h-BN-layer-induced chiral decomposition in the electronic properties of multilayer graphene

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Received 30 October 2017, revised 30 November 2017
Accepted for publication 7 December 2017
Published 5 January 2018

Abstract
We discuss the chiral decomposition of non-symmetric stacking structures. It is shown that the low-energy electronic structure of a Bernal stacked graphene multilayer deposited on h-BN consists of chiral pseudospin doublets. \(N\) layer graphene stacks on the h-BN layer have \(N/2\) effective bilayer graphene systems and one effective h-BN layer if \(N\) is even or \((N - 1)/2\) effective graphene bilayers plus one graphene monolayer modified by an h-BN layer if \(N\) is odd. We present the decomposition procedure and derive the recurrence relations for the effective parameters characterizing the chiral subsystems. In this case, the effective parameters consist of interlayer couplings and on-site potentials in contrast to pure graphene multilayer systems where only interlayer couplings are modified. We apply this procedure to discuss the Klein tunnelling phenomena and quantitatively compare the results with pure graphene multilayer systems.

Keywords: graphene, h-BN, multilayers, chiral decomposition, Klein tunnelling

(Some figures may appear in colour only in the online journal)
by combining them into multilayers [28, 34, 35]. In this context, it is interesting to see how the transport properties of graphene multilayers change via their proximity to an insulator, so that the conducting channels are only through graphene bands. Since graphene and hexagonal boron nitride (h-BN) have identical lattice structures, it is convenient to choose this insulator as a partner for heterogeneous multilayers [36, 37].

The theoretical studies of multilayer graphene reveal that the Hamiltonian of Bernal stacking systems can be block diagonalized into effective bilayer (BLG) and monolayer (MLG) Hamiltonians depending on the parity of the layer numbers [26, 38]. The properties of effective bilayer subsystems are connected with the chirality of charge carriers in each specific multilayer system. This result implies that it may be possible to find different chiral fermions in multilayer graphene on h-BN systems to model tunnelling properties in view of applications in nano-electronics. Although h-BN is only weakly coupled to graphene and graphene bands sit deep within the hBN band gap, it is interesting to see which characteristics are really modified by its presence. In order to achieve this goal, the chiral decomposition procedure is generalized herein for multilayer graphene supported by the h-BN layer. We turn our attention to the tunnelling phenomena in such systems, namely to electron transport through the potential barrier that is higher than the energy of the incident electrons. We consider how the presence of the h-BN layer appears in the electronic properties and in the possibility of observing interband tunnelling when electrons outside the barrier (the conduction band) transform into holes inside it (the valence band), or vice versa [1, 39].

2. Model considerations

Layered materials are predominantly formed in hexagonal symmetries, including different stacking orders of hexagonal layers composed of two triangular sublattices. According to density functional theory (DFT) [40, 41] and the experimental findings [42], it is energetically favourable for the atoms of sublattice A(B) to be displaced along the honeycomb edges in a way that the atom from the sublattice A(B) sits on top of an atom belonging to another sublattice B(A). This stacking rule implies three distinct but equivalent projections of the 3D layered structures onto the xy plane and 2N-2 distinct N-layer stack sequences [27]. It is also known that there are mainly two stacking types for graphite: so-called Bernal stacking, forming the layer sequence 1212... and rhombohedral stacking, which forms the layer sequence 123123... . These two different possibilities for N ≤ 3 are shown in figure 1.

The multilayer systems of these types can be described by the following tight-binding n band Hamiltonian:

\[ H = H_{ML} + H_{inter} \]

where two components account for the intralayer and interlayer hoppings, respectively. The trial wave function for such a multilayer system can be written as:

\[ \Psi_k(\vec{r}) = \sum_{j=1}^{2N} a_j^{(j)} \Psi_j^{(j)}(\vec{r}) \]

where the superscript \( j \) denotes the different atoms per unit cell, \( a_j^{(j)} \) are complex functions of the quasi-momentum \( \vec{k} \) and \( \Psi_j^{(j)} \) are the Bloch functions constructed from the atomic orbital wave functions:

\[ \Psi_j^{(j)}(\vec{r}) = \sum_{\vec{k}} \exp(i\vec{k} \cdot \vec{R}_l) \Psi_j^{(j)}(\vec{r} + \vec{\delta}_l - \vec{R}_l). \]  

\( \vec{\delta}_l \) is the vector which connects the sites of the underlying Bravais lattice to the site of the \( j \) atom within the unit cell. There are \( 2N \) different energy bands and the energy of the \( j \)th band is given by \( E_k^{(j)} = \langle \Psi_k^{(j)} | H | \Psi_k^{(j)} \rangle / | \Psi_k^{(j)} |^2 \).

Minimizing this energy with respect to the \( a_j^{(j)} \) coefficients leads to the eigenvalue equation \( H \Psi_k^{(j)} = E_k^{(j)} \Psi_k^{(j)} \). The transfer integral matrix \( H \) and the overlap integral matrix \( S \) are \( 2N \times 2N \) matrices. The band energies may be determined from the eigenvalue equation by solving the secular equation \( \det(H - E_k^{(j)} I) = 0 \).

We assume that the interaction between two atoms only depends on their distance, and we take into account the nearest neighbour interactions.

The transfer integral matrix that takes into account different stacking sequences and on-site potential energies may be written as:

\[ H_N = \begin{pmatrix}
 ML_1 & \Gamma_{1,2} \\
 \Gamma_{2,1} & ML_2 \\
 \Gamma_{3,2} & ML_3 \\
 \Gamma_{4,3} & \ldots \\
 \ldots & \ldots \\
 ML_{N-1} & \Gamma_{N-1,N} \\
 \Gamma_{N,N-1} & ML_N
\end{pmatrix} \]  

\[ ML_i = \begin{pmatrix}
 \varepsilon_{i,\alpha} & -\gamma_0 f_\alpha(\vec{k}) \\
 -\gamma_0 f_\alpha^*(\vec{k}) & \varepsilon_{i,\beta}
\end{pmatrix} i = 1, 2, \ldots, N \]
\[ \Gamma_{i,i+1} = \gamma_i \begin{pmatrix} 0 & s_i \\ 1 - s_i & 0 \end{pmatrix} \quad i = 1, 2, ..., N - 1 \] (6)

\[ \Gamma_{i,i+1} = \Gamma_{i,i+1}^T. \] (7)

Parameter \( s_i \) equals 0 or 1 depending on the layer sequence in the multilayer system under consideration. The diagonal terms \( \delta_{i\alpha}(\beta) \) denote the on-site electron energy of the atom in layer \( i \) belonging to sublattice A(B). In the first approximation, they can be equal to the energy of an electron in the 2\( p_z \) orbital of an atom. However, this energy is modified as the atoms bond together forming a lattice, and can be considered as a parameter to fit the experimental findings. Two parameters \( \gamma \) describe the strength of the coupling between a specific pair of atoms: \( \gamma_{ij} \) denotes the coupling between the nearest neighbours in each monolayer while \( \gamma \) describes the direct interlayer coupling. The geometrical factor \( f(\vec{k}) \) resulting from a summation over the nearest neighbours in each monolayer can be written in terms of the vectors \( \vec{d}_i \) indicated in figure 1:

\[ f(\vec{k}) \equiv \sum_{i=1}^{N} \exp(\vec{k} \cdot \vec{d}_i) = \exp \left( \frac{k_x a_i}{\sqrt{2}} \right) + \exp \left( \frac{k_y a_i}{\sqrt{2}} \cos \left( \frac{k_z a_i}{2} \right) \right) \] (8)

and can be approximated by: \( f(\vec{k}) \approx -\frac{\sqrt{2} \pi}{\beta} (\xi p_x - ip_y) \) with \( \beta = h^2 - hK^2 \xi \pm 1 \).

The overlapping integrals take into account the fact that the orbitals do not span an orthogonal basis set. In the present approximation we include the overlap between two nearest neighbour atoms in the monolayer and the overlap between the atoms which are directly above/below each other in the neighbouring monolayers. Due to their small value, in all situations under consideration in this paper, even these two integrals are neglected. Then, we obtain the following recurrence relation for the determinant of the N-layer system:

\[ \begin{array}{l}
\det(H_N - E) = D_N = \det(ML_N \cdot D_{N-1}) \\
+ (\varepsilon_{N,\beta} - E) \sum_{k=1}^{N-2} (-1)^k (\varepsilon_{N-k,\alpha} - E) \prod_{i=N-k}^{N-1} (1 - s_i)^2 \gamma_i^2 D_{N-k-1} \\
+ (-1)^{N-1} (\varepsilon_{N,\alpha} - E) \prod_{i=N-1}^{N-1} (1 - s_i)^2 \gamma_i^2 \\
+ (\varepsilon_{N,\alpha} - E) \sum_{k=1}^{N-2} (-1)^k (\varepsilon_{N-k,\beta} - E) \prod_{i=N-k}^{N-1} s_i^2 \gamma_i^2 D_{N-k-1} \\
+ (-1)^{N-1} (\varepsilon_{N,\beta} - E) \prod_{i=1}^{N-1} s_i^2 \gamma_i^2 \\
\end{array} \] (9)

Now, we focus on the transport properties in such multilayer heterostructures. Let us consider the charge carriers incident on a potential barrier. Such a local potential barrier can be created, for example, by the electric field effect coming from local chemical doping. The situation is depicted schematically in figure 2.

Particles travelling from the left (region I) to the right (region III) in the graphene/hBN multilayer system are incident at energy \( E_F > 0 \) on a potential barrier (region II) of height \( U \) and width \( d \).

The Schrödinger equation describing this situation can be written as:

\[ \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \vdots \\ \psi_N \end{pmatrix} = \begin{pmatrix} A_1 \\ B_1 \\ A_3 \\ \vdots \\ B_N \end{pmatrix} \] (10)

where \( A_i \) and \( B_i \) represent the wave functions of sublattice A and B, respectively.

In order to find the eigenvectors one has to solve the following set of recurrence equations:

\[ \begin{align*}
\delta_{1A} \left[ (\varepsilon_{1,\alpha} - E)A_1 - \gamma_{1f}(\vec{k})B_1 + \gamma_1 \gamma_{1f}(\vec{k})A_1 \right] \\
+ (1 - \delta_{1A})(1 - \delta_{1B}) \left[ (1 - \gamma_1)\gamma_{1f}(\vec{k})B_1 - (\varepsilon_{1,\alpha} - E)A_1 - \gamma_{1f}(\vec{k})B_1 + \gamma_1 \gamma_1 \gamma_{1f}(\vec{k})B_1 \right] \\
+ \delta_{1B} \left[ (1 - \gamma_1)\gamma_{1f}(\vec{k})A_1 + (\varepsilon_{1,\alpha} - E)A_1 - \gamma_{1f}(\vec{k})B_1 \right] \\
+ (1 - \delta_{1A})(1 - \delta_{1B}) \left[ (1 - \gamma_1)\gamma_{1f}(\vec{k})B_1 - \gamma_{1f}(\vec{k})A_1 + (1 - \gamma_1)\gamma_{1f}(\vec{k})B_1 \right] \\
+ \delta_{1B} \left[ (1 - \gamma_1)\gamma_{1f}(\vec{k})A_1 - (\varepsilon_{1,\alpha} - E)A_1 - \gamma_{1f}(\vec{k})B_1 \right] \\
\end{align*} \] (12)

for \( k = 1, 2, ..., N \).
The plane-wave solution can be then written as a 2N spinor:

$$\Psi_R = (c_R^1 \Psi_{1,\xi} e^{-i k_{\xi} R} + c_R^2 \Psi_{2,\xi} e^{i k_{\xi} R} + c_R^3 \Psi_{3,\xi} e^{-i k_{\xi} R} + c_R^4 \Psi_{4,\xi} e^{i k_{\xi} R}) e^{i k_x R}$$

(13)

where index R represents three regions: $R = I$ on the left of barrier ($c_R^1 = 0$), $R = II$ inside the barrier and $R = III$ on the right of barrier ($c_R^3 = c_R^4 = 0$). Let $k^2 = 2mE_F/h^2$ be the wave vector for propagating modes in regions I and III, while $(k^\text{II})^2 = 2mE_F - U/\hbar^2$ is the wave vector in region II. We define then $k_x = k \cos \theta$ and $k_y = k \sin \theta$ in regions I and III, while in region II we have $k_x = k^\text{II} \cos \varphi$ and $k_y = k^\text{II} \sin \varphi = k \sin \theta$ last, because the transverse momentum is conserved. To be able to fulfil the boundary conditions for tunnelling through the potential barrier we have to consider the decaying modes which have an imaginary value of the momentum in the x-direction: $k_x = i \kappa_x$. Now the coefficients $c_{R,1,2,3,4}$ have to be found from the continuity of $\Psi_R$ at the boundaries between regions I and II ($x = 0$) and II and III ($x = \ell$). It is well known that the most interesting behaviour is expected for $U > E_F$, where chiral tunnelling can be observed. All the results in the following are discussed in this context.

### 3. Results and discussion

As described in section 2, we assume the nearest neighbour interactions and not locally modified onsite energies. This means we neglect the asymmetry leading to a ‘Mexican hat’ in the band structure, and the trigonal warping and opening up of small energy gaps between the conduction and the valence bands. The details of the band structure including all effects these are a very complicated problem that is yet to be studied. In view of the large uncertainty in the parameters involved, it is meaningless to introduce a more complicated model at this stage. It should be underlined that although inclusion of the other parameters does not cause principal problems, the analysis does become more complicated. For example, the inclusion of a trigonal warping phenomenon does not block the possibility of the chiral decomposition of the Hamiltonian describing the graphene multilayer systems with an arbitrary number of layers [35]. Hence, we believe that the Hamiltonian (4) correctly captures the main features of the present problem.

The values of all parameters employed in the present numerical calculations are taken from the standard set of parameters used in the theoretical analysis of graphene/h-BN multilayer system properties [43, 44]. Within the error bar they agree with the experimentally estimated parameters [45]. Two parameters describing the strength of the coupling between a specific pair of atoms are taken to be: $\gamma_{0,\text{C}-\text{C}} = 3.033\text{ eV}$ and $\gamma_{0,\text{N}-\text{B}} = 2.36\text{ eV}$ for coupling between the nearest neighbours in each graphene and h-BN monolayer, respectively, while $\gamma_{1,\text{C}-\text{C}} \equiv \gamma_1 = 0.39\text{ eV}$ and $\gamma_{1,\text{C}-\text{N}} = \gamma_{1,\text{C}-\text{N}} = 0.25\text{ eV}$ describe the interlayer couplings. Note, that we only consider stackings with carbon–nitrogen interaction [43]. Moreover, it is assumed here that the lattice constant $a$ is common for all monolayers building a system.

Thus, the difference between the lattice constant of graphene and h-BN is not taken into account. However, it seems to be justified by the fact that we consider the ultrathin multilayer systems which are willing to accommodate [46] in contrast to graphene on the h-BN substrate when a moiré pattern is observed [36]. Furthermore, we take the onsite energy to be equal to zero for carbon, 3.36 eV for nitrogen and $-3.66\text{ eV}$ for boron [43].

Transmission probability through a 100 nm wide barrier is calculated as a function of the incident angle for the Fermi energy of incident electrons of 17 meV, which is most typical in experiments with graphene [30, 47]. The barrier height is taken to be 50 meV. For a better comparison, the parameters are kept the same for all considered systems unless other values are stated in the text.

#### 3.1. Homogeneous multilayers

Although the main results of the present paper are connected with graphene/h-BN hybrid systems, we introduce likewise some remarks on pure graphene multilayers which fit in the mainstream discussion about tunnelling effects (48, 49) and the references therein) and seems to be interesting for a better understanding of the interband tunnelling nuances. The results of this subsection serve simultaneously as a background for comparison with the results for heterogeneous multilayers.

Let us start with a few comments on bilayer graphene (BLG). The eigenvalues of the Hamiltonian (4) for BLG are given by:

$$E^\pm_\eta = \pm \frac{\gamma_1}{2} \left( \sqrt{1 + \frac{4\gamma_0^2}{{\gamma_1}^2} |f(k)|^2} + \eta \right), \quad \eta = \pm 1. \quad (14)$$

The eigenvalues $E^\pm_\eta$ describe two bands that split away from the zero energy by $\pm \gamma_1$ at the K point $(f(k) = 0)$. This is because the orbitals on the A2 and B1 sites form a dimer that is coupled by interlayer hopping $\gamma_1$, resulting in a bonding and anti-bonding pair of states $\pm \gamma_1$. The formula $E^\pm_\eta$ interpolates between the linear dispersion at large momenta $(\gamma_1 < \sqrt{\gamma_0^2 + p^2} < \gamma_0)$ and quadratic dispersion near zero energy where the bands touch. These bands arise from the effective coupling between the orbitals on sites A1 and B2, which do not have a counterpart in the other layer. Such a system represents a gapless semiconductor with chiral electrons and holes with a finite mass. The bilayer graphene Hamiltonian, written in a two-component basis [1, 4], yields a parabolic energy spectrum and it is straightforward that we have four possible solutions for a given energy, two of them corresponding to propagating waves and the other two to evanescent waves. This leads to intriguing behaviour in the transport through the potential barrier, which is higher than the incident electron energy: electrons outside the barrier transform into holes inside it, or vice versa [1]. The limit of the validity for the two-band model lies in the condition that two high energy bands are not occupied, which seems to be fulfilled in BLG. However, it is interesting to see that this intriguing behaviour
can also be observed in the four-band description of BLG. In figure 3 we show the band structure (a) and the corresponding dependence of the absolute momentum $k^2$ on energy $E$ (b).

One can notice that in the energy range $0 < E < \gamma_1$ we still have two travelling waves $k^2 > 0$ and two evanescent waves $k^2 = \kappa^2 < 0$, which have an imaginary value of momentum in the propagation direction (holes with wave vectors $i\kappa$). We can now consider the tunnelling phenomena in the four-band approach. We assume that $0 < E_p < \gamma_1$ for the incoming wave, as this is the likely experimental situation. It is straightforward to show that the imaginary value of the momentum in the $x$-direction can be written as: $\kappa_x = \sqrt{k_x^2 - \kappa^2}$, and in the case of BLG it takes a form: $\kappa_x = \sqrt{k_x^2 - \frac{4}{\alpha}(1 - \sqrt{1 + \alpha k^2}) + k_x^2}$ with $\alpha = 3\gamma_0^2 a^2/\gamma_1^2$, which reduces to $\kappa_x = \sqrt{2k_y^2 + k_x^2}$ in the two band approximation. The dispersion relations in both approaches are compared in the bottom panel of figure 3(c). The corresponding transmission probabilities (figure 3(d)) exhibit ‘magic angles’ in the spectrum, at which the total transmission is observed, however the angles differ between these two approaches.

In order to calculate the physical quantities of a multilayer graphene system, it is useful to follow the partition procedure described in paper [27]. This procedure is based on division into smaller multilayer elements in a manner that excludes layers contained within the previously identified partitions. It follows that there is only one way of stacking which allows the chiral decomposition into isolated bilayer systems with some effective interlayer hopping, plus one monolayer if the number of monolayers $N$ is odd. As an example, we present in figures 4(a) and (b) the band structure of trilayer graphene (TLG) stacked as ABA (Bernal) and ABC, respectively.

Only in the case of ABA stacking, the transfer integral matrix:

$$H_{TLG}^{\text{eff}} = \begin{pmatrix} 0 & -\gamma_0 f(\kappa) & 0 & \gamma_1 & 0 & 0 \\ -\gamma_0 f^*(\kappa) & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\gamma_0 f(\kappa) & 0 & 0 \\ \gamma_1 & 0 & -\gamma_0 f^*(\kappa) & 0 & \gamma_1 & 0 \\ 0 & 0 & 0 & \gamma_1 & 0 & -\gamma_0 f(\kappa) \\ 0 & 0 & 0 & 0 & -\gamma_0 f^*(\kappa) & 0 \end{pmatrix}$$

(15)

can be rewritten in terms of two blocks: one representing an effective BLG and another one describing the usual graphene monolayer (MLG):

$$H_{TLG}^{\text{eff}} = \begin{pmatrix} 0 & -\gamma_0 f(\kappa) & 0 & \gamma_{1,\text{eff}} & 0 & 0 \\ -\gamma_0 f^*(\kappa) & 0 & 0 & 0 & 0 & 0 \\ \gamma_{1,\text{eff}} & 0 & -\gamma_0 f^*(\kappa) & 0 & \gamma_1 & 0 \\ 0 & 0 & 0 & 0 & -\gamma_0 f(\kappa) & 0 \\ 0 & 0 & 0 & 0 & -\gamma_0 f^*(\kappa) & 0 \end{pmatrix}$$

(16)

where $\gamma_{1,\text{eff}} = \sqrt{2}\gamma_1$ [26].

As a consequence, in the energy range $0 < E < \gamma_{1,\text{eff}}$, again we have two travelling waves $k^2 > 0$ and two evanescent waves $k^2 \equiv \kappa^2 < 0$, which have an imaginary value of momentum in the propagation direction (see figure 4(c)). The transmission probability of such a TLG has two modes: one connected with the effective BLG and the second one connected with the MLG. Both modes are shown in figure 4(d). It is easily seen that for certain incident angles one can expect the tunnelling through the potential barrier coming both from BLG and MLG. As for the ABC stacked trilayer, we have complex solutions for $k^2$ in the energy range $0 < E < \gamma_1$ with no clear physical interpretation, in contrast to previous cases when we have to deal with hole-like states [1]. Similar conclusions also arise from [26, 38]. Therefore, calculations

![Figure 3](image_url)
in the following are mainly devoted to Bernal stacking systems in which we can study interband tunnelling when the electrons outside the barrier transform into holes inside it, or vice versa. The presence of complex wave vectors instead of pure imaginary wave vectors inside the barrier region is another aspect which is discussed in the context of the tunnelling problem [50]. The influence of these waves, together with the pure oscillating waves, appears as an enhancement of the transmission probabilities at oblique angles when both the oscillating and evanescent wave states participate in the transmission. In the scattering process, the effective positive barrier introduces an evanescent mode which reduces the transmission probability and also causes the oscillating wave to undergo multiple reflections, which yield an angle-dependent Fabry–Pérot resonance. In the tunnelling through the barrier, the discrete bound states of the negative energy serve as transmission channels, resulting in angle-dependent transmission resonances.
3.2. Heterogeneous multilayers

We now consider the problem of chiral decomposition in graphene multilayers supported by the h-BN layer. First of all, let us recall the electronic properties of graphene/h-BN bilayer systems. Due to both the tight-binding [51] and DFT calculations [52], its band structure shows a gap between the valence and conduction bands. However, in the vicinity of the Brillouin-zone corners, the low-energy band structure possesses a near-graphene character, indicating weak interaction between the layers. This last observation has turned our attention towards systems with more graphene layers deposited between the layers. This observation supports the graphene properties. The simplest system, where one might expect chiral decomposition, can consist of 3 ML, which is two graphene layers on one h-BN. The Hamiltonian matrix (4) for a BLG/h-BN system takes the form:

\[
\begin{pmatrix}
    0 & -\gamma_0(\vec{k}) & 0 & \gamma_1 & 0 & 0 \\
    -\gamma_0^* (\vec{k}) & 0 & 0 & 0 & \gamma_0 & 0 \\
    \gamma_1 & 0 & -\gamma_0^* (\vec{k}) & 0 & \gamma_{1C-N} & -\gamma_0^* (\vec{k}) \\
    0 & 0 & 0 & \gamma_{1C-N} & \varepsilon_N & -\gamma_0^* (\vec{k}) \\
    0 & 0 & 0 & 0 & -\gamma_0^* (\vec{k}) & \varepsilon_B \\
\end{pmatrix}
\]

\[ (17) \]

and the effective Hamiltonian, with the same eigenvalues as the original one shown above, can be written as:

\[
\begin{pmatrix}
    \varepsilon & -\gamma_0 (\vec{k}) & 0 & \gamma_{1eff} & 0 & 0 \\
    -\gamma_0^* (\vec{k}) & 0 & 0 & 0 & \gamma_0 & 0 \\
    \gamma_{1eff} & 0 & -\gamma_0^* (\vec{k}) & 0 & \varepsilon_N' & -\gamma_0^* (\vec{k}) \\
    0 & 0 & 0 & \varepsilon_N & -\gamma_0^* (\vec{k}) & \varepsilon_B \\
\end{pmatrix}
\]

\[ (18) \]

The effective Hamiltonian is derived in the same way as for multilayer graphene systems [26], which means by assuming \( \text{det}(H - E I) = \text{det}(H^\text{eff} - E I) \). In the present case, however, the effective Hamiltonian is more complicated, containing not only the effective hoppings but also the effective onsite energies both for bilayer graphene and the h-BN layer. These effective parameters are related to the original parameters by the formulas:

\[
\varepsilon_N = \varepsilon_N' + 2\varepsilon \\
\gamma_1^2 + \gamma_{1C-N}^2 = -2\varepsilon\varepsilon_N' - (\varepsilon^2 - \gamma_{1eff}^2) \\
-\varepsilon_N\gamma_1^2 = \gamma_{1eff}^2 (\varepsilon^2 - \gamma_{1eff}^2)
\]

\[ (19) \]

coming from the factorization procedure applied to the determinant (9). Solving numerically the set of equations (19), all effective parameters can be found, and for the present case they take the values: \( \gamma_{1eff} = 0.389 \text{ eV}, \varepsilon = -0.0094 \text{ eV} \) and \( \varepsilon_N' = 3.3766 \text{ eV} \).

In figure 5, we present the band structure of BLG/h-BN (a) together with the corresponding dependence of the absolute momentum \( k^2 \) on energy \( E \) (b). A simple inspection of these curves indicates that we have to deal with one effective BLG and a single h-BN layer, wherein the band structure of this BLG differs from the band structures of free-standing BLG and the effective BLG in a trilayer graphene system (see figure 5(c)). As a consequence, the transmission probability is also different for these three kinds of BLG. The transmission probability presented in figure 5(d) exhibits perfect tunnelling at some incident angles characteristic for a given system. It is worth noting that the differences in electronic properties of these three BLGs are pronounced better in the Klein paradox phenomena than in the dispersion spectra. As might be expected, the h-BN induced more subtle changes than modifications due to the third graphene monolayer.

It is worth noticing here that the effective on-site potential \( \varepsilon \) induced in graphene layers does not give rise to a gap in the spectrum. It acts rather as a compensation against the imposed asymmetry by h-BN support.

Next, we consider the system composed of three graphene layers and one h-BN layer for which the Hamiltonian matrix is given by:

\[
\begin{pmatrix}
    0 & -\gamma_0 (\vec{k}) & 0 & \gamma_1 & 0 & 0 & 0 & 0 \\
    -\gamma_0^* (\vec{k}) & 0 & 0 & 0 & \gamma_0 & 0 & 0 & 0 \\
    \gamma_1 & 0 & -\gamma_0^* (\vec{k}) & 0 & \gamma & 0 & 0 & 0 \\
    0 & 0 & 0 & \gamma & 0 & -\gamma_0 (\vec{k}) & 0 & \gamma_{1C-N} \\
    0 & 0 & 0 & 0 & 0 & \gamma & 0 & 0 \\
    0 & 0 & 0 & 0 & 0 & 0 & \varepsilon_B & -\gamma_0 (\vec{k}) \\
    \gamma_{1C-N} & 0 & -\gamma_0^* (\vec{k}) & 0 & 0 & 0 & \varepsilon_N & \varepsilon_B \\
\end{pmatrix}
\]

\[ (20) \]
In figure 6, the band structure of a TLG/h-BN system (a) and the corresponding dependence of absolute momentum $k^2$ on the energy $E$ (b) are shown. The BLG bands can be immediately recognized in the spectrum. However, in contrast to homogenous TLG, the graphene monolayer does not conserve its properties. It behaves similarly to the graphene/h-BN system (see inset in figure 6(c)), however, the band gap is twice as small as in the graphene/h-BN bilayer. The electronic properties of bilayer graphene in this system are different from the previous cases. The effective Hamiltonian takes the form:

$$H_{\text{eff}}^\text{TLG/h-BN} = \begin{pmatrix} \varepsilon & -\gamma_0 f(\vec{k}) & 0 & \gamma_{1,\text{eff}} & 0 & 0 & 0 & 0 \\ -\gamma_0 f^*(\vec{k}) & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\gamma_0 f(\vec{k}) & 0 & 0 & 0 & 0 \\ \gamma_{1,\text{eff}} & 0 & -\gamma_0 f^*(\vec{k}) & \varepsilon & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -\gamma_0 f^*(\vec{k}) & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \gamma_{1,\text{C-N,eff}} & 0 \end{pmatrix}$$

with the following dependences between the effective and original parameters, hopping and onsite energies, respectively:

$$\varepsilon'_N = \varepsilon_N - 2\varepsilon$$

$$2\gamma_1^2 + \gamma_{1,\text{C-N}}^2 = -2\varepsilon'_N \varepsilon - (\varepsilon^2 - \gamma_{1,\text{eff}}^2) + \gamma_{1,\text{C-N,eff}}^2$$

$$-2\varepsilon_N \gamma_1^2 = \varepsilon'_N (\varepsilon^2 - \gamma_{1,\text{eff}}^2) - 2\varepsilon \gamma_{1,\text{C-N,eff}}^2$$

$$-\gamma_{1,\text{C-N}}^2 \gamma_1^2 = \gamma_{1,\text{C-N,eff}}^2 (\varepsilon^2 - \gamma_{1,\text{eff}}^2).$$

The following values of the effective parameters:

$$\gamma_{1,\text{eff}} = 0.5509 \text{ eV}, \quad \varepsilon = -0.0047 \text{ eV}, \quad \varepsilon'_N = 3.3674 \text{ eV},$$

$$\gamma_{1,\text{C-N,eff}} = 0.177 \text{ eV}$$

are found for the considered system. Figure 6(d) shows the transmission probability for the effective BLG in the TLG/h-BN system.

In general, the $N$-layer graphene Bernal stacking system deposited on the h-BN layer can be described by $N/2$ isolated bilayer systems with some effective interlayer hopping and onsite energies, and one h-BN with effective onsite energy if $N$ is even or $(N-1)/2$ bilayers plus one MLG modified by h-BN layer if $N$ is odd. In these last cases the MLG/h-BN bilayer is characterized by the effective interlayer hopping and effective onsite energy in the h-BN sublattice, which interacts with the appropriate MLG sublattice. This is appropriate in the sense that the Bernal stacking is conserved in the system. This is the exact mapping of equation (4), without using any approximation during the chiral decomposition procedure. We can easily obtain the recurrence relations for the effective parameters.
If the number of graphene layers is even, \( N = 2N_0 \), we have:

\[
\begin{align*}
\varepsilon_N B_{N_0}^{2N} &= \frac{\varepsilon_N^{\prime} A_{N_0}^{2N} - A_{N_0}^{2N} N_{C,\text{eff}} A_{N_0}^{2N} N_{C,\text{eff}}}{\varepsilon_N^{\prime} B_{N_0}^{2N} N_{C,\text{eff}} A_{N_0}^{2N} N_{C,\text{eff}}} \\
\gamma_1^{\ast} C - N_{C,\text{eff}}^2 B_{N_0}^{2N} - B_{N_0}^{2N} &= \frac{\varepsilon_N^{\prime} A_{N_0}^{2N} - A_{N_0}^{2N} N_{C,\text{eff}} A_{N_0}^{2N} N_{C,\text{eff}}}{\varepsilon_N^{\prime} B_{N_0}^{2N} N_{C,\text{eff}} A_{N_0}^{2N} N_{C,\text{eff}}} \\
\varepsilon_N B_{N_0}^{2N} &= \frac{\varepsilon_N^{\prime} A_{N_0}^{2N} - A_{N_0}^{2N} N_{C,\text{eff}} A_{N_0}^{2N} N_{C,\text{eff}}}{\varepsilon_N^{\prime} B_{N_0}^{2N} N_{C,\text{eff}} A_{N_0}^{2N} N_{C,\text{eff}}}.
\end{align*}
\]

If the number of graphene layers is odd, \( N = 2N_0 + 1 \), we have:

\[
\begin{align*}
\varepsilon_N B_{N_0}^{2N+1} &= \frac{\varepsilon_N^{\prime} A_{N_0}^{2N+1} - A_{N_0}^{2N+1} N_{C,\text{eff}} A_{N_0}^{2N+1} N_{C,\text{eff}}}{\varepsilon_N^{\prime} B_{N_0}^{2N+1} N_{C,\text{eff}} A_{N_0}^{2N+1} N_{C,\text{eff}}} \\
\gamma_1^{\ast} C - N_{C,\text{eff}}^2 B_{N_0}^{2N+1} - B_{N_0}^{2N+1} &= \frac{\varepsilon_N^{\prime} A_{N_0}^{2N+1} - A_{N_0}^{2N+1} N_{C,\text{eff}} A_{N_0}^{2N+1} N_{C,\text{eff}}}{\varepsilon_N^{\prime} B_{N_0}^{2N+1} N_{C,\text{eff}} A_{N_0}^{2N+1} N_{C,\text{eff}}} \\
\varepsilon_N B_{N_0}^{2N+1} &= \frac{\varepsilon_N^{\prime} A_{N_0}^{2N+1} - A_{N_0}^{2N+1} N_{C,\text{eff}} A_{N_0}^{2N+1} N_{C,\text{eff}}}{\varepsilon_N^{\prime} B_{N_0}^{2N+1} N_{C,\text{eff}} A_{N_0}^{2N+1} N_{C,\text{eff}}} \\
\gamma_1^{\ast} C - N_{C,\text{eff}}^2 B_{N_0}^{2N+1} &= \frac{\varepsilon_N^{\prime} A_{N_0}^{2N+1} - A_{N_0}^{2N+1} N_{C,\text{eff}} A_{N_0}^{2N+1} N_{C,\text{eff}}}{\varepsilon_N^{\prime} B_{N_0}^{2N+1} N_{C,\text{eff}} A_{N_0}^{2N+1} N_{C,\text{eff}}} \\
\varepsilon_N &= \varepsilon_N^{\prime} - A_{N_0}^{2N+1}.
\end{align*}
\]

In both the above relations we introduced the following notation:

\[
B_{N_0}^{2N} = \begin{cases} 
\frac{\varepsilon_N^{\prime} A_{N_0}^{2N} - A_{N_0}^{2N} N_{C,\text{eff}} A_{N_0}^{2N} N_{C,\text{eff}}}{\varepsilon_N^{\prime} B_{N_0}^{2N} N_{C,\text{eff}} A_{N_0}^{2N} N_{C,\text{eff}}} & \text{if } l > 0 \\
1 & \text{if } l = 0
\end{cases},
\]

\[
\lambda_{N_0,N_0} = 2\gamma \sin \frac{N_0}{2(N_0 + 1)} \pi,
\]

\[
A_{N_0}^{2N} = \begin{cases} 
\frac{\varepsilon_N^{\prime} A_{N_0}^{2N} - A_{N_0}^{2N} N_{C,\text{eff}} A_{N_0}^{2N} N_{C,\text{eff}}}{\varepsilon_N^{\prime} B_{N_0}^{2N} N_{C,\text{eff}} A_{N_0}^{2N} N_{C,\text{eff}}} & \text{if } l > 0 \\
1 & \text{if } l = 0
\end{cases},
\]

\[
\lambda_i = \begin{cases} 
\varepsilon_i - \gamma_{i,C,C,\text{eff}} & \text{if } i = 2k \\
\varepsilon_i + \gamma_{i,C,C,\text{eff}} & \text{if } i = 2k + 1
\end{cases}.
\]

where \( P_{2N}^{l} \) denotes an \( l \)-element subset of the set \( \{1, 2, \ldots , N\} \) and \( \sum_{l} \) means that the sum is over all \( l \)-element subsets.

In figure 7, we collected the results for multilayer systems with \( N = 4, 5 \). The features that are characteristic of the spectra of gapless bilayers can immediately be recognized in both systems. In the case of 5MLG/h-BN, we observe in addition the typical spectrum of MLG modified by the h-BN layer (see inset with details of the band structure in the vicinity of the Brillouin-zone corner). It is worth noting that the band gap present in this spectrum is smaller than the one observed in the TLG/h-BN system (compare the insets in figures 6(c) and 7).

Finally, let us remark that the ‘magic angles’ for which 100\% transmission is observed are given by the condition \( \sin(\lambda_{i,k} d) = 0 \) [1, 53]. It is interesting that this condition corresponds to the Fabry–Pérot resonances in optics. A potential barrier can be seen as a double interface, so the region inside the barrier creates a cavity, which can accommodate oscillating waves. Accordingly, the incoming wave can interfere with itself between the two interfaces in region II (see figure 5). These Fabry–Pérot resonances are responsible for the petal-like shape of \( T(\varphi) \) when plotted in a polar coordinate system. The h-BN layer influences the values of the ‘magic angles’ (see figure 5(d)) but does not change the width of the resonance peaks. Moreover, the values of the ‘magic angles’ depend on the barrier parameters, but their existence is robust both in the height and width of the barrier.
4. Conclusions

Electrons in monolayer graphene act like massless spin-1/2 Dirac fermions. Backscattering is suppressed due to the pseudospin orthogonality of the forward and reverse scattering modes. The resulting Klein tunnelling provides unit transmission for normally incident electrons at a pn junction, regardless of the barrier height. In contrast, bilayer graphene electrons act like parabolic spin-1 systems with perfect reflection for normal incidence (anti-Klein tunnelling). It has been revealed that the Hamiltonian of Bernal stacking multilayer graphene systems can be block diagonalized into effective BLG and MLG Hamiltonians depending on the parity of the layer numbers [26, 38]. Here, we have extended this technique to the decomposition of the Hamiltonian matrix describing multi-layer graphene systems supported by the h-BN layer, i.e. non-symmetric stacking structures.

We found that the N-layer graphene Bernal stacking system deposited on the h-BN layer can be described by $N/2$ isolated effective bilayer systems with one effective h-BN layer, if N is even or by $(N - 1)/2$ effective bilayers plus one MLG/h-BN effective bilayer if it is odd. The decomposition procedure reveals a non-trivial result connected with the effective on-site potentials $\epsilon$ induced in graphene layers. These parameters act as compensation against the imposed asymmetry by h-BN support and show the physical mechanism that happens in real systems. Moreover, taking into account the impact of h-BN on the properties of graphene seems to be closer to the experimental situation than neglecting it. As examples, we compare the tunnelling properties of effective BLG, which can be recognized in different multilayer systems, both homo- and heterogeneous.

Although only slightly, the h-BN layer modifies the electronic properties of graphene layers present in the system. Thus, it can be regarded not only as insulating support, ensuring pure graphene transport channels, but equally can promote specific BLG properties. This may pave the way for future applications of pseudo-spintronics with bilayer graphene [54, 55]. The unique electronic structure of graphene systems can be used to create pseudo-spin which is analogous of giant magnetoresistance and other established spintronics effects [56].

Acknowledgments

This work is supported in part by the University of Łódź.

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