Quantum Flatland and Monolayer Graphene from a Viewpoint of Geometric Algebra

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Quantum mechanical properties of the graphene are, as a rule, treated within the Hilbert space formalism. However a different approach is possible using the geometric algebra, where quantum mechanics is done in a real space rather than in the abstract Hilbert space. In this article the geometric algebra is applied to a simple quantum system, a single valley of monolayer graphene, to show the advantages and drawbacks of geometric algebra over the Hilbert space approach. In particular, 3D and 2D Euclidean space algebras $Cl_{3,0}$ and $Cl_{2,0}$ are applied to analyze relativistic properties of the graphene. It is shown that only three-dimensional $Cl_{3,0}$ rather than two-dimensional $Cl_{2,0}$ algebra is compatible with a relativistic flatland.

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1. Introduction

Graphene is a two-dimensional crystal made up of carbon atoms. The intense interest in graphene is stimulated by its potential application in the construction of novel nanodevices based on relativistic physics, or at least with a large ingredient of relativity [1-4]. From theoretical aspects the most interesting is the Dirac-like behavior of electrons in 2D lattice, including a linear dispersion law, the Klein tunnelling through potential barriers, confinement and integer Hall effect. The standard mathematical language for this purpose is based on the Hilbert space with such mathematical objects as complex state vectors, matrix operators etc. A pedagogical overview of the single valley graphene within the Hilbert space formalism has recently appeared in [5], which can serve as an introduction to the subject. In this paper a different mathematical language known as geometric or the Clifford algebra [6–10], which is formulated in real spaces, will be used in the analysis of quantum properties of graphene. Examples of applications of geometric algebra (GA) to nanostructures can be found, for example, in [11–15].

As known, the Hilbert space as a such does not carry any attributes of a physical space. The space properties are brought into Lagrangian or Hamiltonian to satisfy symmetry requirements of the space or governing laws for physical objects. In contrast, the selection of a particular GA to solve the physical problem automatically takes into account the dimension, signature and symmetry relations of the space or spacetime. This is best visible from the 8-periodicity table of GA [8], which predetermines types of irreducible matrices, or the Clifford groups that should be used in solving the problem. So, if space dimension has been reduced, one is automatically forced to change the type of Clifford algebra and its irreducible representation.

On the other hand, if the problem was formulated in the Hilbert space terms then, generally, the neglect of one of space dimensions does not spoil the Hilbert space. Of course, one has to reconsider the problem with respect to its symmetry properties from the point of view of group theory, since as a rule a new problem becomes reducible to a simpler one. However, the situations may arise when the mechanical reduction of dimension of the Hilbert space makes the problem ill-posed. For example, this happens with the massless Dirac equation, the basis of which consists of 4×4 complex Dirac matrices, γ^0 and γ^i with i = 1, 2, 3. If one assumes that the electron mass m = 0 and $\gamma^3 = 0$, then one gets the relativistic massless Dirac equation for graphene. However, it appears that in this case one cannot construct the generators of the new algebra [16].

On the other hand, if the Clifford algebra is applied to the problem it will automatically insure correct symmetry of lower dimensional spaces and correct form of generators, because of strict group subordination of lower dimensional subalgebras. Accordingly, the respective lower-dimensional massless Dirac equations, if they exist, will have a correct form.

In this article we shall rely on the GA hierarchy $Cl_{1,3} \rightarrow Cl_{3,0} \rightarrow Cl_{2,0}$ in transforming the equations from the complex matrix representation in the Hilbert space to GA multivectors. The simplest possible case of a single Dirac valley that is described by 2×2 complex matrix is considered. In Sect. 2, the properties of graphene in terms of 3D space algebra $Cl_{3,0}$ are considered. In Sect. 3 the same problem is analyzed in 2D with $Cl_{2,0}$ algebra.

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2. Graphene with Cl_{3,0} 2.1. Graphene Hamiltonian in Cl_{3,0}

 $Cl_{3,0}$ algebra describes Euclidean 3D space and simultaneously is an even subalgebra of relativistic spacetime algebra $Cl_{1,3}$, i.e., the isomorphism $Cl_{1,3}^+ \approx Cl_{3,0}$ is satisfied. The basis vectors of $Cl_{3,0}$ have positive signature: $\sigma_1^2 = \sigma_2^2 = \sigma_3^2 = 1$. The vectors σ_i play the role of space coordinates. The notation reflects the fact that σ_i 's are isomorphic to the Pauli matrices. Therefore, the basis vectors with different indices anticommute, $\boldsymbol{\sigma}_i \boldsymbol{\sigma}_j + \boldsymbol{\sigma}_j \boldsymbol{\sigma}_i = 0$. The orthogonal planes in 3D space are described by bivectors $I\boldsymbol{\sigma}_1 = \boldsymbol{\sigma}_2\boldsymbol{\sigma}_3$, $I\sigma_2 = \sigma_3\sigma_1$, and $I\sigma_3 = \sigma_1\sigma_2$. With scalar and pseudoscalar $I = \sigma_1\sigma_2\sigma_3$ included, there are 8 basis elements in $Cl_{3,0}$. Such algebra is irreducible and closed under geometric multiplication (denoted by spaces between the symbols). A general element of the algebra, usually called a multivector, is a sum of all eight elements $M = a_0 + a_1 \boldsymbol{\sigma}_1 + a_2 \boldsymbol{\sigma}_2 + a_3 \boldsymbol{\sigma}_3 + b_1 I \boldsymbol{\sigma}_1 + b_2 I \boldsymbol{\sigma}_2 + b_3 I \boldsymbol{\sigma}_3 + b_4 I,$ where the coefficients a_i 's and b_i 's are real numbers. The product of any two multivectors gives new multivector that belongs to $Cl_{3,0}$, i.e. $Cl_{3,0}$ is closed under geometric product. If one deletes a basis vector, for example equating $\sigma_3 = 0$, then the remaining set of elements $\{1, \sigma_1, \sigma_2, I\sigma_1, I\sigma_2\}$ will not make up the closed subalgebra. Thus, the GA requires that either all its basis elements, or a closed subalgebra, should be used to get a meaningful result.

In the Hilbert space formalism (in this paper indicated by a hat over the symbol), the massless Dirac Hamiltonian for low energy electrons in the vicinity of critical Kpoint of graphene reduces to [5]:

$$\hat{H}_{\rm g} = \hbar v_{\rm F} \begin{bmatrix} 0 & k_x - \mathrm{i} \, k_y \\ k_x + \mathrm{i} \, k_y & 0 \end{bmatrix},\tag{1}$$

where $v_{\rm F} \approx 10^6$ m/s is the Fermi velocity. The wave vector $\mathbf{k} = (k_x, k_y)$ is measured with respect to valley minimum. In the following the natural units $\hbar = c = 1$ along with $v_{\rm F} = 1$ are used, so that after multiplication of \mathbf{k} by $\hbar v_{\rm F}$ one has the energy. The eigenenergies of the Hamiltonian (1) are

$$E = \pm \sqrt{k_x^2 + k_y^2} = \pm |\mathbf{k}|,\tag{2}$$

where plus/minus sign corresponds to conduction/valence band. Since only two Pauli matrices, $\hat{\sigma}_x$ and $\hat{\sigma}_y$ appear in the Hamiltonian (1), one gets a false impression that the problem is two-dimensional and therefore the problem is limited to graphene plane only. The multiplication table of $Cl_{3,0}$ shows that the third space direction σ_3 which is perpendicular to the graphene plane as well as related GA elements cannot be deleted automatically. As mentioned, similar situation appears in a relativistic case, where 4D massless Dirac equation in momentum representation $\gamma^{\mu}p_{\mu}|\Psi\rangle = 0$, $\mu = 0, 1, 2, 3$ will remain in 4D spacetime even if one limits the equation to two space coordinates ($\mu = 1, 2$) [16].

Now we shall transform the Hamiltonian (1) to $Cl_{3,0}$ algebra using the following mapping rules from the Hilbert

to GA space [9, 17]:

$$|\psi\rangle \longleftrightarrow \psi = a_0 + a_1 I \sigma_1 + a_2 I \sigma_2 + a_3 I \sigma_3,$$

 $\lambda |\psi\rangle \longleftrightarrow \lambda \psi,$
 $\hat{\sigma}_i |\psi\rangle \longleftrightarrow \sigma_i \psi \sigma_3,$
(3)

where λ is the scalar and $\hat{\sigma}_i$ is one of the Pauli matrices. Then, $\hat{H}_{\rm g}|\psi\rangle$, where $\hat{H}_{\rm g}$ is given by (1), maps to the following GA function for spinor ψ :

$$H_{\sigma}(\psi) = \mathbf{k}\psi\boldsymbol{\sigma}_3,\tag{4}$$

where the wave vector $\mathbf{k} = k_x \boldsymbol{\sigma}_1 + k_y \boldsymbol{\sigma}_2$ lies in the graphene plane, Fig. 1. Let us note that in the Hamiltonian function (4) the vector $\boldsymbol{\sigma}_3$ represents the quantization axis, which is perpendicular to graphene plane.



Fig. 1. $Cl_{3,0}$ basis vectors $\boldsymbol{\sigma}_k$ and wave vector \boldsymbol{k} with respect to graphene plane.

The Hamiltonian (4) is a linear function of 2D wave vector \mathbf{k} . The Rashba Hamiltonian and Dresselhaus Hamiltonian for a quantum well that include relativistic corrections are also proportional to 2D wave vector \mathbf{k} . In GA they have the following forms [17]:

$$H_{\rm R}(\psi) = \alpha_{\rm R} \boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2 \boldsymbol{k} \psi \boldsymbol{\sigma}_3, \tag{5}$$

$$H_{\rm D}(\psi) = \alpha_{\rm D} \boldsymbol{\sigma}_1 \boldsymbol{k} \boldsymbol{\sigma}_1 \psi \boldsymbol{\sigma}_3, \tag{6}$$

where $\alpha_{\rm R}$ and $\alpha_{\rm D}$ are, respective, coupling constants. Let us note that the basis vector $\boldsymbol{\sigma}_3$ in all Hamiltonians is perpendicular to the plane $k_x - k_y$ and represents the quantization axis, Fig. 1. Only the factors before ψ , namely $\boldsymbol{k}, \, \boldsymbol{\sigma}_1 \boldsymbol{\sigma}_2 \boldsymbol{k}$, and $\boldsymbol{\sigma}_1 \boldsymbol{k} \boldsymbol{\sigma}_2$, determine the relativistic character of 2D Hamiltonians. Keeping this in mind, simple GA calculations show that there are no new 2D relativistic Hamiltonians. For example, the factor $I\boldsymbol{\sigma}_i \boldsymbol{k} \boldsymbol{\sigma}_i$ before ψ leads to non-Hermitian Hamiltonian which must be discarded. The factors $\boldsymbol{\sigma}_2 \boldsymbol{k} \boldsymbol{\sigma}_2, \, \boldsymbol{\sigma}_3 \boldsymbol{k} \boldsymbol{\sigma}_3, \text{ and } \boldsymbol{\sigma}_2 \boldsymbol{k} \boldsymbol{\sigma}_1$ give already written Hamiltonian functions but with opposite signs or interchanged axes. So, it seems that proportional to \boldsymbol{k} Hamiltonians (4), (5) and (6) are the only ones 2D Hamiltonians that include relativistic effects.

Using GA projectors the Hamiltonian (4) can be rewritten in physically more transparent way. In $Cl_{3,0}$ algebra the elementary projectors that represent the multivector ψ have the form [18]:

$$p_{\pm}(\psi) = \frac{1}{2}(\psi \pm \boldsymbol{\sigma}_{3}\psi\boldsymbol{\sigma}_{3}),$$

$$\psi = p_{+}(\psi) + p_{-}(\psi).$$
(7)

For example, if the projector (7) is applied to basis vectors $\psi = \sigma_1$ or $\psi = \sigma_3$ then one finds $p_+(\pm\sigma_1) = 0$

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and $p_+(\pm \sigma_3) = \pm \sigma_3$, i.e. p_+ selects elements that belong to σ_3 axis. The projector p_- behaves in an opposite manner, $p_-(\pm \sigma_1) = \pm \sigma_1$ and $p_-(\pm \sigma_3) = 0$. The action of the projector on the bivector $I\sigma_3$ that lies in the graphene plane gives $p_+(\pm I\sigma_3) = \pm I\sigma_3$, but $p_-(\pm I\sigma_3) = 0$. The projectors (7), as should be, are idempotent: $p_{\pm}(p_{\pm}(\psi)) = p_{\pm}(\psi)$.

In the terms of projectors the graphene Hamiltonian (4) can be rewritten as a sum of two projectors $P_+(\psi)$ and $P_-(\psi)$ in the following way:

$$H_{g}(\psi) = k \left[\frac{1}{2} \left(\psi + \hat{\boldsymbol{k}} \psi \boldsymbol{\sigma}_{3} \right) - \frac{1}{2} \left(\psi - \hat{\boldsymbol{k}} \psi \boldsymbol{\sigma}_{3} \right) \right]$$
$$= k [h_{+}P_{+}(\psi) + h_{-}P_{-}(\psi)], \qquad (8)$$

where $k = |\mathbf{k}| = \sqrt{k_x^2 + k_y^2}$, $\hat{\mathbf{k}} = \mathbf{k}/k$ is the unit wave vector, and $h_{\pm} = \pm 1$, which as we shall see represents the helicity quantum number. The projectors $P_{\pm}(\psi) = \frac{1}{2}(\psi \pm \hat{\mathbf{k}}\psi\sigma_3)$ select the parts of the multivector ψ that are parallel (plus sign) or antiparallel (minus sign) to \mathbf{k} . If angle φ measured from the basis vector $\boldsymbol{\sigma}_1$ to \mathbf{k} is introduced, Fig. 1, then in polar coordinates the projectors can be written

$$P_{\pm}(\psi) = \frac{1}{2} \left(\psi \pm \cos \varphi \boldsymbol{\sigma}_1 \psi \boldsymbol{\sigma}_3 \pm \sin \varphi \boldsymbol{\sigma}_2 \psi \boldsymbol{\sigma}_3 \right).$$
(9)

The projectors $P_{\pm}(\psi)$ and $P_{-}(\psi)$ are idempotent, i.e. they satisfy $P_{\pm}(P_{\pm}(\psi)) = P_{\pm}(\psi)$. Thus, we find that the simplest graphene Hamiltonian is a sum of two projectors of a multivector spinor onto wave vector \mathbf{k} : the first is related with positive and the second is related with negative helicity. Below we shall see that positive/ negative helicity is related with the conduction/valence band states.

2.2. Eigenenergies and eigenmultivectors

From the projective representation (8) follows that ψ can be written as a sum of two parts having opposite helicities: $\psi = \psi_+ + \psi_-$. Then, the respective eigenenergies E_+ and E_- can be found from two independent multivector eigenequations, $H(\psi_{\pm}) = E_{\pm}\psi_{\pm}$, or in a full form

$$\frac{kh_{\pm}}{2}\left(\psi_{\pm} \pm \hat{\boldsymbol{k}}\psi_{\pm}\boldsymbol{\sigma}_{3}\right) = E_{\pm}\psi_{\pm}.$$
(10)

The equation for positive helicity can be solved in the following way. Remembering that $\hat{k}^2 = 1$, after multiplication from left and right of (10), respectively, by \hat{k} and σ_3 one has

$$kh_+\psi_+ = (2E_+ - kh_+)\hat{\boldsymbol{k}}\psi_+\boldsymbol{\sigma}_3. \tag{11}$$

Expressing $\hat{k}\psi_{\pm}\sigma_3$ from Eq. (10) and inserting back into (11) one gets the scalar equation for eigenenergy

$$(kh_{+})^{2} = (2E_{+} - kh_{+})^{2}.$$
(12)

After squaring of the right hand side and cancellation of similar terms this equation yields conduction band eigenenergy

$$E_+ = h_+ k. \tag{13}$$

Similarly, for the negative helicity one finds valence band eigenenergy

$$E_{-} = h_{-}k. \tag{14}$$

The eigenmultivectors can be deduced from the same Eq. (10) after insertion back of the eigenenergies E_{\pm} . Then, Eq. (10) reduces to

$$\hat{k}\psi_{\pm}\sigma_3 = \pm\psi_{\pm}.\tag{15}$$

As known, in GA the eigenspinor ψ_{\pm} can also be interpreted as a rotor [9] which is very helpful if rotations of vectors, planes etc. in Euclidean or Minkovsky type spaces are needed. Since the rotor satisfies $\tilde{\psi}\psi = \psi\tilde{\psi} = 1$, Eq. (15) can be rewritten in a form of rotation of basis vector $\boldsymbol{\sigma}_3$,

$$\psi_{\pm}\boldsymbol{\sigma}_{3}\tilde{\psi}_{\pm} = \pm \hat{\boldsymbol{k}},\tag{16}$$

where the tilde denotes the reversion involution. Thus, the left hand side represents the equation of rotation of the unit vector $\boldsymbol{\sigma}_3$ perpendicular to graphene plane to other unit vector $\pm \hat{\boldsymbol{k}}$ that lies in the graphene plane, Fig. 1. From all this follows that ψ_{\pm} in (16) can be represented as a rotor in the bivector $\hat{\boldsymbol{k}} \wedge \boldsymbol{\sigma}_3$ plane,

$$\psi_{\pm} = e^{\pm \hat{\boldsymbol{k}} \wedge \boldsymbol{\sigma}_3 \pi/4} = \frac{1}{\sqrt{2}} \Big(1 \pm \hat{\boldsymbol{k}} \wedge \boldsymbol{\sigma}_3 \Big), \tag{17}$$

where the wedge (or outer) product $\mathbf{k} \wedge \sigma_3 = (\mathbf{k}\sigma_3 - \sigma_3 \hat{\mathbf{k}})/2$ represents the bivector. In expansion of the exponential function we have taken into account that $\hat{\mathbf{k}} \wedge \sigma_3$ behaves as an imaginary unit, i.e. $(\hat{\mathbf{k}} \wedge \sigma_3)^2 = -1$. Since $\hat{\mathbf{k}}$ and σ_3 are mutually perpendicular, the outer product may be replaced by geometric, $\hat{\mathbf{k}} \wedge \sigma_3 = \hat{\mathbf{k}}\sigma_3$, or equivalently $\hat{\mathbf{k}}\sigma_3 = -\sigma_3 \hat{\mathbf{k}}$. It should be noted that the eigenspinors (17) are written in a coordinate free way. The states (23) are normalized, $\tilde{\psi}_{\pm}\psi_{\pm} = \psi_{\pm}\tilde{\psi}_{\pm} = 1$, and orthogonal in a sense that the scalar part of the product is equal to zero, $\langle \tilde{\psi}_+\psi_- \rangle = \langle \psi_+\tilde{\psi}_- \rangle = 0$. If the obtained spinors are inserted back into Hamiltonian function (8), the conduction and valence band eigenenergies are found once more

$$\tilde{\psi}_{\pm}H_{\mathrm{g}}(\psi_{\pm}) = h_{\pm}k = \pm k. \tag{18}$$

Finally, we shall note that the Hilbert space eigenstates of the Hamiltonian (1) (the concrete expressions can be found for example in [5]) have no physical meaning and if transformed to the Clifford algebra using the mapping (3) are found to be different from respective GA eigenstates (17). In contrast, the states (17) in GA represent the rotors in 3D physical space [9] and at the same time are related with graphene band eigenenergies.

2.3. Helicity and velocity

In graphene the electron can belong either to A or B sublattice. This property is characterized by pseudo-spin degree of freedom described by operator $\hat{\boldsymbol{\sigma}} = \{\hat{\sigma}_x, \hat{\sigma}_y\}$, where $\hat{\sigma}_x$ and $\hat{\sigma}_y$ are the Pauli matrices. The helicity operator is defined as a projection of the pseudospin operator on the wave vector direction [5]:

$$\hat{C} = \hat{k} \cdot \hat{\sigma}. \tag{19}$$

In geometric algebra the helicity operator (19) transformed by rules (3) becomes

$$C(\psi) = \hat{k}\psi\boldsymbol{\sigma}_3,\tag{20}$$

which can be expressed via Hamiltonian (4)

$$C(\psi) = H(\psi)/k, \tag{21}$$

from which follows that the eigenequation for helicity operator is

$$C(\psi_{\pm}) = h_{\pm}\psi_{\pm} \tag{22}$$

and the respective eigenvalues are $h_{\pm} = \pm 1$.

In conclusion, the same result can be obtained in both the Hilbert space and GA formulations. However, in GA the physics is more transparent since the full system of basis vectors $\boldsymbol{\sigma} = \{\boldsymbol{\sigma}_1, \boldsymbol{\sigma}_2, \boldsymbol{\sigma}_3\}$, which is isomorphic to the Pauli matrices, represents real 3D space. It should be noted that $Cl_{3,0}$ algebra also takes into account the spin quantization axis $\boldsymbol{\sigma}_3$, which can be seen in the Hamiltonian (4) and helicity function (20), although the true spin was not included in the problem. The isospin reflects the property that there are two eigenvalues $(h = \pm 1)$ with respect to \hat{k} axis that is perpendicular to true spin quantization axis $\boldsymbol{\sigma}_3$. Thus, the electron states in a graphene are characterized by two quantum numbers, \boldsymbol{k} and $h = \pm 1$, and can be written as

$$\psi_h(\mathbf{k}) = \frac{1}{\sqrt{2}} \left(1 + h \frac{\mathbf{k}}{|\mathbf{k}|} \wedge \boldsymbol{\sigma}_3 \right).$$
(23)

So, we see that it is preferable to use the term helicity which better reflects the physical meaning rather than the misnomer terms pseudospin, or isospin.

Since the helicity is a good quantum number one can make a superposition of two states having opposite helicities

$$\psi_{\beta} = \cos\beta\psi_{+} + \sin\beta\psi_{-}, \quad \tilde{\psi}_{\beta}\psi_{\beta} = 1, \quad (24)$$

where β is a mixing angle. Then the energy of this state is found to be

$$\psi_{\beta}H(\psi_{\beta}) = k\cos 2\beta. \tag{25}$$

This formula shows that the electron energy can be varied in two ways, either by changing the wave vector magnitude, or by making an appropriate superposition with opposite helicities. At $\beta = \pi/4$ the energy corresponds to the band crossing point, while at $\beta = 0$ and $\beta = \pi/2$ one returns to pure conduction and valence band states. This property is unique to monolayer graphene having a linear dispersion.

In the Hilbert space the electron velocity operator is

$$\hat{\boldsymbol{v}} = \frac{\partial}{\partial \boldsymbol{k}} \hat{H} = v_{\mathrm{F}} \hat{\boldsymbol{\sigma}}.$$
(26)

The corresponding formula in GA is

$$\hat{\boldsymbol{v}}|\psi\rangle \longleftrightarrow \boldsymbol{\nabla}_{\boldsymbol{k}}H(\psi)$$

where the vectorial differential operator was introduced

$$\nabla_{k} = \sigma_{1} \frac{\partial}{\partial k_{x}} + \sigma_{2} \frac{\partial}{\partial k_{y}} + \sigma_{3} \frac{\partial}{\partial k_{z}}.$$
(27)

Then, in GA the average electron velocity is found to be $\langle \boldsymbol{v} \rangle_1 = \dot{\boldsymbol{\nabla}} \langle \tilde{\psi} \dot{H}(\psi) \rangle_0,$ (28)

where the overdot indicates the term which the differentiation vector operator should act upon. We shall remind that such notation comes from a noncommutativity of the GA algebra. Therefore, it is forbidden to swap the symbols ∇ and ψ . In GA terminology the brackets are called grade projectors [9]. The bracket with zero (one) subscript indicates that only the scalar (vector) part of the resulting multivector should be taken. For states (23), the formula (28) gives the average electron velocity

$$\langle \boldsymbol{v} \rangle_1 = h v_{\rm F} \hat{\boldsymbol{k}}.\tag{29}$$

This formula shows that the velocity is independent of wave vector magnitude and its direction in the conduction (h = +1) and valence (h = -1) bands has opposite sense at fixed $\mathbf{k} = k\hat{\mathbf{k}}$.

It is interesting to calculate the average Cartesian components of the velocity, the projection operators of which are defined by equations

$$\hat{v}_{x}|\psi\rangle = v_{\rm F}\hat{\sigma}_{x}|\psi\rangle,
\hat{v}_{y}|\psi\rangle = v_{\rm F}\hat{\sigma}_{y}|\psi\rangle,$$
(30)

or after mapping to GA, by multivector equations

$$v_x(\psi) = v_{\rm F} \boldsymbol{\sigma}_1 \psi \boldsymbol{\sigma}_3,$$

$$v_y(\psi) = v_{\rm F} \boldsymbol{\sigma}_2 \psi \boldsymbol{\sigma}_3.$$
(31)

Simple calculations give the following average projections:

Since commutators of orthogonal components are equal to zero,

$$v_x(v_y(\psi)) = 0,$$

$$v_y(v_x(\psi)) = 0,$$
(33)

we find that for a monolayer graphene we have the same formula as for a classical particle,

$$\langle \boldsymbol{v} \rangle^2 = \langle v_x \rangle^2 + \langle v_y \rangle^2. \tag{34}$$

However, if one includes the spin-orbit interaction the expression (33) and as a result the commutator $v_x(v_y(\psi)) - v_y(v_x(\psi))$ do not become equal to zero [11]. Then, the square of the average velocity (34) will not be equal to the sum of squares of average velocity components.

2.4. Time-dependence

The time-dependent Schrödinger–Pauli equation in $Cl_{3,0}$ reads [17, 19]:

$$\frac{\partial \psi}{\partial t} I \boldsymbol{\sigma}_3 = H(\psi), \tag{35}$$

where the Hamiltonian function $H(\psi)$ is given by (4). Multiplying both sides of (35) by bivector $I\sigma_3$ and noting that the pseudoscalar I commutes with all basis elements, we can rewrite

$$\frac{\partial \psi(t)}{\partial t} = -k I \hat{\boldsymbol{k}} \psi(t), \qquad (36)$$

where $I\hat{k}$ is the unit bivector, the plane of which is perpendicular to k. It satisfies $(I\hat{k})^2 = -1$. The solution of the differential multivector Eq. (36) is

$$\psi(t) = e^{-kIkt}\psi_0 = (\cos kt - I\hat{k}\sin kt)\psi_0, \qquad (37)$$

where ψ_0 is the initial multivector at t = 0. The solution shows that the electron in the monolayer graphene can oscillate only with a single frequency $2k = 2(k_x^2 + k_y^2)^{1/2}$, which is equal to interband transition energy. The multiplier 2 is due to the fact that the rotor $\psi(t)$ should be applied twice in calculating the averages [compare Eq. (18)].

To see how the rotor $\psi(t)$ works, let us apply $\psi(t)$ to an arbitrary unit vector \hat{a} that lies in the graphene plane, $\hat{a} = \cos \gamma \sigma_1 + \sin \gamma \sigma_2$, the direction of which is determined by γ . Assuming that $\psi_0 = 1$, the new vector will be

$$\boldsymbol{a}'(t) = \psi(t)\boldsymbol{a}\tilde{\psi}(t) = a_1'(t)\boldsymbol{\sigma}_1 + a_2'(t)\boldsymbol{\sigma}_2 + a_3'(t)\boldsymbol{\sigma}_3, (38)$$
 where

$$a_1'(t) = \cos^2(kt)\cos\gamma + \sin^2(kt)\cos(\gamma - 2\varphi),$$

$$a_2'(t) = \cos^2(kt)\sin\gamma - \sin^2(kt)\sin(\gamma - 2\varphi),$$

$$a_3'(t) = \sin(2kt)\sin(\gamma - \varphi),$$
(39)

where angle φ is defined in Fig. 1. The module of the vector remains normalized at all times, $(\mathbf{a}'(t))^2 = \hat{\mathbf{a}}^2 = 1$.



Fig. 2. Precession trajectories of an arbitrary vector \boldsymbol{a} . Thick line shows the wave vectors $\pm \boldsymbol{k}$ lying in the graphene plane. If the vector \boldsymbol{a} becomes parallel or antiparallel to electron wave vector the precession trajectories shrink to a point.

Figure 2 illustrates the solution (38), where different curves correspond to different angles γ . The characteristic feature is that an arbitrary \boldsymbol{a} will leave the graphene plane at later moments. However, when $\gamma = \varphi$ or $\gamma = \varphi \pm \pi$, i.e. when $\hat{\boldsymbol{a}}$ is parallel or antiparallel to \boldsymbol{k} , there is no precession and $\boldsymbol{a}'(t) = \hat{\boldsymbol{a}}$. Thus, the in-plane vectors \boldsymbol{a} that are not aligned with \boldsymbol{k} at later moments will stick out from the graphene plane. For such vectors the precession axis coincides with \boldsymbol{k} .

3. Graphene with $Cl_{2,0}$

The $Cl_{3,0}$ algebra is connected with 3D Euclidean space where time is a parameter rather than space-time coordinate. So, apart from a linear dispersion law, no other effects related with relativistic space-time transformations are to be expected. To have a true relativistic graphene flatland we shall address to $Cl_{2,0}$ algebra, where time is assumed to be the bivector [20]. $Cl_{2,0}$ is isomorphic to subalgebra $\{1, \sigma_1, \sigma_2, I\sigma_3\}$ of $Cl_{3,0}$ with equivalence $e_1 = \sigma_1, e_2 = \sigma_2, e_{12} \equiv e_1e_2 = I\sigma_3$. A general multivector of $Cl_{2,0}$ is $A = a_0 + a_2e_1 + a_1e_2 + a_3e_{12}$, where $a_i \in \mathbb{R}$. Before considering the relativistic flatland, however, at first it is instructive to do calculations where time, as in the previous section, is treated as a parameter.

3.1. Real matrix representation

The irreducible matrix representation of $Cl_{2,0}$ algebra consists of the following real matrices [21]:

$$\hat{1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \hat{e}_1 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \tag{40}$$

$$\hat{e}_2 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \hat{e}_{12} = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \tag{41}$$

which satisfy $Cl_{2,0}$ multiplication table. The following mapping rules between the Hilbert space and $Cl_{2,0}$ algebras can be constructed

$$\begin{aligned} |\psi\rangle &= \begin{bmatrix} a_1\\ a_2 \end{bmatrix} \longleftrightarrow \psi = a_1 + a_2 e_{12}, \\ \hat{e}_1 |\psi\rangle &\longleftrightarrow e_1 \psi e_1, \\ \hat{e}_2 |\psi\rangle &\longleftrightarrow - e_2 \psi e_1, \\ \hat{e}_{12} |\psi\rangle &\longleftrightarrow - e_{12} \psi. \end{aligned}$$
(42)

However, it should be noted that real matrices cannot map the complex graphene Hamiltonian (1) onto GA. The mapping becomes possible only after Hamiltonian (1) is brought to diagonal form $\hat{H}_g = \text{diag}(k, -k)$. Then the diagonal Hamiltonian in GA assumes the form

$$H_{\rm g}(\psi) = k \boldsymbol{e}_1 \psi \boldsymbol{e}_1, \quad k = \sqrt{k_x^2 + k_y^2}.$$
 (43)

Taking into account that ψ consists of scalar and pseudoscalar, and using the normalization condition $\tilde{\psi}\psi = 1$, we can express ψ through a single parameter φ ,

$$\psi = e^{\boldsymbol{e}_{12}\varphi/2} = \cos(\varphi/2) + \boldsymbol{e}_{12}\sin(\varphi/2). \tag{44}$$

If the rotor (44) is applied to a vector, for example to e_1 , the new vector will remain in the graphene plane,

$$\psi \boldsymbol{e}_1 \psi = \cos \varphi \boldsymbol{e}_1 - \sin \varphi \boldsymbol{e}_2. \tag{45}$$

The average energy of the state (44) is

$$\langle \tilde{\psi} H_{\rm g}(\psi) \rangle_0 = \sqrt{k_x^2 + k_y^2 \cos \varphi}.$$
 (46)

Thus, at $\varphi = 0$ and $\varphi = \pi$ we have conduction and valence band energies which, as follows from (44), correspond to eigenstates $\psi_{+} = 1$ and $\psi_{-} = e_{12}$, respectively. As in Sect. 2 the energy bands can be related with the helicity quantum numbers h_{\pm} , if the Hamiltonian (43) is rewritten in a form

$$H_{g}(\psi) = k \left[\frac{1}{2} (\psi + e_{1} \psi e_{1}) - \frac{1}{2} (\psi - e_{1} \psi e_{1}) \right]$$

= $k \left[h_{+} P'_{+}(\psi) + h_{-} P'_{-}(\psi) \right],$ (47)

where $h_{\pm} = \pm 1$ and $P'_{\pm}(\psi)$ is the projection operator onto conduction/valence band states,

$$P'_{\pm}(\psi) = \frac{1}{2}(\psi \pm e_1\psi e_1).$$
(48)

Application of (48) to the eigenstates yields $P'_{+}(1) = 1$, $P'_{-}(1) = 0$ and $P'_{+}(e_{12}) = 0$, $P'_{-}(e_{12}) = e_{12}$. Since P'_{\pm} is directly related with the Hamiltonian, one can also introduce the helicity operator similar to (21), although now the concept of the Pauli matrix-vector projection (20) onto \mathbf{k} is not needed altogether. Thus, in contrast to $Cl_{3,0}$ case, the mapping by real matrices yields the Hamiltonian that has no vectors perpendicular to the graphene plane.

In the Hilbert space the dynamics of ψ is governed by equation

$$i\frac{\partial}{\partial t}|\psi\rangle = \hat{H}_{g}|\psi\rangle. \tag{49}$$

Since the imaginary i cannot be mapped onto $Cl_{2,0}$, we are unable to transform the left hand side of this equation to $Cl_{2,0}$ and therefore to construct the equation of motion. In fact, the deadlock here is more serious. Since the GA Hamiltonian (43) is proportional to the module of wave vector \mathbf{k} the transformation from momentum to coordinate representation will result in the square root for a coordinate operator: $k = \sqrt{\mathbf{k}^2} \rightarrow \sqrt{\partial_x^2 + \partial_y^2}$. Thus, we find that the mapping (42) should be rejected from the beginning.

3.2. Complex matrix representation

To circumvent the difficulty the mapping by complex matrices will be addressed. Since $Cl_{2,0}$ is isomorphic to the subalgebra $\{1, \sigma_1, \sigma_2, I\sigma_3\}$ of $Cl_{3,0}$, therefore, its complex matrix representation may be related to the Pauli matrices $\hat{\sigma}_x$ and $\hat{\sigma}_y$ and their product,

$$\hat{1} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \hat{e}_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \tag{50}$$

$$\hat{e}_2 = \begin{bmatrix} 0 & -\mathbf{i} \\ \mathbf{i} & 0 \end{bmatrix}, \quad \hat{e}_{12} = \begin{bmatrix} \mathbf{i} & 0 \\ 0 & -\mathbf{i} \end{bmatrix}.$$
(51)

Now the state vector $|\psi\rangle$ is complex. We shall assume that the following correspondence exists between the complex Hilbert space vector and the general multivector of $Cl_{2,0}$:

$$|\psi\rangle = \begin{bmatrix} a_0 + ia_3 \\ a_2 + ia_1 \end{bmatrix} \longleftrightarrow \psi$$
$$= a_0 + a_2 \mathbf{e}_1 + a_1 \mathbf{e}_2 + a_3 \mathbf{e}_{12}, \tag{52}$$

where $a_i \in \mathbb{R}$. The mapping (52) between the wave function in the Hilbert and GA space allows to construct the following replacement rules for the Pauli matrices and their product

$$\begin{aligned} \hat{\sigma}_x |\psi\rangle &\longleftrightarrow \mathbf{e}_1 \psi, \\ \hat{\sigma}_y |\psi\rangle &\longleftrightarrow \mathbf{e}_2 \psi, \\ \hat{\sigma}_x \hat{\sigma}_y |\psi\rangle &\longleftrightarrow \mathbf{e}_{12} \psi, \end{aligned}$$
(53)

with the help of which the complex graphene Hamiltonian mapped onto $Cl_{2,0}$ becomes

$$H_{\rm g}|\psi\rangle \longleftrightarrow H_{\rm g}(\psi) = k_x \boldsymbol{e}_1 \psi + k_y \boldsymbol{e}_2 \psi = \boldsymbol{k}\psi.$$
 (54)

However, the product $\tilde\psi\psi$ apart from the scalar also contains the vector,

$$\tilde{\psi}\psi = a_0^2 + a_1^2 + a_2^2 + a_3^2 + 2(a_0a_2 - a_1a_3)e_1 + 2(a_0a_1 + a_2a_3)e_2,$$
(55)

and therefore cannot be normalized to unity. The normalization to scalar can be obtained if the following dagged multivector is introduced:

$$\psi^{\dagger} = -\boldsymbol{e}_{12}\psi\boldsymbol{e}_{12} = a_0 - a_2\boldsymbol{e}_1 - a_1\boldsymbol{e}_2 - a_3\boldsymbol{e}_{12}, \qquad (56)$$

then

$$\psi\psi^{\dagger} = \psi^{\dagger}\psi = (a_0^2 + a_3^2) - (a_1^2 + a_2^2).$$
(57)
The formulae become more transparent if they are rewrit-

ten in a form of trigonometric functions $\psi = r(\cos \alpha + e_{12} \sin \alpha) + s(\sin \beta e_1 + \cos \beta e_2)$ (58)

$$\psi = r(\cos \alpha + e_{12} \sin \alpha) + s(\sin \beta e_1 + \cos \beta e_2). \quad (58)$$

Then, we find that

$$\psi^{\dagger}\psi = r^2 - s^2. \tag{59}$$

The ψ -multivector (52) can be decomposed into a product of relativistic boost and rotation in a graphene plane

$$\psi = \rho e^{\phi \hat{\boldsymbol{a}}} e^{\alpha \boldsymbol{e}_{12}},\tag{60}$$

where we require $\rho = \pm \sqrt{r^2 - s^2}$, $\phi = \operatorname{arctanh}(s/r)$ and $\hat{a} = (a_2 e_1 + a_1 e_2)/\sqrt{a_1^2 + a_2^2} = e_1 \sin \beta + e_2 \cos \beta$, and where $a_1 = \cos(\beta - \alpha)$ and $a_2 = \sin(\beta - \alpha)$. The second exponent generates rotation in the graphene plane by angle 2α and is related with trigonometric functions: $e^{\alpha e_{12}} = \cos \alpha + e_{12} \sin \alpha$. The first exponent generates the boost in direction \hat{a} by magnitude ϕ and is related with the hyperbolic functions: $e^{\phi \hat{a}} = \cosh \phi + \hat{a} \sinh \phi$. The scalar ρ defines the magnitude of dilation.

In (3+1) relativistic $Cl_{1,3}$ algebra the event is defined as a sum of four vectors that span the space-time [9, 10]. The metric of this algebra ensures correct invariant interval $(\mathbf{x}^2 - t^2)$ between space \mathbf{x} and time t coordinates. In $Cl_{2,0}$ algebra, the both basis vectors \mathbf{e}_1 and \mathbf{e}_2 were used to construct the spatial vector $\mathbf{x} = x_1\mathbf{e}_1 + x_2\mathbf{e}_2$, therefore, in order to have a correct scalar invariant interval the time will be treated as a bivector. The relativistic event in $Cl_{2,0}$ then can be described by the multivector

$$X = (t + \boldsymbol{x})\boldsymbol{e}_{12},\tag{61}$$

the square of which gives the needed invariant interval $X^2 = x^2 - t^2$.

The spectrum of the Hamiltonian (54) follows from the eigenenergy equation $H_{\rm g}(\psi) = \mathbf{k}\psi = E\psi$. Taking the reverse of this equation $\tilde{\psi}\mathbf{k} = E\tilde{\psi}$ and multiplying both sides by \mathbf{e}_{12} we obtain the dagged form of eigenmultivector equation

$$\psi^{\dagger} \boldsymbol{k} = E \psi^{\dagger}. \tag{62}$$

Once more multiplying the initial and dagged eigenequations from left and right by e_{12} and remembering that $\psi\psi^{\dagger}$ is the scalar, we can write $E^{2}\psi\psi^{\dagger} = \mathbf{k}\psi\psi^{\dagger}\mathbf{k} =$ $\mathbf{k}^{2}\psi\psi^{\dagger}$, which gives the relativistic spectrum E = $\pm\sqrt{\mathbf{k}^{2}} \equiv \pm k$.

Nonetheless, a note of caution is appropriate here. One can check that formally the following mapping holds:

(63)

 $i|\psi\rangle \equiv i\hat{1}|\psi\rangle \longleftrightarrow \psi e_{12},$

which if used with the replacement rules (53) will generate new rules, for example $i\hat{\sigma}_x|\psi\rangle \leftrightarrow e_1\psi e_{12}$ and $i\hat{\sigma}_y|\psi\rangle \leftrightarrow e_2\psi e_{12}$. However, the matrix $i\hat{1}$ is not a member of $Cl_{2,0}$ and therefore it is illegitimate to map it onto $Cl_{2,0}$ algebra. Thus we are facing the same dilemma: the term with time derivative $i\partial_t|\psi\rangle$ in the Schrödinger Eq. (49) cannot be mapped onto $Cl_{2,0}$ algebra.

In the following we shall postulate that $i\partial_t |\psi\rangle$ can be replaced by GA expression $\partial_t \psi e_{12}$, where $e_{12}^2 = -1$ plays the role of the imaginary unit. Then the time-dependent Schrödinger equation in GA will be

$$\frac{\partial \psi}{\partial t} \boldsymbol{e}_{12} = \boldsymbol{k} \psi. \tag{64}$$

This multivector equation can be solved after division of ψ into even (scalar plus bivector) and odd (vector) parts, $\psi = \psi_+ + \psi_-$. This differential equation splits into two equations,

$$\partial_t \psi_+ = \mathbf{k} \mathbf{e}_{12} \psi_-,
\partial_t \psi_- = -\mathbf{k} \mathbf{e}_{12} \psi_+, \tag{65}$$

solutions of which are exponents with positive and negative energies. The general solution will be a sum

$$\psi(t) = e^{\mathbf{e}_{12}kt}\psi_{+0} + e^{-\mathbf{e}_{12}kt}\psi_{-0}.$$
(66)

The initial wave function $\psi(0) = \psi_{+0} + \psi_{-0}$ can be represented as rotation and boost in the graphene plane, Eq. (60). It can be shown that at later moments the relative contribution of even $\psi_+(t) = a_0(t) + \mathbf{e}_{12}a_3(t)$ and odd $\psi_-(t) = a_1(t)\mathbf{e}_1 + \mathbf{e}_2a_2(t)$ parts into the total $\psi(t)$ will not change with time.

3.3. Inclusion of mass term

To obtain full relativistic spectrum $E = \pm \sqrt{k^2 + m^2}$ one should add the diagonal mass term diag(m, -m) to massless relativistic Hamiltonian (1). In $Cl_{3,0}$ such term corresponds to multivector $m\sigma_3\psi\sigma_3$, so that GA Hamiltonian (4) becomes

$$H_{\rm g}(\psi) = (\mathbf{k}^2 + m\boldsymbol{\sigma}_3)\psi\boldsymbol{\sigma}_3. \tag{67}$$

The simplest way to find the spectrum of this relativistic Hamiltonian is to insert the stationary solution $\psi(\mathbf{k}, E) = \psi(\mathbf{k}) e^{-I\boldsymbol{\sigma}_3 E t}$ into (35), which gives

$$E\psi(\mathbf{k}) = (\mathbf{k} + m\boldsymbol{\sigma}_3)\psi(\mathbf{k})\boldsymbol{\sigma}_3.$$
 (68)

Multiplying this algebraic multivector equation by its reverse $E\tilde{\psi}(\mathbf{k}) = \boldsymbol{\sigma}_{3}\tilde{\psi}(\mathbf{k})(\mathbf{k}+m\boldsymbol{\sigma}_{3})$, and remembering that E and $\psi(\mathbf{k})\tilde{\psi}(\mathbf{k})$ are scalars, one finds

$$(E\psi(\mathbf{k}))(E\tilde{\psi}(\mathbf{k}))$$

$$= (\mathbf{k}^2 + m^2 + m\mathbf{k}\boldsymbol{\sigma}_3 + m\boldsymbol{\sigma}_3\mathbf{k})\psi(\mathbf{k})\tilde{\psi}(\mathbf{k}).$$
(69)

Since $\sigma_3 \mathbf{k} = -\mathbf{k}\sigma_3$, we find the correct relativistic dispersion

$$E^2 = k^2 + m^2. (70)$$

In $Cl_{2,0}$, using real matrix representation (40) and (41), one finds the following mapping of the mass term:

$$m\hat{\sigma}_3|\psi\rangle \longleftrightarrow m\boldsymbol{e}_1\psi\boldsymbol{e}_1.$$
 (71)

Then, the Hamiltonian becomes $H_{g} = (\pm k + m) \boldsymbol{e}_{1} \psi \boldsymbol{e}_{1}$.

Since $(\pm k + m)$ is the scalar, the spectrum by analogy with Eq. (43) can be written automatically

$$E = \pm \sqrt{k^2 + m}.\tag{72}$$

If instead of real matrix representation one uses complex representation then one finds exactly the same dispersion (72) for positive as well as for negative states. Thus we find that the geometric algebra $Cl_{2,0}$ which represents the true flatland gives unacceptable relativistic dispersion. In addition, we have seen that we cannot map the imaginary i onto the flatland. These problems do not arise in $Cl_{3,0}$.

4. Conclusion

Two subalgebras of relativistic Clifford algebra $Cl_{1,3}$ were considered as possible candidates for a description of graphene quantum properties in Euclidean spaces without using the Hilbert space concepts. It is shown that in case of a single valley graphene the three-dimensional Euclidean $Cl_{3,0}$ algebra allows to construct Schrödinger--type equation for electron with the relativistic Dirac spectrum. However, it was found impossible to construct such equation with two-dimensional algebra $Cl_{2,0}$, which represents the true Euclidean flatland. The preliminary investigations show that the full relativistic $Cl_{3,1}$ algebra is suitable for description of graphene with two inequivalent K and K' valleys, when electron spin is included.

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