Electronic structure, correlations and excited states of topological quantum materials

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Quantum technologies is a new and very pulsing multidisciplinary research area on the border between physics, chemistry, mathematics, informatics and materials science with a very high technological impact. In order to understand the physical properties of quantum materials on a fundamental level, one needs to explore the corresponding electronic states in detail and disentangle the role of the various interactions. In the past years we saw a big progress in the quantum mechanical description of topological systems and their properties at ideal conditions which are relatively easy so simulate but very hard to achieve in practice, such as, e.g., at zero absolute temperature or ideal structure. However, to directly promote technological progress it is necessary to deepen the theoretical understanding of specific quantum phenomena and/or materials under real conditions such as finite temperatures, structural and chemical disorder, presence of impurities and under the influence of ultrafast light pulses. This way it is important further to develop flexible, material specific theoretical methods which do allow to describe properties of real systems beyond the ground state. In this presentation I will show that fully relativistic multiple scattering Green function KKR theory [1] is the method of choice to include most of these effects as for example correlation effects by means of dynamical mean field theory [2] or the alloy analogy model for the description of spin fluctuations under finite temperatures [3]. Furthermore I will focus on extending our capabilities of performing quantitative calculations of excitations by light ranging from 10 eV up to 10 keV [4]. As an example I will concentrate on the angle-resolved photoemission spectroscopy (ARPES) which is a leading experimental probe for studying the electronic structure and complex phenomena in topological 3D and 2D quantum materials [5,6,7]. As the latest development a theoretical frame for the description of pump-probe photoemission is presented. The approach is based on a general formulation using the Keldysh formalism for the lesser Green function to describe the real-time evolution of the electronic degrees of freedom in the initial state after a strong pump pulse that drives the system out of equilibrium [10].

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