Summary of Professional Accomplishments

1. Paweł Potasz

2. Diplomas, degrees conferred in specific areas of science or arts, including the name of the institution which conferred the degree, year of degree conferment, title of the PhD dissertation

2012	PhD in physical sciences (3.07.2012) Institute of Physics, Wroclaw University of Science and Technology Title of the thesis: Electronic and optical properties of graphene nanostructures Supervisors: prof. Arkadiusz Wójs (Wroclaw University of Science and Technology) prof. Pawel Hawrylak (National Research Council Canada)
2007	MSc in physics (6.07.2007) Faculty of Fundamental Problems of Technology, Wroclaw University of Science and Technology Title: Thermodynamics of paired fermionic systems at BCS–BEC crossover Supervisor: dr Mateusz Krzyżosiak (Wroclaw University of Science and Technology)

3. Information on employment in research institutes or faculties/departments or school of arts

03.2021 –	professor at Department of Quantum Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun
02.2019 – 02.2021	postdoc, The University of Texas at Austin, Department of Physics, Austin, Texas, USA
10.2015 – 10.2020	assistant professor at Department of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wroclaw University of Science and Technology
10.2014 – 09.2015	research assistant at Department of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wroclaw University of Science and Technology
05.2014 – 11.2014	postdoc, Department of Quantum Materials, International Iberian Nanotechnology Laboratory (INL), Braga, Portugal
10.2012 – 09.2014	research assistant in Institute of Physics, Wroclaw University of Science and Technology

4. Description of the achievements, set out in art. 219 para 1 point 2 of the Act

Cycle of scientific articles related thematically, topic of the series: Theoretical research on stability of topological phases in selected two dimensional systems.

The series consists of the following works (in a chronological order):

H1 **P. Potasz**, M. Xie, A. H. MacDonald, *Exact diagonalization for magic-angle twisted bilayer graphene*, Phys. Rev. Lett. **127**, 147203 (2021), 10.1103/PhysRevLett.127.147203

H2 N. Nouri, M. Bieniek, M. Brzezińska, M. Modarresi, S. Zia Borujeni, Gh. Rashedi, A. Wójs, **P. Potasz**, *Topological phases in Bi/Sb planar and buckled honeycomb monolayers*, Phys. Lett. A **382**, 2952–2958 (2018), 10.1016/j.physleta.2018.06.037

H3 B. Jaworowski, A.D Güçlü, P. Kaczmarkiewicz, M. Kupczyński, **P. Potasz**, A. Wójs, *Wigner crystallization in topological flat bands*, New J. Phys. **20**, 063023 (2018), 10.1088/1367-2630/aac690

H4 M. Brzezińska, M. Bieniek, T. Woźniak, **P. Potasz**, A. Wójs, *Entanglement entropy and entanglement spectrum of $Bi_{1-x}Sb_x$ (111) bilayers*, J. Phys.: Condens. Matter **30**, 125501 (2018), 10.1088/1361-648X/aaaf54

H5 M. Bieniek, T. Woźniak, **P. Potasz**, *Stability of topological properties of bismuth (111) bilayer*, J. Phys. Condens. Matter **29**, 155501 (2017), 10.1088/1361-648X/aa5e79

H6 B. Jaworowski, A. Manolescu, **P. Potasz**, *Fractional Chern insulator phase at the transition between checkerboard and Lieb lattices*, Phys. Rev. B **92**, 245119 (2015), 10.1103/PhysRevB.92.245119

H7 **P. Potasz**, J. Fernandez-Rossier, *Orbital magnetization of quantum spin Hall insulator nanoparticles*, Nano Letters **15**, 5799-5803 (2015), 10.1021/acs.nanolett.5b01805

The subject of topological effects is very broad, from the perspective of studied materials and their properties from topological point of view, and together with advanced mathematical tools standing behind them, it is not possible to describe here complete mathematical formulation of the problem, which force me to restrict to the most important issues strictly related to the presented achievement.

Introduction

Research on materials with topologically nontrivial properties is currently one of the main field in condensed matter physics [1, 2]. It is related to crucial importance for understanding of fundamentals laws of physics and huge potential for applications [3-6]. The beginnings start in 80' and discovery of integer quantum Hall effect [7]. Integer quantum Hall effect can be observed in two-dimensional systems under high-magnetic fields. From quantum mechanical point of view, electrons populate so called Landau levels – highly degenerate energy levels. Experimentally measured Hall resistivity forms characteristic plateaus as a function of a magnetic field and conductance as its inverse is precisely defined as an integer number of fundamental constants, despite of defects and other factors affecting idealized predictions of the theory.

Explanation of ideal conductance quantization is possible on the basis of topological interpretation of the phenomena. Topological phases, or in general topologically distinguished objects, are the ones that cannot be transformed one in to the other using continuous transformations. A typical example outside of condensed matter physics, but clearly described the problem, is a sphere and a torus. These are two topologically distinguished objects due to a different number of holes, no holes in case of a sphere and one hole in a torus. Transformation of a sphere into a torus is not possible using continuous transformations because at the end creating a hole in a sphere requires its breaking – noncontinuous transformation. Following this path, objects (or precisely using mathematical terminology, manifolds) without a hole are topologically equivalent between themselves (can be obtain one from the other using continuous transformations like squeezing or stretching), and similarly all objects with a given number of holes are topologically equivalent to each other. Because of that, one can introduce a topological invariant, which distinguishes topologically inequivalent objects. In this case it is a number of holes.

Phases in integer quantum Hall effect are classified by topological invariant called Chern number, which is well defined for energy bands separated by energy gaps from the rest of the spectrum. A value of Chern number reflects on conditions imposed on gauge choice of wave function on a given manifold; in the case of periodic structures our manifold is a reciprocal space (a torus). In the case of nonzero Chern number, one cannot choose one gauge that is continuous on an entire manifold, and also satisfies periodic boundary conditions. Conductance in integer quantum Hall effect is proportional exactly to Chern number, and as a discrete quantity, cannot be changed by tiny deformations or defects in the system. Hence, this is the reason of its peculiar stability observed in the experiment. Nonzero value of Chern number in this case distinguishes topological insulators from trivial insulators (like widely used SiO_2). It is worth to emphasize importance of discovery of integer quantum Hall effect. Hitherto known phases of matter and transitions between them, have been described by Landau theory [9] – phases of matter can be classified by their symmetries and transitions between them requires breaking of that symmetry. Integer quantum Hall effect required a new description, beyond Landau theory, because none of the symmetry is broken in this case. New theory classifies insulators using their topological properties.

The issue related to origin of topologically nontrivial properties in integer quantum Hall effect was considered by Haldane. In this phenomena there are two characteristic factors: existence of Landau levels and breaking of time-reversal symmetry due to a presence of a magnetic field. In 1988

Haldane proposed theoretical model of integer quantum Hall effect without Landau levels [10], proving that crucial for conductance quantization is breaking of time-reversal symmetry. The model, currently known as Haldane model is an example of so called Chern insulator, a system with topologically nontrivial properties without an external magnetic field. Haldane model was crucial in discovery of new systems with topologically nontrivial properties with conserved time-reversal symmetry, called now Z_2 topological insulators. In 2005, C. Kane and E. Mele proposed a model with spin consisting of two copies of Haldane model for each spin [11,12]. Kane-Mele model is a tight-binding model describing crystal structure of graphene with spin-orbit coupling. It is not a good example for realistic realization due to small value of spin-orbit coupling constant, characteristic of light elements, but pioneered the research in a new direction of various crystals with nontrivial topology of energy bands. More realistic model of Z_2 topological insulators, widely known also as quantum spin Hall insulator [12], was proposed by A. Bernevig and collaborators [13], and in 2007 quantized conductance was confirmed experimentally [14]. Currently insulators with nontrivial topology of energy bands are called topological insulators, with integer quantum Hall effect as the first example studied theoretically and experimentally.

Characteristic feature of topological insulators is existence of energy gap between the ground state and excited states in infinite system, and a presence of edge states[1] (or surface states in case of three dimensional materials) crossing the energy gap, if a material is finite in at least one dimension [3, 4]. While the presence of edge states is nothing special and their occurrence is frequent in many materials, in the case of topological insulators, their origin comes from bulk materials properties (topological properties). Additionally, edge states in topological insulators reveal many unique properties related to their topological character. Current flowing through edge states channels is extremely stable against disorder, i.e. energetic dissipation is suppressed - backscattering is forbidden. In integer quantum Hall effect there are so called chiral edge states – current flow through edges has an opposite direction on opposite edges, thus backscattering requires a hop of a scattered carrier to a channel that is macroscopically far. In quantum spin Hall effect, there are so called helical edge states – a direction of current flow is strictly related to spin, and backscattering within a given edge requires a spin flip, which is possible only when time-reversal symmetry is broken, e. g. by a magnetic dopant. Because of this, despite a presence of dopants (nonmagnetic in general) and disorder, current flow like in an ideal, clean, material.

Transport properties of Z_2 topological insulators can be observed in low temperatures because of small energy scale in the systems – an origin of topologically nontrivial effects is most often due to spin-orbit interaction[2], which has relatively small spin-orbit coupling constant – the energy gap in these materials is of the order of few meV. Quantized conductance in topological insulators has been experimentally confirmed in 30 mK temperature [14]. A class of materials with topological properties in two dimensions has been extended to three dimensional materials [3, 4]. Currently, an intensive search of new materials with topologically nontrivial properties is continued, which effects could be observed in higher temperatures, thanks to control of magnitude of the energy gap. Very promising is potential application of such materials to build new, efficient electronic devices.

Integer quantum Hall effect can be explained at the single particles level, without inclusion of electronic correlations. In 1982 plateaus at noninteger values of quantized conductance for partially filled Landau level has been discovered [17], called now fractional quantum Hall effect. Theoretical explanation for 1/3 filling of the lowest Landau level was proposed by Laughlin. Observed plateaus

[1] Within this set of articles I focused on two dimensional materials and topological phases, in which edge states are present, but there are topological phases without edge states [15].

[2] Currently a class of materials with topologically nontrivial properties has been extended to models without spin-orbit coupling, and example is ref. [16].

at other partial fillings can be explained using Haldane-Halperin hierarchical theory [19, 20] and using composite fermions theory proposed by Jain [21, 22].

Haldane model is a single particle model of integer quantum Hall effect on a periodic two-dimensional lattice without external magnetic field and consequently without Landau levels. An interesting issue was if here incompressible liquids for partial filling of energy bands can occur too, i.e. existence of fractional quantum Hall effect with conserved a translational symmetry. In 2011 several theoretical models have been proposed of systems on two dimensional lattices with topologically nontrivial energy bands (with nonzero Chern number), appropriately flatten in order to enhance many-body effects [23-28]. Numerical calculations confirmed existence of incompressible liquids for 1/3 filling of flat topological energy bands, similar to Laughlin state for partially filled lowest Landau level. In consecutive works, appearance of entire family of incompressible strongly correlated liquids for another fillings has been shown [27-32].

In last years twisted atomic layers forming so called moire superlattices have attracted attention of fair number of research groups, experimental and theoretical ones. It is related to experimental confirmation of superconductivity for partial filling of flat bands formed at particular twist angles of bilayer graphene, for angle around 1.1°, named now magic angle [33-35]. In band structure of twisted bilayer graphene, when a twist angle is close to magic angle, a pair of flat bands appear in a vicinity of Fermi energy. These bands can be populated by maximal eight particles per moire unit cell (due to two bands, two valleys characteristic of graphene band structures and two possible spin directions). In the case of integer filling fraction ν (an integer number of electrons per moire unit cell), measured usually in a range $-4 \leq \nu \leq 4$ ($\nu = -4$ corresponds to empty flat bands, $\nu = 0$ to charge neutrality, and $\nu = +4$ fully filled two flat bands), insulating states have been observed, which origin cannot be explained at the level of single particle theory [34-38]. These, so called, Mott states appear because of electronic interactions, which play a major role in the system. By changing a filling fraction of flat bands to noninteger values, one can observe superconducting states, with the highest transition temperature to superconductivity for fillings around $-3 < \nu < -2$. The nature of superconducting states in this material remains to be explained. Essential feature of flat energy bands in twisted bilayer graphene is their nontrivial topology [39-42]. For fillings $\nu = |3|$ (in general also for $\nu = |1|$), appearance of Chern insulators has been theoretically predicted, as a spontaneously broken time-reversal symmetry and occupation of one of two valleys. Anomalous quantum Hall effect has been observed in twisted bilayer graphene aligned with hBN [43,44]. A spontaneously broken time-reversal symmetry together with flat energy bands gives hope to investigate competing effects related to nontrivial topology in the system and electronic interactions.

Band structure and topological phase transition in group IV materials (articles [H2], [H4], [H5])

Electronic and transport properties of materials with a honeycomb lattice (a triangular lattice with two atomic basis) crystal structure were subject of research in publication [H2], [H4] and [H5]. Band structures and electronic properties have been studied by me using tight-binding model, and later by M. Bieniek (that time a PhD student, I was his auxiliary supervisor, he obtained PhD in 2021), who was also responsible for transport calculations, in publication [H5], by N. Nouri (that time a PhD student, she obtained PhD in 2019) in collaboration with S. Zia Borujenie and Gh. Rashedi in publication [H2], and by M. Brzezińska (that time a PhD student, I was her auxiliary supervisor, she obtained PhD in 2021) in publication [H4]. Calculations within density functional theory (DFT) in publication [H5] were done by T. Woźniak (that time a PhD student, he obtained PhD in 2021) and in publication [H2] by M. Modarresi. In order to analyze electronic properties of group IV materials,

I implemented a following multi-orbital tight-binding model, using Slater-Koster approach [45], given by Hamiltonian [46, 47]

$$H = \sum_{i\alpha\sigma} E_{\alpha\sigma} c^{+}_{i\alpha\sigma} c_{i\alpha\sigma} + \sum_{<ij>\alpha\alpha'\sigma} V_{i\alpha j\alpha'\sigma} c^{+}_{i\alpha\sigma} c_{j\alpha'\sigma} + \sum_{\ll ij\gg\alpha\alpha'\sigma} V'_{i\alpha j\alpha'\sigma} c^{+}_{i\alpha\sigma} c_{j\alpha'\sigma} + \sum_j \frac{\lambda}{3}\left(c^{+}_{jz\downarrow} c_{jx\uparrow} - c^{+}_{jz\uparrow} c_{jx\downarrow} + i c^{+}_{jz\uparrow} c_{jy\downarrow} + i c^{+}_{jz\downarrow} c_{jy\uparrow} + i c^{+}_{jx\downarrow} c_{jy\uparrow} - i c^{+}_{jx\uparrow} c_{jy\downarrow}\right) + H.C., \quad (1)$$

where c^{+}, c are creation and annihilation operators of a particle, σ indicates spin, *i,j* are sites indices of a honeycomb lattice, *E* is energy of a given orbital α*=(s, x, y, z)*, where *s* is s-orbital and *x, y, z* are three p-orbitals, *V* is a parametrized hopping integral to nearest neighbors <*i,j*>, to next nearest neighbors <<*i,j*>>, and the last term is spin-orbit coupling with spin-orbit coupling constant λ between orbitals at a given lattice site.

Bismuth monolayer with realistic parameters has the energy gap between the valence and conduction bands. According to ref. [47], it is Z_2 topological insulator. The goal of [H5] was analysis of stability of topologically nontrivial phase against different perturbations, in particular with respect to changes of spin-orbit coupling strength, which can be controlled e.g. using curvature of a monolayer [48]. For small values of spin-orbit coupling, a monolayer is a trivial insulator with topological invariant Z_2=0. Increase of spin-orbit coupling strength leads to an inversion of energy bands and a transition to a topologically nontrivial phase with an invariant Z_2=1. Inversion of bands, closing and reopening of the energy gap one can observe in changes of orbital composition of appropriate energy bands. Before a transition, both valence and conduction bands consist mainly of p_z orbitals, and after reopening there is a significant increase of p_x and p_y contribution to the valence band. Changes in energy spectrum one can see also for calculations in a ribbon geometry, a structure with periodic boundary conditions in one direction, and open boundary conditions in the other. Thanks to that one can observe an evolution of edge states characteristic of a topologically nontrivial phase.

Edge states in Z_2 topological insulator (articles [H2], [H5])

Presence of edge states crossing the energy gap is a characteristic feature of topologically nontrivial properties of a material in a ribbon geometry. Their character can differ when comparing idealized Kane-Mele model [11] with a more realistic multi-orbital models. In articles [H2, H5], I analyzed edge states in bismuth and antimony monolayers, and in their flatten counterparts, bismuthene and antimonene. In both, topologically trivial and nontrivial phases, edge states are present in energy spectrum, but only within a nontrivial phase, these edge states connects valence and conduction bands, which allows conductance through these states – edge states are responsible for quantized conductance, as was shown by analysis of transport properties, electrons moving by them are extremely immune to disorder. It turned out that topological edge states in bismuth, strongly penetrate an interion of the sample. The strongest localization on edges was observed around gamma point of Brillouin zone and increase of delocalization when moving toward edges of one dimensional Brillouin zone. Interestingly, as was shown in transport properties studies, delocalization of edge states do not affect strongly conductance quantization. It is worth to emphasize that the number of edge states is related to the topological character of the material. In systems protected by time-reversal symmetry, Z_2 topological insulator, there is a pair of edge states, while in topological crystalline

insulators protected by reflection symmetry, which correspond to perfectly flat form of bismuth or antimony, bismuthene and antimonene [49], there are two pairs of edge states [H2].

Induced magnetic moment from Edge states (article [H7])

Practical application of topological edge states in nanodevice was proposed in article [7]. In that work, I performed all numerical calculations, and together with J. Fernandez-Rossier, I analyzed the results and edited the manuscript. In quantum dot carved from a material being a topological insulator, edge states form a ladder of, approximately equidistant, energy levels inside the energy gap (this comes from a linear dispersion of edge states as a function of momentum in a ribbon geometry). Each edge state is double degenerate due to Kramers degeneracy. Applied magnetic field causes splitting of energy levels. In tight-binding model, given by Hamiltonian (1), the effect of a magnetic field can be introduced using Peierls substitution [50]

$$\varphi_{ij} = 2\pi \frac{e}{hc} \int_{\boldsymbol{r}_j}^{\boldsymbol{r}_i} \boldsymbol{A}\boldsymbol{d}\boldsymbol{l},$$

where $\boldsymbol{A}$ is a vector potential, a $\varphi_0 = \frac{e}{hc}$ magnetic flux quantum. Changes of a magnetic flux threading a quantum dot surface, induced a current flow through states encircling a structure. In each state of a Kramers pair from edge states, one state carries current flowing clockwise, and the second counterclockwise. Appropriately adjusting Fermi energy, such that only one of these two states was occupied, one generate a magnetic moment proportional to a quantum dot radius. Magnetic moment M_n related to each energy state E_n is defined as

$$M_n = \frac{\partial E_n}{\partial B},$$

where *B* is magnetic field. Analyzing a behavior of energy levels as a function of magnetic field, one can determines an induced magnetic moment. In typical systems described by Schrödinger equation, current *I* coming from electron rotating around a closed circular surface is inversely proportional to square of a radius. Area *S* is also proportional to square of a radius and as a consequence it gives a constant magnetic moment, *M=IS*. Scaling of a magnetic moment with a radius is a characteristic feature of topological insulators. Low energy properties (edge states) can be described using Dirac equation. In systems described by Dirac equation, current is inversely proportional to radius of a circular area and this causes a linear scaling of a magnetic moment with system size. Indeed, in work [H7] I considered two models of topological insulators, Kane-Mele model and bismuth monolayer, and in each case we observed a linear dependence of induced magnetic moment as a function of a quantum dot radius. Additionally, I have shown that due to topological character of edge states, current going along a perimeter are extremely robust against perturbation. Generated magnetic moment was stable with respect to Anderson disorder (random potential on lattice sites), with a disorder strength much exceeding the energy gap, and still present in finite temperatures, at the order of few Kelvins for a quantum dot with 18 nm radius. Presence of edge states, and in consequence induced magnetic moment is a universal features of topological quantum dots, regardless of their shape and defects on edges.

Characterization of topological properties of a material using entanglement spectrum (articles [H2], [H4])

A useful tool for identification of topologically nontrivial phases is entanglement spectrum [51-56]. Z_2 topological insulators, Chern insulators, or topological crystalline insulators are systems of noninteracting fermions belonging to so called topological phases with short-range entanglement

[57]. Entanglement properties of states with nontrivial topology can be studied dividing a system into two parts, two subsystems, and analyzing an effect of one of the part on the second one, in analogy to quantum mechanical open systems, the systems interacting with the environment. In the case of noninteracting fermions, so called entanglement Hamiltonian can be obtained from correlation matrix, which corresponds to reduced density matrix of one of subsystems [51]. Diagonalization of entanglement Hamiltonian matrix gives so called entanglement spectrum, which corresponds to a realistic spectrum of a system in one dimensional geometry, with edge states along a cut, but with flattened energy bands, where states from the conduction band are projected to 1 and states from the valence band to 0. Nontrivial topology is revealed by spectral flow, a set of eigenvalues continuously connecting eigenvalues 0 and 1, indexed by momentum along the cut. Additionally, to identify topological phases, one can use trace index, which can be related to topological invariant [55]. Trace index can be calculated by taking a trace of entanglement Hamiltonian matrix for each momentum and counting a number of discontinuities in one dimensional Brillouin zone.

Entanglement spectrum and trace index I used to study bismuth and antimony monolayer [H2, H4]. In both articles, analysis of topological properties using these tools is based on my initial numerical calculations and next on calculations performed by M. Brzezińska (that time a PhD student, I was her auxiliary supervisor, she obtained PhD in 2021). Bismuth monolayer is Z_2 topological insulator but antimony monolayer is a trivial insulator. Entanglement spectrum of bismuth monolayer has features of ribbon geometry spectrum, which means, has a pair of edge states crossing the energy gap – a spectral flow. In entanglement spectrum of antimony monolayer spectral flow does not occur, but a flat band around 0.5 appears. It has been connected with a presence of so called dangling bonds, which form a flat band of localized edge states inside the energy gap. Topologically nontrivial character of the system has been confirmed by calculating trace index. One has to calculate a number of discontinuities in half of one dimensional Brillouin zone, which is an odd number in the case of Z_2 topological insulators (bismuth), and even in the case of a trivial insulator (antimony).

Using entanglement entropy, as a sum over all eigenvalues of entanglement spectrum, a transition from a topologically nontrivial phase to a trivial phase was analyzed, which can be induced using external electric field, changes of concentration x of bismuth in relation to antimony in $Bi_{1-x}Sb_x$ compound and by applying strain. A topologically nontrivial phase is stable for a compound with above 75% bismuth concentration and in pure antimony for strain above 14%. Determining entanglement entropy in a vicinity of a topological phase transition, one can analyze its character. We have noticed that in the case of a transition induced by a concentration change x, and by applying strain, there is a finite discontinuity in the entanglement entropy. In the case of a transition induced by an external electric field, a phase transition seems to have a different character as entanglement entropy remains a continuous function of the electric field strength, while its first derivative, $\frac{\partial S_A}{\partial V_{field}}$, where S_A is entanglement entropy and V_{field} is a potential from external electric field, is discontinuous, which suggests first order phase transition (in the first case) and second order phase transition (in the second case) but more careful analysis is still required.

Many-body effects
(articles [H1], [H3], [H6])

A part of Hamiltonian with two-body interaction term to study many-body effects has a general form

$$H_{MB} = \sum_{i\sigma} E_i c_{i\sigma}^{+} c_{i\sigma} + \frac{1}{2} \sum_{\substack{i,j,k,l \\ \sigma,\sigma'}} \langle ij|v|kl\rangle c_{i\sigma}^{+} c_{j\sigma'}^{+} c_{k\sigma'} c_{l\sigma}, \qquad (2)$$

where $\langle ij|v|kl\rangle$ are Coulomb matrix elements, and i, j, k, l are indices of occupied states with energy E_i. In exact diagonalization method, Hamiltonian matrix is written and diagonalized in a basis of configurations of particles populating energy states. A total number of possible configurations is determined by binomial coefficient, $\binom{n}{k}$, where n is a number of energetic states to populate and k is a number of particles. Because of exponential growth of Hilbert space with a system size and a number of possible states to populate, calculations within exact diagonalization method are restricted in systems with periodic boundary conditions to discretized Brillouin zone with a finite number of states with a given momentum. Two-body scattering given by Hamiltonian (2) conserves total momentum, thus Hamiltonian matrix has a block diagonal form and each block can be diagonalized independently. Additionally, Coulomb scattering conserves a number of particles with a given spin, thus a spin projection on a given axis is a good quantum number (Hamiltonian (2) also commutes with square of total spin operator S^2, but due to an additional cost related to a basis rotation, it was not implemented). In our calculations, we considered systems sizes with up to several millions per subspace of full Hilbert space. It corresponds to systems with 12 particles maximally for half-filling of single particle energy states.

Fractional Chern Insulators (article [H6])

In [H6] we analyzed stability of fractional Chern insulators using Laughlin type of state (filling 1/3) realized in topologically nontrivial band on a checkerboard lattice. In that work, I proposed to consider this problem together with A. Manolescu, and performed initial analysis of single particle spectrum as a function of model parameters and performed calculations of many-body effects using self-implemented exact diagonalization method. Numerical calculations were continued by B. Jaworowski (that time a PhD student, I was her auxiliary supervisor, he obtained PhD in 2019).

In work [H6] we restricted analysis to spinless particles and interaction of a density-density type between neighbors on a given lattice, $\langle ij|v|ji\rangle = V_{ij}$, with a parametrized interaction between nearest neighbors $V_{ij} = V_{nn}$ for $< i, j >$, and second nearest neighbors $V_{ij} = V_{nnn}$ for $\ll i, j \gg$. Stability of topologically nontrivial phases was studied with respect to a transition between checkerboard lattice and Lieb lattice. Checkerboard lattice can be treated as one sublattice, and a transition to Lieb lattice is done by adding a second sublattice, with a coupling between the two sublattices controlled by a value of a potential on each sublattices so called staggered potential. In this work, we analyzed evolution of three energy bands forming a band structure of Lieb lattice (due to three lattice sites in a unit cell) and changes of their topological properties. For Lieb lattice with zero value of staggered potential, Chern insulator model gives two topologically nontrivial bands with opposite Chern numbers, C=-1 and C=1, separated by the energy gap, and the third trivial flat energy band lying between them with energy E=0. Changes of values of staggered potential induces a topological phase transition and the middle band, now quasi-flat, exchanges Chern number with a lower band, getting C=-1. A small dispersion of the band and its nontrivial topology allows to realize fractional Chern insulator. There are several conditions, needed to be satisfied, in order to quantum incompressible liquid analogical to Laughlin state could appear. One of them is uniform Berry curvature [32]. Because of that we analyzed Berry curvature of the middle flat band in a wide range of model parameters. Area on a phase diagram with a small standard deviation of Berry curvature should coincide with the region of the most stable fractional Chern insulator phase. Existence of Laughlin state for filling 1/3 has been confirmed by analyzing degeneracy of the many-body ground state in a wide range of parameter space, analyzing spectral flow between three states forming the ground state and using counting rule of quasiholes. Indeed we were able to observe strong correlation between an

area of uniform Berry curvature and a value of the many-body energy gap between three-fold degenerate ground state and excited states. Because of that, we concluded that a main mechanism of Laughlin state stabilization due to a presence of extra lattice sites is by modification of Berry curvature.

Wigner crystallizaion in topological bands (article [H3])

For small filling fractions of electrons populating flat energy bands, overlap between wavefunctions of different electrons decreases, which weakens a role of electronic correlations. Long range part of Coulomb interaction gives minimal value of energy for a configuration in which interparticle distances of localized electrons is maximized. In particular, the lowest energy can be achieved when electrons form a two dimensional periodic lattice, crystallize to form Wigner crystal [58]. Because of that, incompressible quantum liquids on partially filled flat bands compete with Wigner crystals when filling factor is decreased [59-62]. In work [H3] we analyzed possible appearance of Wigner crystallization on partially filled topological flat energy bands obtained from various lattices: kagome, checkerboard and honeycomb. Within extensive numerical calculations (done by B. Jaworowski) using exact diagonalization method we considered wide range of filling factors, ranging from 1/3 to 1/11. In that work, I proposed to analyze this problem together with A. Wójs and A. D. Guclu, I performed initial calculations of many-body effects using codes implemented by me for exact diagonalization method, which were next improved by P. Kaczmarkiewicz (that time a postdoc in A. Wójs group).

Wigner crystals were characterized using cartesian and angular Fourier transform of pair correlation function of the ground state. As one could expect, a degree of crystallization, measured by high of Fourier peaks, increased with decrease of particle densities. The results from numerical calculations were compared with a model for classical point-like particles obtaining satisfactory agreement. Observed crystallization was present for all studied lattice models, in a wide range of interaction parameters and filling factors. Because of a small number of particles taken in the calculations (between 4 and 7 particles, this restriction comes from exponential growth of Hilbert space size with a particle number), we were not able to determine a critical value of filling factor for which crystallization occurs, but it was clearly evident that a level of crystallization drastically increases below 1/7 filling. Additionally, a type of Wigner crystallization was strongly dependent on boundary conditions of chosen plaquette (all calculations were performed on finite fragments of a lattice with periodic boundary conditions in both directions). Because of that, it was not possible to uniquely determine a type of a crystallized lattice in a thermodynamic limit. Nevertheless, we were able to generally conclude that Wigner crystal is mainly independent on an underlying lattice, including topology of the bands and reflects behavior of classical point-like particles.

Correlation on flat topological bands in twisted bilayer graphene (article [H1])

In work [H1] I studied correlation effects on flat bands in twisted bilayer graphene as a function of filling factor. I did not succeed in getting personal statements about contribution to work [H1], but confirmation of my significant contribution to this work is that (i) I am the first author of this work, (ii) I was PI of the research project related to this work (Research on correlation effects in twisted bilayer crystals, NAWA grant, Bekker's program), (iii) most of the calculations were done using exact diagonalization method (the name of the method is in the title of this work), which is the method

used by me in the past, and this method has never been used by the second author, and the last author A. H. MacDonald is a group leader, with which this article was created, and he is mainly the person standing behind the ideas and do not currently perform numerical calculations (in the past A. H. MacDonald used exact diagonalization method, in '80 and '90). M. Xie, the second author, was mainly responsible for initial calculations using Hartree-Fock method and preparation of inputs for many-body calculations.

Because of huge sizes of Hilbert spaces in studied system, which is related to additional eight degrees of freedom in twisted bilayer graphene flat bands (2 valleys, 2 bands, 2 spins), I performed calculations on a discretized Brillouin zone with M=9 momentum states. These states were populated by particles and I investigated a behavior of the ground state as a function of filling fraction for every possible distribution of particles. Many-body Hamiltonina (2) was diagonalized using Lanczos method in subspaces for total spin within valley S_K and $S_{K'}$ (scattering between valleys can be neglected in the first approximation because valleys are far in a reciprocal space, thus a number of particles within a valley is conserved), and in subspace with total momentum *K*. We have shown that for filling factor $\nu = |3|$ there is a spontaneous breaking of time-reversal symmetry and only one valley is occupied with maximum total spin, obtaining Chern insulator. Spin polarization is characteristic of for fillings above critical electronic density on flat bands, where the effect of interactions start to dominate over single particle effects due to finite band dispersion of energy bands. For fillings $\nu > |3|$, valley depolarization is observed, which is in agreement with experimental findings of Landau levels degeneracy around filling $\nu = -2$ [36-38]. The results obtained using exact diagonalization method I compared with mean-field calculations (Hartree-Fock method), which allowed me to determine the role of electronic correlations. We have noticed that for integer filling $\nu = |3|$, correlation energy has the lowest value, which increases when going farther from integer fillings. Additionally, the results within Hartree-Fock method were extrapolated to a thermodynamic limit, confirming their validity for a finite number of single particle states. We have shown that for integer fillings exchange interaction plays a crucial role in the system, which is responsible for spin polarization. Spin and valley polarization for filling $\nu = -3$ is stable in a range of angles of twisted bilayer graphene between 1.06° and 1.15° (in that range an energy band dispersion is not sufficient to overcome the energy of exchange interaction).

Summary

The results described in this set of scientific articles present different methods of analysis of topological phase properties and their stability with respect to parameters that potentially can be controlled experimentally. A common factor of these works is preparation of theoretical tools, including mainly appropriate models for numerical calculations on two dimensional lattices, analysis of topological properties using various topological invariants or analysis of helical edge states in these systems. A set of articles can be divided into two complementary groups. The first group contain results about single particle properties, containing studies of electronic properties and topological effects in multi-orbital tight-binding models of realistic materials like bismuth Bi and antimony Sb, or graphene (articles H1, H2, H4, H5, H7). The second group contains articles about correlations, which means including many-body effects (articles H1, H3, H6). In the case of H3 and H6, abstract models were considered with parametrically controlled interactions, which allows one to analyze phenomena in a wide range of values and creation of appropriate stability phase diagrams. Article H1 contains research within both groups

Obtained results can help in practical application of topological effects in modeling and potential building of more efficient optoelectronic devices in the future. In articles [H1, H2, H4, H5, H7], we have studied properties various realistic materials, which were determined by topological properties of energy bands. Articles [H2, H4, H5, H7] are about bismuth and antimony monolayer and mixed crystals. In articles [H2], [H4], [H5], stability of topological phases and their potential observation when model parameters are changed was analyzed, which can be caused by perturbations present in realistic materials (e.g. dopants, crystal deformations), interaction with a substrate, or external fields. Antimony dopants effects was considered [H4], deformation of a perfect crystal [H4, H5], or changes in spin-orbit coupling constant [H5]. Additionally, in articles [H2, H5] analysis of transport properties was performed, in particular describing conditions in which quantized conductance can be observed, which is related to a topological character of edge states. In article [H7] it was shown how one can use topologically nontrivial properties in practical application – building nanomagnet. Articles [H2] and [H4] show how one can use entanglement spectrum to identify topologically nontrivial phases. In article [H1] role of correlation effects in a real material, twisted bilayer graphene, was investigated. Research within this set of articles allowed one to deeper understand nature of topological properties in selected systems, by determining conditions for their stability.

Literatura

[1] S.-Q. Shen, Natl. Sci. Rev. **1**, 49 (2014).
[2] F. Duncan M. Haldane, Rev. Mod. Phys. **89**, 040502 (2017).
[3] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. **82**, 3045 (2010).
[4] X.-L. Qi and S.-C. Zhang, Rev. Mod. Phys. **83**, 1057 (2011).
[5] J. E. Moore, Nature (London) **464**, 194 (2010).
[6] X. L. Qi and S. C. Zhang, Phys. Today **63**, 33 (2010).
[7] K. von Klitzing, G. Dorda, and M. Pepper, Phys. Rev. Lett, **45**, 494 (1980).
[8] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982).
[9] L. D. Landau, Phys. Z. Sowjetunion **11**, 26 (1937).
[10] F. D. M. Haldane, Phys. Rev. Lett. **61**, 2015 (1988).
[11] C. L. Kane and E. J. Mele Phys. Rev. Lett. **95**, 226801 (2005).
[12] C. L. Kane and E. J. Mele, Phys. Rev. Lett. **95**, 146802 (2005).
[13] A. Bernevig, T. Hughes, and S. C. Zhang, Science **314**, 1757 (2006).
[14] M. König et al., Science **318**, 766 (2007).
[15] B. A. Bernevig and T. L. Hughes, Topological Insulators and Topological Superconductors (Princeton University Press, Princeton, NJ, 2013).
[16] A. Alexandradinata and B. A. Bernevig, Physica Scripta **2015**, 014013 (2015).
[17] D. C. Tsui, H. L. Stormer, and A. C. Gossard, Phys. Rev. Lett. **48**, 1559 (1982).
[18] R. B. Laughlin, Phys. Rev. Lett. **50**, 1395 (1983).
[19] D. M. Haldane, Phys. Rev. Lett. **51**, 605 (1983).
[20] B. I. Halperin, Phys. Rev. Lett. **52**, 1583 (1984).
[21] J. K. Jain, Phys. Rev. Lett. **63**, 199 (1989).
[22] J. K. Jain, Composite fermions (Cambridge University Press, 2007).
[23] K. Sun, Z. Gu, H. Katsura, and S. Das Sarma, Phys. Rev. Lett. **106**, 236803 (2011).
[24] E. Tang, J.-W.Mei, and X.-G.Wen,Phys. Rev. Lett. **106**, 236802 (2011).
[25] T. Neupert, L. Santos, C. Chamon, and C. Mudry, Phys. Rev.Lett. **106**, 236804 (2011).
[26] Y.-F.Wang, Z.-C. Gu, C.-D. Gong, and D. N. Sheng, Phys. Rev. Lett. **107**, 146803 (2011).
[27] D. Sheng, Z.-C. Gu, Gu, K. Sun, and L. Sheng, Nat. Commun. **2**, 389 (2011).

[28] N. Regnault and B. A. Bernevig, Phys. Rev. X **1**, 021014 (2011).
[29] T. Liu, C. Repellin, B. Andrei Bernevig, and N. Regnault, Phys. Rev. B **87**, 205136 (2013).
[30] A. M. Lauchli, Z. Liu, E. J. Bergholtz, and R. Moessner, Phys. Rev. Lett. **111**, 126802 (2013).
[31] S. A. Parameswaran, R. Roy, and S. L. Sondhi, C. R. Phys. **14**, 816 (2013).
[32] E. J. Bergholtz and Z. Liu, Int. J. Mod. Phys. B **27**, 1330017 (2013).
[33] R. Bistritzer and A. H. MacDonald, Proc. Natl. Acad. Sci.U.S.A. **108**, 12233 (2011).
[34] Y. Cao et al., Nature(London) **556**, 80 (2018).
[35] Y. Cao et al., Nature (London) **556**, 43(2018).
[36] M. Yankowitz et al., Science **363**, 1059 (2019).
[37] X. Lu et al., Nature(London) **574**, 653 (2019).
[38] A. Uri et al., Nature (London) **581**, 47 (2020).
[39] H. C. Po, L. Zou, A. Vishwanath, and T. Senthil, Phys. Rev.X **8**, 031089 (2018).
[40] Z. Song et al., Phys. Rev. Lett. **123**, 036401 (2019).
[41] N. Bultinck, S. Chatterjee, and M. P. Zaletel, Phys. Rev.Lett. **124**, 166601 (2020).
[42] N. Bultinck et al., Phys. Rev. X **10**, 031034 (2020).
[43] A. L. Sharpe et al., Science **365**, 605 (2019).
[44] M. Serlin et al., Science **367**, 900 (2020).
[45] J. C. Slater and G. F. Koster, Phys. Rev. **94** 1498 (1954).
[46] Y. Liu and R. E. Allen, Phys. Rev. B **52** 1566 (1995).
[47] S. Murakami, Phys. Rev. Lett. **97** 236805 (2006).
[48] S. Fratini, et al. Phys. Rev. B88 115426 (2013).
[49] C.-H. Hsu et al., Sci. Rep. **6**, 18993 (2016).
[50] R. Peierls, Z. Phys. **80**, 763–791 (1933).
[51] I. Peschel, J. Phys. A: Math. Gen. **36**, L205 (2003).
[52] D. Gioev and I. Klich, Phys. Rev. Lett. **96**, 100503 (2006).
[53] I. Klich, J. Phys. A: Math. Gen. **39**, L85 (2006).
[54] S. Ryu and Y. Hatsugai, Phys. Rev. B **73**, 245115 (2006).
[55] A. Alexandradinata, T. L. Hughes, and B. A. Bernevig, Phys. Rev. B **84**, 195103 (2011).
[56] T. L. Hughes, E. Prodan and B. A. Bernevig Phys. Rev. B **83**, 245132 (2011).
[57] Y.-M. Lu and A. Vishwanath, Phys. Rev. B **86**, 125119 (2012).
[58] E. Wigner, Phys. Rev. **46**, 1002 (1934).
[59] D. Yoshioka and H. Fukuyama, J. Phys. Soc. Japan **47**, 394 (1979).
[60] K. Maki and X. Zotos, Phys. Rev. B **28**, 4349 (1983).
[61] P. Maksym J. Phys.: Condens. Matter **4**, L97 (1992).
[62] K. Yang, F. D. M. Haldane, and E. H. Rezayi, Phys. Rev. B **64**, 081301 (2001).

5. Presentation of significant scientific or artistic activity carried out at more than one university, scientific or cultural institution, especially at foreign institutions.

The primary place, where I carry out the scientific activity is Department of Quantum Physics, Faculty of Physics, Astronomy and Informatics, Nicolaus Copernicus University in Torun, where I am employed as a professor since March 2021.

During years 2012-2020 I was employed at Department of Theoretical Physics, Faculty of Fundamental Problems of Technology, Wroclaw University of Science and Technology, where in

2002-2007 years I have realized unified master studies in physics, and after finished, I realized in 2008-2012 years PhD studies, and Council of Institute of Physics of Wroclaw University of Science and Technology 7th July 2012 gave me PhD degree. In years 2008-2011, during my PhD studies, I realized 4 internships at National Research Council in Ottawa, Canada, with a total length of 12 months. In years 2012-2017 I had several short term scientific consultations (lasting 1-3 weeks), visiting Spain (University of Alicante), Iceland (Reykjavik University), Canada (University of Ottawa) and Turkey (Izmir Institute of Technology). I also had 6 months postdoc in Portugal (International Iberian Nanotechnology Laboratory (INL), Braga) within Mobilność Plus programm from Ministry of Science and Higher Education of Poland. Additionally, in years 2019-2021 I had a postdoc in USA, The University of Texas at Austin, Department of Physics, Austin, Texas, with financial support for the first year by The Polish National Agency for Academic Exchange NAWA, Bekker's program and for the second year employed by The University of Texas at Austin. As the results of these visits and collaborations are following published articles:

Canada (in total 14 publications):	D1-D10, E16-E19, monography M1
Turkey (1):	E5
Iceland (1):	E14
Portugal and Spain (1):	E15
USA (3):	E1 – E3

Currently, I mainly Focus on maintaining collaboration with A. H. MacDonald from The University of Texas at Austin, who is my main co-PI in Opus grant, National Science Centre of Poland (NCN), Twistronics - research on new quantum simulators.

6. Presentation of teaching and organizational achievementsas as well as achievements in popularization of science

6.1. Popularization of physics

8.05.2013 r.	Lecture: „Graphene – material of the XXI century. Nobel Prize in Physics in 2010 r.", XX set of lectures popularizing physics, Wrocław
19.04.2013	Promotion of Institute of Physics Wroclaw University of Science and Technology, presentation in Zespol Szkół Ponadgimnazjalnych, ul. J. Słowackiego 4 57-500 Bystrzyca Kłodzka,

6.2. Supervision of students

1. Michał Kupczyński, MSc, the title of the thesis: Topological effects in two dimensional systems, period of supervision: 2015-2017, Wroclaw University of Science and Technology **(supervisor)**

6.3. Supervision of PhD students

1. MSc. Błażej Jaworowski, the title of the thesis: Electron correlations in topological flat bands, Wroclaw University of Science and Technology (**auxiliary supervisor**). Date of obtaining the doctoral degree: 26.02.2019.

2. MSc. Marta Brzezińska, the title of the thesis: Topological phases and topological phase transitions in low-dimensional systems, Wroclaw University of Science and Technology (**auxiliary supervisor**). Date of obtaining the doctoral degree: 21.01.2021.

3. MSc. Maciej Bieniek, the title of the thesis: Electronic and optical properties of two-dimensional transition metal dichalcogenide crystals, Wroclaw University of Science and Technology (**auxiliary supervisor**). Date of obtaining the doctoral degree: 21.04.2021.

4. MSc. Michał Kupczyński, the title of the thesis: Many-body effects in topological materials and structures, Wroclaw University of Science and Technology (**auxiliary supervisor**). Planning date of obtaining the doctoral degree: December 2022.

6.4. Didactics

Courses:

Wroclaw University of Science and Technology:

Physics 1 (exercises, 20 semesters, 4h/week)
Physics 1 (labs, 2 semesters, 2h/week)
Computer modelling (labs, 1 semester, 2h/week)
Topological effects in low dimensional systems (lecture, 1 semester, 2h/week)

Nicolaus Copernicus University in Torun:

Programming, Matlab (labs, 1 semester, 2h/week)
Programming, Fortran (labs, 2 semesters, 1h/week)

7. Other information important from the point of view of my professional career

In my opinion, positive impact on my entire scientific achievements during my career had many international collaborations, which ended with many scientific articles. I also participated in realization of many national grants, from National Science Centre of Poland (NCN), Ministry of Science and Higher Education of Poland, as PI (3) and Co-Investigator (4). I was awarded for my scientific achievements at local and nationwide level:

7.1. Awards

05.11.2017	Dionizy Smoleński Award for exceptional scientific achievements in interdisciplinary sciences, Rector of Wroclaw University of Science and Technology
03.11.2016	Rector's Award for exceptional contribution to university development, Head of Wroclaw University of Science and Technology

10.12.2015	Rector's Award for exceptional contribution to university development, Head of Wroclaw University of Science and Technology
10.2013 – 04.2014	III edition of competition for young PhDs within Human Capital Operational Programme *„Human Capital 2015 Plus. Enhancement of educational offer of Wroclaw University of Science and Technology for university-wide courses offer and new interdisciplinary PhD studies".*
04.2013 – 04.2014	START scholarship from Foundation for Polish Science (FNP) for 2013
10.2012 – 09.2013	II edition of competition for young PhDs within Human Capital Operational Programme *„Human Capital 2015 Plus. Enhancement of educational offer of Wroclaw University of Science and Technology for university-wide courses offer and new interdisciplinary PhD studies".*
11.2011 – 07.2012	Max Born scholarship
10.2011 – 03.2012	V edition of competition in Project *„Enhancement of scientific-educational potential development of young faculty of Wroclaw University of Science and Technology"*
15.11.2011	Deans's Award for scientific achievements, Dean of Faculty of Fundamental Problems of Technology, Wroclaw University of Science and Technology
10.2010 – 03.2011	III edition of competition in Project *„Enhancement of scientific-educational potential development of young faculty of Wroclaw University of Science and Technology"*