Bloch Wavefunction Reconstruction using Multidimensional XUV Photoemission Spectroscopy

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Angle-resolved photoemission spectroscopy is the most powerful technique to investigate the electronic band structure of crystalline solids. To completely characterize the electronic structure of topological materials, one needs to go beyond band structure mapping and probe the texture of the Bloch wavefunction in momentum-space, associated with Berry curvature and topological invariants. Because phase information is lost in the process of measuring photoemission intensities, retrieving the complex-valued Bloch wavefunction from photoemission data has yet remained elusive. In this talk, I will introduce a novel measurement methodology and observable in extreme ultraviolet (XUV) angle-resolved photoemission spectroscopy, based on continuous modulation of the XUV polarization axis. By tracking the energy- and momentum-resolved amplitude and phase of the photoemission modulation upon polarization variation, we reconstruct the Bloch wavefunction of prototypical semiconducting transition metal dichalcogenide 2H-WSe_2 with minimal theory input. This novel experimental scheme, which is articulated around the manipulation of the photoionization transition dipole matrix element, in combination with a simple tight-binding theory, is general and can be extended to provide insights into the Bloch wavefunction of many relevant crystalline solids. Our approach is also compatible with ultrafast time-resolved measurements: we envision using this new observable to directly follow the dynamical evolution of the Bloch wavefunction of materials undergoing light-induced ultrafast topological phase transitions.

[1] S. Beaulieu, J. Schusser, S. Dong, M. Schüler, T. Pincelli, M. Dendzik, J. Maklar, A. Neef, H. Ebert, K. Hricovini, M. Wolf, J. Braun, L. Rettig, J. Minár and R. Ernstorfer, *"Revealing Hidden Orbital Pseudospin Texture with Time-Reversal Dichroism in Photoelectron Angular Distributions,"* Physical Review Letters **125**, 216404 (2020).

[2] M. Schüler, T. Pincelli, S. Dong, T. P. Devereaux, M. Wolf, L. Rettig, R. Ernstorfer, and S. Beaulieu, *"Bloch Wavefunction Reconstruction using Multidimensional Photoemission Spectroscopy,"* arXiv:2103.17168 (2021).

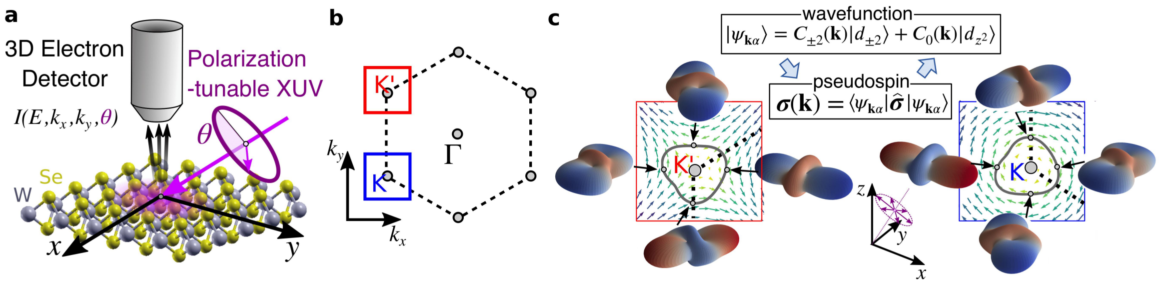

Figure 1 : Experimental setup: (a) A polarization-axis-tunable linearly polarized femtosecond XUV pulse (21.7 eV) is focused onto a 2H-WSe_2 crystal ejecting photoelectrons which are detected by a time-of-flight momentum microscope, allowing to measure the energy- and momentum-resolved photoemission intensity as a function of the polarization axis angle θ. (b) Sketch of the first Brillouin zone of 2H-WSe_2. (c) Bloch wavefunction of the top valence band of monolayer WSe_2. There is a one-to-one map of the complex wavefunction coefficients to the orbital pseudospin; the corresponding texture is represented by the vector field.