Universal electronic structure of layered nickelates via oxygen-centered planar orbitals

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In a series of groundbreaking discoveries, superconductivity has recently been demonstrated in $La_3Ni_2O_7$ up to 91 K under moderate pressure in bulk crystals, and up to 48 K at ambient pressure in thin films grown under compressive strain. Key questions remain open regarding the crystal structure and low-energy electronic states that support superconductivity in these compounds. Here we take advantage of the natural polymorphism between bilayer (2222) or alternating monolayer-trilayer (1313) stacking sequences that arises in bulk $La_3Ni_2O_7$ crystals to identify universal features in this family of materials. Employing angle-resolved photoemission spectroscopy (ARPES) we observe the fingerprint of a spin-density wave (SDW) instability, strong and coherent enough to modify the electronic structure[1]. We demonstrate that this feature is a 'translated' β Fermi surface associated with a scattering vector $Q_{t\beta}$ which matches the Q_{SDW} detected by neutron and x-ray scattering experiments. This observation provides an important link between surface and bulk probes, and demonstrates a universal connection between magnetism and fermiology in $La_3Ni_2O_7$ as well as $La_4Ni_3O_{10}$. Using an effective tight-binding model, we simulate the spectral weight distribution observed in our ARPES dichroism experiments and establish that the low-energy electronic phenomenology is dominated by oxygen-centered planar orbitals, which – upon moving along the Fermi surface away from the Ni-O-Ni bond directions – evolve from the $d3x^2-r^2$ and $d3y^2-r^2$ symmetry characteristic of 3-spin polarons to the familiar dx^2-y^2 Zhang-Rice singlets that support high-temperature superconductivity in cuprates. Despite the multiorbital nature of the nickelates, our work establishes an empirical correspondence between the low-energy electronic structure of cuprates and nickelates, thus suggesting a common origin for their unconventional superconductivity[1].

[1] Christine C. Au-Yeung, X. Chen, S. Smit, M. Bluschke, et al., arXiv:2502.20450 (2025).

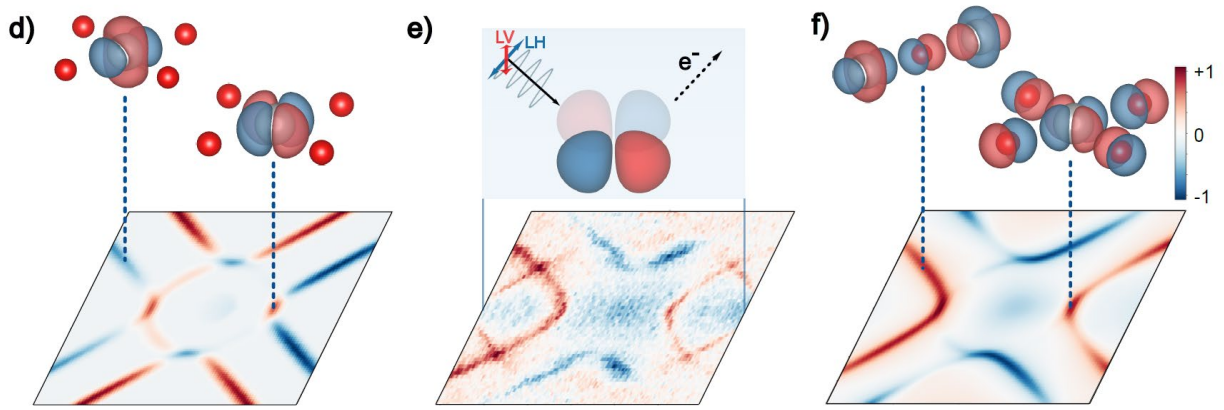

Figure 1. (d,f) (top) Schematic representation of wavefunctions at the indicated momenta along the FS with relative phases in red and blue (O and Ni sites in red and silver, respectively), along with (bottom) the simulated ARPES dichroism (LV-LH). (e) (top) Experimental geometry, showing the polarization vector of the light with respect to the in-plane orbitals, along with (bottom) the experimental dichroism measured by ARPES on LNO327.