Thesis of doctoral (PhD) dissertation:

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

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1 Introduction

Chiral electrons of single layer graphene and helical electronic states of second-generation topological insulators are both well described by linear energy dispersion, called as Dirac-cone. On the one hand, analogy between theory of graphene and quantum mechanics of relativistic particles, provides opportunity to study effects known long ago from relativistic dynamics. Topological insulators, on the other hand, seem to be promising on the field of spintronics. Both physical systems are ideal to be studied by surface sensitive experimental methods like photoemission spectroscopy or scanning probe microscopy.

Photoemission spectroscopy is an excellent experimental method to study electronic band structure of materials of different phases. The great history of photoemission spectroscopy started with experimental and theoretical work of Einstein in 1905. According to theoretical description of the photoemission effect, electrons can be emitted from the sample as a consequence of the interaction with photons of higher energy than the work function of the sample. The emitted electrons are called *photoelectrons*. During experiments, samples were illuminated by a monochromatic beam of light in high quality vacuum tube. In our days similar technique is in use, however, the detection of photoelectrons went under notable improvements. Recent electron detectors are designed to be able to measure the whole distribution of photoelectron in the energy and momentum space.

Recent developments of spintronics generated photoemission spectroscopy techniques to be expanded in order to detect the spin polarization of photoelectrons as well. The spin polarization is measured by two spin sensitive Mott detectors. Each detector can determine the projection of the spin polarization onto the plane of the detector. The three-dimensional polarization of photoelectrons can than be restored from data of the two-dimensional projections.

Scanning probe microscope methods, similarly to photoemission spectroscopy, are excellent in studying surface physics, like topography, chemical bonds, electronic and magnetic properties, etc. However, to study different physical properties of samples, one needs experimental equipments designed in different ways. The most frequently used techniques are the scanning tunneling microscope (STM) and the scanning force microscope (SFM) methods. In booth cases, thin conducting tips are used to examine the interaction between the tip and surface. In STM measurements the central physical quantity is the tunneling current, while SFM technique are based on the force between the tip and surface. Another important quantity in STM measurements is the bias voltage on the STM point contact. Numerous properties of electronic states of the sample can be deduced from the tunneling current (I) - bias voltage (V) curve. In addition, deriving the $\mathrm{d}I/\mathrm{d}V$ differential conductivity, one can examine electronic states directly as a function of

the energy.

STM technique, compared to photoemission spectroscopy, can be used at both lower and higher energies than the Fermi energy of the sample. On defect free, regular crystal surface one can measure the $\rho_0(E)$ density of surface states (and the density of bulk states which gives lower contributions to the tunneling current) of the sample. Close to point and line defects on the surface, the local density of states differs substantially from $\rho_0(E)$. Oscillations appear in the local density of states as a function of the distance from the defect, which characteristics (such as wavelength or decaying) can be understood via properties of the energy dispersion of electronic states.

2 Objectives of the study

2.1 Interaction between photons and the sample. Modeling the photoemission effect.

In order to explain experimental results on graphene and topological insulators, we reviewed the theoretical models of the photoemission effect. The intensity of photoelectrons is closely related to the density of states, while the anisotropy in the distribution of photoelectrons is characterized by the transition matrix elements. The peaks in energy (or momentum) distribution curves are broadened by finite energy and momentum resolution of experimental equipment and by the interaction between the quasiparticles.

2.2 Theoretical description of intensity distribution of photoelectrons

In graphene the intensity distribution of photoelectrons shows two-folded symmetry related to the interference of photoelectrons emitted from the two sublattice. In our work we aimed to develop a relation to describe the distribution of photoelectrons, which could be evaluated for arbitrary translational invariant (one electron) interaction, and would be related directly to the matrix elements of the Hamiltonian. Derived expression can then be used to study various interactions via the changes in the distribution of photoelectrons.

2.3 Theoretical description of spin polarization of photoelectrons

Detection of spin polarization in spin and angle resolved photoemission spectroscopy has been markedly improved during recent years. Generalizing the relation developed for the distribution

of photoelectrons, one can determine the expectation value for general physical operator. The spin polarization can be computed from the expectation value of spin operators.

2.4 Spin-orbit interaction in graphene

Spin and angle resolved photoemission spectroscopy revealed finite spin-orbit interaction in graphene placed on special substrates. In contrast with isotropic models we propose anisotropic effective Hamiltonian to describe Rashba-type spin-orbit coupling, taking into account the symmetry properties of the graphene lattice. We compare theoretical predictions to experimental data.

2.5 Review of models of three-dimensional topological insulators

Topological properties of the band structure play important role in physics of insulators. Surface states in insulators with nontrivial topological properties are protected against defects in the crystal. Furthermore, energy dispersion of surface states in second-generation topological insulators can be described with two-dimensional Dirac-cone. In order to study surface states we reviewed the effective models of second-generation topological insulators.

2.6 Higher order corrections in the effective model of Bi_2Te_3 crystal

All the second-generation topological insulators have the same crystal lattice structure, but different chemical composition. Due to identical crystal lattice, surface states of second-generation topological insulators can be described with the same effective model regardless of the chemical composition. For each composition the parameters of the effective model can be obtained by fitting the energy dispersion and the density of states to experimental data. Accurate description of the energy dispersion may plays important role in modeling many physical effects, like electronic standing waves around defects. Among the samples, Bi_2Te_3 crystal shows the most pronouncing hexagonal warping effect in the energy dispersion of surface states. Therefore, we examined the influence of higher order corrections in the effective model on the band dispersion of surface states.

2.7 Review of scanning tunneling microscope methods

Scanning tunneling microscope is an excellent experimental tool to study electronic states on the surface. In order to study electronic standing waves on the surface of graphene and topological

insulators, we reviewed the theoretical models of tunneling currents.

2.8 Modeling electronic standing waves around line defects

Asymptotic description of standing waves around line defects has been already studied in various publications. However, at closer distances to the defect, standing waves might show different behavior compared to the asymptotic tendency. Notable differences can be found between experimental data on Bi_2Te_3 crystal and asymptotic theoretical predictions for standing waves. We aim at develop a more accurate model of standing waves, which can be applied at closer distances to the line defect as well.

3 Applied methods

3.1 Models of electron systems

Bloch states of electrons in the tight binding model are expressed as a coherent superposition of atomic orbitals localized on the sites in the crystal lattice. Most of the physical responses of the sample to perturbations are characterized by electronic states close to the Fermi energy. Hence it is frequently applied method to use an effective continuous model of electronic states around the Fermi energy. The continuous model, as a long wave approximation of the tight binding model, can be used to study interactions with characteristic lengths much longer than the lattice constant.

The wavefuction of an elastically scattered electron (at surface defect for example) can be written as a coherent superposition of the incident and scattered electronic states. The total spatial distribution of the electrons with a given energy can then be computed as a sum of wavefunctions of scattered electrons related to each incident states weighted by the local density of states of the homogeneous system in the momentum space.

3.2 Models for experimental methods

In the three-step model of the photoemission effect the distribution of photoelectrons is calculated via the Fermi's golden rule, considering the interaction between photons and electrons as a perturbation.

According to the Tersoff-Hamann model of scanning tunneling microscope, the tunneling current is proportional to the integral of the local density of states on the surface at the STM

contact in the energy window determined by the bias voltage on the STM contact, and shows exponential dependence on the distance between the surface and the scanning tip.

3.3 Fourier analysis of oscillations in the local density of states

Fourier analysis provides excellent tools to explore fundamental properties of decaying oscillations (like electronic standing waves on the surface of topological insulators). Singularity in the Fourier spectrum, for example, indicates power-low decay of the oscillation. The lack of singularities, on the other hand, indicates decaying rate other than power-law.

4 Results and conclusions

4.1 Anisotropic model of Rashba-type spin-orbit coupling in graphene

Electrons in graphene with energy close to the Dirac-point are usually described by isotropic models where the lattice induced hexagonal warping effect has influence on electron dynamics only at higher energies. However, we worked out a low energy Hamiltonian for Rashba-type spin-orbit coupling that describes anisotropic behavior of electronic states even close to the Dirac-point. We presented our results in publication [1].

a Continuous model of Rashba-type spin-orbit interaction

We showed, that the effective continuous model of Rashba-type spin-orbit interaction in graphene describes unitary equivalent dynamics of electrons as the low energy Hamiltonian of bilayer graphene with trigonal warping. This conclusion is surprising since the two systems are physically very different [1].

b Symmetry properties of band structure and spin-polarization of Bloch-states

Although the low energy spectrum in graphene with Rashba-type spin-orbit coupling consists of four Dirac-cones, the spin-polarization of electronic states remains isotropic in the momentum space with vanishing perpendicular component to the plane of graphene. The trigonal warping effect has influence on the spin-polarization only in higher order corrections of the momentum [1].

c Relationship of intrinsic and Rashba-type spin-orbit interaction in graphene

Although the energy scale of the trigonal warping effect in the low energy dispersion of electronic states is comparable with the strength of the intrinsic spin-orbit coupling (based on measurements and realistic simulations), we showed that the intrinsic spin-orbit coupling does not break the trigonal warping effect in the low energy spectrum caused by the Rashba-type spin-orbit interaction [1].

4.2 Influence of sublattice asymmetry on the spin-polarization of photoelectrons

The spin-polarization of photoelectrons can be affected by any interaction coupled to the Bloch electron spin. In case of graphene the sublattice asymmetry is coupled to the electron spin via spin-orbit interaction. We presented our results in publication [2].

a Theoretical description of the spin-polarization of photoelectrons

In order to study spin-polarization of photoelectrons we derived a general expression for the to compute expectation value of arbitrary physical operator in terms of the matrix elements of the Hamiltonian. This method omits the computation of the wavefunctions, hence one can resolve the problem of discontinuity in the phase of wavefunctions [2].

b Sublattice asymmetry induced out-of-plane the spin-polarization of Bloch electrons

While for equivalent sublattices the the spin-polarization of the Bloch states lies in the plane of graphene, we showed, that sublattice asymmetry induces finite out-of-plane spin-polarization. The half width of the peak in the distribution of out-of-plane spin-polarization is independent of the magnitude of the sublattice asymmetry, it is characterized by the strength of the spin-orbit coupling [2].

c Effect of sublattice asymmetry on the spin-polarization of photoelectrons

Due to sublattice interference, the distribution of spin-polarization of photoelectrons is very different from the spin-polarization resulted from Bloch-electrons. In the direction of minimal intensity of photoelectrons (called dark corridor) the out-of-plane component of the spin-polarization becomes finite due to the presence of sublattice asymmetry [2]. We also studied the rapid variation of the spin-polarization (as a function of the momentum) across the dark corridor.

The effect of sublattice asymmetry on the spin-polarization might play crucial role in physical systems where both sublattice asymmetry and spin-orbit interaction are strong, as in the case of recently produced samples of silicene.

4.3 Description of electronic standing waves around line defects

Electronic standing waves around defects on the surface of topological insulators have been studied both experimentally and theoretically. Deviation between experimental results and recent theoretical predictions are most pronounced in case of Bi_2Te_3 crystal where the energy dispersion of surface states differs most from the ideal Dirac-cone. We developed a new approach to explain characteristic features of electronic standing waves along line defects obtained in recent experiments. We presented our results in publication [3].

a Parameters in the effective model of surface states for Bi_2Te_3 crystal

Theoretical description of oscillations in the local density of states strongly depends on the accuracy of computing constant energy contours of the dispersion of surface states. Two fitting parameters in the effective Hamiltonian already describe the feature of the hexagonal warping of constant energy contours, however the agreement between the theoretical energy dispersion curves along high symmetry sections in the Brillouin zone and experimental data is still not satisfactory. In order to compute the energy dispersion curves and the density of states more accurately we fitted two more parameters allowed by symmetry considerations relevant in the effective model to the experimental data [3].

b Derivation of unitary scattering matrix of the scattering on quasi-one-dimensional potential barrier on the surface of second generation topological insulators

In most studies on electronic standing waves around line defect on the surface of Bi_2Te_3 crystal, an important ingredient is missing, namely the scattering matrix is not unitary. We extended these calculations by taking into account evanescent states localized on the line defect leading to a unitary scattering matrix. Due to the unitarity of the scattering matrix, oscillation components that were considered to be dominant in the asymptotic theory cancels each other independently of the shape of the potential barrier [3].

c Pre-asymptotic contribution to electronic standing waves on the surface of Bi_2Te_3 crystal

We showed that our theoretical results agree well to experimental data on electronic standing waves around line defects on the surface of Bi_2Te_3 crystal, unless we limit our calculation to asymptotic behavior of the oscillation, but we also consider contributions to the oscillation that can be dominant at closer distances to the line defect. The wavelength of the standing waves – for orientation found in experiments – is characterized by the point on the constant energy contour where the group velocity component parallel to the line defect is minimal. According to Fourier analysis of numerical data, we showed that despite of the asymptotic limit, standing waves closer to the line defect decays rather exponentially than polynomially [3]. For other orientations of the line defect, when there exist nesting segments on the constant energy contour, our results coincide with predictions of the asymptotic theory of oscillations in the local density of states. Since we demonstrated that the oscillation behavior of the electron density of states is encoded only in the dispersion relation, we expect that our results are not dependent on the shape of the potential barrier. Hence we expect that our results are valid for arbitrary potential profile.

5 Publications related to the thesis

1. P. Rakyta, A. Kormányos, and J. Cserti, *Trigonal warping and anisotropic band splitting in monolayer graphene due to Rashba spin-orbit coupling*, Phys. Rev. B **82**, 113405 (2010).

2. P. Rakyta, A. Kormányos, J. Cserti, *Effect of sublattice asymmetry and spin-orbit interaction on out-of-plane spin polarization of photoelectrons*, Phys. Rev. B **83**, 155439 (2011).

3. P. Rakyta, A. Palyi, J. Cserti, *Electronic standing waves on the surface of the topological insulator Bi_2Te_3*, arXiv:1111.6184 (2011).