron systems. Often, superconductivity is accompagnied by competing phases such as charge ordering and magnetism. As a direct consequence, these systems display complex phase diagrams. In the quest to understand the guiding principles, studying the non-superconducting phases is a common strategy. Scattering techniques, develloped at large scale facilities, provide powerful methodology to reveal broken symmetries as well as excitations of order parameters.

Layered copper-oxides (cuprates) are perhaps the most famous example of superconductivity in conjunction with a complex set of competing orders. In fact, these systems display, in addition to high-temperature (high-T_c) superconductivity, several competing phases. With the discovery of charge-density-wave ordering in $YBa_2Cu_3O_{7-x}$ back in 2011-2012, it was established that charge ordering is a universal property of hole doped cuprates. This lead to a boom of experimental and theoretical work producing more than 500 scientific publications. In addition to direct studies of the cuprates, it also motivated more general studies of charge order in connection with superconductivity. Another reaction was to return to the fundamental questions of the mysterious pseudogap phase and the mechanism of high-temperature superconductivity.

In essense, this was the scientific landscape of this field when Oleh Ivashko started his PhD thesis work in May 2015. In the past 3.5 years, Oleh has been working on a broad set of unconventional superconductors: $YBa_2Cu_3O_{7-x}$, $La_{2-x}Sr_xCuO_4$, URu_2Si_2, $Pr_4Fe_2As_2Te_{0.88}O_4$, $Ir_{1-x}Pt_xTe_2$ and Ca_2RuO_4 that superconducts under high-pressure conditions. These systems has been studied by hard x-ray diffraction (XRD) and resonant inelastic x-ray scattering (RIXS). Oleh is by now an expert on both these two techniques and masters different sample environments such as magnetic fields, hydrostatic pressure and ultra-high vacuum (UHV) conditions. Oleh has therefore educated himself broadly both in terms of materials, experimental techniques and sample enviroment.

The PhD thesis of Oleh focuses on the $Ir_{1-x}Pt_xTe_2$ and $La_{2-x}Sr_xCuO_4$ systems. The thesis is structured as follows.

- Chapter 1-3 provides a breif introductions to (a) the materials and their phenomenology, (b) the experimental techniques and sample environment applied, and (c) some conceptual backgrounds underlying either analysis or experimental methodology. Chapter 2 contains Laue diffraction patterns of the square and hexagonal lattices found in $Ir_{1-x}Pt_xTe_2$ and La_{2-}

$_{x}Sr_{x}CuO_4$. During his PhD, Oleh helped to install a commercial Laue back-scattering instrument and he develloped exercises that are now used in a praktikum for the bachelor students. Chapter 3 contains an original (simplified) expression of the spin-excitation (magnon) dispersion derived from the U-t-t'-t'' Hubbard model.

- Chapter 4 presents a hard x-ray diffraction of $Ir_{1-x}Pt_xTe_2$ with x=0.04 and 0.05. The experiments where carried out under hydrostatic pressures up to 17 kbar. Several new results are reported. (a) In $Ir_{1-x}Pt_xTe_2$ with x=0.04, charge ordering was known to exist under ambient pressure. Oleh could, however, show directly by XRD that in contrary to IrTe2 with 1/8 modulation, a 1/5 modulation is develloped in $Ir_{0.96}Pt_{0.04}Te_2$. (b) The system $Ir_{0.95}Pt_{0.05}Te_2$ is superconducting in ambient pressure. Application of hydrostatic pressure however triggers a sequence of symmetry breakings. First, the hexagonal lattice symmetry breaks above p_{c1} = 11 kBar, followed by a 1/5 charge modualtion for $p > p_{c2}$ = 16 kbar. From this sequence, it is argued that the charge ordering is lattice driven. Combining (a) and (b), a global phase diagram was constructed. On this basis, the relation between charge ordering and superconductivity is discussed. The work has been published in Scientific Reports (2017).

- Chapter 5 shifts the focus to hole-doped cuprate superconductors. This chapter presents a RIXS study of the high-energy magnetic excitations in $La_{2-x}Sr_xCuO_4$ with x = 0.12 and x = 0.145. The work, carried out at the ADRESS-RIXS instrument at the Swiss Light Source (SLS), benefitted from a newly installed manipulator that allowed flexible scans in the kinematically allowed reciprocal space. In this fashion, Oleh could study the spin-excitations along the underlying antiferromagnetic zone boundary. It is demonstrated that the zone boundary dispersion, compared to the parent compound La_2CuO_4, is dispersing much stronger. As a result, the „magnon" dispersion along the nodal direction is strongly softened. This result was interpreted within the U-t-t'-t'' Hubbard model. Oleh could demonstrate that the zone boundary dispersion is controlled by t', the next-nearest hopping integral. To reach this conclusion, it was necessary to understand the crystal field splittings. With doping, the d_{z2} level moving to lower energy. This lead to a larger hybridization between d_{x2-y2} and d_{z2} orbitals which in term complicated the extraction of t'. Having understood the role of the d_{z2} crystal field splitting, the intrinsic value of t' was unmasked. Oleh work provides a clear picture of how the spin excitation dispersion evolves with doping. This work has been published in Phys. Rev. B (2017).

- Chapter 6 is similar to chapter 5 in terms of methodology. Thin MBE films of La_2CuO_4 grown on different substrates were studied. The substrate provides an in-plane strain on the La_2CuO_4 films and hence controls the in-plane lattice parameter. In this fashion Oleh has been the first to study the magnon dispersion as a function of externally applied pressure. The results are beautifully clear and several key conclusions are reached. (a) From the XAS study oft he Cu L-edge, it can be concluded the the Coulomb interaction U is increasing with the in-plane lattice parameter. (b) RIXS reveals that the magnon band width is controllable by strain. In fact, the band is tuned by as much as 50 meV. Without any analysis, this demonstrates that the magnetic exchange interaction is controlled by strain. Emperically, it is thus demonstrated that the substrate giving the larger T_c upon doping also have the largest magnetic exchange interaction. As such, the work of Oleh goes in the direction to establish a magnetic isotrope effect for cuprate superconductivity. These conclusions are backed up with more detailed analysis through the U-t-t'-t'' Hubbard model. It is demonstrated that the magnon dispersion can be described by a single parameter – namely nearest neighbor hopping t that is intuitively controlled by in-plane pressure. This work has been submitted to Nature Communications (2018) and has recieved positive feedback from the referees.

In addition to the work presented in chapter 3-6, Oleh has been highly involved in several other projects. For example, Oleh has been working on the charge ordering in YBCO. This work deals with the field-induced three-dimensional charge ordering. One paper is already published in Nat. Comm. 2016 with Oleh as third author. Another manuscript, with Oleh as second author, is in preparation. To conclude his XRD work, Oleh has also been working on URu_2Si_2 and $Pr_4Fe_2As_2Te_{0.88}O_4$. This work is also going to be published in near future with Oleh as second author on both these papers. Finally, Oleh has contributed to RIXS studies on pnictides and ruthenate systems. The latter mentioned work is published in PRX 2018 while the first mentioned work is submitted to PRL. Generally, the scientific contributions of Oleh Ivashko demonstrate that he is capable of taking the lead on specific projects while at the same time helping and contributing to projects of group members. Oleh has in this fashion during his PhD produced in total nine publications (published, submitted or in the pipeline). The quality of Oleh's experimental work has also been noticed by our international collaborators and competitors. Oleh has for example been head-hunted for a postdoctoral instrument scientist job at PETRA-III, Desy-Hamburg.

The breath of Oleh's PhD thesis work is impressive. I can therefore recommend this dissertation without hesitation to be accepted by the Faculty of Sciences of UZH.

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