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Analysis of Dirac materials with the methods of mathematical physics

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1 Dirac materials

Dirac equation was derived by Paul Dirac in 1928 in his seek for a consistent description of quantum relativistic particles [1]. The first-order differential equation with matrix coefficients proved to be an indispensable tool for description of the fermions with spin- $\frac{1}{2}$. It was originally intended to describe dynamics in four-dimensional space-time. However, the equation with reduced spatial dimensions emerges in description of surprising variety of both classical and quantum systems. These physical settings were coined as Dirac materials or Dirac matter in the literature [2], [3].

Experimental isolation of graphene marked a milestone in physics. It proved that genuinely two-dimensional crystals can exist in the Nature. It confirmed theoretical prediction that the dynamics of low-energy charge carriers in graphene is governed by two-dimensional Dirac-type equation. This breakthrough ignited intensive, both theoretical and experimental, investigation of planar quantum systems where the quasi-particles exhibit relativistic-like properties. Besides graphene, the $(2 + 1)$ dimensional Dirac fermions were predicted or observed in silicene, germanene or dichalcogenides [4], [5], [6], [7], [8]. Dirac materials were also prepared artificially. Relativistic dynamics of quasi-particles was reported in hexagonal lattices assembled by positioning carbon oxide molecules on the copper surface [9], in hexagonal arrays of ultra cold atoms in optical lattices [10].

In description of these systems, Dirac equation appears in great variety of modifications that reflect diverse physical situations. Dirac fermions in graphene and other planar crystals are described by two-dimensional Dirac equation. The one-dimensional Dirac equation emerges naturally in description of the relativistic quasi-particles in carbon nanotubes [12]. Interaction with external electromagnetic field is incorporated into the stationary equation in the form of minimal coupling. Qualitatively similar Hamiltonian is obtained when the mechanical deformations of the crystal are taken into account; the nontrivial strain tensor gives rise to the effective vector and scalar

potential [11], [12], [6]. This way, the mechanical deformations mimic presence of (electro-)magnetic field. Dirac fermions with position-dependent mass appear in the heterostructures where the graphene sheet is posed on the substrate (e.g. on hexagonal boron-nitride) [13], [14]. Dirac equation with nontrivial metric tensor describes fermions on the curved sheets or on carbon macromolecules (e.g. fullerenes) [15] [16], [17]. Nontrivial boundary conditions reflect termination of the crystal lattice and its orientation with respect to the lattice structure [18].

Relativistic quasi-particles in Dirac materials possess several degrees of freedom. Pseudo-spin is related to the crystal structure where the elementary cell is formed by two atoms. Valley degree of freedom emerges as there are two inequivalent Dirac points in the first Brillouin zone where the dispersion relation is approximately linear in momentum. The electrons in the lattice have spin degree of freedom. In dependence on the considered physical situation, some of these degrees of freedom can be neglected as they are not involved in dynamics. For instance, only the pseudo-spin is relevant when smooth electromagnetic fields are considered as the interaction does not change spin of the particles and does not cause flipping of the states between the two Dirac valleys. In this case, the effective Dirac Hamiltonian has the form of 2×2 matrix operator. When either the spin-orbit interaction [19] or the interaction mixing the valley index is considered [20], then the Dirac operator is given in terms of either 4×4 or 8×8 matrices.

When few layers of the two-dimensional crystals are stuck together, the new intriguing properties arise that were absent in single layer crystals [21]. Graphene has no gap between conductance and valence bands and its opening is nontrivial. It represents major complication for its use in electronics; the electronic transport in gapless Dirac material cannot be controlled easily by the electrostatic field¹.

¹This is related to the Klein tunneling known in relativistic quantum mechanics. The (relativistic) massless electron can tunnel through the electrostatic

In bilayer graphene, the gap can be opened by application of the electrostatic field such that the two layers have different electrostatic potential [22]. The low energy excitations of electrons in the bilayer graphene can be effectively described by the Hamiltonian given in terms of 4×4 matrices.

In the selected papers [Jak1]-[Jak17], I focused on the analysis of two-dimensional Dirac equation describing quasi-particles in presence of electromagnetic interaction [Jak1], [Jak5], [Jak6], [Jak7], [Jak10], [Jak12], mechanical deformations [Jak2], [Jak3], [Jak6], [Jak11], or spin-orbital coupling [Jak13], [Jak14], [Jak15]. The spectral and transport (scattering) properties were of the main interest. The obtained results have broader applicability due to the variety of systems described by the considered dynamical equation. Nevertheless, I mostly interpreted the results in the context of carbon nanotubes [Jak1], [Jak2], [Jak3], [Jak5], [Jak6], graphene nanoribbons [Jak16], or graphene and bi-layer graphene [Jak1], [Jak6], [Jak7], [Jak9], [Jak10], [Jak11], [Jak12], [Jak13], [Jak14], [Jak15], and [Jak16]. In [Jak8], we analyzed a system described by Dirac equation in the context of classical optics. In the paper [Jak4], we discuss construction of reflectionless systems and compared the results with the known integrable models associated with the known solutions of integrable AKNS hierarchies.

2 The methods

In the presented research, I followed two complementary strategies. In the first one, I focused on construction of exactly solvable models with desirable physical characteristics, with bound states or specific scattering properties in particular. The second one was the qualitative spectral analysis where the relevant information on the energy spectrum and transport properties of Dirac fermions was de-

barrier of any height without being reflected.

rived without the need to solve dynamical equation explicitly. Let me comment on the two directions in more detail:

- Analytical solvability (partial at least) of the evolution equation is the distinctive property of any solvable model. Nevertheless, the family of analytically solvable differential equations is not very populated. It is true for ordinary differential equations and even more for partial differential equations that describe higher-dimensional systems.

We used diverse techniques that allow us to exploit this family. They share the same philosophy: analytically solvable equation is transformed into another one that can be interpreted as an evolution equation of the new physical system. Let me mention a simple example: the operator $H_0 = -i\sigma_1\partial_x$ can be transformed into $H_1 = U^{-1}H_0U = -i\sigma_1\partial_x + V(x)\sigma_0$ via a unitary transformation $U = e^{i\sigma_1\int V(x)dx}$, where σ_1 is the Pauli matrix and σ_0 is the identity matrix. The initial operator corresponds to free Dirac fermion on the line, whereas H_1 describes dynamics of the particle in presence of an electrostatic potential $V(x)$. As H_1 inherits the trivial scattering characteristics of the free particle, the link between the two operators provides a simple explanation of the Klein tunneling of Dirac fermions in graphene through electrostatic barriers in normal direction [Jak1]. The same technique was used for construction of solvable models of Dirac fermions in electromagnetic field [Jak7]. We used a unitary transformation also in [Jak13], [Jak14], [Jak15], and [Jak17], where construction of the systems with extended degrees of freedom was of the main interest.

Change of coordinates (point transformation) alters the form of evolution equation. When the altered equation can describes evolution of the new physical system, the point transformation can provide interesting predictions. For example, the point

transformation served well to show that the wave packets of Dirac fermions in graphene can be focused by unidirectional strains [Jak11].

The last example is Darboux transformation. It is represented by a differential operator [24] whose kernel is typically formed by some fixed eigenstates of the initial Hamiltonian. The transformation is neither unitary nor invertible. It intertwines two Hamiltonians, let us call them again H_0 and H_1 , as $LH_0 = H_1L$. When an eigenstate Ψ of H_0 is known, we can obtain its analogue $L\Psi$ for H_1 . The inverse-like transformation to L can be obtained by conjugation of the intertwining relation (provided that H_0 and H_1 are hermitian). Indeed, L^\dagger satisfies $H_0L^\dagger = L^\dagger H_1$. The transformation can be generalized by considering intertwining operators of higher-order whose kernel can also consist of generalized eigenstates (Jordan states) [25]. The construction for Dirac operators via intertwining relations was discussed both for one-dimensional [26] and higher-dimensional models [27], [28]. Darboux transformation is particularly suitable for construction of systems with bound states as the Hamiltonian H_1 can possess discrete energies that were absent in the spectrum of H_0 . We used Darboux transformation for construction of the systems where Dirac fermions in graphene or carbon nanotubes were in presence of mechanical deformations [Jak2], [Jak3]. It was employed in construction of the new systems with antilinear symmetry (PT -symmetry) that find their application in optics [Jak8].

Darboux transformation is not limited to stationary systems, it can be used for construction of time-dependent settings [29]. It can also serve for construction of partially solvable planar systems [Jak12]. In the context of physics of graphene, Darboux transformation was mostly used for Dirac equation given in terms of 2×2 matrices. In [Jak15], and [Jak17], we employed Darboux transformation for construction of solvable systems in

terms of 4×4 systems where inhomogeneous spin-orbital interaction in graphene or interlayer interaction in bilayer graphene were of interest.

In our research, we frequently identified the initial known equation with the dynamical equation of the free particle, reflectionless Pöschl-Teller (Rosen-Morse) model, or with the Lamé finite-gap equation. These solvable systems share one remarkable property, they belong to the family of finite-gap systems. Their potentials are solutions of specific non-linear differential equations that belong to the AKNS (KdV) hierarchy of integrable systems. They have nontrivial integral of motion that can be identified with the Lax operator. Its presence implied nontrivial algebraic structure coined as hidden supersymmetry, where grading operator was identified with a space reflection operator and the supercharges were based on the Lax operator. The superalgebraic structure was showed to reflect spectral properties of the considered systems in [Jak2], [Jak3], [Jak5].

The new concepts and constructions were frequently illustrated with the use of the either massive or massless free-particle model. Fixing H_0 in this manner, the new models represented by H_1 inherited some of its peculiar properties, e.g. reflectionless scattering on the potential barriers [Jak2], [Jak4], [Jak8], [Jak15], [Jak17]. With this choice of the initial system, we were got the new insight into the Klein tunneling or omnidirectional Klein tunneling in diverse physical systems [Jak1], [Jak12].

- When analytic solution of evolution equation is not feasible, one can employ qualitative methods to derive valuable information on the system without the need of explicit solutions. Variational principle for Schrödinger operators tells us that the expectation value of energy for any state from the domain of the Hamiltonian is equal or greater than the ground state ener-

gy. When the asymptotic behavior of the potential allows us to fix the threshold of the essential spectrum, the variational principle can be used to prove existence of bound states with discrete energies in the system. The knowledge of the eigenstates is not essential as the variational principle allows us to work with auxiliary functions belonging to the domain of the Hamiltonian (or of its quadratic form).

It is possible to use this framework for a class of Dirac operators with chiral symmetry whose squares are diagonal and coincide with Schrödinger Hamiltonians. Dirac operators with magnetic field possessing translational symmetry belong into this class. We investigated their spectral properties in a series of works [Jak6], [Jak9], [Jak10], [Jak11] where inhomogeneous magnetic field, effective mass or strains were associated with the vector potential.

3 Structure of the thesis

3.1 Review of concepts and techniques

I will provide a short review basic concepts that are useful in description of graphene and carbon nanotubes. I will show how Dirac equation emerges in dynamics of the condensed matter systems, how it reflects crystal properties. The origin of degrees of freedom possessed by Dirac fermions in graphene will be discussed as well as different types of interactions. Electromagnetic interaction and mechanical deformations as well as the interactions that can change spin or valley degrees of freedom will be of particular interest.

Then I will provide a brief introduction into the methods and concepts that I used in the analysis of the mentioned systems. In particular, I will review Darboux transformations both for Schrödinger and Dirac Hamiltonians, their role in supersymmetric quantum mechanics, and the extensions based on higher-order Darboux trans-

formation and confluent Darboux transformation. Advantages and weaknesses of the framework will be pointed out. I will discuss basics definitions and concepts on finite-gap integrable systems, e.g. Lax operators and AKNS hierarchies. The basic concepts and definitions for the qualitative analysis will be presented as well.

The next part will contain the selected papers [Jak1]-[Jak17], grouped by the discussed topics. The anticipated structure of this part is as follows²:

3.2 Physics of Dirac fermions in graphene-based systems via Darboux transformations

Darboux transformation is defined both for one-dimensional Schrödinger and Dirac operators. It can be used for analysis of Dirac operators in both cases. Yet, in the first case, it is to be applied to the square of Dirac Hamiltonian that should coincide with the Schrödinger operator. In our works, we preferred to employ direct Darboux transformation that intertwines two Dirac Hamiltonians. It was used for the analysis of confined Dirac fermions in twisted carbon nanotubes, calculation of their Green's functions, and local density of states [Jak2], [Jak3]. Darboux transformation of Dirac operator was also utilized in [Jak4] where a family of reflectionless models was discussed in the context of finite-gap integrable models. A confluent Darboux transformation for Dirac Hamiltonians was proposed in [Jak8] and utilized for generation of PT -symmetric Hamiltonians applicable in the context of classical optics.

Darboux transformation of Dirac Hamiltonian cannot alter electrostatic field. We proposed an alternative construction in [Jak7] where we used gauge transformation to generate the new Hamiltonian of the required form. In [Jak2], [Jak3], [Jak5], we focused on the relation between the superalgebra, generated by the Hamiltonian

²in each subsection, a brief review of the results is followed by extended abstracts of the presented works

and its integrals of motion, and the spectral properties of considered models. In [Jak5], we approximated the effect of homogeneous magnetic field in carbon nanotube by a solvable finite-gap potential.

Finally, let me comment on our effort in the analysis of the electrostatic confinement and Klein tunneling of Dirac fermions in electrostatic barriers. In [Jak1], rather simple but useful construction based on unitary transformation was used to provide an alternative explanation for Klein tunneling in carbon nanotubes and in planar graphene for specific (normal) direction of incidence. In [Jak12], we employed time-dependent Darboux transformation and Wick rotation of coordinates to construct a model where all-angle Klein tunneling emerges in presence of two-dimensional electrostatic field. We also discussed confinement of Dirac fermions by the potential. These results were employed in [Jak16] where we studied confinement by Dirac fermions by the electrostatic field in arm-chair nanoribbons.

Interactions in carbon nanotubes via supersymmetry

[Jak2] Supersymmetric twisting of carbon nanotubes

Vector potential in one-dimensional Dirac equation can be related to the radial twist of the nanotube. Darboux transformation was used in the analysis of twisted carbon nanotubes for the first time. We focused on two different frameworks where Darboux transformation provides us with Dirac Hamiltonian of 1D fermion in a twisted carbon nanotube. We showed that the twists can confine Dirac fermions. We calculated the Green's function and local density of states (LDOS) of the new systems with the use of Darboux transformation. We found that LDOS decreases in the space where bound states are localized. Two explicit models of twisted carbon nanotubes were discussed, both with asymptotically inverted (single-kink) and asymptotically vanishing (double-kink) twists. They were supersymmetric partners of the free particle model, therefore, they possessed nontrivial integral of motion. It allowed us to

define hidden nonlinear supersymmetry of the new model. The bound state energies were found in dependence of the twist. Darboux transformations was proposed as a useful tool for deformation-induced spectral engineering.

[Jak3] Finite-gap twists of carbon nanotubes and an emergent hidden supersymmetry

In the work, we focused on the specific class of systems where the vector potential belongs into the family of finite-gap potentials. These potentials are solutions of one of the nonlinear differential equations of the AKNS hierarchy. They have remarkable properties. When being periodic functions, the Dirac Hamiltonian has finite number of energy gaps in its spectrum. It has an integral of motion, Lax operator, whose kernel is spanned by the states corresponding to the band-edge energies. We reviewed the known result, e.g. closed analytical form for diagonal Green's function (also called Gorkov resolvent) and the analytic formula for local density of states LDOS as well as the integrated density of states (DOS). We discussed explicit examples of two-, three- and four-gap potentials. Three-gap model has a gap between positive and negative energies. We introduced the quantity called average twist and demonstrated that it is related to the spectral gap. It was vanishing in case of two- and four-gap systems, whereas it was non-vanishing in case of three-gap model. The extended Hamiltonian, which describes Dirac fermions in both Dirac valleys, commutes with the time-reversal operator. It is in contrary to the magnetic field as the pseudo-magnetic field does not break time-reversal symmetry. All the energy levels are doubly degenerate in accordance with Kramer's theorem. We showed that there exists hidden nonlinear supersymmetry that reflects spectral properties, the number of bands and degeneracy of energy levels in particular. The square of the supercharges gets factorized in terms of the band-edge energies.

[Jak5] Carbon nanotubes in an inhomogeneous transverse magnetic field: exactly solvable model

When in presence of a magnetic field, Dirac fermions in graphene are affected by the perpendicular to the surface component of the field only. Due to this fact, the magnetic field "felt" by the Dirac fermions in carbon nanotubes (small cylinders of graphene) is altered by the curved surface of the nanotube. In case of homogeneous magnetic field, the component of the field perpendicular to the surface of the nanotube is inhomogeneous and the stationary equation is not exactly solvable. We proposed an exactly solvable model where the homogeneous field is approximated in terms of finite-gap Lamé potential. Inhomogeneity of the external field (also interpretable as a deviation from the perfectly circular profile of the nanotube) made the stationary equation solvable for the vanishing longitudinal the momentum. We utilized exact solutions of Lamé equation to get the eigenstates of the Hamiltonian. The integral of motion associated with the finite-gap Lamé equation can be interpreted as the supercharge of the superalgebra. We show that for the metallic and maximally semiconducting nanotubes, we can define grading operator that gives rise to $N = 2$ supersymmetry. In the last section, we show that the energy levels are stable with respect to the fluctuations of the momentum parallel with the symmetry axis.

Extensions of Darboux transformations, reflectionless models and classical optics

[Jak4] Twisted kinks, Dirac transparent systems, and Darboux transformations

We applied Darboux transformation on the model of one-dimensional free particle with constant mass. The transformed Hamiltonians formed a four-parametric family with singula-

rity-free potentials consisting of inhomogeneous vector potential and a mass term. We showed that these reflectionless potentials satisfy corresponding equations of the AKNS hierarchy. For specific choices of the parameters, it was possible to identify them with the reflectionless models known in the realm of finite-gap integrable systems. We also discussed reflectionless Schrödinger operators with matrix potential defined as the squares of the reflectionless Dirac operators. The associated algebra of integrals of motion was of our interest.

[Jak7] Spectrally isomorphic Dirac systems: Graphene in an electromagnetic field

Darboux transformation does not allow to alter the electrostatic interaction in Dirac Hamiltonian. I proposed an alternative construction of solvable models that allows for manipulation with the electrostatic field. It is based on an inhomogeneous gauge (unitary) transformation. I discussed the explicit form of the transformation and the range of its applicability. I showed that solvability of stationary equation is not altered by addition of a constant mass term. I illustrated the construction on examples of localized electromagnetic barriers based on Rosen-Morse II and Scarf II potentials as well as on the periodic electromagnetic potential based on two-gap Lamé model.

[Jak8] Confluent Crum-Darboux transformations in Dirac Hamiltonians with PT-symmetric Bragg gratings

Counter-propagating waves in Bragg gratings can be described within the framework of coupled mode theory, where the Maxwell equations turn into Dirac-type equation for zero energy. The role of the vector potential and the mass term is played by quantities that fix the refractive index. In the article, we provided confluent extension of Darboux transformations for Dirac equation. The confluent Darboux transformation is defined in terms of a single eigenstate and associated Jordan

state. We discussed construction of the Jordan states. We presented formulas for both the higher-order Darboux transformation and the associated new Hamiltonians in terms of Wronskians. We discussed the mapping between eigenstates and Jordan states mediated by the Darboux transformation. In the application of the framework, the settings with PT-symmetric interaction were of our interest. We showed that they can be obtained when the seed solutions (kernel of Darboux transformation) have definite PT-parity. We used the confluent transformation to construct two explicit reflectionless models obtained from the free particle system. In the first example, the free particle was massive and the seed solutions of zero energy were exponentially expanding. The potential term as well as the bound states in the new system were exponentially decreasing. In the second case, the particle was massless. We fixed the zero mode and its Jordan state as the seed eigenstates for Darboux transformation. We show that the new potential as well as the bound states have $1/x$ decay. The second case illustrates the advantage of confluent transformation that allows us to produce singularity-free potentials in case where the standard transformation would fail. In both cases, the complex refractive index is calculated.

Klein tunneling and confinement of Dirac fermions by electrostatic field

[Jak1] **Klein tunneling in carbon nanostructures:**

A free-particle dynamics in disguise

Dirac fermions in metallic carbon nanotubes are remarkably inert with respect to backscattering on the impurities. It is understood as the manifestation of Klein tunneling of the quasi-particles through electrostatic barriers. In non-relativistic quan-

tum mechanics, reflection-less systems are related with free-particle system via supersymmetric (Darboux) transformation. It inspired us to find similar structure for Dirac operator with electrostatic barrier. The intertwining operator was found in the form of a unitary operator, the associated superalgebra was of the zero-order³. The framework was also used to calculate s-waves of generic systems with rotational symmetry.

[Jak12] Super-Klein tunneling of Dirac fermions through electrostatic gratings in graphene

Super-Klein tunneling is a phenomenon where the particle goes through the barrier without reflection, independently on the incidence angle. We constructed a model of a comb of scatterers where absence of backscattering was independent on the incidence angle, provided that the particle had specific energy. The result demonstrated that the super-Klein tunneling does not rely on translational symmetry. We constructed the model with the use of time-dependent Darboux transformation applied on the free particle model and Wick rotation of coordinates. It was granted by construction that the new model was reflectionless at specific energy, i.e. that it possessed the super-Klein tunneling. We also found that there are bound states confined at the electrostatic barrier.

[Jak17] Dirac fermions in armchair graphene nanoribbons trapped by electric quantum dots

The edge properties of graphene nanoribbons are encoded into the boundary conditions imposed on the solutions of the dynamical equation. We proposed an elegant way how to construct wave functions that comply with boundary conditions, with the use of specific projection operators. We applied this

³Anticommutator of the supercharges is a typically a polynomial in the Hamiltonian. In the standard supersymmetric quantum mechanics, it is of the first order. It is a polynomial in case of higher-order quantum mechanics.

technique in construction of bound states confined by electrostatic field in armchair nanotubes. The energy gap of armchair nanoribbons can be both vanishing or finite, dependently on the boundary condition. We considered two situations where the energy gap was either vanishing or maximal. We used solvable model of Dirac fermions in structured electric field and the explicit formulas for the bound states. The electric field did not alter essential spectrum. Therefore, we could show that the energy of bound states was either discrete or it belonged to the essential spectrum. In the later case, we dealt with the bound states in the continuum.

3.3 Qualitative analysis of energy spectrum and transport properties of Dirac fermions

It is not necessary to solve dynamical equation in order to guarantee existence of bound states in the system. In [Jak6], we focused on a one-dimensional stationary equation for Dirac fermion in presence of inhomogeneous vector potential or mass term. We found a set of criteria for existence of bound states (discrete energies) in the system. In [Jak9], we considered two-dimensional systems with translational invariance. We showed that discrete energy levels and associated bound states of the effective one-dimensional Hamiltonian can be used to construct (partially) dispersionless wave packets of specific group velocity. In [Jak10], we used the previous results to analyze transport properties in the wave guides in graphene formed by the magnetic field. We proposed a simple device based on a set of electric wires that allowed to change quantum transport of dispersionless wave packets by simple changes of currents in the wires. We further extended the analysis by considering planar systems under unidirectional strains [Jak11]. We found that the strains lead naturally to essentially unidirectional transport of dispersionless wave packets.

[Jak6] Qualitative analysis of trapped Dirac fermions in graphene

We found sufficient conditions for existence of bound states in the spectrum of one-dimensional Dirac equation with asymptotically constant vector potential. The criteria were found with the use of variational principle. It was applied on the square of Dirac Hamiltonian that coincides with Schrödinger operator. We discussed three different scenarios where this type of interaction can trap Dirac fermions: magnetic traps, effective mass traps and mechanical deformations. We discussed radial twists of carbon nanotubes, effective mass trenches caused by folded substrate and magnetic field trap generated by the wire with electric current.

[Jak9] Dispersionless wave packets in Dirac materials

We focused on two-dimensional systems with translational symmetry in one direction. The energy operator was written as direct integral of effectively one-dimensional Hamiltonians acting on the spaces with fixed value of longitudinal momentum. We showed that discrete energies of the effective Hamiltonians form specific bands in the energy spectrum. We constructed wave packets from the bound states corresponding to these energies and showed that they are dispersionless in perpendicular direction to the barrier. We discussed influence of perturbations on the propagation of the (partially) dispersionless wave packets. We presented experimentally realizable system with inhomogeneous mass term where dispersionless wave packets with different valley index could be observed.

[Jak10] Qualitative analysis of magnetic waveguides for two-dimensional Dirac fermions

We considered systems described by 2×2 two dimensional Dirac equation with constant mass in presence of an inhomogeneous magnetic field. We focused on the qualitative analysis

of confinement and transport of the wave packets by magnetic traps with translational symmetry. Separability of the system in the Cartesian coordinates allowed us to use qualitative criteria for existence of bound states of one-dimensional Dirac operator derived in [Jak6]. Dependence of the discrete energies of the effective 1D Dirac Hamiltonians on longitudinal momentum k was of our interest as it implied formation of energy bands of the two-dimensional energy operator. In dependence on the asymptotic properties of the vector potential, we provided some estimates for the intervals of k where the existence of the discrete energy bands is either granted or they cannot exist at all. We discussed existence of bidirectional or (essentially) unidirectional dispersionless wave packets. We investigated transport properties of the dispersionless wave packets in the field generated by a set of current wires and by magnetized strips. We proposed a simple device based on a bunch of electric wires that allowed for an easy manipulation of the magnetic field and for the control of transport properties of the dispersionless wave packets.

[Jak11] On the propagation of Dirac fermions in graphene with strain-induced inhomogeneous Fermi velocity

We analyzed the effect of unidirectional strain of graphene on dynamics of the wave packets. We showed that the trajectory of the wave packet gets curved and the wave packet is squeezed in direction of the strain. The effects are explained both qualitatively and quantitatively by the link with the free-particle system via suitable point transformation. When the unidirectional strain was inhomogeneous along both Cartesian axes, the link with the free particle was no longer applicable. Nevertheless, the point transformation was used to show that the wave packets get focused (more localized) in the region with the strain. Additionally it was possible to map the Hamiltonian with strains into the Dirac operator with an effective

magnetic field. This effective energy operator allowed for qualitative spectral analysis with the use of the criteria derived in [Jak10]. We showed that unidirectional strain gives rise naturally to essentially unidirectional transport of dispersionless wave packets. We showed that combination of an external magnetic field and unidirectional strain can generate valley-distinguished transport of the wave packets with possible application in valleytronics.

3.4 Coupled systems of Dirac fermions

In dependence on the involved interactions, it can be necessary to use 4×4 matrices in description of Dirac fermions in graphene as the additional degrees of freedom get coupled. In addition to the pseudospin, there can be also involved valley- or spin-degrees of freedom. In bilayer graphene, the additional degree of freedom reflects presence of the two interacting graphene sheets.

It can be considerably more difficult to solve the corresponding dynamical equations than those given in term of 2×2 matrices. In the series of articles [Jak13], [Jak14], and [Jak15], we discussed a family of 4×4 Hamiltonians describing such interactions that can be uncoupled by a suitable unitary transformation. The evolution equation is reduced into two, lower-dimensional Dirac equations with auxiliary interactions. The general family was described in [Jak13]. In [Jak14], the scheme was employed for the analysis of bilayer graphene with interlayer or intralayer interactions. In [Jak15], Darboux transformation of the reducible systems was discussed and its advantages in design of quantum systems demonstrated. Finally, we used Darboux transformation and the associated supersymmetric structure of the involved operator for construction of coupled system where two Dirac fermions with different Fermi velocities can exist [Jak17].

[Jak13] Reduction scheme for coupled Dirac systems

In the work, we focused on the class of 4×4 Dirac oper-

ators where the associated dynamical equation could be reduced into two auxiliary equations of lower dimension, and therefore, made the calculations more feasible. We found the multi-parametric class of energy operators that complied with the condition of reducibility. They find their application in description of distortion scattering or spin-orbit interaction in graphene, as well as in bilayer graphene. We presented explicit examples with interactions dependent on two spatial coordinates or on time.

[Jak14] Confinement in bilayer graphene via intra- and inter-layer interactions

We focused on the analysis of spectral properties of Dirac fermions in graphene. We considered 4×4 Dirac Hamiltonian with possibly inhomogeneous vector potential, on-site interaction and interlayer interaction. The Hamiltonian also comprises nonvanishing trigonal warping interaction. We analyzed how the stationary equation can be solved, dependently on the mentioned interactions. The stationary equation can be decoupled into Schrödinger-like form with energy-dependent potential. Its analytic solution was not feasible in general, nevertheless, there were detected specific cases that could be treated analytically. They were analyzed in detail for three scenarios where either vector potential, on-site interaction, or interlayer coupling were inhomogeneous. We found in all these cases that local fluctuations of the interaction can confine Dirac fermions. We demonstrated this effect on explicit examples, where the decoupled, energy-dependent equation was matched with the one of harmonic oscillator, Rosen-Morse or Pöschl-Teller model.

[Jak15] Form preserving Darboux transformations for 4×4 Dirac equation

Darboux transformation is a powerful tool for construction of

the new solvable models. Nevertheless, it can be difficult to keep control over the form of the potential in the Darboux-transformed Hamiltonian. This problem grows rapidly with dimension of the involved matrices. Using our previous results [Jak13], we showed that Darboux transformation can be used for construction of 4×4 Dirac operators where the potential terms have specific form given either by spin-orbit interaction or distortion scattering. The key point was reducibility of the stationary equation into two, lower-dimensional, stationary equations for 2×2 Dirac operators with auxiliary interactions. Performing Darboux transformation of the reduced Dirac operators made it possible to construct the new 4×4 Hamiltonians describing distortion scattering of spin-orbit interaction. We discussed in detail this class of form-preserving Darboux transformations. We found Darboux partners of a one-dimensional 2×2 Dirac Hamiltonian with constant matrix potential (i.e. a slight generalization of our previous results in [Jak4]). Then we used them in construction of Darboux transformed 4×4 Dirac operator describing spin-orbit interaction or distortion scattering. We worked with the systems with translational symmetry. The construction provided results for the normal incidence of the particles on the barrier. The presented models were reflectionless by construction. To extend applicability of our results, we employed perturbation analysis for small nonvanishing values of the momentum parallel with the axis of translational symmetry. We showed that the perturbation preserves bound states and, therefore, the system could host partially dispersionless wave packets as defined in [Jak9]. In the last section, we discussed issues related with the use of the non-reducible Darboux transformations; the transformed Dirac operator is non-hermitian. We showed that there can be strong link between hermiticity of the new operator and its reducibility.

[Jak17] Coupled system of Dirac fermions with different Fermi velocities via composites of SUSY operators

Supersymmetric quantum mechanics provides the framework for construction of the new solvable models from the known ones. Its backbone is Darboux transformation, a differential operator that intertwines Hamiltonians of the new and the old system. Darboux (supersymmetric) transformation together with the new and the old Hamiltonian can be used to define (nonlinear) superalgebra that consists of supersymmetric Hamiltonian and two supercharges. In the work, we showed that the supersymmetric Hamiltonian and one of the supercharges can be used to compose the new extended Hamiltonian. We showed that the new operator can be interpreted as the energy operator of the coupled system of Dirac fermions with two different Fermi velocities. We discussed in detail spectral properties of the composite Hamiltonian, we showed that they differ substantially from the spectral characteristics of the original systems, e.g. by level crossing of energy level or existence of bound states in the continuum. We illustrated the construction on two examples of the reflectionless and massive Pöschl-Teller models.

References

- [Jak1] V. Jakubský, L. -M. Nieto and M. S. Plyushchay, “Klein tunneling in carbon nanostructures: A Free particle dynamics in disguise,” *Phys. Rev. D* **83**, 047702 (2011).
- [Jak2] V. Jakubský and M. S. Plyushchay, “Supersymmetric twisting of carbon nanotubes,” *Phys. Rev. D* **85**, 045035 (2012).
- [Jak3] F. Correa and V. Jakubský, “Finite-gap twists of carbon nanotubes and an emergent hidden supersymmetry,” *Phys. Rev. D* **87**, 085019 (2013).
- [Jak4] F. Correa and V. Jakubsky, “Twisted kinks, Dirac transparent systems and Darboux transformations,” *Phys. Rev. D* **90**, 125003 (2014).
- [Jak5] V. Jakubsky, S. Kuru and J. Negro, “Carbon nanotubes in an inhomogeneous transverse magnetic field: exactly solvable model,” *J. Phys. A* **47**, 115307 (2014).
- [Jak6] V. Jakubský and D. Krejčířík, “Qualitative analysis of trapped Dirac fermions in graphene,” *Annals Phys.* **349**, 268 (2014); erratum **353**, 340 (2015).
- [Jak7] V. Jakubský, “Spectrally isomorphic Dirac systems: Graphene in an electromagnetic field,” *Phys. Rev. D* **91**, 045039 (2015).
- [Jak8] F. Correa and V. Jakubský, “Confluent Crum-Darboux transformations in Dirac Hamiltonians with PT -symmetric Bragg gratings,” *Phys. Rev. A* **95**, 033807 (2017).
- [Jak9] V. Jakubský and M. Tušek, “Dispersionless wave packets in Dirac materials,” *Annals Phys.* **378**, 171 (2017).

- [Jak10] M. Fialová, V. Jakubský and M. Tušek, “Qualitative analysis of magnetic waveguides for two-dimensional Dirac fermions,” *Annals of Physics* **395**, 219-237 (2018).
- [Jak11] A. Contreras-Astorga, V. Jakubský, A. Raya, “On the propagation of Dirac fermions in graphene with the strain-induced inhomogeneous Fermi velocity,” *J. Phys.: Condens. Matter* **32**, 295301 (2020).
- [Jak12] A. Contreras-Astorga, F. Correa and V. Jakubský, “Super-Klein tunneling of Dirac fermions through electrostatic gratings in graphene,” *Phys. Rev. B* **102**, 115429 (2020)
- [Jak13] M. Castillo-Celeita, V. Jakubský, ”Reduction scheme for coupled Dirac systems,” *J. Phys. A* **54**, 455301 (2021).
- [Jak14] M. Castillo-Celeita, V. Jakubský, K. Zelaya, Confinement in bilayer graphene via intra- and inter-layer interactions, *J. Phys. A* **55**, 035202 (2022).
- [Jak15] M. Castillo-Celeita, V. Jakubský, K. Zelaya, ”Form-preserving Darboux transformations for 4×4 Dirac equations,” *Eur. Phys. J. Plus* **137**, 389 (2022).
- [Jak16] V. Jakubský, S. Kuru, J. Negro, ”Dirac fermions in armchair graphene nanoribbons trapped by electric quantum dots,” *Phys. Rev. B* **105**, 165404 (2022).
- [Jak17] V. Jakubský, K. Zelaya, ”Coupled system of Dirac fermions with different Fermi velocities via composites of SUSY operators,” *Phys. Lett. A* **435**, 128053 (2022).

- [1] P. A. M. Dirac, Proc. Roy. Soc. A **117**, 610 (1928).
- [2] T. O. Wehling, A. M. Black-Schaffer, A. V. Balatsky, Advances in Physics **63**, 1 (2014).
- [3] B. Duplantier, “Dirac Matter”, Birkhauser Verlag AG (2017)
- [4] P. R. Wallace, Phys. Rev. **71**, 622 (1947).
- [5] G. W. Semenoff, Phys. Rev. Lett. **53**, 2449 (1984).
- [6] M. A. H. Vozmediano, M. I. Katsnelson and F. Guinea, Phys. Rept. **496**, 109 (2010).
- [7] S. Cahangirov et. al., Phys. Rev. Lett. **102**, 236804 (2009).
- [8] Di Xiao et al., Phys. Rev. Lett. **108**, 196802 (2012).
- [9] K. Gomes, W. Mar, W. Ko, F. Guinea, H. C. Manoharan, Nature **483**, 306 (2012).
- [10] Dan-wei Zhang, Zi-dan Wang, Shi-liang Zhou, Front. Phys. **7**, 31 (2012).
- [11] J. C. Charlier, X. Blase, and S. Roche, Rev. Mod. Phys. **79**, 677 (2007).
- [12] C. L. Kane, E. J. Mele, Phys. Rev. Lett. **78**, 1932 (1997).
- [13] B. Hunt, et.al., Science **340**, 1427 (2013).
- [14] N. M. R. Peres, A. H. Castro Neto, and F. Guinea, Phys. Rev. B **73**, 241403 (2006).
- [15] J. González, F. Guinea, and M. A. H. Vozmediano, Phys. Rev. Lett. **69**, 172 (1992).
- [16] F. de Juan, A. Cortijo, and M. A. H. Vozmediano, Phys. Rev. B **76**, 165409 (2007).

- [17] A. Iorio and G. Lambiase, Phys. Lett. B **716**, 334 (2012).
- [18] L. Brey and H. A. Fertig, Phys. Rev. B **73**, 235411 (2006).
- [19] C. L. Kane and E. J. Mele, Phys. Rev. Lett. **95**, 226801 (2005).
- [20] Chang-Yu Hou, C. Chamon, Ch. Mudry, Phys. Rev. Lett. **98**, 186809 (2007).
- [21] K. Novoselov et al, Nature Physics **2**, 177180 (2006).
- [22] Zhenhua Qiao et al, Nano Lett. **11**, 34533459 (2011).
- [23] M. I. Katsnelson, *Graphene: Carbon in Two Dimensions*, (Cambridge University Press, 2012).
- [24] F. Cooper, A. Khare and U. Sukhatme, *Supersymmetry in quantum mechanics*, (World Scientific, Singapore, 2001).
- [25] A. A. Andrianov and F. Cannata, J. Phys. A **37**, 10297 (2004).
- [26] L. M. Nieto et al, Annals Phys. **305**, 151 (2003).
- [27] E. Pozdeeva et al, J. Math. Phys. **51**, 113501 (2010).
- [28] A. Schulze-Halberg, Open Physics **11**, 457 (2013).
- [29] A. A. Pecheritsyn et al, Russian Physics Journal **48**, 365 (2005).

