Summary of PhD thesis:

Theoretical description of photoemission and scanning tunneling microscope measurements on Dirac-like electrons

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To study Dirac-like electronic states in single layer graphene and three-dimensional topological insulators I have applied theoretical models of photoemission spectroscopy and scanning tunneling microscopy (STM). I have calculated the intensity distribution of photoelectrons and the local density of states, which is proportional to the differential conductivity of the STM point contact.

For single layer graphene I have developed a general formula to determine the intensity distribution of photoelectrons, which can be used to study arbitrary translational invariant one-electron interaction in graphene. I worked out an anisotropic effective Hamiltonian to describe Rashba-type spin-orbit coupling in graphene. I showed that the low energy Hamiltonian of single layer graphene with Rashba-type spin-orbit coupling is unitary equivalent to the Hamiltonian of bilayer graphene with trigonal warping. Despite of the three folded symmetry of the low energy dispersion, the spin polarization of the Bloch states is isotropic in the momentum space with vanishing out-of-plane component. My theoretical predictions are consistent with experimental results.

Generalizing the expression developed for the intensity distribution of photoelectrons, one can determine the expectation value of arbitrary physical operator. Thus the spin polarization can be calculated from the expectation value of spin operators. I showed that sublattice asymmetry in graphene coupled to the electron spin via spin-orbit coupling, induces finite out-of-plane spin polarization in the distribution of both Bloch electrons and photoelectrons.

Finally I have studied surface states of second-generation topological insulators by modeling electronic standing waves induced by line defects on the surface. According to my results, standing waves at line defects oriented along ΓK direction on the surface of Bi_2Te_3 crystal, are characterized by different properties as predicted by the theory describing asymptotic tendency: (i) the wavelength of standing waves close to the line defect is determined by the point on the constant energy contour where the group velocity parallel to the line defect is minimal. This finding is in contrast with the asymptotic behavior of standing waves, where the characteristic wavelength is determined by nesting segments on the constant energy contour in the momentum space. (ii) The decaying characteristics of standing waves, in the spatial range studied in experiments, is rather exponential than polynomial. My results agrees very well with recent experiments.