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Elastic Deformations and Wigner–Weyl Formalism in Graphene

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Received: 21 January 2020; Accepted: 17 February 2020; Published: 23 February 2020

Abstract: We discuss the tight-binding models of solid state physics with the Z_2 sublattice symmetry in the presence of elastic deformations in an important particular case—the tight binding model of graphene. In order to describe the dynamics of electronic quasiparticles, the Wigner–Weyl formalism is explored. It allows the calculation of the two-point Green's function in the presence of two slowly varying external electromagnetic fields and the inhomogeneous modification of the hopping parameters that result from elastic deformations. The developed formalism allows us to consider the influence of elastic deformations and the variations of magnetic field on the quantum Hall effect.

Keywords: graphene; integer quantum hall effect; Wigner–Weyl calculus

1. Introduction

Recently there has been a revival of interest in Wigner–Weyl formalism in both condensed matter and high energy physics. It was proposed long ago by H. Groenewold [1] and J. Moyal [2], primarily in the context of one-particle quantum mechanics. The main notions of this formalism are those of the Weyl symbol of the operator and the Wigner transformation of the functions. Correspondingly, the formalism accumulated the ideas of H. Weyl [3] and E. Wigner [4]. In quantum mechanics, the Wigner–Weyl formalism substitutes the notion of the wave function by the so called Wigner distribution, that is, the function of both coordinates and momenta. The operators of physical quantities are described by their Weyl symbols (that are also the complex-valued functions of momenta and coordinates). The product of the operators on the language of Wigner–Weyl formalism becomes the Moyal product of their Weyl symbols [5,6]. The Wigner–Weyl formalism has been applied to several problems in quantum mechanics [7,8]. Notice that certain modifications of this formalism were proposed [9–16], where the main notions were changed somehow.

Let us recall the basic notions of Wigner–Weyl formalism in quantum mechanics with the example of the one dimensional model. The Wigner distribution $W(x,p)$ is a function of coordinate x and momentum p. It gives the probability that the coordinate x belongs to the interval $[a,b]$ in the following way:

$$P[a \leq x \leq b] = \frac{1}{2\pi}\int_a^b \int_{-\infty}^{\infty} W(x,p)\, dp\, dx.$$

Let $\hat{A}$ be operator of a certain physical observable. Its Weyl symbol $A_W(x,p)$ is defined as the function in phase space, which gives the expectation value of the given quantity with respect to the Wigner distribution $W(x,p)$ as follows [2,17]:

$$\langle \hat{A} \rangle = \frac{1}{2\pi} \int A_W(x,p) W(x,p)\, dp\, dx.$$

For the pure quantum state, the Wigner function is given by:

$$W(x,p) = \int dy\, e^{-ipy} \psi^*(x+y/2)\psi(x-y/2),$$

where $\psi(x)$ is the wave function of the state. The formalism is readily generalized to multidimensional $\boldsymbol{x}$ and $\boldsymbol{p}$.

The Schrodinger equation in the language of the Wigner–Weyl formalism acquires the form:

$$i\partial_t W(\boldsymbol{x},\boldsymbol{p},t) = H_W(\boldsymbol{x},\boldsymbol{p}) * W(\boldsymbol{x},\boldsymbol{p},t) - W(\boldsymbol{x},\boldsymbol{p},t) * H_W(\boldsymbol{x},\boldsymbol{p}).$$

The Moyal product of two functions f and g is given here by:

$$f * g = f \, \exp\left(\frac{i}{2}(\overleftarrow{\partial}_{\boldsymbol{x}} \overrightarrow{\partial}_{\boldsymbol{p}} - \overleftarrow{\partial}_{\boldsymbol{p}} \overrightarrow{\partial}_{\boldsymbol{x}})\right) g.$$

The left arrow above the derivative shows that the derivative acts on f while the right arrow assumes the action of the derivative on g.

The definition of the Weyl symbol of an arbitrary operator $\hat{A}$ is:

$$A_W(\boldsymbol{x},\boldsymbol{p}) = \int d\boldsymbol{y}\, e^{-i\boldsymbol{p}\boldsymbol{y}} \langle \boldsymbol{x}+\boldsymbol{y}/2|\hat{A}|\boldsymbol{x}-\boldsymbol{y}/2\rangle.$$

We denote by $H_W(\boldsymbol{x},\boldsymbol{p})$ the Weyl symbol of Hamiltonian $\hat{H}$.

The Wigner–Weyl formalism was also modified somehow in order to be applied to quantum field theory. The analogue of the Wigner distribution was introduced in QCD [18,19]. It has been used in field-theoretic kinetic theory [20,21] and noncommutative field theories [22,23]. Certain applications of the Wigner–Weyl formalism were proposed to several fields of theoretical physics including cosmology [24–26]. Using this formalism, quantum field theory has been discussed in this aspect in relation to quantum information theory (see [27–29] and references therein).

Wigner–Weyl formalism has been widely applied to the study of nondissipative transport phenomena [30–35]. Using this formalism it has been shown that the response of nondissipative currents to the external field strength is expressed through the topological invariants that are robust to the smooth deformation of the system. This allows the calculation of nondissipative currents for certain complicated systems within the more simple ones connected to the original systems by a smooth deformation. Using this method, the absence of the equilibrium chiral magnetic effect [36] was demonstrated within lattice regularized field theory [34]. The anomalous quantum Hall effect was studied using Wigner–Weyl formalism for the Weyl semimetals and topological insulators [35]. In addition, Wigner–Weyl formalism allows one to derive the chiral separation effect [37] within lattice models [30,32]. The same method was also applied to the investigation of the hypothetical color-flavor locking phase in QCD [33], where the fermion zero modes on vortices were discussed. The scale magnetic effect [38] has also been investigated using the same technique [31].

Historically the momentum space topological invariants were treated mainly in the context of condensed matter physics theory [39–43]. They protect gapless fermions on the edges of topological insulators [44,45] and the gapless fermions in the bulk of Weyl semi-metals [43,46]. The fermion zero modes of various topological defects in ^{3}He are also governed by momentum space topology [47]. In high energy physics, the topological invariants in momentum space were considered in [46,48–55]. The Wigner–Weyl formalism in [30,32,34,35] was developed in the context of lattice field theory. The one-particle fermion Green's function $G(\boldsymbol{p},\boldsymbol{q})$ was considered in momentum space $\mathcal{M}$ ($\boldsymbol{p},\boldsymbol{q} \in \mathcal{M}$).

It has been shown that the introduction of an Abelian external gauge field $\boldsymbol{A}(x)$ resulting in the Peierls substitution leads to the following equation:

$$\hat{Q}(\boldsymbol{p} - \boldsymbol{A}(i\partial_{\boldsymbol{p}})))G(\boldsymbol{p}, \boldsymbol{q}) = \delta(\boldsymbol{p} - \boldsymbol{q}).$$

Here $\hat{Q}(\boldsymbol{p})$ is the lattice Dirac operator. Notice that in lattice field theory, the imaginary time is discretized on the same ground as space coordinates.

The Wigner transformation of Green's function is defined as follows:

$$G_W(\boldsymbol{x}, \boldsymbol{p}) \equiv \int d\boldsymbol{q}\, e^{i\boldsymbol{x}\boldsymbol{q}} G(\boldsymbol{p} + \boldsymbol{q}/2, \boldsymbol{p} - \boldsymbol{q}/2) \tag{1}$$

It was shown [30] that for slowly varying external fields it obeys the Groenewold equation:

$$G_W(\boldsymbol{x}, \boldsymbol{p}) * Q_W(\boldsymbol{x}, \boldsymbol{p}) = 1 \tag{2}$$

with the above defined Moyal product $*$ extended to the D-dimensional vectors of coordinates $\boldsymbol{x}$ and momentum $\boldsymbol{p}$. Here Q_W is the Weyl symbol of operator $\hat{Q}(\boldsymbol{p} - \boldsymbol{A}(i\partial_{\boldsymbol{p}}))$.

In [56–58], the approach of [30,32,34,35] was further developed. In [56], the lattice model with Wilson fermions was investigated in detail. The precise expression for the Weyl symbol of the Wilson Dirac operator was derived in the presence of an arbitrarily varying external gauge field. In addition, the complete iterative solution of the Groenewold equation, Equation (2), was given. As a result the fermion propagator in the background of the arbitrary external electromagnetic field was calculated. We refer to [56] for the technical details of the Wigner–Weyl formalism in lattice models, which will be used in the present paper as well. In [57] it was shown that in the lattice models (i.e., in the tight-binding models) of solid state physics with essential inhomogeneity (caused by the varying external magnetic field), the Hall conductance integrated over the whole space is given by a topological invariant in phase space. This quantity is expressed through the Wigner transformation of the one-fermion Green's functions. The expression for the phase space topological invariant repeats the form of the momentum space topological invariants of [30,44,45,59,60]. The difference is that Green's functions entering this expression depend on both momenta and coordinates, and the ordinary product is substituted by the Moyal product, while the extra integration over the whole space is added (The topological invariants of [44–46,59,60] repeat the structure of the degree of mapping of the three-dimensional manyfold to a group of matrices). It has been shown that the value of the topological invariant in phase space responsible for the Hall conductance is robust to the introduction of disorder. Certain indications were found that it is also robust to weak Coulomb interactions.

The topological description of the Quantum Hall Effect (QHE) started from the discovery of the Thouless - Kohmoto - Nightingale - den Nijs (TKNN) invariant [61] defined in two-dimensional systems. Three dimensional topological invariants for the QHE were considered in [62]. This formalism allows one to deal with the intrinsic Anomalous Quantum Hall Effect (AQHE) and with the QHE in the presence of a constant magnetic field [63]. Unfortunately, the formalism that is based on the notion of Berry curvature does not admit the direct generalization to the QHE in the presence of a varying external magnetic field and elastic deformations when the system becomes essentially inhomogeneous. It is widely believed that the total QHE conductance is robust to the introduction of disorder and weak interactions. Expression for QHE conductivity through one-particle Green's functions has been invented in [59,60]. In the presence of interactions the full two-point Green's function should be substituted to the corresponding expression. It has been checked in [58], that the leading order contributions due to the Coulomb interactions do not change expression for AQHE conductivity in topological insulators. This expression has the form of an integral in momentum space over the certain composition of the interacting two-point Green's function. It is worth mentioning, however, that there is still no proof in a general case to all orders in the perturbation theory that higher order full

Green's functions do not give contributions to the QHE. For a discussion of this issue see also [44,45]. The AQHE conductivity discussed in [58] may be applied, in particular, to Weyl semimetals [64–69].

It is difficult to overestimate the role of disorder in the Quantum Hall Effect [63,70–72]. One of its effects is the elimination of the Hall current from the bulk, and its concentration along the boundary. The formalism developed in [57] allows one to give an alternative to prove that the total conductance remains robust to the introduction of disorder in the majority of systems although the total current remains only along the boundary of the sample. However, for graphene there are certain complications to be discussed in the Conclusions section. Namely, when the Hall current remains only along the boundary, the QHE is absent at the half filling (neutrality point). According to the common lore, the Hall conductance is assumed to be robust to the introduction of weak interactions, at least in the presence of the sufficient amount of disorder. However, Coulomb interactions are able to give rise to the fractional QHE [63,72,73] for clean systems at very small temperatures. This, however, is out of the scope of the present paper.

Graphene [74–82] represents the two-dimensional Weyl semimetal. The low energy physics of its electronic quasiparticles is described by the massless Dirac equation. Therefore, it allows one to simulate in the contect of a laboratory certain features of high energy physics that cannot be observed directly. Examples of such effects are the Schwinger pair production and gravitational effects in the quantum-mechanical motion of particles. Gravity appears in graphene in the presence of elastic deformations [79]. One more exceptional feature of graphene is that (unlike the later discovered three-dimensional Weyl semimetals) it is described with a very good accuracy by the simple tight-binding model defined on the honeycomb lattice. The investigation of various features of this model (including the QHE) based on the Wigner–Weyl formalism constitutes the subject of the present paper. It is worth noting here that many phenomena in graphene can be adequately treated even with low energy continuum approximation, within appropriate (pseudo-relativistic) field-theoretical methods [83,84].

In graphene, the elastic deformations lead both to the appearance of the emergent gauge field and emergent gravitational field (see, for example, [53,79,85–89]). The emergent gauge field appears as the variation of the Fermi point position in momentum space while the emergent gravitational field comes as the slope's variation of the dependence of energy on momentum (i.e., the anisotropic Fermi velocity).

Although our main aim is to investigate the tight-binding model of monolayer graphene, the paper is organized in such a way, that many of the obtained expressions may be applied to some other lattice models of solid state physics (though, only the model of graphene from this class describes quantitatively the really existing physical system). The paper is organized as follows. We start from the description of the almost arbitrary non-homogeneous lattice model in Section 2. We represent the formulation of such models in momentum space. Next, we reduce the considered class to the tight-binding models with the jumps of electrons between only the adjacent lattice sites. This section ends with the consideration of non-homogeneous tight-binding models with Z_2 sublattice symmetry. The tight-binding model of graphene belongs to this class. However it is much wider, in particular the tight-binding models defined on rectangular lattices in $2D$ and $3D$ remain in this class.

In Section 3, we introduce Wigner–Weyl formalism in nonhomogeneous lattice models with Z_2 sublattice symmetry. We explore the definition of the Weyl symbol of the lattice Dirac operator (entering the fermion action), which is defined through the integral in momentum space. We calculate the Weyl symbol of the Dirac operator for the considered models both in the presence of inhomogeneous hopping parameters and in the presence of the varying external electromagnetic field. Both the electromagnetic field and the hopping parameters are assumed to vary slowly, i.e., we neglect their variations on the distance of the lattice spacing. Next, we turn directly to the physics of graphene. We recall the relation between elastic deformations and the non-homogeneous hopping parameters. After that, we express the Weyl symbol of the lattice Dirac operator in graphene in the presence of

elastic deformations and the electromagnetic field through the electromagnetic potential and tensor of elastic deformations.

In Section 4, we consider the relation between the Weyl symbol of the lattice Dirac operator in the considered systems and the Wigner transformation of Green's functions. Additionally, we express the electric current through the quantities of the Wigner–Weyl formalism.

In Section 5, we again consider the lattice models of the general type. The corresponding calculations are of course applied to the case of graphene directly. Namely, we extend the results of [56] for the calculation of the Wigner transformation of the fermion Green's function (obtained for lattice Wilson fermions on rectangular lattice) to the case of the non-homogeneous tight-binding models of the arbitrary form. It is also explained how to reconstruct the Green's function both in momentum and coordinate representations from its known Weyl symbol.

In Section 6 we extend the consideration of [57] to the case when elastic deformations are present. Namely, we prove that for the noninteracting $2D$ condensed matter model with slowly varying electromagnetic fields and elastic deformations, the Hall conductivity integrated over the whole area of the sample is given by the topological invariant in phase space composed of the Wigner transformed one-particle Green's function. It is the same topological invariant proposed in [57]. It remains robust to the smooth modification of the model (if the modification remains local and bounded to the smooth modification of the Hamiltonian in the limited region of the sample that remains far from its boundary).

In Section 7, we apply the results of the previous sections to the discussion of Hall conductivity in graphene in the presence of both elastic deformations and inhomogeneous magnetic field. First, we recall the standard derivation of Hall conductance in the noninteracting $2D$ models with constant magnetic field and constant hopping parameters. Next, this standard derivation is extended to the case of the weakly varying elastic deformations that cause varying hopping parameters that remain isotropic (i.e., their values are equal for all directions in the given point though they vary from point to point). We obtain the formula for the Hall conductance that allows one to express it through the total number of electrons in the occupied energy levels and external magnetic field. Next, we apply the topological invariant in phase space defined in Section 3 to the consideration of the QHE in graphene. The very existence of such a representation for the QHE conductance allows one to prove that it remains robust to the weak elastic deformations of arbitrary form and weak modification of magnetic field unless the topological phase transition is encountered. Both are assumed to be localized in the region that remains far from the boundaries of the sample. Finally, in this section we notice that the elastic deformations in graphene that do not cause the emergent magnetic field give rise to the isotropic hopping parameters. The corresponding displacement appears to be the analytical function of the atom coordinates of the unperturbed honeycomb lattice. For the constant external magnetic field, this allows one to derive the simple relation between the number of electrons in the occupied branches of spectrum and the value of magnetic field.

In Section 8, we end with the conclusions, discuss the obtained results, and directions for future research.

Throughout the paper the following notational conventions are used. Latin letters in subscript a, b, c numerate the spatial components of vectors. The Latin letters in superscript i, j enumerate the elementary translations. All momenta vectors are bold italic $\boldsymbol{l}, \boldsymbol{k}, \boldsymbol{p}, \boldsymbol{q}$ from the middle of the alphabet, coordinate vectors are from its end, $\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{u}, \boldsymbol{v}$. Operators are denoted by the Latin letters with hat $\hat{Q}, \hat{G}$ and their matrix elements of operators by functions of two variables $Q(\boldsymbol{p}, \boldsymbol{q})$. The Weyl symbols of operators are denoted by the sub-index W: $(\hat{Q})_W \equiv Q_W$.

2. Hamiltonian for the Nonlocal Tight–Binding Model

2.1. General Case

We start our discussion with a general case of the non-local tight-binding model in the presence of the external electromagnetic field A. The discussion of the present section is applicable, in principle,

not only to the tight-binding model of graphene, but also to other $2+1$D and $3+1$D tight-binding models of solid state physics.

The Hamiltonian under consideration has the form:

$$\begin{aligned}\mathcal{H} &\equiv \sum_{\boldsymbol{x},\boldsymbol{y}} \bar{\Psi}(\boldsymbol{y}) f(\boldsymbol{y},\boldsymbol{x}) e^{\mathrm{i}\int_x^y dv \boldsymbol{A}(v)} \Psi(\boldsymbol{x}) \\ &= \frac{1}{|\mathcal{M}|^2} \int d\boldsymbol{p} d\boldsymbol{q} d\boldsymbol{l} d\boldsymbol{k}\ \bar{\Psi}(\boldsymbol{p}) f(\boldsymbol{q},\boldsymbol{l}) \Psi(\boldsymbol{k}) \sum_{\boldsymbol{x},\boldsymbol{y}} e^{\mathrm{i}\int_x^y dv \boldsymbol{A}(v)} e^{\mathrm{i}\boldsymbol{y}(\boldsymbol{q}-\boldsymbol{p})+i\boldsymbol{x}(-\boldsymbol{l}+\boldsymbol{k})}\end{aligned} \tag{3}$$

and here the sum is over the lattice sites $\boldsymbol{x},\boldsymbol{y}$, while $f(\boldsymbol{x},\boldsymbol{y})$ is the matrix of hopping parameters. The lattice is assumed to be infinite, which means that we neglect the finite volume effects as well as the finite temperature corrections. Thus, the integrals in the second line are over momentum space $\mathcal{M}$, which is the first Brillouin zone specific for the given lattice model.

In the following, we may absorb the electromagnetic field to the definition of f. Therefore, we omit it temporarily and will restore it in appropriate expressions.

Now let us consider a less general situation of the tight-binding model with the jumps of electrons between the adjacent sites only—the nearest neighbor approximation. We discuss the case of the inhomogeneous hopping parameters, which will allow us to discuss elastic deformations. Now,

$$f(\boldsymbol{y},\boldsymbol{x}) = \sum_{j=1}^{M} \delta(\boldsymbol{y} - (\boldsymbol{x} + \boldsymbol{b}^{(j)})) f^{(j)}(\boldsymbol{y}) \tag{4}$$

where $\boldsymbol{b}^{(j)}$ are the vectors connecting each atom to its nearest M neighbors, $j = 1, ..., M$, and $f^{(j)}(\boldsymbol{y})$ is the non-uniform varying hopping parameter.

Then,

$$\begin{aligned}f(\boldsymbol{q},\boldsymbol{l}) &= \frac{1}{|\mathcal{M}|} \sum_{j=1}^{M} \sum_{\boldsymbol{x},\boldsymbol{y}} e^{-\mathrm{i}\boldsymbol{q}\boldsymbol{x}+\mathrm{i}\boldsymbol{l}\boldsymbol{y}} \delta(\boldsymbol{y} - (\boldsymbol{x} + \boldsymbol{b}^{(j)})) f^{(j)}(\boldsymbol{y}) \\ &= \frac{1}{|\mathcal{M}|} \sum_{j=1}^{M} \sum_{\boldsymbol{y}} e^{-\mathrm{i}(\boldsymbol{q}-\boldsymbol{l})\boldsymbol{y}+\mathrm{i}\boldsymbol{q}\boldsymbol{b}^{(j)}} f^{(j)}(\boldsymbol{y}) \\ &= \sum_{j=1}^{M} f^{(j)}(\boldsymbol{q}-\boldsymbol{l}) e^{\mathrm{i}\boldsymbol{q}\boldsymbol{b}^{(j)}}\end{aligned} \tag{5}$$

and

$$\mathcal{H} = \frac{1}{|\mathcal{M}|} \sum_{j=1}^{M} \int_{\mathcal{M}} d\boldsymbol{p} d\boldsymbol{q}\, \bar{\Psi}(\boldsymbol{p}) \left[f^{(j)}(\boldsymbol{p}-\boldsymbol{q}) e^{\mathrm{i}\boldsymbol{q}\boldsymbol{b}^{(j)}} \right] \Psi(\boldsymbol{q}). \tag{6}$$

2.2. The Z_2 Sublattice Symmetry

Our next simplification is the consideration of a particular case, when crystal lattice exhibits Z_2 sublattice symmetry, i.e., there are two sublattices $\mathcal{O}_{1,2}$ that constitute the crystal, and there is the one to one correspondence between them generated by shift $\boldsymbol{x} \to \boldsymbol{x} + \boldsymbol{b}^{(j)}$ for any $j = 1, ..., M$ and $\boldsymbol{x} \in \mathcal{O}_1$ or $\boldsymbol{x} \to \boldsymbol{x} - \boldsymbol{b}^{(j)}$ for $\boldsymbol{x} \in \mathcal{O}_2$.

The points of those two sublattices are to be considered independently, which gives the sublattice index $\alpha = 1, 2$ to Ψ. We identify $\Psi(t,\boldsymbol{x})$, where $\boldsymbol{x} \in \mathcal{O}_1$, with $\Psi_1(t,\boldsymbol{x})$, and $\Psi(t,\boldsymbol{x})$ for $\boldsymbol{x} \in \mathcal{O}_2$ is identified with $\Psi_2(t,\boldsymbol{x})$. We set $\Psi_1(t,\boldsymbol{x}) = 0$ for $\boldsymbol{x} \in \mathcal{O}_2$ and $\Psi_2(t,\boldsymbol{x}) = 0$ for $\boldsymbol{x} \in \mathcal{O}_1$. Then,

$$\Psi_\alpha(\boldsymbol{p}) = \frac{1}{|\mathcal{M}|^{1/2}} \sum_{\boldsymbol{x} \in \mathcal{O}_\alpha} \Psi_\alpha(\boldsymbol{x}) e^{-\mathrm{i}\boldsymbol{p}\boldsymbol{x}}, \qquad \alpha = 1, 2.$$

The inverse transform is similar:

$$\Psi_\alpha(\boldsymbol{x}) = \frac{1}{|\mathcal{M}|^{1/2}} \int_{\mathcal{M}} d\boldsymbol{p}\, \Psi_\alpha(\boldsymbol{p}) e^{i\boldsymbol{p}\boldsymbol{x}}, \qquad \alpha = 1,2.$$

Note, that Brillouin zone $\mathcal{M}$ is the same for both sublattices since both of them are built over the same basis vectors, and thus have the same periodicity. $\mathcal{M}$ is formed as space of vectors $\boldsymbol{p}$ defined by modulo transformations:

$$\boldsymbol{p} \to \boldsymbol{p} + \boldsymbol{g}^{(k)}$$

where $\boldsymbol{g}^{(k)}$ are vectors of inverse lattice that solve the system of equations:

$$e^{i\boldsymbol{g}^{(k)}\boldsymbol{m}^{(j_1 j_2)}} = 1, \quad j_1, j_2 = 1, ..., M \tag{7}$$

while $\boldsymbol{m}^{(j_1,j_2)} = \boldsymbol{b}^{(j_1)} - \boldsymbol{b}^{(j_2)}$ form each of the two sublattices $\mathcal{O}_{1,2}$. Then the hoping parameters $f^{(j)}$ become 2×2 matrices. Besides, we assume that the spatial hoping parameters are coordinate dependent,

$$f_{21}^{(j)}(\boldsymbol{x} + \boldsymbol{b}^{(j)}) = -t^{(j)}(\boldsymbol{x} + \boldsymbol{b}^{(j)}), \tag{8}$$

i.e., the values of $t^{(j)}$ may vary independently but not with time. The diagonal ones are vanishing, $f_{11}^{(j)} = f_{22}^{(j)} = 0$.

The Hamiltonian then receives the form:

$$\mathcal{H} = \sum_{j=1}^{M} \sum_{\substack{\boldsymbol{x}\in\mathcal{O}_1 \\ \boldsymbol{y}=\boldsymbol{x}+\boldsymbol{b}^{(j)}}} \left(t^{(j)}(\boldsymbol{y}) \bar{\Psi}_2(t,\boldsymbol{y}) \Psi_1(t,\boldsymbol{x}) + t^{(j)}(\boldsymbol{y}) \bar{\Psi}_1(t,\boldsymbol{x}) \Psi_2(t,\boldsymbol{y}) \right). \tag{9}$$

In what follows we will omit the temporal argument of the wave function whenever no confusion is provoked.

3. Weyl Symbol for the Lattice Dirac Operator

3.1. Lattice Dirac Operator

Let us rewrite Equation (9) in the following way:

$$\begin{aligned} \mathcal{H} &= \sum_{\substack{\boldsymbol{x}\in\mathcal{O}_1 \\ \boldsymbol{y}\in\mathcal{O}_2}} \left(\bar{\Psi}_1(\boldsymbol{x}),\, \bar{\Psi}_2(\boldsymbol{y})\right) \boldsymbol{H}(\boldsymbol{x},\boldsymbol{y}) \left(\Psi_1(\boldsymbol{x}),\, \Psi_2(\boldsymbol{y})\right)^T \\ &\equiv \sum_{\substack{\boldsymbol{x}\in\mathcal{O}_1 \\ \boldsymbol{y}\in\mathcal{O}_2}} \left(\bar{\Psi}_2(\boldsymbol{y}) H_{21}(\boldsymbol{y},\boldsymbol{x}) \Psi_1(\boldsymbol{x}) + \bar{\Psi}_1(\boldsymbol{x}) H_{12}(\boldsymbol{x},\boldsymbol{y}) \Psi_2(\boldsymbol{y}) \right) \end{aligned} \tag{10}$$

where

$$\begin{aligned} H_{21}(\boldsymbol{y}_2,\boldsymbol{y}_1) &= -\sum_{j=1}^{M} \delta\left(\boldsymbol{y}_2 - (\boldsymbol{y}_1 + \boldsymbol{b}^{(j)})\right) t^{(j)}\left(\frac{\boldsymbol{y}_1+\boldsymbol{y}_2}{2}\right), \qquad \begin{matrix} \boldsymbol{y}_1 \in \mathcal{O}_1 \\ \boldsymbol{y}_2 \in \mathcal{O}_2 \end{matrix} \\ H_{12}(\boldsymbol{y}_1,\boldsymbol{y}_2) &= H_{21}(\boldsymbol{y}_2,\boldsymbol{y}_1). \end{aligned} \tag{11}$$

Note that we define the hoping parameter by its values in the middle of the lattice links, $t^{(j)}\left(\frac{\boldsymbol{y}_1+\boldsymbol{y}_2}{2}\right)$ for better readability of consequent formulas.

We will refer to the 2 by 2 matrix operator $\boldsymbol{H}$ as to the lattice Dirac Hamiltonian, although its geometrical symmetries will only be defined after specifying $\boldsymbol{b}^{(j)}$. Along with Hamiltonian, we also

introduce the Dirac operator, which enters the action and consequently will be useful for an analysis of the system's partition function:

$$Q \equiv \mathrm{i}\omega - \boldsymbol{H} = \begin{pmatrix} \mathrm{i}\omega & -H_{12} \\ -H_{21} & \mathrm{i}\omega \end{pmatrix}. \tag{12}$$

Let us consider the off-diagonal term 21 in the Hamiltonian. It can be written in terms of the Fourier transformation as:

$$\mathcal{H}_{21} = \frac{1}{|\mathcal{M}|} \int_{\mathcal{M}} d\boldsymbol{p} d\boldsymbol{q}\, \bar{\Psi}_2(\boldsymbol{p}) H_{21}(\boldsymbol{p}, \boldsymbol{q}) \Psi_1(\boldsymbol{q}) \tag{13}$$

modifying Equation (5) for two sublattices, we have:

$$\begin{aligned} H_{12}(\boldsymbol{q}, \boldsymbol{p}) &= \frac{1}{|\mathcal{M}|} \sum_{j=1}^{M} \sum_{\substack{\boldsymbol{y}_1 \in \mathcal{O}_1 \\ \boldsymbol{y}_2 \in \mathcal{O}_2}} e^{-\mathrm{i}\boldsymbol{q}\boldsymbol{y}_1 + \mathrm{i}\boldsymbol{p}\boldsymbol{y}_2} \delta\left(\boldsymbol{y}_2 - (\boldsymbol{y}_1 + \boldsymbol{b}^{(j)})\right) t^{(j)}\left(\frac{\boldsymbol{y}_1 + \boldsymbol{y}_2}{2}\right) \\ &= \frac{1}{|\mathcal{M}|} \sum_{j=1}^{M} \sum_{\boldsymbol{y}_1 \in \mathcal{O}_1} e^{-\mathrm{i}(\boldsymbol{q}-\boldsymbol{p})\boldsymbol{y}_1 + \mathrm{i}\boldsymbol{q}\boldsymbol{b}^{(j)}} t^{(j)}\left(\boldsymbol{y}_1 + \boldsymbol{b}^{(j)}/2\right) \end{aligned}. \tag{14}$$

We can identify now the points $\boldsymbol{y}_1 + \boldsymbol{b}^{(j)}/2$, $\boldsymbol{y}_1 \in \mathcal{O}_1$ with those situated in the middle of the lattice links along the j-th direction. We call these sets of points by $\mathcal{O}^{(j)}_{1/2}$. Now we can write,

$$H_{21}(\boldsymbol{p}, \boldsymbol{q}) = \sum_{j=1}^{M} t^{(j)}(\boldsymbol{p} - \boldsymbol{q}) e^{\mathrm{i}(\boldsymbol{p}+\boldsymbol{q})\boldsymbol{b}^{(j)}/2} \tag{15}$$

where

$$t^{(j)}(\boldsymbol{p}) = \frac{1}{|\mathcal{M}|} \sum_{\boldsymbol{x} \in \mathcal{O}^{(j)}_{1/2}} t^{(j)}(\boldsymbol{x}) e^{-\mathrm{i}\boldsymbol{x}\boldsymbol{p}}. \tag{16}$$

Note, that the above expression is simply a Fourier transformation of a function shifted by $\boldsymbol{b}^{(j)}/2$ since $t^{(j)}$ are only defined in the middle of the links. In this particular case, when $t^{(j)}(\boldsymbol{x}) = t^{(j)}$, i.e., if it does not depend on $\boldsymbol{x}$, we obtain:

$$t^{(j)}(\boldsymbol{p}) = t^{(j)} \delta(\boldsymbol{p} \mod \boldsymbol{g}^{(j)}).$$

3.2. The Definition of the Weyl Symbol in Momentum Space

We propose the following definition of the Weyl symbol of operator $\hat{A}$:

$$(\hat{A})_W(\boldsymbol{x}, \boldsymbol{p}) = \int_{\mathcal{M}} d\boldsymbol{q}\, A(\boldsymbol{p} + \boldsymbol{q}/2, \boldsymbol{p} - \boldsymbol{q}/2) e^{\mathrm{i}\boldsymbol{q}\boldsymbol{x}}. \tag{17}$$

Here, the integral is over momentum space $\mathcal{M}$, in which the two vectors are equivalent if they differ by $\boldsymbol{g}^{(j)}$. In particular this means that $\boldsymbol{p} \pm \boldsymbol{q}/2$ do not span the whole Brillouin zone $\mathcal{M}$.

For off-diagonal components of $\boldsymbol{H}$ from the above it gives:

$$H_{21,W}(\boldsymbol{x}, \boldsymbol{p}) = \int_{\mathcal{M}} d\boldsymbol{q}\, e^{\mathrm{i}\boldsymbol{q}\boldsymbol{x}} \sum_{j=1}^{M} t^{(j)}(\boldsymbol{q})\, e^{\mathrm{i}\boldsymbol{p}\boldsymbol{b}^{(j)}} = \sum_{j=1}^{M} e^{\mathrm{i}\boldsymbol{p}\boldsymbol{b}^{(j)}} \int_{\mathcal{M}} d\boldsymbol{q}\, t^{(j)}(\boldsymbol{q}) e^{\mathrm{i}\boldsymbol{q}\boldsymbol{x}}. \tag{18}$$

If the hopping parameters are homogeneous, then:

$$H_{21,W}(\boldsymbol{x}, \boldsymbol{p}) = e^{\mathrm{i}\boldsymbol{p}\boldsymbol{b}^{(j)}} t^{(j)}.$$

On the other hand, when the hopping parameters vary, we use Equation (16):

$$\begin{aligned} H_{21,W}(\boldsymbol{x},\boldsymbol{p}) &= \frac{1}{|\mathcal{M}|}\sum_{j=1}^{M} e^{\mathrm{i}\boldsymbol{p}\boldsymbol{b}^{(j)}} \sum_{\boldsymbol{y}\in\mathcal{O}_{1/2}^{(j)}} t^{(j)}(\boldsymbol{y}) \int_{\mathcal{M}} d\boldsymbol{q}\; e^{\mathrm{i}\boldsymbol{q}(\boldsymbol{x}-\boldsymbol{y})} \\ &= \sum_{j=1}^{M} e^{\mathrm{i}\boldsymbol{p}\boldsymbol{b}^{(j)}} \sum_{\boldsymbol{y}\in\mathcal{O}_{1/2}^{(j)}} t^{(j)}(\boldsymbol{y})\mathcal{F}(\boldsymbol{x}-\boldsymbol{y}), \end{aligned} \tag{19}$$

where

$$\mathcal{F}(\boldsymbol{x}) = \frac{1}{|\mathcal{M}|}\int_{\mathcal{M}} d\boldsymbol{q}\, e^{\mathrm{i}\boldsymbol{q}\boldsymbol{x}}. \tag{20}$$

Notice that for $\boldsymbol{x},\boldsymbol{y}\in\mathcal{O}_{1/2}^{(j)}$, we have $\boldsymbol{y}-\boldsymbol{x}\in\mathcal{O}$ and thus, the function $\mathcal{F}(\boldsymbol{y}-\boldsymbol{x})$ vanishes for all $\boldsymbol{x}\in\mathcal{O}_{1/2}^{(j)}$ except for $\boldsymbol{x}=\boldsymbol{y}$. However, it remains nonzero and oscillates for all other values of $\boldsymbol{x}$, including continuous ones, and gives unity if summed over $\mathcal{O}_{1/2}^{(j)}$ for any $\boldsymbol{x}$,

$$\sum_{\boldsymbol{y}\in\mathcal{O}_{1/2}^{(j)}} \mathcal{F}(\boldsymbol{x}-\boldsymbol{y}) = 1. \tag{21}$$

Each term of the j-sum in Equation (19) receives a particular form if $\boldsymbol{x}\in\mathcal{O}_{1/2}^{(j)}$ (with the same value of j):

$$H_{21,W}^{(j)}(\boldsymbol{x},\boldsymbol{p})\Big|_{\boldsymbol{x}\in\mathcal{O}_{1/2}^{(j)}} = e^{\mathrm{i}\boldsymbol{p}\boldsymbol{b}^{(j)}} t^{(j)}(\boldsymbol{x}) \tag{22}$$

However, Equation (19) also defines H_W for continuous values of $\boldsymbol{x}$.

The presence of an external electromagnetic field with a vector potential $\boldsymbol{A}$ may be introduced to the model via the modification of a hopping parameter in the term H_{21}:

$$t^{(j)}(\boldsymbol{x}) \to t^{(j)}(\boldsymbol{x}) e^{-\mathrm{i}\int_{\boldsymbol{x}-\boldsymbol{b}^{(j)}/2}^{\boldsymbol{x}+\boldsymbol{b}^{(j)}/2}\boldsymbol{A}(\boldsymbol{y})d\boldsymbol{y}}.$$

In H_{12} there should be a complex conjugate substitution:

$$t^{(j)}(\boldsymbol{x}) \to t^{(j)}(\boldsymbol{x}) e^{-\mathrm{i}\int_{\boldsymbol{x}+\boldsymbol{b}^{(j)}/2}^{\boldsymbol{x}-\boldsymbol{b}^{(j)}/2}\boldsymbol{A}(\boldsymbol{y})d\boldsymbol{y}}$$

From Equation (19) we see that it is simply the Pieirls substitution in the language of Weyl symbols.

Combining this substitution with Equation (12) we get:

$$Q_W = \sum_{j=1}^{M} Q_W^{(j)}$$

where

$$Q_W^{(j)}(\boldsymbol{x},\boldsymbol{p})\Big|_{\boldsymbol{x}\in\mathcal{O}_{1/2}^{(j)}} = \begin{pmatrix} \mathrm{i}\omega/M & -t^{(j)}(\boldsymbol{x})\, e^{\mathrm{i}(\boldsymbol{p}\boldsymbol{b}^{(j)}-A^{(j)}(\boldsymbol{x}))} \\ -t^{(j)}(\boldsymbol{x})\, e^{-i(\boldsymbol{p}\boldsymbol{b}^{(j)}-A^{(j)}(\boldsymbol{x}))} & \mathrm{i}\omega/M \end{pmatrix}, \tag{23}$$

and M is the number of the nearest neighbours. Here:

$$A^{(j)}(\boldsymbol{x}) = \int_{\boldsymbol{x}-\boldsymbol{b}^{(j)}/2}^{\boldsymbol{x}+\boldsymbol{b}^{(j)}/2} \boldsymbol{A}(\boldsymbol{y})d\boldsymbol{y}.$$

For both $t^{(j)}$ and A that almost do not vary at the distances of order of lattice spacing we may use Equation (23) for arbitrary values of $\boldsymbol{x}$, and get:

$$Q_W(\boldsymbol{x},\boldsymbol{p}) = \sum_{j=1}^{M} \begin{pmatrix} \mathrm{i}\omega/N & -t^{(j)}(\boldsymbol{x})\, e^{\mathrm{i}(\boldsymbol{p}\boldsymbol{b}^{(j)} - A^{(j)}(\boldsymbol{x}))} \\ -t^{(j)}(\boldsymbol{x})\, e^{-\mathrm{i}(\boldsymbol{p}\boldsymbol{b}^{(j)} - A^{(j)}(\boldsymbol{x}))} & \mathrm{i}\omega/N \end{pmatrix}. \tag{24}$$

This approximation corresponds to the situation, when the typical wavelength of electromagnetic field is much larger than the lattice spacing.

3.3. Elastic Deformation and Modification of Hoping Parameters

Now we are in the position to consider elastic deformations and Wigner–Weyl formalism in graphene. In this section we discuss the graphene monolayer in the presence of elastic deformations. The sheet of graphene is parametrized by coordinates $x_k, k = 1, 2$. The displacements of each point have three components $u_a(\boldsymbol{x})$, where $a = 1, 2, 3$. The resulting coordinates of the graphene sheet embedded into three-dimensional space y_a are given by:

$$\begin{aligned} y_k(\boldsymbol{x}) &= x_k + u_k(\boldsymbol{x}), \quad k = 1, 2 \\ y_3(\boldsymbol{x}) &= u_3(\boldsymbol{x}). \end{aligned} \tag{25}$$

In the absence of the displacements, when $u_a = 0$, the graphene is flat. The metric of elasticity theory is given by:

$$g_{ik} = \delta_{ik} + 2u_{ik}, \;\; u_{ik} = \frac{1}{2}\Big(\partial_i u_k + \partial_k u_i + \partial_i u_a \partial_k u_a\Big), \quad a = 1, 2, 3, \quad i, k = 1, 2. \tag{26}$$

When the distance between the given atom and its neighbor is changed, and the change of the distance is in δr, then the corresponding hopping parameter is modified as $t \to t(1 - \beta\delta r)$, where β is the so-called Gruneisen parameter. As a result the elastic deformations change the spatial hopping parameters, which enter Equation (11), as follows:

$$t^{(j)}(\boldsymbol{x}) = t\left(1 - \beta u_{ik}(\boldsymbol{x}) b_i^{(j)} b_k^{(j)}\right). \tag{27}$$

Here,

$$\{\boldsymbol{b}^{(j)}\}_{j=1}^{3} = \{(-1, 0); (1/2, \sqrt{3}/2); (1/2, -\sqrt{3}/2)\}. \tag{28}$$

We imply that $\beta|u_{ij}| \ll 1$.

The standard expression for the emergent electromagnetic potential has the form:

$$\begin{aligned} A_1 &= -\frac{\beta}{a}\, u_{12} \\ A_2 &= \frac{\beta}{2a}\,(u_{22} - u_{11}). \end{aligned} \tag{29}$$

For the arbitrarily varying field u we obtain the following expression for Q_W:

$$Q_W(\omega, p; \tau, \boldsymbol{x}) = \mathrm{i}\omega - t\sum_{j=1}^{3}\left(1 - \beta u_{ik}(\boldsymbol{x}) b_i^{(j)} b_k^{(j)}\right) \begin{pmatrix} 0 & e^{\mathrm{i}(\boldsymbol{p}\boldsymbol{b}^{(j)} - A^{(j)}(\boldsymbol{x}))} \\ e^{-\mathrm{i}(\boldsymbol{p}\boldsymbol{b}^{(j)} - A^{(j)}(\boldsymbol{x}))} & 0 \end{pmatrix}. \tag{30}$$

4. Green's Function and the Groenewold Equation

4.1. Appearance of the Moyal Product

Our definition of the Weyl symbol of operator $\hat{A}$ in Equation (17) can also be written as:

$$A_W(\boldsymbol{x},\boldsymbol{p}) = \int_{\mathcal{M}} d\boldsymbol{\mathcal{P}} e^{i\boldsymbol{x}\boldsymbol{\mathcal{P}}} \left\langle \boldsymbol{p} + \frac{\boldsymbol{\mathcal{P}}}{2} \middle| \hat{A} \middle| \boldsymbol{p} - \frac{\boldsymbol{\mathcal{P}}}{2} \right\rangle. \tag{31}$$

The integral over $\boldsymbol{\mathcal{P}}$ is over the Brillouin zone $\mathcal{M}$, i.e., in $\mathcal{M}$ we identify the points that differ by a vector of reciprocal lattice $\boldsymbol{g}^{(j)}$.

Now let us consider the Weyl symbol $(AB)_W(\boldsymbol{x},\boldsymbol{p})$ of the product of two operators $\hat{A}$ and $\hat{B}$ such that their matrix elements $\left\langle \boldsymbol{p}+\frac{\boldsymbol{q}}{2}\right| \hat{A} \left|\boldsymbol{p}-\frac{\boldsymbol{q}}{2}\right\rangle$ and $\left\langle \boldsymbol{p}+\frac{\boldsymbol{q}}{2}\right| \hat{B} \left|\boldsymbol{p}-\frac{\boldsymbol{q}}{2}\right\rangle$ are nonzero only when $\boldsymbol{q}$ remains in the small vicinity of zero. Then:

$$\begin{aligned}
(AB)_W(\boldsymbol{x},\boldsymbol{p}) &= \int_{\mathcal{M}} d\boldsymbol{\mathcal{P}} \int_{\mathcal{M}} d\boldsymbol{\mathcal{R}}\, e^{\mathrm{i}\boldsymbol{x}\boldsymbol{\mathcal{P}}} \left\langle \boldsymbol{p}+\tfrac{\boldsymbol{\mathcal{P}}}{2}\right| \hat{A} \left|\boldsymbol{\mathcal{R}}\right\rangle \left\langle \boldsymbol{\mathcal{R}}\right| \hat{B} \left|\boldsymbol{p}-\tfrac{\boldsymbol{\mathcal{P}}}{2}\right\rangle \\
&= \frac{1}{2^D} \int_{\mathcal{M}} d\boldsymbol{\mathcal{P}} d\boldsymbol{\mathcal{K}}\, e^{\mathrm{i}\boldsymbol{x}\boldsymbol{\mathcal{P}}} \left\langle \boldsymbol{p}+\tfrac{\boldsymbol{\mathcal{P}}}{2}\right| \hat{A} \left|\boldsymbol{p}-\tfrac{\boldsymbol{\mathcal{K}}}{2}\right\rangle \left\langle \boldsymbol{p}-\tfrac{\boldsymbol{\mathcal{K}}}{2}\right| \hat{B} \left|\boldsymbol{p}-\tfrac{\boldsymbol{\mathcal{P}}}{2}\right\rangle \\
&= \frac{2^D}{2^D} \int_{\mathcal{M}} d\boldsymbol{q} d\boldsymbol{k}\, e^{\mathrm{i}\boldsymbol{x}(\boldsymbol{q}+\boldsymbol{k})} \left\langle \boldsymbol{p}+\tfrac{\boldsymbol{q}}{2}+\tfrac{\boldsymbol{k}}{2}\right| \hat{A} \left|\boldsymbol{p}-\tfrac{\boldsymbol{q}}{2}+\tfrac{\boldsymbol{k}}{2}\right\rangle \left\langle \boldsymbol{p}-\tfrac{\boldsymbol{q}}{2}+\tfrac{\boldsymbol{k}}{2}\right| \hat{B} \left|\boldsymbol{p}-\tfrac{\boldsymbol{q}}{2}-\tfrac{\boldsymbol{k}}{2}\right\rangle \\
&= \int_{\mathcal{M}} d\boldsymbol{q} d\boldsymbol{k} \left[e^{\mathrm{i}\boldsymbol{x}\boldsymbol{q}} \left\langle \boldsymbol{p}+\tfrac{\boldsymbol{q}}{2}\right| \hat{A} \left|\boldsymbol{p}-\tfrac{\boldsymbol{q}}{2}\right\rangle\right] e^{\frac{\boldsymbol{k}}{2}\overleftarrow{\partial}_p - \frac{\boldsymbol{q}}{2}\vec{\partial}_p} \left[e^{\mathrm{i}\boldsymbol{x}\boldsymbol{k}} \left\langle p+\tfrac{\boldsymbol{k}}{2}\right| \hat{B} \left|\boldsymbol{p}-\tfrac{\boldsymbol{k}}{2}\right\rangle\right] \\
&= \left[\int_{\mathcal{M}} d\boldsymbol{q}\, e^{\mathrm{i}\boldsymbol{x}\boldsymbol{q}} \left\langle \boldsymbol{p}+\tfrac{\boldsymbol{q}}{2}\right| \hat{A} \left|\boldsymbol{p}-\tfrac{\boldsymbol{q}}{2}\right\rangle\right] e^{\frac{\mathrm{i}}{2}\left(-\overleftarrow{\partial}_p\vec{\partial}_x + \overleftarrow{\partial}_x\vec{\partial}_p\right)} \left[\int_{\mathcal{M}} d\boldsymbol{k}\, e^{\mathrm{i}\boldsymbol{x}\boldsymbol{k}} \left\langle \boldsymbol{p}+\tfrac{\boldsymbol{k}}{2}\right| \hat{B} \left|\boldsymbol{p}-\tfrac{\boldsymbol{k}}{2}\right\rangle\right]
\end{aligned} \tag{32}$$

Here the bra- and ket- vectors in momentum space are defined modulo vectors of reciprocal lattice $\boldsymbol{g}^{(j)}$, as it is inflicted by the periodicity of the lattice. In the second line we change variables:

$$\boldsymbol{\mathcal{P}} = \boldsymbol{q}+\boldsymbol{k}, \quad \boldsymbol{\mathcal{K}} = \boldsymbol{q}-\boldsymbol{k}$$

$$\boldsymbol{q} = \frac{\boldsymbol{\mathcal{P}}+\boldsymbol{\mathcal{K}}}{2}, \quad \boldsymbol{k} = \frac{\boldsymbol{\mathcal{P}}-\boldsymbol{\mathcal{K}}}{2}$$

with the Jacobian:

$$J = \begin{vmatrix} 1 & 1 \\ -1 & 1 \end{vmatrix} = 2^D.$$

This results in the factor 2^D in the third line. Here D is the dimension of space. In the present paper it may be either 2 or 3.

Hence, the Moyal product may be defined similarly to the case of continuous space:

$$(AB)_W(\boldsymbol{x},\boldsymbol{p}) = A_W(\boldsymbol{x},\boldsymbol{p}) e^{\frac{\mathrm{i}}{2}\left(\overleftarrow{\partial}_x\vec{\partial}_p - \overleftarrow{\partial}_p\vec{\partial}_x\right)} B_W(\boldsymbol{x},\boldsymbol{p}) \tag{33}$$

Notice, that for the chosen form of the Wigner transformation on a lattice above the equality is approximate and works only if the operators $\hat{A}$, $\hat{B}$ are close to diagonal.

4.2. Lattice Groenewold Equation

Let us define the Fourier components of field $\Psi(\tau,\boldsymbol{x})$ that depends on both space coordinates $\boldsymbol{x}$ and imaginary time τ as:

$$\Psi_\alpha(\tau,\boldsymbol{x}) = \frac{1}{\sqrt{2\pi}|\mathcal{M}|^{1/2}} \int_{\mathbb{R}\otimes\mathcal{M}} d\boldsymbol{p} d\omega\, \Psi_\alpha(\omega,\boldsymbol{p}) e^{\mathrm{i}\boldsymbol{p}\boldsymbol{x}}, \qquad \alpha = 1,2.$$

The partition function of the considered models has the form:

$$Z = \int D\bar{\Psi} D\Psi\; e^{S[\Psi,\bar{\Psi}]} \qquad S[\Psi,\bar{\Psi}] = \int_{\mathbb{R}\otimes\mathcal{M}} \frac{d\omega d^D\boldsymbol{p}}{2\pi|\mathcal{M}|}\, \bar{\Psi}^T(\omega,\boldsymbol{p}) \hat{Q} \Psi(\omega,\boldsymbol{p}). \tag{34}$$

As usual, we relate operators $\hat{Q}$ and $\hat{G} = \hat{Q}^{-1}$ defined in Hilbert space $\mathcal{H}$ of functions (on $\mathbb{R}\otimes\mathcal{M}$) with their matrix elements $Q(p,q)$ and $G(p,q)$, where the $D+1$ dimensional vectors consist of the spatial parts $\boldsymbol{p},\boldsymbol{q}$ and frequencies p_{D+1}, q_{D+1}:

$$Q(p,q) = \langle p|\hat{Q}|q\rangle, \quad G(p,q) = \langle p|\hat{Q}^{-1}|q\rangle.$$

It is implied that the basis of $\mathcal{H}$ is normalized as $\langle p|q\rangle = \delta(p_{D+1} - q_{D+1})\delta^{(D)}(\boldsymbol{p} - \boldsymbol{q})$. The mentioned operators satisfy:

$$\hat{Q}\hat{G} = 1 \tag{35}$$

or, equivalently,

$$\langle p|\hat{Q}\hat{G}|q\rangle = \delta^{(D+1)}(p - q).$$

Equation (34) may be rewritten as follows;

$$S[\Psi, \bar{\Psi}] = \int_{\mathbb{R}\otimes\mathcal{M}} \frac{d^{D+1}p_1}{\sqrt{2\pi|\mathcal{M}|}} \int_{\mathbb{R}\otimes\mathcal{M}} \frac{d^{D+1}p_2}{\sqrt{2\pi|\mathcal{M}|}}\, \bar{\Psi}^T(p_1) Q(p_1, p_2) \Psi(p_2) \tag{36}$$

while the Green's function is:

$$G_{ab}(k_2, k_1) = \frac{1}{Z} \int D\bar{\Psi} D\Psi\, W_{ab}(k_2, k_1)\; e^{S[\Psi,\bar{\Psi}]} \tag{37}$$

where we introduced the Grassmann-valued Wigner function:

$$W_{ab}(p,q) = \frac{\Psi_b(p)}{\sqrt{2\pi|\mathcal{M}|}} \frac{\bar{\Psi}_a(q)}{\sqrt{2\pi|\mathcal{M}|}}. \tag{38}$$

Formally we may also define operator $\hat{W}_{ab} \equiv \hat{W}_{ab}[\Psi, \bar{\Psi}]$, whose matrix elements are equal to the Wigner function, $W_{ab}(p,q) = \langle p|\hat{W}_{ab}[\Psi, \bar{\Psi}]|q\rangle$. Indices a, b enumerate the components of the fermionic fields and we will omit them for brevity.

We may consider the $D+1$ dimensional version of the Wigner transformation of $\hat{G}$ in a similar way to that of Equation (17):

$$G_W(x,p) \equiv G_W(\tau, \boldsymbol{x}; p_{D+1}, \boldsymbol{p}) = \int_{\mathbb{R}} dq_{D+1} \int_{\mathcal{M}} d\boldsymbol{q}\, e^{\mathrm{i}(\tau q_{D+1} + \boldsymbol{x}\boldsymbol{q})} G(p + q/2, p - q/2). \tag{39}$$

Its inverse then is:

$$G(p + q/2, p - q/2) = \frac{1}{2\pi|\mathcal{M}|} \int_{\mathbb{R}} d\tau \sum_{\boldsymbol{x}\in\mathcal{O}_1} e^{-\mathrm{i}(\tau\omega + \boldsymbol{x}\boldsymbol{q})} G_W(\tau, \boldsymbol{x}; \omega, \boldsymbol{p}). \tag{40}$$

In the same way the $D+1$ dimensional Weyl symbol of $\hat{Q}$ may be defined. For $\hat{Q} = -\partial_\tau - \mathbf{H}$ we obtain:

$$Q_W(x,p) = \mathrm{i}\omega - H_W(\boldsymbol{x}, \boldsymbol{p})$$

where H_W is the D-dimensional Weyl symbol of the Hamiltonian that was defined above.

For the slowly varying external electromagnetic field and/or in the presence of weak elastic deformations the function $Q_W(x,p)$ varies slowly as a function of $\boldsymbol{x}$ on the distances of order of lattice spacing. As a result, matrix elements $\left\langle p + \frac{q}{2}\right| \hat{Q} \left| p - \frac{q}{2}\right\rangle$ and $\left\langle p + \frac{q}{2}\right| \hat{G} \left| p - \frac{q}{2}\right\rangle$ are both nonzero in the small vicinity of $\boldsymbol{q} = 0$. This imposes the bounds on the value of external magnetic field B: It should be much smaller than $1/a^2$ (where a is the typical lattice spacing). In practice this means $B \ll 1000$ Tesla. Then we are able to use Equations (33) and (35) becomes a lattice version of the Groenewold equation:

$$G_W(x,p) * Q_W(x,p) = 1 \tag{41}$$

that is,

$$1 = G_W(x,p) e^{\frac{\mathrm{i}}{2}\left(\overleftarrow{\partial}_x \vec{\partial}_p - \overleftarrow{\partial}_p \vec{\partial}_x\right)} Q_W(x,p). \tag{42}$$

The Weyl symbol Q_W of operator $\hat{Q}$ has been calculated above and is given by Equation (30). For external fields that vary slowly on the distances of the order of lattice spacing, we are able to represent it as a function of $t^{(j)}(x)$ and combination $p - A(x)$:

$$Q_W(x,p) = Q_W(t^{(j)}(x), p - A(x)).$$

4.3. Expression for the Electric Current

Let us consider the variation of the partition functionin Equation (34), corresponding to the variation of the external field A.

We note first that the action can be written as an operator trace,

$$S[\Psi,\bar{\Psi}] = \mathrm{Tr}\left(\hat{W}[\Psi,\bar{\Psi}]\hat{Q}\right), \tag{43}$$

where $\hat{W}[\Psi,\bar{\Psi}]$ is the Wigner operator corresponding to Equation (38). Vacuum expectation value, defined in the usual way,

$$\langle\hat{O}\rangle = \frac{1}{Z}\int D\bar{\Psi}D\Psi\,\hat{O}e^{S[\Psi,\bar{\Psi}]}, \tag{44}$$

gives then for the variation of the action:

$$\langle\delta S\rangle = \int_{\mathbb{R}\otimes\mathcal{M}}\frac{dp}{2\pi|\mathcal{M}|}\mathrm{tr}\left[G_W(p,x)*\partial_{p_k}Q_W(t^{(j)}(x),p-A(x))\right]\delta A_k(x) \tag{45}$$

where we used Equation (37) for the expectation value of $\hat{W}$ and expressed trace of (almost diagonal) operators through a trace of their Weyl symbols:

$$\mathrm{Tr}\hat{A}\hat{B} = \mathrm{Tr}(A_W * B_W) = \sum_x\int\frac{dp}{(2\pi)^{D+1}}\,\mathrm{tr}(A_W * B_W).$$

Now we obtain:

$$\delta\log Z = -\int_{\mathbb{R}^{D+1}}dx\int_{\mathbb{R}\otimes\mathcal{M}}\frac{dp}{2\pi|\mathcal{M}|}\,\mathrm{tr}\left[G_W(p,x)*\partial_{p_k}Q_W(t^{(j)}(x),p-A(x))\right]\delta A_k(x). \tag{46}$$

We used that for the slow varying fields:

$$\sum_{x\in\mathcal{O}_1}\approx\int_{\mathbb{R}^D}\frac{dx}{|\mathcal{V}|} \tag{47}$$

where $|\mathcal{V}|$ is the volume of the lattice cell. Additionally, we used the following relation between $|\mathcal{V}|$ and $|\mathcal{M}|$:

$$|\mathcal{V}||\mathcal{M}| = (2\pi)^D.$$

The total current, i.e., the current density integrated over the whole volume of the system, appears as the response to the variation of $A(x)$ integrated over the whole space–time:

$$\langle J^k\rangle \;=\; -T\int_{\mathbb{R}^{D+1}}dx\int_{\mathbb{R}\otimes\mathcal{M}}\frac{dp}{(2\pi)^{D+1}}\,\mathrm{tr}\left[G_W(p,x)\partial_{p_k}Q_W(p,x)\right] \tag{48}$$

Here T is temperature that is assumed to be small. We rewrite the last equation in the following way:

$$\langle J^k\rangle = -\frac{T}{(2\pi)^{D+1}}\,\mathrm{Tr}\left[G_W(p,x)\partial_{p_k}Q_W(p-A(\boldsymbol{x}))\right]. \tag{49}$$

This expression for the total current is a topological invariant, i.e., it is not changed when the system is modified continuously and provided that there are periodic boundary conditions in space. Here Tr of a Weyl symbol of an operator stands for integration over whole phase space and summation over spinor indices, if any:

$$\mathrm{Tr}\, A_W(x,p) \equiv \int_{\mathbb{R}^{D+1}} dx \int_{\mathbb{R}\otimes\mathcal{M}} dp\ \mathrm{tr}\, A_W(x,p). \tag{50}$$

5. Calculation of the Green's Function in the Inhomogeneous Lattice Models

5.1. Calculation of the Wigner Transformation of the Green's Function

In this section, we propose method of calculation of electronic Green's function in lattice models. This method is based on solving the Groenewold equation of Equation (42):

$$Q_W * G_W = 1 \tag{51}$$

for the Wigner transformation G_W as defined in Equation (39). In the following we use Equation (30) as the definition of the Weyl transform of $\hat{Q}$. Let us also introduce the following notation:

$$\overleftrightarrow{\Delta} = \frac{i}{2}\left(\overleftarrow{\partial}_x\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial}_x\right).$$

The solution may be written as follows:

$$\begin{aligned} G_W =& Q_W^{-1} + \sum_{n=1}^{\infty} \sum_{\substack{M=1 \\ \sum_j k_j = n \\ k_i \neq 0}}^{n} \frac{(-1)^M}{\Pi_{i=1}^M k_i!} \left[\ldots\left[Q_W^{-1}\overleftrightarrow{\Delta}^{k_1}Q_W\right]Q_W^{-1}\overleftrightarrow{\Delta}^{k_2}Q_W\right]Q_W^{-1}\ldots\overleftrightarrow{\Delta}^{k_M}Q_W\Big]Q_W^{-1} \\ =& \sum_{M=0}^{\infty} \underbrace{\left[\ldots\left[Q_W^{-1}(1-e^{\overleftrightarrow{\Delta}})Q_W\right]Q_W^{-1}(1-e^{\overleftrightarrow{\Delta}})Q_W\right]\ldots(1-e^{\overleftrightarrow{\Delta}})Q_W\Big]}_{M\ \ brackets} Q_W^{-1} \\ =& \sum_{M=0}^{\infty} \underbrace{\left[\ldots\left[Q_W^{-1}(1-*)Q_W\right]Q_W^{-1}(1-*)Q_W\right]Q_W^{-1}\ldots(1-*)Q_W\Big]}_{M\ \ brackets} Q_W^{-1} \end{aligned} \tag{52}$$

In the first row, the sum may be extended to the values $M = n = 0$, then the first term will be equal to Q_W^{-1}. Let us introduce the product operator $\bullet$, which works as follows being combined with the star product introduced above:

$$A \bullet B * C = (AB) * C, \quad A * B \bullet C = (A * B) \bullet C.$$

In the first equation, $*$ acts both on AB and on C while in the second equation it acts only on A and B. These rules allow us to write the above equation in a compact way:

$$\begin{aligned} G_W(x,p) =& \sum_{M=0}^{\infty} \underbrace{Q_W^{-1}(1-*)Q_W \bullet Q_W^{-1}(1-*)Q_W \bullet Q_W^{-1}\ldots(1-*)Q_W\bullet}_{M\ \bullet-products} Q_W^{-1} \\ =& \sum_{M=0}^{\infty} \left(Q_W^{-1}(1-*)Q_W \bullet\right)^M Q_W^{-1} \end{aligned} \tag{53}$$

We may write symbolically:

$$G_W(x,p) = \Big(1 - Q_W^{-1}(1-*)Q_W \bullet\Big)^{-1} Q_W^{-1} = \Big(Q_W^{-1} * Q_W \bullet\Big)^{-1} Q_W^{-1} \quad . \tag{54}$$

In order to show that Equation (52) is indeed the solution of the Groenewold equation, let us substitute Equation (55) to the star product $G_W * Q_W$ and obtain:

$$\begin{aligned} G_W * Q_W &= \sum_{M=0}^{\infty} \Big(Q_W^{-1}(1-*)Q_W \bullet\Big)^M Q_W^{-1} * Q_W \\ &= -\sum_{M=0}^{\infty} \Big(Q_W^{-1}(1-*)Q_W \bullet\Big)^M Q_W^{-1}(1-*)Q_W + \sum_{M=0}^{\infty} \Big(Q_W^{-1}(1-*)Q_W \bullet\Big)^M \\ &= -\sum_{M=0}^{\infty} \Big(Q_W^{-1}(1-*)Q_W \bullet\Big)^M + \sum_{M=0}^{\infty} \Big(Q_W^{-1}(1-*)Q_W \bullet\Big)^M \\ &= \Big(Q_W^{-1}(1-*)Q_W \bullet\Big)^0 = 1 \end{aligned} \quad . \tag{55}$$

5.2. Reconstruction of Fermion Propagator from Its Wigner Transformation

Using the definitions of the Wigner transform in Equation (39) and its inverse in Equation (40), we find the Green's function in discrete coordinate space:

$$\begin{aligned} G(x_1,x_2) &= \frac{1}{2\pi|\mathcal{M}|}\int_{\mathbb{R}\otimes\mathcal{M}} dp_1 dp_2\, G(p_1,p_2) e^{\mathrm{i}p_1x_1 - \mathrm{i}p_2x_2} \\ &= \frac{1}{4\pi^2|\mathcal{M}|^2}\int d\omega_1 d\omega_2 \int_{\mathcal{M}} d\boldsymbol{p}_1 d\boldsymbol{p}_2 \int d\tau \\ &\qquad \sum_{\boldsymbol{x}\in\mathcal{O}_1} e^{-\mathrm{i}(p_1-p_2)x + \mathrm{i}p_1x_1 - \mathrm{i}p_2x_2} G_W\left(x, \tfrac{p_1+p_2}{2}\right) \\ &= \frac{1}{2\pi|\mathcal{M}|}\int d\omega \int_{\mathcal{M}} d\boldsymbol{p} \sum_{\boldsymbol{x}\in\mathcal{O}_1} D(\boldsymbol{x} - (\boldsymbol{x}_1+\boldsymbol{x}_2)/2|\boldsymbol{p}) G_W(x,p) e^{\mathrm{i}p(x_1-x_2)}. \end{aligned} \tag{56}$$

It is assumed that $p_i = (\omega_i, \boldsymbol{p}_i)$ and $x = (\tau, \boldsymbol{x})$. Here,

$$\begin{aligned} D(\boldsymbol{y}|\boldsymbol{p}) &= \frac{1}{|\mathcal{M}|}\int_{\mathcal{M}} d\boldsymbol{p}_1 d\boldsymbol{p}_2 \int_{\mathbb{R}^D} d\boldsymbol{q}\, e^{-\mathrm{i}\boldsymbol{q}\boldsymbol{y}} \delta(\boldsymbol{p} - (\boldsymbol{p}_1+\boldsymbol{p}_2)/2)\delta(\boldsymbol{q} - (\boldsymbol{p}_1 - \boldsymbol{p}_2)) \\ &= \frac{1}{|\mathcal{M}|}\int_{\mathcal{M}} d\boldsymbol{p}_1 d\boldsymbol{p}_2\, e^{-\mathrm{i}(\boldsymbol{p}_1-\boldsymbol{p}_2)\boldsymbol{y}} \delta(\boldsymbol{p} - (\boldsymbol{p}_1+\boldsymbol{p}_2)/2). \end{aligned} \tag{57}$$

Notice, that function $D(\boldsymbol{y}|\boldsymbol{p})$ is not equal to the lattice delta function.

In this particular case, when both hopping parameters and the external electromagnetic field vary slowly, we may substitute the sum over $\boldsymbol{x}$ by an integral, and $D(\boldsymbol{y}|\boldsymbol{p})$ by $\delta(\boldsymbol{y})$. This gives:

$$G(x_1,x_2) \approx \frac{1}{2\pi|\mathcal{M}|}\int_{\mathbb{R}\otimes\mathcal{M}} dp\, G_W((x_1+x_2)/2, p) e^{\mathrm{i}p(x_1-x_2)}. \tag{58}$$

6. Total Hall Conductance as the Topological Invariant in Phase Space

6.1. Derivation in the Framework of Wigner–Weyl Formalism

We discuss here the case when $D = 2$ and slightly modify the derivation presented in [57]. Let us start from Equation (49) for the electric current. We represent the electromagnetic potential as a sum of the two contributions:

$$A = A^{(M)} + A^{(E)}$$

where $A^{(E)}$ is responsible for the electric field while $A^{(M)}$ is responsible for the magnetic field. The former is assumed to be weak, and we will keep in Equation (49) the term linear in $A^{(E)}$.

The Groenewold equation for G_W may be solved iteratively. We will keep in this solution the terms linear in $A^{(E)}$ and in its first derivative. The zeroth order term (that does not contain $A^{(E)}$ at all) is denoted $G_W^{(0)}$. Then,

$$G_W \approx G_W^{(0)} + G_W^{(0)} * (\partial_{p_m} Q_W A_m) * G_W^{(0)}. \tag{59}$$

Next, we further expand the second term in derivatives of A and write symbolically:

$$G_W \approx G_W^{(0)} + G_W^{(1)} + G_W^{(2)} \tag{60}$$

where,

$$\begin{aligned} G_W^{(1)} &= (G_W^{(0)} * \partial_{p_m} Q_W^{(0)} * G_W^{(0)}) A_m^{(E)} \\ G_W^{(2)} &= \frac{\mathrm{i}}{2}(G_W^{(0)} * \partial_{p_m} Q_W * \partial_{p_l} G_W^{(0)}) \partial_{x_l} A_m^{(E)} - \frac{\mathrm{i}}{2}(\partial_{p_l} G_W^{(0)} * \partial_{p_m} Q_W^{(0)} * G_W^{(0)}) \partial_{x_l} A_m^{(E)} \\ &= \frac{\mathrm{i}}{2}(G_W^{(0)} * \partial_{p_l} Q_W^{(0)} * G_W^{(0)} * \partial_{p_m} Q_W^{(0)} * G_W^{(0)}) F_{lm}^{(E)} \end{aligned} \tag{61}$$

where we used that $\partial_{p_l} G_W^{(0)} = -G_W^{(0)} * \partial_{p_l} Q_W^{(0)} * G_W^{(0)}$. The Q_W does not depend on the derivatives of A, therefore, it is given by:

$$Q_W = Q_W^{(0)} + \partial_{p_m} Q_W^{(0)} A_m^{(E)} \tag{62}$$

Upon the substitution of Equations (60) and (62) in Equation (49) the terms proportional to $A^{(E)}$ (i.e., with no derivatives) cancel each other. The remaining term proportional to the field strength $F^{(E)}$ is:

$$\begin{aligned} \mathrm{Tr}\left(G_W^{(2)} \partial_k Q_W^{(0)}\right) &= \frac{\mathrm{i}}{2}\mathrm{Tr}\left((G_W^{(0)} * \partial_{p_l} Q_W^{(0)} * G_W^{(0)} * \partial_{p_m} Q_W^{(0)} * G_W^{(0)}) F_{lm}^{(E)} \partial_k Q_W^{(0)}\right) \\ &= \frac{\mathrm{i}}{2}\mathrm{Tr}\left((G_W^{(0)} * \partial_{p_l} Q_W^{(0)} * G_W^{(0)} * \partial_{p_m} Q_W^{(0)} * G_W^{(0)} * \partial_k Q_W^{(0)}) F_{lm}^{(E)}\right). \end{aligned} \tag{63}$$

Here we assume that the periodic boundary conditions in space are imposed in the absence of the electric field. Then the star may be inserted to the product inside the integral: $G_W^{(2)} \partial_k Q_W^{(0)} \to G_W^{(2)} * \partial_k Q_W^{(0)}$. We come to the following representation of the average Hall current (i.e., the Hall current integrated over the whole area of the sample divided by this area $\mathcal{A}$) in the presence of electric field along the x_2 axis:

$$\langle J_1 \rangle = \frac{\mathcal{N}}{2\pi} E_2$$

Here,

$$\mathcal{N} = \frac{T\epsilon_{ijk}}{\mathcal{A}\, 3!\, 4\pi^2}\ \mathrm{Tr}\left[G_W(x,p) * \frac{\partial Q_W(x,p)}{\partial p_i} * \frac{\partial G_W(x,p)}{\partial p_j} * \frac{\partial Q_W(x,p)}{\partial p_k}\right]_{A^{(E)}=0} \tag{64}$$

with Tr defined in Equation (50). This expression for $\mathcal{N}$ is a topological invariant in phase space, i.e., it is not changed if the system is modified smoothly within a finite region distant from the boundary of the sample or from infinity if the sample is infinite. This may be checked via the direct consideration of a variation of Equation (64) with respect to the variation of Q_W.

Note that Equation (64) is distinct and has a wider application than the classical TKNN invariant [61] since it is also applicable to non homogeneous systems.

6.2. From Topological Invariant in Phase Space Expressed Through G_W, Q_W to the Standard Expression for Hall Conductance

In the previous section we showed that Hall conductance (i.e., the conductivity integrated over the whole area of the sample) is given by $\sigma_{xy} = \mathcal{N}/2\pi$ where $\mathcal{N}$ is the topological invariant in phase space. Our derivation is applicable to the general case of the inhomogeneous one-particle Hamiltonian including the case when elastic deformations are present. Our next purpose is to bring Equation (64) to the conventional expression for the Hall conductance in the case, when the non-interacting charged fermions have Hamiltonian $\mathcal{H}$.

First of all, one may show that Equation (64) is equivalent to the following representation for $\mathcal{N}$ in terms of the Green's 's function written in momentum representation:

$$\begin{aligned}\mathcal{N} &= \frac{T\,(2\pi)^3}{\mathcal{A}\,3!\,4\pi^2}\,\epsilon_{ijk}\int\prod_{l=1}^{4}d^3p^{(l)}\,\mathrm{tr}\left[G(p^{(1)},p^{(2)})\left([\partial_{p_i^{(2)}}+\partial_{p_i^{(3)}}]Q(p^{(2)},p^{(3)})\right)\right.\\ &\left.\times\left([\partial_{p_j^{(3)}}+\partial_{p_j^{(4)}}]G(p^{(3)},p^{(4)})\right)\left([\partial_{p_k^{(4)}}+\partial_{p_k^{(1)}}]Q(p^{(4)},p^{(1)})\right)\right]_{A=0}.\end{aligned}\tag{65}$$

This may be proved noticing that the functional trace of a product of two operators is expressed through their Weyl symbols as follows:

$$\mathrm{Tr}\hat{A}\hat{B} = \mathrm{Tr}(A_W * B_W) = \int d^3x \int \frac{d^3p}{(2\pi)^3}\,\mathrm{tr}(A_W * B_W).$$

Again, we need the matrix elements $\left\langle p+\frac{q}{2}\right|\hat{A}\left|p-\frac{q}{2}\right\rangle$ and $\left\langle p+\frac{q}{2}\right|\hat{B}\left|p-\frac{q}{2}\right\rangle$ to be nonzero only when q remains in the small vicinity of zero. Applying this formula several times to Equation (64) we come to Equation (65).

Secondly, for non-interacting fermions described by $\mathcal{H}$ with energy eigenstates $|n\rangle$: $\mathcal{H}|n\rangle = \mathcal{E}_n|n\rangle$, function $Q(p^{(1)},p^{(2)})$ in momentum space has the following form:

$$Q(p^{(1)},p^{(2)}) \equiv \langle p^{(1)}|\hat{Q}|p^{(2)}\rangle = \left(\delta^{(2)}(\boldsymbol{p}^{(1)}-\boldsymbol{p}^{(2)})\mathrm{i}\omega^{(1)} - \langle \boldsymbol{p}^{(1)}|\mathcal{H}|\boldsymbol{p}^{(2)}\rangle\right)\delta(\omega^{(1)}-\omega^{(2)})\tag{66}$$

where $p = (p_1,p_2,p_3) = (\boldsymbol{p},\omega)$. At the same time:

$$G(p^{(1)},p^{(2)}) = \sum_n \frac{1}{\mathrm{i}\omega^{(1)}-\mathcal{E}_n}\langle \boldsymbol{p}^{(1)}|n\rangle\langle n|\boldsymbol{p}^{(2)}\rangle\delta(\omega^{(1)}-\omega^{(2)})$$

This way we obtain:

$$\begin{aligned}\mathcal{N} = -\frac{\mathrm{i}\,(2\pi)^2}{8\pi^2\,\mathcal{A}}\sum_{n,k}\int_{\mathbb{R}} \quad & d\omega\prod_{l=1}^{4}d^2\boldsymbol{p}^{(l)}\epsilon_{ij}\\ & \mathrm{tr}\left[\frac{1}{(\mathrm{i}\omega-\mathcal{E}_n)^2}\langle \boldsymbol{p}^{(1)}|n\rangle\langle n|\boldsymbol{p}^{(2)}\rangle\left([\partial_{p_i^{(2)}}+\partial_{p_i^{(3)}}]\langle \boldsymbol{p}^{(2)}|\mathcal{H}|\boldsymbol{p}^{(3)}\rangle\right)\right.\\ & \left.\frac{1}{(\mathrm{i}\omega-\mathcal{E}_k)}\langle \boldsymbol{p}^{(3)}|k\rangle\langle k|\boldsymbol{p}^{(4)}\rangle\left([\partial_{p_j^{(4)}}+\partial_{p_j^{(1)}}]\langle \boldsymbol{p}^{(4)}|\mathcal{H}|\boldsymbol{p}^{(1)}\rangle\right)\right]_{A=0}.\end{aligned}$$

One may represent:

$$[\partial_{p_j^{(4)}}+\partial_{p_j^{(1)}}]\langle \boldsymbol{p}^{(4)}|\mathcal{H}|\boldsymbol{p}^{(1)}\rangle = i\langle \boldsymbol{p}^{(4)}|\mathcal{H}\hat{\boldsymbol{x}}_j - \hat{\boldsymbol{x}}_j\mathcal{H}|\boldsymbol{p}^{(1)}\rangle = i\langle \boldsymbol{p}^{(4)}|[\mathcal{H},\hat{\boldsymbol{x}}_j]|\boldsymbol{p}^{(1)}\rangle.$$

By operator $\hat{\boldsymbol{x}}$ we understand $i\partial_{\boldsymbol{p}}$ acting on the wavefunction written in momentum representation:

$$\hat{x}_j\Psi(\boldsymbol{p}) = \langle \boldsymbol{p}|\hat{x}_j|\Psi\rangle = i\partial_{p_j}\langle \boldsymbol{p}|\Psi\rangle = \mathrm{i}\partial_{p_j}\Psi(\boldsymbol{p}).$$

Then, for example,

$$\hat{x}_j\delta^{(2)}(\boldsymbol{q}-\boldsymbol{p}) = \langle \boldsymbol{p}|\hat{x}_j|\boldsymbol{q}\rangle = \mathrm{i}\partial_{p_j}\langle \boldsymbol{p}|\boldsymbol{q}\rangle = \mathrm{i}\partial_{p_j}\delta^{(2)}(\boldsymbol{p}-\boldsymbol{q}) = -\mathrm{i}\partial_{p_j}\langle \boldsymbol{q}|\boldsymbol{p}\rangle.$$

Therefore, we can write

$$\hat{x}_j|\boldsymbol{p}\rangle = -\mathrm{i}\partial_{p_j}|\boldsymbol{p}\rangle.$$

Notice, that the sign minus here is counter-intuitive because the operator $\hat{\boldsymbol{x}}$ is typically associated with $+\mathrm{i}\partial_{\boldsymbol{p}}$. We should remember, however, that with this latter representation the derivative acts on $\boldsymbol{p}$ in the bra-vector $\langle \boldsymbol{p}|$ rather than on $\boldsymbol{p}$ in $|\boldsymbol{p}\rangle$. Above we have shown that the sign is changed when the derivative is transmitted to $\boldsymbol{p}$ of $|\boldsymbol{p}\rangle$.

Thus we have:

$$\begin{aligned}\mathcal{N} &= \frac{\mathrm{i}\,(2\pi)^2}{8\pi^2\,\mathcal{A}}\sum_{n,k}\int_{\mathbb{R}} d\omega\,\epsilon_{ij}\,\frac{\langle n|[\mathcal{H},\hat{x}_i]|k\rangle\langle k|[\mathcal{H},\hat{x}_j]|n\rangle}{(\mathrm{i}\omega-\mathcal{E}_n)^2(\mathrm{i}\omega-\mathcal{E}_k)}\\ &= -\frac{2\mathrm{i}\,(2\pi)^3}{8\pi^2\,\mathcal{A}}\sum_{n,k}\epsilon_{ij}\,\frac{\theta(-\mathcal{E}_n)\theta(\mathcal{E}_k)}{(\mathcal{E}_k-\mathcal{E}_n)^2}\langle n|[\mathcal{H},\hat{x}_i]|k\rangle\langle k|[\mathcal{H},\hat{x}_j]|n\rangle. \qquad (67)\end{aligned}$$

The last expression is just the conventional expression for the Hall conductance (multiplied by 2π) for the given system. Notice, that it is valid for the slowly varying electromagnetic potential only (the potential almost does not vary at the distance of order of lattice spacing). Then operator $\hat{\boldsymbol{x}} = i\frac{\partial}{\partial \boldsymbol{p}}$ has the meaning of the coordinate operator.

7. Integer Quantum Hall Effect in the Presence of Varying Magnetic Field and Elastic Deformations

7.1. Constant Magnetic Field and Constant Hopping Parameters

In this subsection we repeat the standard derivation of the Hall conductance in the noninteracting $2D$ models with a constant magnetic field perpendicular to the surface, and constant hopping parameters. It is assumed here that the magnetic field $\boldsymbol{B}$ is sufficiently weak, so that $|\boldsymbol{B}|a^2 \ll 1$, where a is the lattice spacing. Then the Hall conductivity may be represented as $\mathcal{N}/(2\pi)$, where $\mathcal{N}$ is given above in Equation (67).

In order to calculate the value of $\mathcal{N}$ we decompose the coordinates x_1, x_2 in relative coordinates ξ_i (with bounded values) and center coordinates X_i (the unbounded part):

$$\hat{x}_1 = \hat{\xi}_1 + \hat{X}_1, \qquad \hat{x}_2 = \hat{\xi}_2 + \hat{X}_2 \qquad (68)$$

where,

$$\hat{\xi}_1 = -\frac{\hat{p}_2 - Bx_1}{B}, \qquad \hat{X}_1 = \frac{\hat{p}_2}{B} \qquad (69)$$

$$\hat{\xi}_2 = -\frac{\hat{p}_1}{B}, \qquad \hat{X}_2 = \frac{\hat{p}_1 - Bx_2}{B}. \qquad (70)$$

Then the commutation relations follow:

$$[\hat{\xi}_1,\hat{\xi}_2] = \frac{i}{B}, \quad [\hat{X}_1,\hat{X}_2] = -\frac{i}{B}, \qquad [\hat{\xi}_i,\hat{X}_j] = 0 \quad \forall i,j. \qquad (71)$$

Since the Hamiltonian is a function of ξ_i only (in Landau gauge)

$$\mathcal{H} \equiv \mathcal{H}(\xi_1,\xi_2), \qquad (72)$$

its commutator with X_j vanishes:

$$[\mathcal{H},\hat{X}_1] = [\mathcal{H},\hat{X}_2] = 0. \qquad (73)$$

We use these relations to obtain:

$$\begin{aligned}\mathcal{N} &= -\frac{2\mathrm{i}\,(2\pi)^3}{8\pi^2\,\mathcal{A}}\sum_{n,k}\Big[\frac{1}{(\mathcal{E}_k-\mathcal{E}_n)^2}\langle n|[\mathcal{H},\hat{\xi}_i]|k\rangle\langle k|[\mathcal{H},\hat{\xi}_j]|n\rangle\Big]_{A=0}\epsilon_{ij}\,\theta(-\mathcal{E}_n)\theta(\mathcal{E}_k)\\ &= \frac{2\mathrm{i}\pi}{\mathcal{A}}\sum_{n,k}\epsilon_{ij}\Big[\langle n|\hat{\xi}_i|k\rangle\langle k|\hat{\xi}_j|n\rangle\Big]_{A=0}\theta(-\mathcal{E}_n)\theta(\mathcal{E}_k)\\ &= \frac{2\mathrm{i}\pi}{\mathcal{A}}\sum_{n}\Big[\langle n|[\hat{\xi}_1,\hat{\xi}_2]|n\rangle\Big]_{A=0}\theta(-\mathcal{E}_n)\\ &= -\frac{2\mathrm{i}\pi}{\mathcal{A}\,B}\sum_{n}\langle n|n\rangle\theta(-\mathcal{E}_n).\end{aligned} \tag{74}$$

Momentum p_2 is a good quantum number, and it enumerates the eigenstates of the Hamiltonian:

$$\mathcal{H}|n\rangle = \mathcal{H}(\hat{p}_1,\hat{p}_2-B\hat{x}_1)|p_2,m\rangle = \mathcal{E}_m(p_2)|p_2,m\rangle,\ m\in Z.$$

We assume that the size of the system is $L\times L$. This gives,

$$\mathcal{N} \;=\; -\frac{(2\pi)}{\mathcal{A}}\sum_m\int\frac{dp_2L}{2\pi}\,\frac{1}{B}\theta(-\mathcal{E}_m(p_2)). \tag{75}$$

Average value $\langle\boldsymbol{x}\rangle = p_y/B$ plays the role of the center of orbit, and this center should belong to the interval $(-L/2,L/2)$. This gives,

$$\mathcal{N} \;=\; N\,\mathrm{sign}(-B). \tag{76}$$

Here $\mathcal{A}=L^2$ is the area of the system while N is the number of occupied branches of the spectrum. In conventional systems they are counted from the neutrality point, and this way we come to the standard expression for the Hall conductance of the fermionic system in the presence of constant magnetic and electric fields. On the other hand, in the exact treatment of the honeycomb lattices (e.g., for graphene) the levels are to be counted from the edge of the band. This introduces into consideration levels with large negative Chern numbers [90]. As a result, close to half filling the conductivity is given by the 'Dirac-Landau level index' [91] counted from zero energy.

However, our approximation in Equation (47) is probably valid only up to $|E_F|\sim t$, i.e., in the region between the innermost van Hove singularities [91]. Thus we cannot correctly take into account the above mentioned deep lying levels. On the other hand, for the constant magnetic field in the absence of elastic deformations their contribution is known as it cancels precisely that of $\mathcal{N}/(2\pi)$ at the half filling. We denote this term by $\sigma_{xy}^{(0)} = \mathcal{N}^{(0)}/(2\pi)$, and the final expression for the Hall conductivity becomes:

$$\sigma_{xy} = \frac{\mathcal{N}}{2\pi} - \sigma_{xy}^{(0)}, \tag{77}$$

which we can also rewrite as:

$$\sigma_{xy} = \frac{N'}{2\pi}\mathrm{sign}(-B) \tag{78}$$

where N' is counted from the half filling (the LLL being occupied contributes with the factor $1/2$).

7.2. Constant Magnetic Field and Weakly Varying Hopping Parameters

Let us consider the case when:

$$t^{(j)}(\boldsymbol{x}) = t_0^{(j)}e^{\boldsymbol{x}\boldsymbol{f}},$$

(with some constant spatial vector $\boldsymbol{f}$) for specific Hamiltonian, which we define by its Weyl symbol:

$$\mathcal{H}_W(\boldsymbol{x},\boldsymbol{p}) = \sum_{j=1}^{M} \begin{pmatrix} -\mu/N & t^{(j)}(\boldsymbol{x})\, e^{\mathrm{i}(p\boldsymbol{b}^{(j)} - A^{(j)}(x))} \\ t^{(j)}(\boldsymbol{x})\, e^{-\mathrm{i}(p\boldsymbol{b}^{(j)} - A^{(j)}(\boldsymbol{x}))} & -\mu/N \end{pmatrix} \tag{79}$$

and here μ is the chemical potential. As above, we decompose the coordinates x_1, x_2 into relative coordinates ξ_i and the center coordinates X_i using Equation (68). We still have the commutation relations in Equation (71). However, since $t^{(j)}(\boldsymbol{x})$ now depend on coordinates, the Hamiltonian does not commute anymore with X_1, X_2. Instead we have:

$$\mathcal{H}_W * X_{W,j} - X_{W,j} * \mathcal{H}_W = \frac{i}{2B}\epsilon^{ji} f_i\,(\mathcal{H}_W - \mu). \tag{80}$$

Here,

$$\hat{X}_1 = \frac{\hat{p}_2}{B}, \qquad \hat{X}_2 = \frac{\hat{p}_1 - B\hat{x}_2}{B} \tag{81}$$

and $X_{W,i}$ is their Weyl symbols. This gives,

$$\mathcal{H}\hat{X}_j - \hat{X}_j\mathcal{H} = \frac{\mathrm{i}}{2B}\epsilon^{ji} f_i\,(\mathcal{H} - \mu). \tag{82}$$

Then for $n \neq k$ we obtain:

$$\langle n|\mathcal{H}\hat{X}_j - \hat{X}_j\mathcal{H}|k\rangle = 0$$

and we come again to Equation (74)

$$\mathcal{N} = -\frac{2\pi}{\mathcal{A}\,B}\sum_n \langle n|n\rangle\theta(-\mathcal{E}_n) = -\frac{2\pi}{B}\,\rho \tag{83}$$

where now ρ is the average density of occupied states.

If we require, in addition, that $t^{(j)}$ does not depend on y and depends on x only, then momentum p_y is still a good quantum number, and Equation (75) is applicable. As above, we will obtain:

$$\mathcal{N} \quad = \quad N\,\mathrm{sign}(-B). \tag{84}$$

Recall that $\mathcal{A} = L^2$ is the area of the system while N is the number of the occupied branches of spectrum. One can see, that in the presence of constant magnetic field and the hopping parameters that depend on x_1 and do not depend on x_2 (i.e., $t^{(j)}(\boldsymbol{x}) = t_0^{(j)} e^{x_1 f_1}$) the Hall conductivity is given by the same standard value as for the constant hopping parameters. Here we also assume that weak elastic deformations are not able to modify the contribution $\sigma_{xy}^{(0)}$ of the deep Landau Levels, so that Equation (77) remains valid, and we come finally to the conductivity (averaged over the area of the sample) as:

$$\sigma_{xy} \quad = \quad \frac{N'}{2\pi}\,\mathrm{sign}(-B), \tag{85}$$

where the number of occupied branches of spectrum N' is counted from the half-filling.

7.3. Weak Variations of Magnetic Field and Hopping Parameters

Without elastic deformations the constant external magnetic field results in the appearance of Landau Levels. Each Landau level is highly degenerate. Weak elastic deformations result in the appearance of the emergent gauge field and anisotropic Fermi velocity. Both emergent gauge field and anisotropic Fermi velocity vary in space. The latter may be interpreted, in addition, as the emergent gravitational field (see [80,81]). Both emergent fields result in a certain modification of

the band structure. It is discussed, for example, in [82], where particular cases were considered. In these particular cases the elastic deformations modify the Fermi velocity and degeneracy of Landau Levels. In a general case it is expected that the degeneracy of the Landau Levels may be lifted by both spatial variations of magnetic field and elastic deformations, so that the energy levels become thick. The overall number of the one-electron states in each Landau Level may be affected as well. When the elastic deformations and variations of magnetic field become more strong, we expect that the band structure may be modified more crucially. In particular, certain Landau Levels may merge and form the common strip of the states. The gaps between different strips may disappear and, possibly, appear again in the different ranges of energies if the variations of fields become stronger.

In Section 7.1 we considered a constant magnetic field and hopping parameters. It was noticed there that although the deep LL of the honeycomb lattices (those near the edge of the band) could not be taken correctly in our approximation, their contribution was known and could be used, given by the value of Equation (64) at half filling. Since those levels are deep, they cannot be affected by weak elastic deformations and weak variations of magnetic field, which modify only the contributions of the energy levels sufficiently close to half filling.

Let us suppose, that the magnetic field is slowly varying in the limited region of the sample, such that it approaches constant value B close to the boundary of the sample. Then we come to the following result valid in the presence of varying elastic deformations as well. The total average Hall conductivity (i.e., the Hall conductivity integrated over the area $\mathcal{A}$ of the sample and divided by this area) has the form of:

$$\sigma_{xy} = \frac{1}{2\pi}\left(\mathcal{N} - \mathcal{N}^{(0)}\right) \tag{86}$$

where $\mathcal{N}$ is the topological invariant in phase space:

$$\mathcal{N} = \frac{T}{\mathcal{A}\, 3!\, 4\pi^2}\,\epsilon_{ijk}\int_{\mathbb{R}^{D+1}} dx \int_{\mathbb{R}\otimes\mathcal{M}} dp\ \mathrm{tr}\left[G_W(p,x) * \frac{\partial Q_W(p,x)}{\partial p_i} * \frac{\partial G_W(p,x)}{\partial p_j} * \frac{\partial Q_W(p,x)}{\partial p_k}\right]. \tag{87}$$

In graphene, $\mathcal{N}^{(0)}$ is the value of Equation (87) at half filling and unlike $\mathcal{N}$ it is to be calculated with a constant magnetic field and without elastic deformations.

The value of $\mathcal{N}$ may be affected by variations of magnetic field and by elastic deformations. The resulting Hall conductivity becomes vanishing at half filling when those variations of magnetic field are sufficiently weak as well as the elastic deformations. At the same time, we do not have any reasons to suppose that the sufficiently strong elastic deformations/variations of magnetic field cannot lead to the deviation of Hall conductivity from zero at half filling.

7.4. Analytical Elastic Deformations In Graphene

In graphene, the relation between t, A, and u is given by [79],

$$t^{(j)}(\boldsymbol{x}) = t[1 - \beta u_{kl}(\boldsymbol{x}) b_k^{(j)} b_l^{(j)}], \qquad A_1 = -\frac{\beta}{a}\, u_{12} \quad A_2 = \frac{\beta}{2a}\,(u_{22} - u_{11}). \tag{88}$$

With elementary translations given by Equation (28), the nontrivial part of $t^{(j)}$ is:

$$u_{kl}(\boldsymbol{x}) b_k^{(j)} b_l^{(j)} = \frac{a^2}{4}\begin{pmatrix} 4u_{11} \\ u_{11} + 2\sqrt{3}u_{12} + 3u_{22} \\ u_{11} - 2\sqrt{3}u_{12} + 3u_{22} \end{pmatrix}. \tag{89}$$

Requiring that,

$$t^{(1)}(\boldsymbol{x}) = t^{(2)}(\boldsymbol{x}) = t^{(3)}(\boldsymbol{x}), \tag{90}$$

is consistent with Section 7.2, thus we come to the Cauchy–Riemann conditions:

$$\frac{\partial u_1}{\partial x_1} = \frac{\partial u_2}{\partial x_2}, \qquad \frac{\partial u_2}{\partial x_1} = -\frac{\partial u_1}{\partial x_2}$$

that is $h(z) \equiv u_1(z) + \mathrm{i}u_2(z)$ is analytic as a function of $z = x_1 + \mathrm{i}x_2$. (There is another solution of (90)

$$\partial_1 u_1 = -2 - \partial_2 u_2, \quad \partial_1 u_2 = \partial_2 u_1,$$

which however brakes the smallness condition $\beta|u_{ij}| \ll 1$.)

In this case we have a vanishing emergent gauge field, while up to the terms linear in the derivatives of the hopping parameters the results of Section 7.2 give:

$$\mathcal{N} = -\frac{2\pi}{B}\rho \tag{91}$$

where ρ is the average density of occupied states. On the other hand, the results of Section 7.2 ensure that any weak variations of both hopping parameters and magnetic field give:

$$\mathcal{N} = -N \operatorname{sign} B$$

where N is the number of occupied Landau Levels (now instead of the degenerate Landau level we may have the energy band parametrized by certain parameters). Comparing this result with Equation (91) we obtain:

$$\rho = \frac{|B|}{2\pi}N$$

for the elastic deformations given by an analytical function of coordinates (i.e., when the emergent magnetic field is absent).

8. Conclusions and Discussions

In the present paper we proceeded with the development of Wigner–Weyl formalism for tight-binding models of solid state physics (or, equivalently, for the lattice regularized quantum field theory). We extended the previous works made in this direction [30–35,56–58]. The developed technique was applied to the class of inhomogeneous models that include, in particular, the tight-binding model of graphene in the presence of both inhomogeneous magnetic field and nontrivial elastic deformations. It is worth mentioning that the majority of our results may be applied to other models of solid state physics. Apart from the family of two-dimensional honeycomb lattice materials (graphene, germanene, silicene, etc), all rectangular lattice crystals, both in two and three dimensions could be treated with developed methods, if described within nearest-neighbor approximation. In these cases the electrons may jump only between the nearest neighbors, and there is the Z_2 sublattice symmetry. The lattice consists of the two sublattices $\mathcal{O}_1$ and $\mathcal{O}_2$. For each $\boldsymbol{x} \in \mathcal{O}_1$ site $\boldsymbol{x} + \boldsymbol{b}^{(j)} \in \mathcal{O}_2$ with fixed vectors $\boldsymbol{b}^{(j)}$, where $j = 1, 2, ..., M$. For the honeycomb lattice $M = 3$, for the $2D$ rectangular lattice $M = 4$, for the $3D$ rectangular lattice $M = 8$. Among the mentioned models only the two-dimensional model on the honeycomb lattice sufficiently and accurately describe the real system (graphene). Therefore, the emphasis is on the application to the physics of graphene. The particular interest in our study was the consideration of the arbitrarily varying external magnetic field and nonhomogeneous elastic deformations.

We obtained the following main results:

1. We calculated the Weyl symbol of the lattice Dirac operator (i.e., the operator $\hat{Q}$ that enters the action $\sum_{x,y} \bar{\Psi}_x Q_{x,y} \Psi_y$) in the presence of both elastic deformations and slowly varying external electromagnetic field:

$$Q_W = i\omega - t \sum_j \left(1 - \beta u_{kl}(\boldsymbol{x}) b_k^{(j)} b_l^{(j)}\right) \begin{pmatrix} 0 & e^{\mathrm{i}(\boldsymbol{p}\boldsymbol{b}^{(j)} - A^{(j)}(\mathbf{r}))} \\ e^{-i(\boldsymbol{p}\boldsymbol{b}^{(j)} - A^{(j)}(\mathbf{r}))} & 0 \end{pmatrix} \tag{92}$$

where u_{ij} is the tensor of elastic deformations while,

$$A^{(j)}(\boldsymbol{x}) = \int_{\boldsymbol{x}-\boldsymbol{b}^{(j)}/2}^{\boldsymbol{x}+\boldsymbol{b}^{(j)}/2} \boldsymbol{A}(\boldsymbol{y}) d\boldsymbol{y}.$$

It was assumed that the variation of electromagnetic field $A(\boldsymbol{x})$ at the distances of order of the lattice spacing may be neglected. In practice this corresponded to magnetic fields B that obeyed $Ba^2 \ll 1$. In practice this bound read $B \ll 1000$ Tesla. Additionally, we required that the typical wavelenth of the external electromagnetic field was much larger than the lattice spacing. This did not allow the use of Equation (92) for matter interacting with the X-rays with the wavelengths of the order of several Angstroms and smaller;

2. The Wigner transformation of the electron propagator in the presence of the slowly varying magnetic field and arbitrary elastic deformations may be calculated using the following expression:

$$G_W(x,p) = \sum_{M=0\ldots\infty} \underbrace{\left[\ldots\left[Q_W^{-1}(1 - e^{\overleftrightarrow{\Delta}})Q_W\right]Q_W^{-1}(1 - e^{\overleftrightarrow{\Delta}})Q_W\right]\ldots(1 - e^{\overleftrightarrow{\Delta}})Q_W\Big]}_{M \;\; brackets} Q_W^{-1} \tag{93}$$

where

$$\overleftrightarrow{\Delta} = \frac{i}{2}\left(\overleftarrow{\partial}_x \overrightarrow{\partial}_p - \overleftarrow{\partial}_p \overrightarrow{\partial}_x\right);$$

3. The electron propagator in the presence of a slowly varying electromagnetic field and elastic deformations may be expressed through the Wigner transformed Green's function as follows:

$$G(x_1, x_2) \approx \frac{1}{2\pi|\mathcal{M}|} \int dp G_W((x_1 + \boldsymbol{x}_2)/2, p) e^{-ip(x_1 - \boldsymbol{x}_2)} \tag{94}$$

where $|\mathcal{M}|$ is the area of the Brillouin zone.

4. The total average Hall conductivity (i.e., the Hall conductivity integrated over the area of the sample and divided by this area) in the presence of varied weak magnetic field $\mathcal{B} \ll 1/a^2$ and elastic deformations had the form of:

$$\sigma_{xy} = \frac{\mathcal{N}}{2\pi} - \frac{\mathcal{N}^{(0)}}{2\pi} \tag{95}$$

where $\mathcal{N}$ is the topological invariant in phase space, which is the generalization of the classical TKNN invariant [61] since it is also applicable to non homogeneous systems:

$$\mathcal{N} = \frac{T}{\mathcal{A}\, 3!\, 4\pi^2} \epsilon_{ijk} \int_{\mathbb{R}^{D+1}} dx \int_{\mathbb{R}\otimes\mathcal{M}} dp \; \mathrm{tr}\left[G_W(p,x) * \frac{\partial Q_W(p,x)}{\partial p_i} * \frac{\partial G_W(p,x)}{\partial p_j} * \frac{\partial Q_W(p,x)}{\partial p_k}\right], \tag{96}$$

here $\mathcal{A}$ is the area of the sample. For the conventional systems, like those with the one particle Hamiltonian $p^2/2m$ (in the absence of magnetic field), when the spectrum was bounded from below, $\mathcal{N}^{(0)} = 0$, but in graphene it was given by the value of $\mathcal{N}$ at half filling (with a constant magnetic field and without elastic deformations). Thus, in the presence of a constant magnetic field at half filling the Hall conductivity vanished. The value of $\mathcal{N}^{(0)}$ originated from the

contribution of the deep Landau Levels was not affected by variations of magnetic field and by elastic deformations. At the same time, the value of $\mathcal{N}$ may, in principle, be affected by them. The resulting expression worked for the magnetic field slowly varying in the limited region of the sample, such that it approached constant value B close to the boundary of the sample. The applied electric field resulted from the electric potential varying in space. The latter may be considered also as a variation in space of chemical potential or Fermi energy. Voltage U appeared as the difference of the Fermi energy between the edges of the sample. Then the Hall current is given by:

$$I_{xy} = \frac{\mathcal{N} - \mathcal{N}^{(0)}}{2\pi} U \tag{97}$$

(Recall that we used the relativistic system of units. To obtain expression for the Hall current in an ordinary system of units we have to multiply the above expression by the unity of conductance $\frac{e^2}{\hbar}$);

5. The above mentioned representation of the average Hall conductivity through the topological invariant in phase space allowed us to prove that in graphene it was robust to both sufficiently weak variations of magnetic field and sufficiently weak elastic deformations. It is worth mentioning that both mentioned variations of magnetic field and elastic deformations were to be concentrated within the finite region far from the boundary of the sample. Under these conditions Equation (96) was not changed for the smooth variations of lattice Hamiltonian (for the proof see Appendix D in [57]);
6. The special case of elastic deformations was considered, when the emergent gauge field in graphene was absent. It was shown that the corresponding deformations were given by the arbitrary analytical functions of coordinates. Namely, the condition of the absence of emergent gauge field was equivalent to the Riemann–Cauchy conditions for the displacement function u_i, $i = 1, 2$. As a result the function $u(z) = u_1(z) + iu_2(z)$ appeared to be an analytical function of $z = x_1 + i\boldsymbol{x}_2$, where $\boldsymbol{x}_i$ were the coordinates of the carbon atoms in the unperturbed honeycomb lattice. Under these circumstances for the constant magnetic field B the Hall current was given by:

$$I_{xy} = -\frac{N' U}{2\pi} \operatorname{sign} B \tag{98}$$

where U is voltage while N' is the number of occupied Landau Levels (counted from the half filling). Now unlike the case of the unperturbed graphene the Landau Levels may already not be degenerated.

It is worth mentioning that our results were obtained in the absence of both disorder and Coulomb interactions. In the presence of disorder the Hall current density is pushed towards the boundary. However, its total value is generally believed to remain the same. This is proved, at least, in the absence of elastic deformations when the magnetic field is homogeneous It appears that the neutrality point (when chemical potential is in the middle of the Lowest Landau Level) corresponds to vanishing Hall conductivity. Again, the Landau Levels (LL) participate in the QHE being counted from the neutrality point. This occurs now because close to the boundary, the branches of energy spectrum above and below the neutrality point behave differently. Energies of those branches above the neutrality point are increased while energies of the branches situated below it are decreased. As a result there is no crossing of the energy levels with the Fermi level on the boundary at neutrality point [72], and, consequently, there are no gapless edge states that are to be the carriers of the Hall current. This shows that weak disorder does not cause a jump in the value of total conductance. The average conductivity (the conductivity integrated over the area of the sample divided by this area) is given by $\sigma_{xy} = \frac{N'}{2\pi} \operatorname{sign} B$, where N' is the number of occupied electronic energy levels counted from the half filling. Therefore, for graphene, N' may be both negative and positive. Moreover, for the chemical potential just above zero only half of the Lowest Landau Level contributed to the Hall conductance. Therefore, in this case $N' = \frac{1}{2} g_s g_v = \frac{4}{2} = 2$. We also supposed that weak variations of magnetic field and weak elastic deformations do not change this property, and the value of the average Hall conductivity

should remain the same until the topological phase transition to the state with a different value of Hall conductivity is encountered. For sufficiently strong elastic deformations and/or variations of magnetic field the very notion of Landau Levels may lose its sense, but the values of Hall conductivity may still remain nonzero.

We expected that the Hall current would be robust to the weak Coulomb interactions (at least in the presence of a sufficient amount of disorder) although the detailed investigation of this issue is still to be performed (see [58] and references therein), especially in the presence of elastic deformations and variations of magnetic field. At the same time, the clean samples of graphene (very weak disorder) exhibit the Fractional Quantum Hall Effect (FQHE) due to the Coulomb interactions. The investigation of this issue remains out of the scope of the present paper although we expect that Equation (96) may still be related somehow to the description of the FQHE.

We suppose that the results obtained here may be used further in the investigation of various properties of graphene. In particular, Equations (92) and (93) determined electron propagator in the complete tight-binding model in the presence of both elastic deformations and slowly varying external electromagnetic field. This propagator may be used in those investigations of transport properties that require use of the complete tight-binding model, i.e., when the low energy effective continuum field theory of graphene is not sufficient for the solution of a particular problem. Since the form of the obtained expressions is rather complicated, and the result of Equation (93) is represented in the form of the infinite series, the practical applications of the obtained formulas are likely to require certain numerical techniques.

We also expect that the practical calculation of Hall conductivity using Equation (96) may require the application of certain numerical procedures. The possible problem to be solved using this expression is the calculation of Hall conductivity in the presence of varying magnetic field and/or varying elastic deformations. For the constant external magnetic field and without elastic deformations the result for the Hall conductance is well known. According to our results, weak elastic deformations and weak variations of magnetic field could not affect the value of the total Hall current. However, when the variations become stronger, the system may undergo a topological phase transition to the state with different value of Hall conductance. We may determine the critical values of magnetic field variation and/or deformation tensor variation using the direct evaluation of an integral in Equation (96). Both numerical and analytical methods of this evaluation await for their development.

It is worth mentioning, that the simplified version of Equation (96) (discussed in [30]) that appeared when G_W did not depend on coordinates, represents the generator of the co-homology group $\mathcal{H}^{(3)}(\mathcal{M})$, where $\mathcal{M}$ is momentum space. Equation (96) also awaits for the interpretation using the language of algebraic topology. At the present moment we noticed only that this topological invariant certainly played a role in the classification of the homotopic classes of maps $G : \mathcal{M} \otimes \mathcal{R} \to GL(2, C)$, where $\mathcal{R}$ is the coordinate space with certain boundary conditions while $\mathcal{M}$ is momentum space.

We would like to notice again, that the theory presented here is valid for the slowly varying potentials, which is consistent with the requirement $Ba^2 \ll 1$. It would be interesting to extend the Wigner–Weyl formalism to the precise consideration of the tight-binding model of graphene in the presence of strong magnetic fields $B \sim 1/a^2$. Another challenge is an extension of our results to the investigation of the fractional Hall effect.

The authors are grateful for the ideas and comments, as well as the collaboration in the adjacent fields, of M. Suleymanov, Xi Wu, and Chunxu Zhang. M.A.Z. is indebted for the valuable discussions to G.E.Volovik.

Author Contributions: Authors contribute equally to this work.

Funding: The present research received no external funding.

Conflicts of Interest: The authors declare no conflict of interest.

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