Electron with arbitrary pseudo-spins in multilayer graphene*

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Using the low-energy effective Hamiltonian of the ABC-stacked multilayer graphene, the pseudo-spin coupling to real orbital angular momentum of electrons in multilayer graphene is investigated. We show that the electron wave function in N-layer graphene mimics the behavior of a particle with a spin of $N \times (\hbar/2)$, where $N = \{1,2,3,\ldots\}$. It is said that for $N > 1$ the low-energy effective Hamiltonian for ABC-stacked graphene cannot be used to describe pseudo-spin-1/2 particles. The wave function of electrons in multilayer graphene may behave like fermionic (or bosonic) particle for N being odd (or even). In this paper, we propose a theory of graphene serving as a host material of electrons with arbitrary pseudo-spins tunable by changing the number of graphene layers.

Keywords: multilayer graphene, exotic particles, particle physics

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1. Introduction

Since graphene was discovered,[1] it has become a promising material for nanotechnology. It has also become a wonder material carrying several interesting physics properties that may connect the condensed matter to high energy physics.[2] In graphene, its carriers mimic the behavior of Dirac fermions. This may lead to Klein tunneling observed in the graphene p–n junction.[3] Zitterbewegung, trembling motion, could be studied in a graphene system.[2–4] Observation of atomic collapse in artificial nuclei on graphene was recently reported.[5] This is related to the relativistic quantum effect in grapheme, which causes charged impurities to exhibit resonances due to atomic collapse states.[5] Being significant for building a quantum computer, the fractional quantum Hall effect, which is tunable by the electric field in bilayer graphene, has been observed recently.[6] Related to the electron in graphene behaving like relativistic fermions, the fundamental physical property of such a pseudo-relativistic particle needs to be clarified. One of the important topics is the physical property of a pseudo-spin, which is generated by the presence of its two sublattices, A and B, instead of the usual (real) spin.[7] In this paper, the property of the pseudo-spin of an electron coupling to the real orbital angular momentum in ABC-stacked multilayer graphene will be investigated. We propose new pseudo-spin operators for the number of layers being greater than one.

2. The pseudo-spin-1/2 electron in monolayer graphene

Monolayer graphene, a two-dimensional (2D) honeycomb-like atomic structure formed by carbon atoms, has two sublattices A and B in a unit cell. The wave function of electrons may be described by two-component wave states ψ_A and ψ_B of electrons in the A- and B-sublattices, which act as the pseudo-spin states, i.e., $\psi_A \approx \psi_\uparrow$ and $\psi_B \approx \psi_\downarrow$, respectively. Graphene yields the low excited energy dispersion similar to a 2D Dirac fermion where the speed of light is replaced by the Fermi velocity $v_F \cong 10^6$ m/s. The momentum–energy relation obeys the relativistic-like relation

$$E = \sqrt{(pv_F)^2 + (mv_F^2)^2},$$

where E and p are energy and momentum, respectively. The pseudo-Dirac mass "m" may be generated due to breaking the symmetry of sublattice energy.[8] Since the pseudo-spin in graphene is generated by the presence of sublattice states, it was previously understood that the pseudo-spin generated by the presence of the sublattice states in monolayer graphene may not be associated with angular momentum.[9,10] Recently, some fundamental physical properties of the pseudo-spin in monolayer graphene have been investigated.[11,12] Mecklenburg and Regan[11] showed that the pseudo-spin of an electron in graphene is associated with real angular momentum, although it is not a real spin. This is because the total angular momentum $J_{z,1} = L_z + S_{z,1}$, which is perpendicular to the graphene plane, is conserved, i.e.,

$$[\hat{H}_1, \hat{L}_z + \hat{S}_{z,1}] = 0. \quad (1)$$

The $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$ is the angular momentum operator perpendicular to the graphene plane where $\langle \hat{x}, \hat{y} \rangle$ and $\langle \hat{p}_x, \hat{p}_y \rangle$ are operators of positions and momentum of the electron moving in the graphene plane, respectively. The intrinsic pseudo-spin of the electron in monolayer is found to be in the form of[11]

$$\hat{S}_{z,1} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \approx \frac{\hbar}{2}\sigma_z. \quad (2)$$

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Here σ_z is known as the Pauli spin matrix in the z direction. Since H_1 is the Hamiltonian acting on a pseudo-spinor field $\psi = (\psi_A, \psi_B)^T$ in monolayer graphene, it may be said that an effective electron field in monolayer graphene mimics the behavior of "spin-1/2 particle" because the spin operator in Eq. (2) yields an eigenvalue of $\hbar/2$.[11,12] The pseudo-spin in graphene may be defined as a usual Pauli spin operator, and it is given by

$$\hat{S}_1 = \hat{S}_{x,1}\hat{i} + \hat{S}_{y,1}\hat{j} + \hat{S}_{z,1}\hat{k}, \tag{3}$$

where $\hat{S}_{x,1} = (\hbar/2)\sigma_x$ and $\hat{S}_{y,1} = (\hbar/2)\sigma_y$ with $\sigma_{x(y)}$ being the Pauli matrice in the x (y) direction. The unit vectors parallel to the x, y, and z directions are $\hat{i}$, $\hat{j}$, and $\hat{k}$, respectively. In general, as all spin operators must satisfy "the commutation rule of an angular momentum",[13] it is found that the pseudo-spin operator of an electron in monolayer graphene defined in Eq. (3) obeys this rule to obtain

$$\begin{aligned} &[\hat{S}_{x,1}, \hat{S}_{y,1}] = \mathrm{i}\hbar\hat{S}_{z,1}, \quad [\hat{S}_{y,1}, \hat{S}_{z,1}] = \mathrm{i}\hbar\hat{S}_{x,1}, \\ &[\hat{S}_{z,1}, \hat{S}_{x,1}] = \mathrm{i}\hbar\hat{S}_{y,1}. \end{aligned} \tag{4}$$

The pseudo-spin only in the z direction is associated with the real angular momentum because there is no orbital angular momentum in the xy plane. It can be said that in-plane pseudo-spin may not be considered as a real angular momentum, since $[\hat{H}_1, \hat{L}_x + \hat{S}_{x,1}] \neq 0$ and $[\hat{H}_1, \hat{L}_y + \hat{S}_{y,1}] \neq 0$ in a 2D system, which has been discussed in Ref. [12].

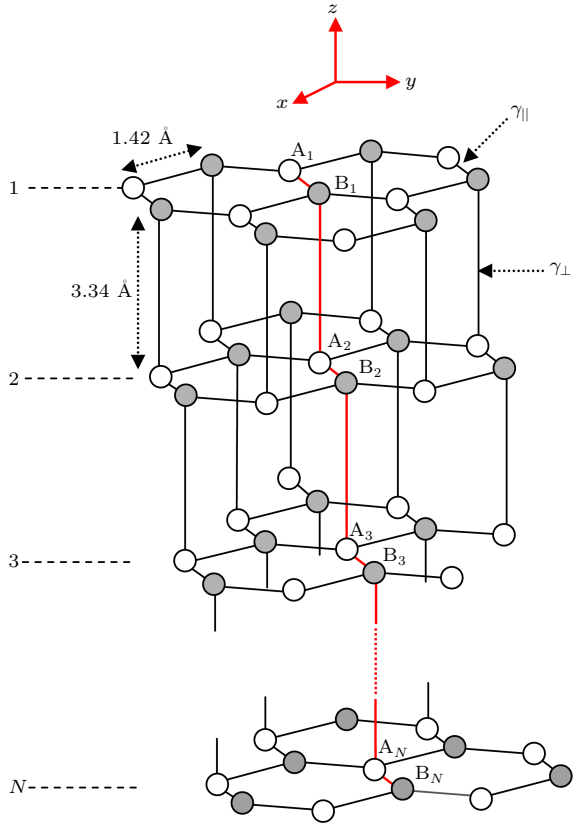


Fig. 1. (color online) Atomic structure of ABC-stacked N-layer graphene where A_N and B_N are denoted as the two sublattices in the N-th layer. The in-plane-nearest neighbor hopping energy $\gamma_{\parallel} \cong 2.8$ eV and the interlayer hopping energy $\gamma_{\perp} \cong 0.4$ eV are approximated.[15]

In the next section we will study the pseudo-spin operator coupling to orbital angular momentum $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$ for an electron in ABC-stacked multilayer graphene (see Fig. 1). We will show that the low energy electrons in N-layer graphene may not behave like spin-1/2 particles for $N > 1$.

3. Pseudo-spin and its angular momentum property in multilayer graphene

We start with the Hamiltonian derived based on the tight-binding model for the ABC-stacked N-layer graphene at the k point as given by[14]

$$\hat{H}_N = \hbar v_F \begin{pmatrix} \boldsymbol{\sigma}\cdot\boldsymbol{k} & \tau & 0 & 0 & 0 & \cdots & 0 \\ \tau^T & \boldsymbol{\sigma}\cdot\boldsymbol{k} & \tau & 0 & 0 & 0 & \vdots \\ 0 & \tau^T & \boldsymbol{\sigma}\cdot\boldsymbol{k} & \ddots & 0 & 0 & 0 \\ 0 & 0 & \ddots & \ddots & \ddots & 0 & 0 \\ 0 & 0 & 0 & \ddots & \boldsymbol{\sigma}\cdot\boldsymbol{k} & \tau & 0 \\ \vdots & 0 & 0 & 0 & \tau^T & \boldsymbol{\sigma}\cdot\boldsymbol{k} & \tau \\ 0 & \cdots & 0 & 0 & 0 & \tau^T & \boldsymbol{\sigma}\cdot\boldsymbol{k} \end{pmatrix}, \tag{5}$$

where

$$\tau^T = \begin{pmatrix} 0 & \gamma_{\perp} \\ 0 & 0 \end{pmatrix} / \hbar v_F, \text{ and } \tau = \begin{pmatrix} 0 & 0 \\ \gamma_{\perp} & 0 \end{pmatrix} / \hbar v_F,$$

with $t_{\perp}$ being the interlayer hopping energy.[15] Here, $\hat{\boldsymbol{k}} = \hat{k}_x\hat{i} + \hat{k}_y\hat{j}$ is the operator of the wave vector, and $\boldsymbol{\sigma} = \sigma_x\hat{i} + \sigma_y\hat{j} + \sigma_z\hat{k}$. The above Hamiltonian would act on a $2N$-component wave function of

$$\psi_N = \begin{pmatrix} \psi_{A,1} & \psi_{B,1} & \psi_{A,2} & \psi_{B,2} & \cdots & \psi_{A,N} & \psi_{B,N} \end{pmatrix}^T. \tag{6}$$

Near the Dirac point, we have $\psi_{B,1} = \psi_{A,2} = \psi_{B,2} = \cdots = \psi_{A,N} \cong 0$, the wave functions for electrons may be approximately given as a two-component wave function of the form

$$\psi_N \to \psi_{N,eff} = \begin{pmatrix} \psi_{A,1} \\ \psi_{B,N} \end{pmatrix}. \tag{7}$$

The two-component low energy effective Hamiltonian reduced form of Eq. (5) is usually obtained as[14,16–18]

$$\hat{H}_N \to \hat{H}_{N,\mathrm{eff}} = \frac{(\hbar v_F)^N}{(-\gamma_{\perp})^{N-1}} \begin{pmatrix} 0 & (\hat{k}_x - \mathrm{i}\hat{k}_y)^N \\ (\hat{k}_x + \mathrm{i}\hat{k}_y)^N & 0 \end{pmatrix}. \tag{8}$$

This two-component Hamiltonian would act on the two-component pseudo-spin state i.e., $\hat{H}_{N,\mathrm{eff}}\psi_{N,\mathrm{eff}} = E\psi_{N,\mathrm{eff}}$, where E is the excitation energy of the electron.

Next, we consider the pseudo-spin operator $\hat{S}_{z,N}$ which is associated with orbital angular momentum operator $\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x$ for the low energy electron in the N-layer ABC-stacked graphene. We may define the total angular momentum for the low energy electron as being in the form of $\hat{J}_{z,N} = \hat{L}_z + \hat{S}_{z,N}$. The pseudo-spin operator for the N-layer graphene must satisfy the conservation of the total angular momentum

condition of $[\hat{H}_{N,\text{eff}}, \hat{J}_{z,N}] = 0$. We thus calculate pseudo-spin operators via this condition, i.e.,

$$[\hat{H}_{N,\text{eff}}, \hat{L}_z] = \frac{(\hbar v_\text{F})^N}{(-\gamma_\perp)^{N-1}} \begin{pmatrix} 0 & N\hbar(\hat{k}_x - \text{i}\hat{k}_y)^N \\ -N\hbar(\hat{k}_x + \text{i}\hat{k}_y)^N & 0 \end{pmatrix} = -[\hat{H}_{N,\text{eff}}, \hat{S}_{z,N}],$$

where

$$\hat{S}_{z,N} = N\frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = N\frac{\hbar}{2}\sigma_z. \tag{9}$$

This result is unusual and very surprising, because the eigenvalue of the pseudo-spin in the z direction has a value of $\hbar/2$ only for $N = 1$ or in the case of monolayer graphene. For the case of $N = \{1,2,3,4,5,\ldots\}$, the pseudo-spin operator yields its eigenvalue of $\{\hbar,\ \frac{3}{2}\hbar,\ 2\hbar,\ \frac{5}{2}\hbar,\ \ldots\}$, respectively. It is said that the effective pseudo-spin for an electron in N-layer graphene behaves like the spin of a fermionic- (bosonic-) particle when N is odd (even). The lattice wave state may be equivalent to the pseudo-spin state of the form

$$\psi_{N,\text{eff}} = \begin{pmatrix} \psi_{\text{A},1} \\ \psi_{\text{B,N}} \end{pmatrix} \to \begin{pmatrix} \psi_{+N/2} \\ \psi_{-N/2} \end{pmatrix},$$

where

$$\hat{S}_{z,N}\begin{pmatrix} \psi_{+N/2} \\ 0 \end{pmatrix} = +(N\hbar/2)\begin{pmatrix} \psi_{+N/2} \\ 0 \end{pmatrix},$$
$$\hat{S}_{z,N}\begin{pmatrix} 0 \\ \psi_{-N/2} \end{pmatrix} = -(N\hbar/2)\begin{pmatrix} 0 \\ \psi_{-N/2} \end{pmatrix}. \tag{10}$$

Unfortunately, the two-component pseudo-spin state in Eq. (10) may be usual only in the case of $N = 1$ (monolayer), because there are two equivalent spin states $\psi_{\text{A},1} \to \psi_{+1/2}$ and $\psi_{\text{B},1} \to \psi_{-1/2}$ for the spin of $\hbar/2$. In monolayer graphene, spin operators $\hat{S}_{x,1}$, $\hat{S}_{y,1}$, and $\hat{S}_{z,1}$ do satisfy the "the commutation rule of an angular momentum", while for $N > 1$, there are no two-component spin operators $\hat{S}_{x,N}$, $\hat{S}_{y,N}$, and $\hat{S}_{z,N}$ to satisfy such a rule. If we define the spin operators as

$$\hat{S}_{x,N} = N\frac{\hbar}{2}\sigma_x \ \text{ and } \ \hat{S}_{y,N} = N\frac{\hbar}{2}\sigma_y \tag{11}$$

for the N-layer, we will obtain

$$[\hat{S}_{x,N}, \hat{S}_{y,N}] = \text{i}N\hbar\hat{S}_{z,N}, \quad [\hat{S}_{y,N}, \hat{S}_{z,N}] = \text{i}N\hbar\hat{S}_{x,N},$$
$$[\hat{S}_{z,N}, \hat{S}_{x,N}] = \text{i}N\hbar\hat{S}_{y,N}. \tag{12}$$

The result in Eq. (12) violates "the commutation rule of an angular momentum", except for $N = 1$. It is said that for $N > 1$, the pseudo-spin operators defined in Eq. (11) do not exhibit angular momentum operators. It will be better if we describe the pseudo-spin state in N-layer graphene as a real spin angular momentum state, because $\hat{S}_{z,N}$ should be a real angular momentum of eigenspin $N\hbar/2$. This is related to the property that it obeys the conservation of total angular momentum $[\hat{H}_{N,\text{eff}}, \hat{J}_{z,N}] = 0$.[11,12]

4. New pseudo-spin operator presentation

Since the pseudo-spin operator given in Eq. (9) violates "the commutation rule of an angular momentum" for $N > 1$, despite it being an angular momentum in the z direction, it must be wrong if it is an angular momentum and it does not obey the commutation rule of an angular momentum. In this work, we thus propose new pseudo-spin states $\tilde{\psi}_N$ for effective electrons in N-layer graphene analogous to real spin states.[19] We may have

$$\tilde{\psi}_{N=\text{even}} = (\psi_{+N/2},\ \psi_{+(N-2)/2},\ \cdots, \psi_0,\ \ldots, \psi_{-(N-2)/2},\ \psi_{-N/2})^\text{T} \tag{13}$$

$$\tilde{\psi}_{N=\text{odd}} = (\psi_{+N/2},\ \psi_{+(N-2)/2}, \cdots, \psi_{+1/2},\ \psi_{-1/2}, \ldots, \psi_{-(N-2)/2},\ \psi_{-N/2})^\text{T}. \tag{14}$$

The associated pseudo-spin in the z direction may be defined as being similar to a real spin angular momentum operator[19] and given by

$$\hat{\tilde{S}}_{z,N=\text{even}} = \frac{\hbar}{2}\begin{pmatrix} +N & & & & & & 0 \\ & +(N-1) & & & & & \\ & & \ddots & & & & \\ & & & 0 & & & \\ & & & & \ddots & & \\ & & & & & -(N-1) & \\ 0 & & & & & & -N \end{pmatrix}, \tag{15}$$

and

$$\hat{\tilde{S}}_{z,N=\text{odd}} = \frac{\hbar}{2}\begin{pmatrix} +N & & & & & & 0 \\ & +(N-1) & & & & & \\ & & \ddots & & & & \\ & & & +1 & & & \\ & & & & -1 & & \\ & & & & & \ddots & \\ & & & & & -(N-1) & \\ 0 & & & & & & -N \end{pmatrix}. \tag{16}$$

As we have seen from Eq. (13) to Eq. (16), the condition of $\psi_{\text{A},1} = \psi_{+N/2}$ and $\psi_{\text{B,N}} = \psi_{-N/2}$ satisfies the eigenvalues of spin $+N\hbar/2$ and $-N\hbar/2$, respectively. Also $\{\psi_0, \ldots, \psi_{\pm(N-6)/2}, \psi_{\pm(N-4)/2}, \psi_{\pm(N-2)/2}\}$ and $\{\psi_{\pm1/2}, \ldots, \psi_{\pm(N-6)/2}, \psi_{\pm(N-4)/2}, \psi_{\pm(N-2)/2}\}$ are introduced to serve as the eigenstates of $\hat{\tilde{S}}_{z,N=\text{even}}$ and $\hat{\tilde{S}}_{z,N=\text{odd}}$, respectively. We may set their amplitudes to be zero because there are no such states in multilayer graphene.

The Hamiltonian in Eq. (8) may be replaced by an $(N+1)\times(N+1)$ matrix because it must act on $\tilde{\psi}_N$, and is given by

$$\hat{\tilde{H}}_N = \begin{pmatrix} 0 & & & h_N \\ & & 0 & \\ & \iddots & & \\ & 0 & & \\ h_N^* & & & 0 \end{pmatrix},$$

where

$$h_N = \frac{(\hbar v_{\rm F})^N}{(-\gamma_\perp)^{N-1}}(\hat{k}_x - {\rm i}\hat{k}_y)^N. \tag{17}$$

Since we define the total angular momentum operator $\hat{\tilde{J}}_{z,N} = \hat{L}_z + \hat{\tilde{S}}_{z,N}$, the conservation of the total angular momentum remains the same, i.e.,

$$[\hat{\tilde{H}}_N, \hat{L}_z + \hat{\tilde{S}}_{z,N}] = 0. \tag{18}$$

As mentioned above, the bosonic-like wave states $\{\psi_0, \ldots, \psi_{\pm(N-6)/2}, \psi_{\pm(N-4)/2}, \psi_{\pm(N-2)/2}\}$ and the fermionic-like wave states $\{\psi_{\pm 1/2}, \ldots, \psi_{\pm(N-6)/2}, \psi_{\pm(N-4)/2}, \psi_{\pm(N-2)/2}\}$ were introduced due to the fact that the eigenstates associated with the revised pseudo-spin operators in Eqs. (15) and (16) may be required to preserve "the commutation rule of an angular momentum" for $N > 1$, because the spin operator must be an $(N+1)\times(N+1)$ matrix. In the equation of motion, it would play no role, because there are no matrix elements in the Hamiltonian $\hat{\tilde{H}}_N$. The term for describing the motion may disappear in the Hamiltonian. The condition, under which the motions of $\psi_{\rm A,1} = \psi_{+N/2}$ and $\psi_{\rm B,N} = \psi_{-N/2}$ with using the new Hamiltonian in Eq. (17) remains the same as the one calculated via Eq. (8), is also required.

From Eqs. (14)–(18) we may obtain, for instance, the results for pseudo-wave states, pseudo-spin operators, and modified Hamiltonians which have been revised as follows.

For $N = 1$ (spin-1/2 particle), the pseudo-spin state reads

$$\tilde{\psi}_1 = \begin{pmatrix} \psi_{+1/2} \\ \psi_{-1/2} \end{pmatrix}, \quad \psi_{\rm A,1} = \psi_{+1/2}, \quad \psi_{\rm B,1} = \psi_{-1/2},$$

and the spin operators are

$$\hat{\tilde{S}}_{z,1} = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \hat{\tilde{S}}_{x,1} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{\tilde{S}}_{y,1} = \frac{\hbar}{2}\begin{pmatrix} 0 & -{\rm i} \\ {\rm i} & 0 \end{pmatrix},$$

the Hamiltonian is

$$\hat{\tilde{H}}_1 = \begin{pmatrix} 0 & \hbar v_{\rm F}(\hat{k}_x - {\rm i}\hat{k}_y) \\ \hbar v_{\rm F}(\hat{k}_x + {\rm i}\hat{k}_y) & 0 \end{pmatrix}.$$

The conservation of the total angular momentum

$$\hat{\tilde{J}}_{z,1} = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x + \hat{\tilde{S}}_{z,1} : [\hat{\tilde{H}}_1, \hat{\tilde{J}}_{z,1}] = 0. \tag{19}$$

For $N = 2$ (spin-1 particle), the pseudo-spin state reads

$$\tilde{\psi}_2 = \begin{pmatrix} \psi_{+1} \\ \psi_0 \\ \psi_{-1} \end{pmatrix}, \quad \psi_{\rm A,1} = \psi_{+1}, \quad \psi_{\rm B,2} = \psi_{,-1},$$

the spin operators are

$$\hat{\tilde{S}}_{z,2} = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \hat{\tilde{S}}_{x,2} = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\hat{\tilde{S}}_{y,2} = \frac{\hbar}{\sqrt{2}}\begin{pmatrix} 0 & -{\rm i} & 0 \\ {\rm i} & 0 & -{\rm i} \\ 0 & {\rm i} & 0 \end{pmatrix}.$$

The Hamiltonian is

$$\hat{\tilde{H}}_2 = \begin{pmatrix} 0 & 0 & \dfrac{(\hbar v_{\rm F})^2}{-\gamma_\perp}(\hat{k}_x - {\rm i}\hat{k}_y)^2 \\ 0 & 0 & 0 \\ \dfrac{(\hbar v_{\rm F})^2}{-\gamma_\perp}(\hat{k}_x + {\rm i}\hat{k}_y)^2 & 0 & 0 \end{pmatrix}$$

and the conservation of the total angular momentum is

$$\hat{\tilde{J}}_{z,2} = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x + \hat{\tilde{S}}_{z,2} : [\hat{\tilde{H}}_2, \hat{\tilde{J}}_{z,2}] = 0. \tag{20}$$

For $N = 3$ (spin 3/2 particle), the pseudo-spin state reads

$$\tilde{\psi}_3 = \begin{pmatrix} \psi_{+3/2} \\ \psi_{+1/2} \\ \psi_{-1/2} \\ \psi_{-3/2} \end{pmatrix}, \quad \psi_{\rm A,1} = \psi_{+3/2}, \quad \psi_{\rm B,3} = \psi_{-3/2},$$

the spin operators are expressed as

$$\hat{\tilde{S}}_{z,3} = \frac{\hbar}{2}\begin{pmatrix} 3 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -3 \end{pmatrix},$$

$$\hat{\tilde{S}}_{x,3} = \frac{\hbar}{2}\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix},$$

$$\hat{\tilde{S}}_{y,3} = \frac{\hbar}{2}\begin{pmatrix} 0 & -{\rm i}\sqrt{3} & 0 & 0 \\ {\rm i}\sqrt{3} & 0 & -{\rm i}2 & 0 \\ 0 & {\rm i}2 & 0 & -{\rm i}\sqrt{3} \\ 0 & 0 & {\rm i}\sqrt{3} & 0 \end{pmatrix}.$$

The Hamiltonian has the form of

$$\hat{\tilde{H}}_3 = \begin{pmatrix} 0 & 0 & 0 & \dfrac{(\hbar v_{\rm F})^3}{(-\gamma_\perp)^2}(\hat{k}_x - {\rm i}\hat{k}_y)^3 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \dfrac{(\hbar v_{\rm F})^3}{(-\gamma_\perp)^2}(\hat{k}_x + {\rm i}\hat{k}_y)^3 & 0 & 0 & 0 \end{pmatrix},$$

and the conservation of the total angular momentum reads

$$\hat{\tilde{J}}_{z,3} = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x + \hat{\tilde{S}}_{z,3} : [\hat{\tilde{H}}_3, \hat{\tilde{J}}_{z,3}] = 0. \tag{21}$$

All the pseudo-spin operators satisfy the commutation rule of an angular momentum to obtain

$$\begin{aligned} &\left[\hat{\tilde{S}}_{x,N}, \hat{\tilde{S}}_{y,N}\right] = {\rm i}\hbar\hat{\tilde{S}}_{z,N}, \quad \left[\hat{\tilde{S}}_{y,N}, \hat{\tilde{S}}_{z,N}\right] = {\rm i}\hbar\hat{\tilde{S}}_{x,N}, \\ &\left[\hat{\tilde{S}}_{z,N}, \hat{\tilde{S}}_{x,N}\right] = {\rm i}\hbar\hat{\tilde{S}}_{y,N}. \end{aligned} \tag{22}$$

5. Gap-induced pseudo-Larmor precession for pseudo-spin-1/2 and spin-1 particles

In this section, we investigate the pseudo-Larmor precession of the total angular momentum, which is associated with pseudo-spin $\hat{\tilde{S}}_N = \hat{\tilde{S}}_{x,N}\hat{i} + \hat{\tilde{S}}_{y,N}\hat{j} + \hat{\tilde{S}}_{z,N}\hat{k}$ in the cases of $N = 1$ and $N = 2$, in order to compare the Larmor frequencies of pseudo-spin-1/2 and spin-1 particles. The 2D angular momentum operators must satisfy $\hat{L}_x = (\hat{y}\hat{p}_z - \hat{z}\hat{p}_y) = \hat{L}_y = (\hat{z}\hat{p}_x - \hat{x}\hat{p}_z) = 0$, thus we obtain

$$\hat{L} = \begin{pmatrix} \hat{y}\hat{p}_z - \hat{z}\hat{p}_y \\ \hat{z}\hat{p}_x - \hat{x}\hat{p}_z \\ \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \hat{x}\hat{p}_y - \hat{y}\hat{p}_x \end{pmatrix}. \tag{23}$$

Hence, the total angular momentum operator may be defined as

$$\hat{\tilde{J}}_N = \begin{pmatrix} \hat{\tilde{J}}_{x,N} \\ \hat{\tilde{J}}_{y,N} \\ \hat{\tilde{J}}_{z,N} \end{pmatrix} = \begin{pmatrix} \hat{\tilde{S}}_{x,N} \\ \hat{\tilde{S}}_{y,N} \\ (\hat{x}\hat{p}_y - \hat{y}\hat{p}_x) + \hat{\tilde{S}}_{z,N} \end{pmatrix}. \tag{24}$$

The torque of the total angular momentum operator may be determined using the Heisenberg picture as follows:

$$\frac{\mathrm{d}\hat{\tilde{J}}_N}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}\left[\hat{\tilde{H}}_N, \hat{\tilde{J}}_N\right]. \tag{25}$$

We will first determine the torque of the pseudo-spin-1/2 particle in monolayer graphene. The Hamiltonian for an electron in monolayer graphene in the case of gap opening may be usually given as[11,12]

$$\hat{\tilde{H}}_1 = \begin{pmatrix} 0 & \hbar v_{\mathrm{F}}(\hat{k}_x - \mathrm{i}\hat{k}_y) \\ \hbar v_{\mathrm{F}}(\hat{k}_x + \mathrm{i}\hat{k}_y) & 0 \end{pmatrix} + \begin{pmatrix} \Delta & 0 \\ 0 & -\Delta \end{pmatrix}, \tag{26}$$

where 2Δ is denoted as the energy gap between the valance band and the conduction band. We consider the precession of the rest electron, which satisfies $k_x = k_y = 0$.

$$\frac{\mathrm{d}\hat{\tilde{J}}_1}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}[\hat{\tilde{H}}_1, \hat{\tilde{J}}_1] = \begin{pmatrix} \dfrac{\mathrm{d}\hat{\tilde{J}}_{x,1}}{\mathrm{d}t} = -\left(\dfrac{2\Delta}{\hbar}\right)\hat{\tilde{J}}_{y,1} \\ \dfrac{\mathrm{d}\hat{\tilde{J}}_{y,1}}{\mathrm{d}t} = +\left(\dfrac{2\Delta}{\hbar}\right)\hat{\tilde{J}}_{x,1} \\ \dfrac{\mathrm{d}\hat{\tilde{J}}_{z,1}}{\mathrm{d}t} = 0 \end{pmatrix}. \tag{27}$$

The above result indicates that the frequency of the Larmor precession of the pseudo-total angular momentum about the z axis is $\omega_{\mathrm{Larmor}} = 2\Delta/\hbar$ for the electron in monolayer graphene.

We will first determine the torque of the spin-1 particle in bilayer graphene. The modified Hamiltonian for the electron in bilayer graphene in the case of gap opening may be given as

$$\hat{\tilde{H}}_2 = \begin{pmatrix} 0 & 0 & \dfrac{(\hbar v_{\mathrm{F}})^2}{-\gamma_\perp}(\hat{k}_x - \mathrm{i}\hat{k}_y)^2 \\ 0 & 0 & 0 \\ \dfrac{(\hbar v_{\mathrm{F}})^2}{-\gamma_\perp}(\hat{k}_x + \mathrm{i}\hat{k}_y)^2 & 0 & 0 \end{pmatrix} + \begin{pmatrix} \Delta & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\Delta \end{pmatrix}. \tag{28}$$

When the precession of the rest electron is considered, we obtain

$$\frac{\mathrm{d}\hat{\tilde{J}}_2}{\mathrm{d}t} = \frac{\mathrm{i}}{\hbar}[\hat{\tilde{H}}_2, \hat{\tilde{J}}_2] = \begin{pmatrix} \dfrac{\mathrm{d}\hat{\tilde{J}}_{x,2}}{\mathrm{d}t} = -\left(\dfrac{\Delta}{\hbar}\right)\hat{\tilde{J}}_{y,2} \\ \dfrac{\mathrm{d}\hat{\tilde{J}}_{y,2}}{\mathrm{d}t} = +\left(\dfrac{\Delta}{\hbar}\right)\hat{\tilde{J}}_{x,2} \\ \dfrac{\mathrm{d}\hat{\tilde{J}}_{z,2}}{\mathrm{d}t} = 0 \end{pmatrix}. \tag{29}$$

The Larmor precession of the pseudo-total angular momentum about the z axis is $\omega_{\mathrm{Larmor}} = \Delta/\hbar$ for the electron in bilayer grapheme, which is lower than that in monolayer graphene. It is said that both gaps in mono- and bilayer-graphene would behave like a pseudo-magnetic field leading to the Larmor precessions. The magnetic-like interaction Hamiltonians in mono- and bilayer-graphene resulting from the gap opening may be written respectively as

$$\hat{\tilde{H}}_{1,\mathrm{int}} = \begin{pmatrix} \Delta & 0 \\ 0 & -\Delta \end{pmatrix} = \mu_{\mathrm{B}}\boldsymbol{B}_1 \cdot \hat{\tilde{S}}_1 = \mu_{\mathrm{B}}B_{z,1}\hat{\tilde{S}}_{z,1}$$

and

$$\hat{\tilde{H}}_{2,\mathrm{int}} = \begin{pmatrix} \Delta & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -\Delta \end{pmatrix} = \mu_{\mathrm{B}}\boldsymbol{B}_2 \cdot \hat{\tilde{S}}_2 = \mu_{\mathrm{B}}\boldsymbol{B}_2\hat{\tilde{S}}_{z,2}, \tag{30}$$

where

$$\boldsymbol{B}_{1(2)} = (0)\hat{i} + (0)\hat{j} + B_{z,1(2)}\hat{k}.$$

As we have seen in the above equations, the gap-induced magnetic interaction strength in monolayer graphene is twice that in bilayer graphene, i.e.,

$$\mu_{\mathrm{B}}B_{z,1} = 2 \times \mu_{\mathrm{B}}B_{z,2} = \Delta/\hbar,$$

where μ_{B} and B_z are equivalent to the Bohr magneton and magnetic field, respectively.

6. Summary and conclusion

In this work, we studied the pseudo-spin coupling to the real orbital angular momentum in an ABC-stacked N-layer graphene. The pseudo-spin operator perpendicular to the graphene sheet is calculated using the conservation of the total angular momentum of the z direction.[11,12] It is found that at the low energy limit, the pseudo-spin of the electron in an N-layer ABC-stacked graphene does not exhibit a spin-1/2 particle when $N > 1$. The pseudo-spin of the electron is found to be of $N \times \hbar/2$. In this work, we introduced new pseudo-spin operators for electrons in multilayer graphene satisfying "the commutation rule of an angular momentum". We proposed graphene serving as a host material of electrons with arbitrary pseudo-spin, tunable by the number of layers.

References

[1] Novoselov K S, Geim A K, Morozov S V, Jiang D, Zhang Y, Dubonos S V, Grigorieva I V and Firsov A A 2004 *Science* **306** 666

[2] Sarma S D, Geim A K, Kim P and MacDonald A H 2007 *Solid State Commun.* **143** 1

[3] Stander N, Huard B and Gordon D G 2009 *Phys. Rev. Lett.* **102** 026807

[4] Katsnelson M I, Novoselov K S and Geim A K 2006 *Nat. Phys.* **2** 620

[5] Wang Y, Wong D, Shytov A V, Brar V W, Choi S, Wu Q, Tsai H Z, Regan W, Zettl A, Kawakami R K, Louie S G, Levitov L S and Crommie M F 2013 *Science* **340** 734

[6] Maher P, Wang L, Gao Y, Forsythe C, Taniguchi T, Watanabe K, Abanin D, Papić Z, Zimansky P C, Hone J, Kim P and Dean C R 2014 *Science* **345** 61

[7] Wallace P R 1947 *Phys. Rev.* **71** 622

[8] Giovannetti G, Khomyakov P A, Brocks G, Kelly P J and Brink J V D 2007 *Phys. Rev. B* **76** 073103

[9] Divincenzo D P and Male E J 1984 *Phys. Rev. B* **29** 1685

[10] Gusynin V P, Sharapov S G and Carbotte J P 2007 *Physica B* **21** 4611

[11] Mecklenburg M and Regan B C 2011 *Phys. Rev. Lett.* **106** 116803

[12] Soodchomshom B 2013 *Chin. Phys. Lett.* **30** 126201

[13] Desai B R 2009 *Quantum Mechanics with Basic Field Theory* (New York: Cambridge University Press)

[14] van Duppen B and Peeters F M 2013 *Europhys. Lett.* **102** 27001

[15] Neto A H C, Guinea F, Peres N M R, Novoselov K S and Geim A K 2009 *Rev. Mod. Phys.* **81** 109

[16] Min H and Macdonald A H 2008 *Phys. Rev. B* **77** 155416

[17] Nakamura M and Hirasawa L 2008 *Phys. Rev. B* **77** 045429

[18] Barlas Y, Yang K and MacDonald A H 2012 *Nanotechnology* **23** 052001

[19] Chiff L I 1968 *Quantum Mechanics*, 3rd edn. (New York: McGraw-Hill)