Calculation of quantum eigens with geometrical algebra rotors

A. Dargys and A. Acus

Abstract. A practical computational method to find the eigenvalues and eigenspinors of quantum mechanical Hamiltonian is presented. The method is based on reduction of the eigenvalue equation to well known geometrical algebra rotor equation and, therefore, allows to replace the usual $\det(H - E) = 0$ quantization condition by much simple vector norm preserving requirement. In order to show how it works in practice a number of examples are worked out in $\text{Cl}_{3,0}$ (monolayer graphene and spin in the quantum well) and in $\text{Cl}_{3,1}$ (two coupled two-level atoms and bilayer graphene) algebras.

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1. Introduction

The standard approach to quantum mechanical eigenvalue problems is based on matrix representation of the operator defined in a complex Hilbert space and its subsequent diagonalization in a chosen basis. A modern approach to quantum mechanics [1, 2, 3, 4] is based on Clifford’s geometric algebra (GA), where the Clifford space filled with geometric objects such as oriented lines, planes etc is used instead of abstract Hilbert space. Selection of a particular GA to solve the physical problem, in contrast to Hilbert space approach, automatically then takes into account Clifford space properties such as dimension, signature and symmetry relations of the physical space or spacetime.

Despite the advantages that GA offers to quantum mechanics, in practice the methods needed to solve concrete problems are not elaborated enough. So, for the physicists and engineers the GA may appear a nice but exotic theory only. In this report a practical method to calculate eigenvalues and eigenvectors is proposed that is based on the reduction of the multivector eigenvalue equation to well known rotor equation. In particular the primary goal of this paper is to shown by fully elaborated examples how GA can be
used to find eigenvalues and eigenmultivectors in 3D Euclidean space with $Cl_{3,0}$ and in relativistic Minkowski space with $Cl_{3,1}$ algebra without explicitly involving Hamiltonian matrix diagonalization procedure. Both mentioned algebras are of paramount importance in physics. An overview on eigenvalue problems in the framework of Clifford analysis is given in Ref. [5]. Some examples of GA approach to eigenblades can be found in books [2, 3, 4, 6].

In the Sec. 2 we shall remind the pertinent properties of rotors and methods used to find the eigens. In Sec. 3 we demonstrate how the proposed method works in practice where we solve four problems of increasing complexity. Relations with matrix representation and symbols are summarized in Appendix. The following fonts are used to denote GA elements: $a$ or $\mathbf{a}$ – vector, $A$ – bivector, $A$ – multivector, $A$ – transformation.

2. Rotors and eigens in GA

Rotation of vector. In GA the rotation of vector $\mathbf{a}$ to vector $\mathbf{c}$ is described by a linear transformation

$$R(\mathbf{a}) = R\mathbf{a}R^{-1} = \mathbf{c},$$

(1)

where $R$ is the rotor that satisfies $RR^{-1} = R^{-1}R = 1$, $R^{-1} = \bar{R}$, with tilde denoting the reversion operation. Since $c^2 = a^2$ the inverse transformation is $\mathbf{a} = \bar{R}\mathbf{c}R$. Usually the rotor $R$ is constructed applying two reflections in planes perpendicular to unit vectors $\mathbf{m}$ and $\mathbf{n}$,

$$R = \mathbf{m}\mathbf{n}, \quad \bar{R} = \mathbf{n}\mathbf{m}, \quad \hat{m}^2 = \hat{n}^2 = 1.$$

(2)

In this way defined rotor can be put into more convenient exponential form

$$R = \hat{m}\hat{n} = \hat{m} \cdot \hat{n} + \frac{\hat{m} \wedge \hat{n}}{|\hat{m} \wedge \hat{n}|} |\hat{m} \wedge \hat{n}| = \cos \frac{\theta}{2} + \hat{B} \sin \frac{\theta}{2} = e^{\hat{B} \theta/2},$$

(3)

where $\theta$ is the angle of rotation in a plane made up of $\hat{m}$ and $\hat{n}$, $\cos(\theta/2) = \hat{m} \cdot \hat{n}$ and $\sin(\theta/2) = |\hat{m} \wedge \hat{n}|$. $\hat{B} = \frac{\hat{m} \wedge \hat{n}}{|\hat{m} \wedge \hat{n}|}$ denotes the unit bivector, $\hat{B}^2 = -1$.

In practice, however, it is required to have a rotor which brings the end of a unit radius-vector $\hat{a}$ to a new position $\hat{b}$. If $\theta$ is the angle between $\hat{a}$ an $\hat{b}$ then the rotation plane can be written as the outer product $\hat{a} \wedge \hat{b} = (\hat{a}\hat{b} - \hat{b}\hat{a})/2$ and angle $\theta$ can be expressed through the inner product $\hat{a} \cdot \hat{b} = (\hat{a}\hat{b} + \hat{b}\hat{a})/2 = \cos \theta$.

The rotor in this case takes the following form

$$R = e^{\pm \frac{\hat{a} \wedge \hat{b}}{|\hat{a} \wedge \hat{b}|} \theta} = \cos \frac{\theta}{2} \pm \frac{\hat{a} \wedge \hat{b}}{|\hat{a} \wedge \hat{b}|} \sin \frac{\theta}{2},$$

(4)

The trigonometric functions of half angle, $\cos(\theta/2) = 2^{-1/2}(1 + \cos \theta)^{1/2}$ and $\sin(\theta/2) = 2^{-1/2}(1 - \cos \theta)^{1/2}$, appear in the formulas (3) and (4). If $\hat{a}$ and $\hat{b}$ are mutually orthogonal, then the equation (4) simplifies to

$$R = e^{\pm \hat{a}\hat{b} \pi/4} = (1 \pm \hat{a}\hat{b})/\sqrt{2}, \quad \hat{a} \perp \hat{b}.$$

(5)

The rotor can also be put [3] in the form $R = (1 + \hat{a}\hat{b})/(|\hat{a} + \hat{b}|)$, which reduces to (4) after half angle formulas are applied.
It is important to note, that two successive rotations can be always described by the composite rotation \( R_3(a) = R_2(R_1(a)) \equiv R_2R_1a \). However, the result of product of two rotors is not necessarily a rotor. The exception happens, in particular, when \( R_1 \) and \( R_2 \) belong to nonintersecting subspaces.

**Rotation of blade and multivector.** The rotation of a blade relies on the extension of the outermorphism from vectors to multivectors [7]. Since the outermorphism preserves the outer product and as a result the shape of geometric objects, this transformation induces a more general linear transformation in the full Clifford space. For example, the rotation of the bivector \( a \wedge b \) gives new bivector \( R(a \wedge b) = R(a) \wedge R(b) \) having the same properties. To rotate general blade \( A_r = a_1 \wedge a_2 \wedge \cdots \wedge a_r \) one rotates all the vectors \( a_i \) in it \( \bar{R}(A_r) = \bar{R}(a_1) \wedge \bar{R}(a_2) \wedge \cdots \wedge \bar{R}(a_r) \) (the underbar denotes the outermorphism), so the rotation formula for blade \( A_r \) has the same structure as for vector (1), \( R(A_r) = RA_r\bar{R} = B_r. \) In particular, the pseudoscalar is rotationally invariant \( RIR^{-1} = I. \) The formula remains valid if the blade is replaced by any multivector. General properties of rotation transformation \( R \) of multivectors \( M \) and \( N \) are listed below.

1. \( R(aM) = aR(M) \) \hspace{1cm} Preserves scalar multiplication
2. \( R(M + N) = R(M) + R(N) \) \hspace{1cm} Preserves multivector addition
3. \( R(M \cdot N) = R(M) \cdot R(N) \) \hspace{1cm} Preserves inner product
4. \( R(M \wedge N) = R(M) \wedge R(N) \) \hspace{1cm} Preserves outer product
5. \( R(MN) = R(M)R(N) \) \hspace{1cm} Preserves geometric product
6. grade\((R(A_r)) = \) grade\((A_r) \) \hspace{1cm} Preserves grade \( r \)

An important property of the outermorphism is that the outermorphism of the product of two functions \( F \) and \( G \) is the product of the outermorphisms,

\[
FG(a \wedge b \cdots \wedge c) = FG(a) \wedge FG(b) \cdots \wedge FG(c). \tag{6}
\]

**Blade eigens.** The outermorphism allows to characterize the invariant subspaces under linear transformations. In particular, it allows to generalize the concept of the eigenblade [7]. Indeed, if \( F \) is a linear function then the equation

\[
F(A_r) = \lambda A_r \tag{7}
\]

is called the eigenblade equation or collineation transformation, where blade \( A_r \) of grade \( r \) is called eigenblade and \( \lambda \) is a real eigenvalue. Frequently the outermorphism symbol (underbar) is omitted. For example, if \( a \) and \( b \) are vectors and function \( F \) satisfies \( F(a) = b \) and \( F(b) = a \), then by outermorphism extension we have \( F(a \wedge b) = F(a) \wedge F(b) = b \wedge a = -a \wedge b, \) or \( F(a \wedge b) = -a \wedge b. \) Thus \( a \wedge b \) is the eigenbivector with eigenvalue \( -1. \)

If applied to pseudoscalar \( I \) the outermorphism can be used to define the determinant \( \det(F) \) of linear transformation \( F, \)

\[
F(I) = \det(F)I, \tag{8}
\]

without any need of matrices. For example, in \( \mathbb{Cl}_{3,0} \) the determinant of \( F \) as follows from (8) is \( \det(F) = (F(e_1) \wedge F(e_2) \wedge F(e_3))(e_3 \wedge e_2 \wedge e_1) = \text{scalar}. \)
The eigenvalue equation (7) can be rewritten in the form

\[(F - \lambda)(A_r) = 0\]  

(9)

showing that the operator \((F - \lambda)\) is singular. Every singular operator has a vanishing determinant:

\[\det(F - \lambda)(A_r) = (F (I_r) - \lambda I_r) I_r^{-1} = 0,\]

(10)

where the last expression follows from (8), the \(I_r\) being \(r\)-grade pseudoscalar.

This equation is called the secular equation for \(F\), the solution of which with respect to \(\lambda\) gives the eigenvalues. For example, let \(F\) be a vector-valued function \(f(x)\) of vector \(x\) in \(Cl_{3,0}\). If \(f_i = f(e_i)\), then

\[\det(f - \lambda)(x) = (f_1 - \lambda e_1) \wedge (f_2 - \lambda e_2) \wedge (f_3 - \lambda e_3) I_3^{-1} = 0,\]

where \(I_3 = e_1 \wedge e_2 \wedge e_3 = e_1 e_2 e_3\) and \(I_3^{-1} = -I_3\). After expansion this equation reduces to scalar cubic equation

\[\lambda^3 + \alpha_2 \lambda^2 + \alpha_1 \lambda + \alpha_0 = 0\]

where the scalar coefficients are \(\alpha_0 = (f_1 \wedge f_2 \wedge f_3) \cdot I_3, \alpha_1 = -(f_1 \wedge f_2 \wedge e_3 + f_1 \wedge e_2 \wedge f_3 + e_1 \wedge f_2 \wedge f_3) \cdot I_3,\) and \(\alpha_2 = (f_1 \wedge e_2 \wedge e_3 + e_1 \wedge f_2 \wedge e_3 + e_1 \wedge e_2 \wedge f_3) \cdot I_3\). After the eigenvalues have been determined, the eigenblade equation (7) becomes algebraic multivector equation with respect to \(A_r\) which can be solved by GA methods. Example of applications of this approach can be found, for example, in the textbook [6]. The described method, however, is not a coordinate free, and is based on expansion of the transformation in a particular frame.

Spinor eigens. The eigens, however, in many cases could be calculated in a compact way without any reference to determinant equation (10). In particular, as we shall see, this is easy to do if the eigenequation

\[H(\psi) = E\psi\]  

(11)

for spinor \(\psi\) that consists of a sum of even-grade blades can be transformed to an eigenequation for a corresponding rotor. In quantum mechanics the transformation \(H\) is called the Hamiltonian and \(E\) is the energy (scalar). The reformulation of eigen problem (11) may be realized if one observes that in many quantum mechanical problems there is a specific direction called the quantization axis (\(z\)-axis). As we shall see this allows to reduce quantum mechanical eigenmultivector equation to a single rotor equation, where the quantization axis is rotated to some final direction determined by the Hamiltonian of the problem. It is important to note that, in contrast to Hilbert space formulation where the quantization axis is hidden in the structure of the Hamiltonian, in GA this axis appears explicitly. In other words the quantization axis, represented below by \(e_3\) basis vector, appears directly in the Hamiltonian function. The proposed method is based on this quantum mechanical Hamiltonian property and allows us to construct a single optimal rotor expressed in coordinate-free way, which is very similar to rotor (4) or (5), where the vectors \(a = e_3\) and \(b\) are given by eigenequation (11).

The realization of the described procedure is straightforward in case of \(Cl_{3,0}\) algebra (Schrödinger-Pauli equation). In relativistic \(Cl_{3,1}\) and \(Cl_{1,3}\)
algebras the spinor of Dirac equation is the sum of eight terms: scalar, six bivectors and pseudoscalar. The reduction of relativistic spinors to rotors of 3D Euclidean space can be accomplished after splitting of $\psi$ into even $\psi_+$ and odd $\psi_-$ parts with the help of spatial inversion operator described in Appendix 4,

$$\psi = \psi_+ + \psi_-, \quad \bar{\psi} = \psi_+ - \psi_-.$$  

As we shall see the eigenvalue equations $H(\psi_+ + \psi_-) = (\psi_+ + \psi_-)E$ and $\overline{H}(\psi_+ + \psi_-) = (\psi_+ - \psi_-)E$ in this case reduce to two multivector equations for even $\psi_+$ and odd $\psi_-$ (or $I\psi_-$) parts. Reduced equations then can be interpreted as rotors which rotate quantization axis $e_3$ to the final direction determined by the Hamiltonian.

### 3. Examples from quantum mechanics

In this section four characteristic examples from quantum mechanics are considered to illustrate how the proposed method works in practice. The spectra of all considered Hamiltonians are shown in Fig. 1.
3.1. Monolayer graphene

Monolayer graphene is a 2D crystal consisting of a single layer of carbon atoms. The intense interest in graphene was stimulated by 2010 Nobel prize in physics (A. Geim and K. Novoselov) and potential application of graphene in construction of novel 2D nanodevices [8]. From theoretical point of view the most interesting problem is the ultrarelativistic electron behavior in 2D lattice at very small energies (< 1 eV), Fig. 1a. The spectrum represents an ultrarelativistic limit of eigenenergy \( E = (p^2 + m^*)^{1/2} \) of the solution of the Dirac equation in the case when fraction of electron energy due to kinetic momentum \( p \) is much larger than effective electron mass, \( p^2 \gg m^* \), where \( m^* \approx 0.012m_0 \) (\( m_0 \) being free electron mass).

In the Hilbert space formalism the massless (ultrarelativistic) Hamiltonian in the vicinity of critical \( K \) point of graphene (the momentum space point where electron transport takes place) reduces to simple form

\[
\hat{H}_{MG} = \hbar v_F \begin{bmatrix} 0 & k_x - i k_y \\ k_x + i k_y & 0 \end{bmatrix},
\]

where \( v_F \approx 10^6 \) m/s is the Fermi velocity. The wave vector \( \mathbf{k} = (k_x, k_y) \) lies in the graphene plane and is measured with respect to \( K \) valley minimum. In the following the natural units \( \hbar = 1 \) along with \( v_F = 1 \) are used. The eigenenergies of the Hamiltonian (13) are

\[
E_{\pm} = \pm \sqrt{k_x^2 + k_y^2} = \pm |\mathbf{k}|,
\]

where plus/minus sign corresponds to conduction/valence bands shown in Fig. 1a. As discussed in [9] a minimal algebra needed to describe the monolayer Hamiltonian is \( Cl_{3,0} \), where the basis vectors \( \mathbf{e}_i \) play the role of space coordinates and satisfy \( \mathbf{e}_1^2 = \mathbf{e}_2^2 = \mathbf{e}_3^2 = 1 \), Fig. 2. The orthogonal oriented planes are described by bivectors \( \mathbf{le}_1 = \mathbf{e}_2 \mathbf{e}_3 \), \( \mathbf{le}_2 = \mathbf{e}_3 \mathbf{e}_1 \), and \( \mathbf{le}_3 = \mathbf{e}_1 \mathbf{e}_2 \). With scalar and pseudoscalar \( I = \mathbf{e}_1 \mathbf{e}_2 \mathbf{e}_3 \) included, there are 8 basis elements.

Now we shall transform the Hamiltonian (13) to \( Cl_{3,0} \) algebra using the following mapping rules from Hilbert to Clifford space [3],

\[
|\psi\rangle \leftrightarrow \psi = a_0 + a_1 \mathbf{e}_1 + a_2 \mathbf{e}_2 + a_3 \mathbf{e}_3, \\
\lambda |\psi\rangle \leftrightarrow \lambda \psi, \quad \hat{\sigma}_i |\psi\rangle \leftrightarrow \mathbf{e}_i \psi \mathbf{e}_3,
\]

where \( \lambda \) is the scalar and \( \hat{\sigma}_i \) is one of \( 2 \times 2 \) complex Pauli matrices \( \hat{\sigma}_1 = \hat{\sigma}_x \), \( \hat{\sigma}_2 = \hat{\sigma}_y \) or \( \hat{\sigma}_3 = \hat{\sigma}_z \). Then, \( \hat{H}_{MG} |\psi\rangle \) maps to the following simple GA function of spinor \( \psi \)

\[
H_{MG}(\psi) = \mathbf{k} \psi \mathbf{e}_3,
\]

where the wave vector \( \mathbf{k} = k_x \mathbf{e}_1 + k_y \mathbf{e}_2 \) lies in the graphene plane, Fig. 2.

It should be noted that the Hamiltonian function (16) has a coordinate-free form. The appearance of vector \( \mathbf{e}_3 \) in Hamiltonian (16) follows from the existence the pseudospin quantization axis, which is perpendicular to graphene plane, Fig. 2. This is not so evident from the Hilbert space Hamiltonian (13).

The eigenvalue equation for monolayer graphene then reads

\[
\mathbf{k} \psi \mathbf{e}_3 = \psi E,
\]
Figure 2. 2D electron (dot) moving with velocity $\mathbf{v}$ and coordinate system $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$. The planes represent either two graphene layers, or in the case of quantum well, two potential walls so that the electron is squeezed between the planes. $\mathbf{k}$ is the wave vector, $\theta = \pi/2$, $\cos \varphi = k_1/|\mathbf{k}|$, $\sin \varphi = k_2/|\mathbf{k}|$.

which can be easily rewritten in a form of the rotor equation

$$\frac{\psi^* \mathbf{e}_3 \psi}{\psi \psi} = \frac{\mathbf{k}}{|\mathbf{k}|^2} E,$$

(18)

where $|\mathbf{k}| \equiv k = \sqrt{k_x^2 + k_y^2}$ is the magnitude of the wave vector. Since $\mathbf{e}_3$ is a unit vector, it follows that after rotation by $\psi$ the right hand side of (18) must be unit vector too. This means that the square of it satisfies algebraic equation $(E/k)^2 = 1$, which in fact represents the quantization condition, and from which the dispersion law, $E_\pm = \pm k$, immediately follows.

The corresponding eigenmultivectors can be deduced from the same equation (18) after insertion of $E_\pm$ values and requiring the rotor to satisfy $\psi \bar{\psi} = 1$. Then, the equation (18) reduces to

$$\psi_\pm \mathbf{e}_3 \bar{\psi}_\pm = \pm \hat{\mathbf{k}},$$

(19)

where $\hat{\mathbf{k}} = \mathbf{k}/|\mathbf{k}|$ is the unit vector. Thus, according to GA the eigenspinors $\psi_\pm$ of a monolayer graphene are simply rotors that bring the unit vector $\mathbf{e}_3$ which is parallel to the quantization axis to new direction $\pm \hat{\mathbf{k}}$, which is either parallel, as shown in Fig. 2, or antiparallel to the electron wave vector $\mathbf{k}$. No such clear-cut geometrical interpretation for eigenspinors exists in the Hilbert space. Using (14), solution of the rotor equation (19) can be written automatically as a rotation of $\mathbf{e}_3$ in the unit bivector plane $\hat{\mathbf{k}} \wedge \mathbf{e}_3$ by angle $\theta = \pi/2$ [see Eq. (5)],

$$\psi_\pm = e^{\pm \hat{\mathbf{k}} \wedge \mathbf{e}_3 \pi/4} = \frac{1}{\sqrt{2}} \left(1 \pm \hat{\mathbf{k}} \wedge \mathbf{e}_3\right) = \frac{1}{\sqrt{2}} \left(1 \pm \hat{\mathbf{k}} \mathbf{e}_3\right).$$

(20)

It should be noted that the eigenspinors (20) are coordinate-independent. The appearance of $\mathbf{e}_3$ in (20) is indispensable since the quantum mechanics requires to indicate the direction of the pseudospin (or spin) quantization axis which in our case was selected to be $\mathbf{e}_3$. If, as shown in Fig. 2, angle $\varphi$ between $\mathbf{e}_1$ and $\mathbf{k}$ is introduced the equation (20) can be written in coordinate form as $\psi_\pm = (1 \pm \sin \varphi \mathbf{e}_1 \mp \cos \varphi \mathbf{e}_2) / \sqrt{2}$. 

From quantum mechanical point of view the pseudospin in graphene has the same properties as spin. However, the spin is an intrinsic property of electron, while the pseudospin is the property of interacting $p$-orbitals of carbon atoms that make up the lattice. Thus, the average of pseudospinvector
may be found in exactly the same way as for electron spin [3],
\[
\langle P \rangle = \psi_+ \epsilon_3 \tilde{\psi}_+ = \pm k/|k| = \pm (\cos \varphi \epsilon_1 + \sin \varphi \epsilon_2).
\] (21)
We see, that the pseudospin is either parallel or antiparallel to electron propagation direction, Fig. 1a. This allows to introduce the helicity operator [9].

### 3.2. Electron in a quantum well (QW)

Let us now consider a potential well where the electron is squeezed between two stepped-potential planes. The Hamiltonian for electron in the QW is
\[
\hat{H}_{QW} = \left( \frac{\hbar^2}{2m^*} \right) (k_x^2 + k_y^2) \mathbf{\hat{1}} + \alpha_R (k_y \hat{\sigma}_x - k_x \hat{\sigma}_y)
\] (22)
where \(m^*\) is the effective mass of electron, \(k_x\) and \(k_y\) are the in-plane components and \(\mathbf{\hat{1}}\) denotes \(2 \times 2\) identity matrix. The first term is the kinetic energy and the second term describes interaction of electron spin with its orbital motion via spin-orbit interaction constant \(\alpha_R\). For simplicity we shall assume that \(m^* = \hbar = 1\). Using the replacement rules (15) the Hamiltonian (22) can be mapped into \(Cl_{3,0}\),
\[
H_{QW}(\psi) = k^2/2 + \alpha_R \epsilon_{12} k \psi \epsilon_3, \quad k = k_x \epsilon_1 + k_y \epsilon_2.
\] (23)
This expression is a coordinate-free. The blades \(\epsilon_{12}\) and \(\epsilon_3\) represent the QW plane and spin quantization axis which may be arbitrary.

To find the eigen one has to solve the multivector equation \(H_{QW}(\psi) = E\psi\), where \(E\) is the eigenenergy. Assuming that the spinor is normalized \(\psi\tilde{\psi} = 1\), the equation (23) can be rearranged into the rotor form
\[
\psi \epsilon_3 \tilde{\psi} = \frac{k^2/2 - E}{\alpha_R k^2} \epsilon_{12},
\] (24)
where \(k \epsilon_{12} = k \cdot \epsilon_{12}\) is the vector and \(k = |k|\) is \(k\) norm. Since the right hand side of (24) must be unit vector, its square must be equal to 1. This again results in a scalar equation (the quantization condition) the solution of which gives the spectrum (solid and dashed lines in Fig. 1b),
\[
E_\pm = k^2/2 \pm k\alpha_R.
\] (25)
Insertion of eigenenergies \(E_\pm\) back into (24) then gives
\[
\psi_\pm \epsilon_3 \tilde{\psi}_\pm = \pm (k_y \epsilon_1 - k_x \epsilon_2)/k \equiv \mathbf{\hat{a}}_\pm.
\] (26)
Since \(\epsilon_3\) is perpendicular to, while \(\mathbf{\hat{a}}_\pm\) lies in the quantum well plane the rotation angle is \(\theta = \pm \pi/2\). Then the solution of equation (26) is the rotor
\[
\psi_\pm = \exp \left( \pm \frac{\epsilon_3 \wedge \mathbf{\hat{a}}_\pm}{|\epsilon_3 \wedge \mathbf{\hat{a}}_\pm|} \frac{\pi}{4} \right).
\] (27)
In coordinate form the eigenspinors are \(\psi_\pm = (1 \mp \cos \varphi \epsilon_{23} \mp \sin \varphi \epsilon_{31})/\sqrt{2}\). The eigenspinors \(\psi_\pm\) can be used to calculate the average spin \(\langle s_\pm \rangle = \psi_\pm \epsilon_3 \tilde{\psi}_\pm\),
\[
\langle s_\pm \rangle = \pm (\sin \varphi \epsilon_1 - \cos \varphi \epsilon_2).
\] (28)
Thus the spins of SO split energy bands, as shown in Fig. 1b, are parallel to confining planes and have opposite directions, and at the same time (since \(k \cdot \langle s \rangle = 0\)) they are perpendicular to the wave vector.
3.3. A pair of coupled two-level atoms

In $Cl_{3,0}$ algebra, a single two-level atom Hamiltonian is $\hat{H}_1 = \hbar \omega \hat{\sigma}_z / 2$ which can be coupled to dipole moment $\mathbf{d}_1 = \mu \hat{\sigma}_x$, where $\hbar \omega$ is the energy difference between the energy levels and $\mu$ is the vectorial coupling constant. Let us take a pair of two-level atoms coupled to each other through dipole-dipole interaction. This kind of interaction may produce entanglement. Let the dipole coupling interaction energy be of the form $\Gamma \hat{\sigma}^{(1)} \hat{\sigma}^{(2)}$, where $\Gamma$ is the coupling constant and the superscript indicates the first and second two-level atom. Since the coupling energy is proportional to $\mu$, the coupling constant $\Gamma$ depends on angle $\theta$ between the vectors $\mu^{(1)}$ and $\mu^{(2)}$.

The composite Hamiltonian describing two two-level atom then is

$$\hat{H}_2 = \frac{\hbar \omega}{2} \left( \hat{\sigma}_z^{(1)} \otimes \hat{1} + \hat{1} \otimes \hat{\sigma}_z^{(2)} \right) + \Gamma \hat{\sigma}_x^{(1)} \otimes \hat{\sigma}_x^{(2)}. \quad (29)$$

The eigenvalues of $\hat{H}_2$ form four energy levels, $\pm \Gamma$ and $\pm \sqrt{\Gamma^2 + \omega^2}$, as shown in Fig. 1c.

Since $Cl_{3,0}$ algebra is too small for the four level system, the $Cl_{3,1}$ algebra will be used in the following. Its matrix representation by $4 \times 4$ complex matrices is given in the Appendix 4. After mapping of matrix equation (29) onto $Cl_{3,1}$ algebra one finds the respective GA Hamiltonian ($\hbar = 1$)

$$H_2(\psi) = \frac{\omega}{2} e_{34} \psi e_{34} - \Gamma e_2 \psi e_3 + \frac{\omega}{2} e_3 \psi e_3. \quad (30)$$

To find the eigens of the equation $H_2(\psi) = E\psi$ we will utilize spatial inversion operation $\bar{\psi} = -e_4 \psi e_4$ (see Appendix 4). With the help of it the spinor can be split into a sum of even $\bar{\psi}_+ = \psi_+$ and odd $\bar{\psi}_- = -\psi_-$ parts. Since $e_{34} \psi e_{34} = e_3 \bar{\psi} e_3$ and the eigenequation $H_2(\psi) = E\psi$ and its inversion $\overline{H}_2(\bar{\psi}) = \overline{E\psi}$ give $(H_2(\psi) + \overline{H}_2(\psi))/2 = E\psi_+$ and $(H_2(\psi) - \overline{H}_2(\psi))/2 = E\psi_-$, we find that the equations for even and odd states decouple into two independent equations,

$$-\Gamma e_2 \psi_+ e_3 = E\psi_+, \quad (31)$$

$$\omega e_3 \psi_- e_3 - \Gamma e_2 \psi_- e_3 = E\psi_. \quad (32)$$

Assuming that $\psi_+ \bar{\psi}_+ = 1$, the first equation (31) can be rearranged into rotor form

$$\psi_+ e_3 \bar{\psi}_+ = -\frac{E}{\Gamma} e_2, \quad (33)$$

from which we find the eigenvalues and respective rotor equation

$$E^{(1,2)} = \pm \Gamma, \quad \psi_+ e_3 \bar{\psi}_+ = \mp e_2. \quad (34)$$

The solution of the latter gives the first pair of spinor-rotors

$$\psi_+^{(1,2)} = e^{\pm e_{23} \pi/4} = (1 \pm e_{23}) / \sqrt{2}. \quad (35)$$

The rotor $\psi_+^{(1)}$ gives the eigenenergy $E_+^{(1)} = \langle \psi_+^{(1)} | \hat{H} | \psi_+^{(1)} \rangle = -\Gamma$ and rotates $e_3$ to $e_2$, while $\psi_+^{(2)}$ gives $E_+^{(2)} = \langle \psi_+^{(2)} | \hat{H} | \psi_+^{(2)} \rangle = \Gamma$ and rotates $e_3$ to $-e_2$. 


Figure 3. Basis vectors \( \{ \mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3 \} \), the wave vector \( \mathbf{k} \), and the rotation plane \( \hat{\mathbf{B}} = \mathbf{e}_3 \wedge \mathbf{a} \). The vector \( \mathbf{e}_3 \) is perpendicular to bilayer graphene plane (square). The line that connects \( K \) and \( K' \) valleys in the Brillouin zone is perpendicular to \( \mathbf{e}_2 \).

In a similar fashion from the second eigenequation (32) one finds

\[
E^{(3,4)} = \pm \sqrt{\omega^2 + \Gamma^2}, \quad \psi_- \mathbf{e}_3 \bar{\psi}_- = \pm \frac{\omega \mathbf{e}_3 - \Gamma \mathbf{e}_2}{\sqrt{\omega^2 + \Gamma^2}} \equiv \mathbf{a}.
\]

The solution of the second equation gives the second pair of spinor-rotors

\[
\psi_{-,3}^{(3,4)} = \exp \left( \pm \frac{\mathbf{e}_3 \wedge \hat{\mathbf{a}}}{|\mathbf{e}_3 \wedge \hat{\mathbf{a}}|} \theta \right) = \cos \frac{\theta}{2} \pm \frac{\mathbf{e}_3 \wedge \hat{\mathbf{a}}}{|\mathbf{e}_3 \wedge \hat{\mathbf{a}}|} \sin \frac{\theta}{2},
\]

where \( \cos \theta = \mathbf{e}_3 \cdot \hat{\mathbf{a}} \), \( \cos(\theta/2) = \frac{1 + \cos \theta}{2} \) and \( \sin(\theta/2) = \frac{1 - \cos \theta}{2} \). In our case \( \cos \theta = \omega / \sqrt{\omega^2 + \Gamma^2} \) and \( \frac{\mathbf{e}_3 \wedge \hat{\mathbf{a}}}{|\mathbf{e}_3 \wedge \hat{\mathbf{a}}|} = \mathbf{e}_{23} \), therefore, the rotation acts in \( \mathbf{e}_{23} \) plane.

3.4. Bilayer graphene

In previous example the rotors \( \psi_+ \) and \( \psi_- \) were decoupled. Here we shall consider more complex case of bilayer graphene (BG) where the rotors are coupled. A unique feature of the BG is its tunable energy band structure [8].

In \( Cl_{3,1} \) the BG Hamiltonian function reads [10]

\[
H_{BG}(\psi) = \eta \mathbf{k} \psi \mathbf{l} \mathbf{e}_3 - \frac{\gamma_1}{2} \mathbf{e}_2 (\psi - \bar{\psi}) \mathbf{e}_3 + \eta U \mathbf{e}_3 \psi \mathbf{e}_3,
\]

where \( \gamma_1 \) is the interlayer coupling energy (constant), \( 2U \) is the potential difference between the layers, and \( \eta = +1 \) is for \( K \)-valley and \( \eta = -1 \) for \( K' \)-valley, i.e. the points in the momentum space where electron transport takes place. The presence of two basis vectors in (38) comes from the geometry. One of them represents pseudospin quantization axis which is aligned with \( \mathbf{e}_3 \), the other being \( K - K' \) axis which is perpendicular to \( \mathbf{e}_2 \), Fig. 3. Thus, the geometry again comes explicitly in GA formulation of quantum problems.

To transform the eigenequation \( H_{BG}(\psi) = E \psi \) into rotors the spinor is again split into even and odd parts, \( \psi = \psi_+ + \psi_- \), and then the eigenequation is decomposed into two coupled multivector equations for \( \psi_+ \) and \( \psi_- \),

\[
E \psi_+ = \eta \mathbf{k} \psi_- \mathbf{l} \mathbf{e}_3 + \eta U \mathbf{e}_3 \psi_+ \mathbf{e}_3,
E \psi_- = \eta \mathbf{k} \psi_+ \mathbf{l} \mathbf{e}_3 + \eta U \mathbf{e}_3 \psi_- \mathbf{e}_3 - \gamma_1 \mathbf{e}_2 \psi_- \mathbf{e}_3.
\]

The method of solution of the coupled system (39) uses the fact that \( \psi_+ \) and \( \mathbf{i} \psi_- \), where \( \mathbf{i} \) is the pseudoscalar of \( Cl_{3,1} \), are rotors in 3D Euclidean space. If \( \psi_- \) is solved from the first equation and inserted into the second equation of (39) then after some algebraic manipulations one can construct the following rotor equation \( \psi_+ \mathbf{e}_3 \psi_+ = \mathbf{a} \) for \( \psi_+ \) (and analogous equation.
for $I \psi_{-}$. The requirement that the final vector $\hat{a}$ in Fig. 3 after rotation will not change its length is expressed by condition $\hat{a}^2 = 1$ which gives [10]

$$\hat{a}^2 = \frac{(E^2 - k^2 + U^2)^2 + U^2 \gamma_1^2}{E^2(4U^2 + \gamma_1^2)} = 1.$$  \hspace{1cm} (40)

This fourth order polynomial equation yields BG spectrum shown in Fig. 1d,

$$E^{(i)} = \pm \sqrt{k^2 + U^2 + \gamma_1^2} \pm \frac{1}{2} \sqrt{\gamma_1^4 + 4k^2(4U^2 + \gamma_1^2)}.$$  \hspace{1cm} (41)

Knowing $\hat{a}^{(i)} = a^{(i)}/|a^{(i)}|$ and $E^{(i)}$, one can construct the rotor for the $i$-th energy band. For details and properties of Berry’s phase calculated in terms of GA the reader should refer to [10].

In conclusion, we have shown that presence of a specific direction called the quantization axis in the Hamiltonian can be employed to solve quantum problems in GA. Since GA approach is coordinate-free the formulas found in this way appear to be compact and may be interpreted geometrically.

4. Appendix

Matrix representation. The basis vectors $e_i$ of $Cl_{3,1}$ algebra satisfy $e_i^2 = e_i^2 = e_i^2 = 1$ and $e_i^2 = -1$. The following $4 \times 4$ matrix representation of $e_i$ was used in transforming Hilbert space Hamiltonians to GA

$$\hat{e}_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \hat{e}_2 = i \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}, \quad \hat{e}_3 = \begin{bmatrix} \hat{\sigma}_y & 0 \\ 0 & -\hat{\sigma}_y \end{bmatrix}, \quad \hat{e}_4 = i \begin{bmatrix} \hat{\sigma}_z & 0 \\ 0 & -\hat{\sigma}_z \end{bmatrix},$$  \hspace{1cm} (42)

where $i = \sqrt{-1}$. $\hat{I}$ is $2 \times 2$ unit matrix and $\hat{\sigma}_x$, $\hat{\sigma}_y$, $\hat{\sigma}_z$ are Pauli matrices. Representations of higher blades can be found from matrix products, for example, $e_{12} \rightarrow \hat{e}_{12} = \hat{e}_1 \hat{e}_2$.

Replacement rules. The following mapping is assumed between the complex spinor $|\psi\rangle$ in a form of column and GA spinor $\psi$,

$$|\psi\rangle = \begin{bmatrix} a_0 + ia_3 \\ -b_3 + ib_0 \\ -b_2 - ib_1 \\ -a_1 + ia_2 \end{bmatrix} \leftrightarrow \begin{cases} \psi = a_0 + a_1 e_{23} - a_2 e_{31} + a_3 e_{12} \\ -b_0 I - b_1 e_{14} + b_2 e_{24} + b_3 e_{34}, \end{cases}$$  \hspace{1cm} (43)

where $a_i$’s and $b_i$’s are scalars. Matrix representation of basis elements (42) and rule (43) allow to construct the following replacement rules between the action of matrices on column vectors and $Cl_{3,1}$ multivector functions,

$$\hat{e}_i |\psi\rangle \leftrightarrow e_i \psi I e_3, \quad \hat{e}_{ij} |\psi\rangle \leftrightarrow e_{ij} \psi, \quad \hat{I} \hat{e}_i |\psi\rangle \leftrightarrow I e_i \psi I e_3,$$  \hspace{1cm} (44)

where $i, j = 1, 2, 3, 4$. Also, additional replacement rules may be useful

$$i |\psi\rangle \leftrightarrow I \psi e_{34}, \quad \langle \psi | \phi \rangle \leftrightarrow \langle \psi | \phi \rangle, \quad \langle \psi | \phi \rangle \leftrightarrow \langle \phi | \psi \rangle - \langle \phi | \psi \rangle e_{12}.$$  \hspace{1cm} (45)

As always, in GA the angled brackets, for example $\langle M \rangle$, indicate that only the scalar part of the multivector $M$ should be taken.

Spatial inversion, reversion and dagger operations. The spatial inversion (denoted by overbar) changes signs of all spatial vectors to opposite but leaves
“time” vector $e_4$ invariant: $e_i = -e_i$ for $i=1,2,3$ and $e_4 = e_4$. In $Cl_{3,1}$ the inversion of general multivector $M$ is defined by

$$\bar{M} = -e_4Me_4.$$  \hspace{1cm} (46)

Properties of inversion: $\bar{M_1 + M_2} = \bar{M_1} + \bar{M_2}$, and $\bar{M_1 M_2} = \bar{M_1} \bar{M_2}$. The spatial inversion allows to split the general spinor (43) into even and odd parts, $\psi = \psi_+ + \psi_-$, which satisfy $\bar{\psi}_+ = \psi_+$ and $\bar{\psi}_- = -\psi_-$. The reversion (denoted by tilde) changes the order of basis vectors in the multivector. The dagger operation is a combination of the reversion and spatial inversion

$$\psi^\dagger = -e_4 \tilde{\psi} e_4.$$ \hspace{1cm} (47)

If applied to a general bispinor it allows to find the square of the module

$$\langle \psi^\dagger \psi \rangle = a_0^2 + a_1^2 + a_2^2 + a_3^2 + b_0^2 + b_1^2 + b_2^2 + b_3^2.$$ \hspace{1cm} (48)

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A. Dargys
Center for Physical Sciences and Technology, Semiconductor Physics Institute, A. Goštauto 11, LT-01108 Vilnius, Lithuania
e-mail: adolfas.dargys@ftmc.lt

A. Acus
Institute of Theoretical Physics and Astronomy, Vilnius University, A. Goštauto 12, LT-01108 Vilnius, Lithuania
e-mail: arturas.acus@tfai.vu.lt