We review the energy spectrum and transport properties of several types of one-dimensional superlattices (SLs) on single-layer and bilayer graphene. In single-layer graphene, for certain SL parameters an electron beam incident on an SL is highly collimated. On the other hand, there are extra Dirac points generated for other SL parameters. Using rectangular barriers allows us to find analytical expressions for the location of new Dirac points in the spectrum and for the renormalization of the electron velocities. The influence of these extra Dirac points on the conductivity is investigated. In the limit of δ-function barriers, the transmission $T$ through and conductance $G$ of a finite number of barriers as well as the energy spectra of SLs are periodic functions of the dimensionless strength $P$ of the barriers, $P\delta(x) = V(x)/\hbar v_F$, with $v_F$ the Fermi velocity. For a Kronig–Penney SL with alternating sign of the height of the barriers, the Dirac point becomes a Dirac line for $P = \pi/2 + n\pi$ with $n$ an integer. In bilayer graphene, with an appropriate bias applied to the barriers and wells, we show that several new types of SLs are produced and two of them are similar to type I and type II semiconductor SLs. Similar to single-layer graphene SLs, extra ‘Dirac’ points are found in bilayer graphene SLs. Non-ballistic transport is also considered.

Keywords: graphene; electron transport; two-dimensional crystals

1. Introduction

Since the experimental realization of graphene (Novoselov et al. 2004), this one-atom-thick layer of carbon atoms has attracted the attention of the scientific world. This interest was created by the prediction that the carriers in graphene behave as massless relativistic fermions moving in two dimensions. The latter particles, which are described by the Dirac–Weyl Hamiltonian, possess interesting
properties such as a gapless and linear-in-wave vector electronic spectrum, a perfect transmission, at normal incidence, through any potential barrier, i.e. the Klein paradox (Klein 1929; Katsnelson et al. 2006; Pereira et al. 2010; Roslyak et al. 2010), which was recently addressed experimentally (Huard et al. 2007; Young & Kim 2009), the zitterbewegung (Schliemann et al. 2005; Zawadzki 2005; Winkler et al. 2007), and so on (see Castro Neto et al. (2009) and Abergel et al. (2010) for recent reviews). On the other hand, in bilayer graphene, the carriers exhibit a very different but extraordinary electronic behaviour, such as being chiral (Katsnelson et al. 2006; McCann 2006) but with a different pseudospin ($=1$) than in single-layer graphene ($=1/2$). Although the spectrum is parabolic in wave vector and also gapless, it is possible to create an energy gap by applying a perpendicular electric field on a bilayer graphene sample (Castro et al. 2007). This allows one to electrostatically create quantum dots in bilayer graphene (Pereira et al. 2007b) and enrich its technological capabilities.

In previous work, we studied the band structure and other properties of single-layer and bilayer graphene (Barbier et al. 2008, 2009b) in the presence of a one-dimensional periodic potential, i.e. a superlattice (SL). SLs are known to be useful in altering the band structure of materials and thereby broadening their technological applicability.

The already peculiar, cone-shaped band structure of single-layer graphene can be drastically changed in an SL. An interesting feature is that for certain SL parameters, the carriers are restricted to move along one direction, i.e. they are collimated (Park et al. 2009a). Furthermore, it was found that for other parameters of an SL instead of the single-valley (the $K$ or $K'$-point) Dirac cone, ‘extra Dirac points’ appeared at the Fermi level in addition to the original one (Ho et al. 2009). The latter extra Dirac points are interesting because of their accompanying zero modes (Brey & Fertig 2009) and their influence on many physical properties, such as the density of states (Ho et al. 2009), the conductivity (Barbier et al. 2010; Wang & Zhu 2010) and the Landau levels upon applying a magnetic field (Park et al. 2009b; Sun et al. 2010).

One can also obtain extra Dirac points in bilayer graphene SLs. The possibility of locally altering the gap (Castro et al. 2007) of bilayer graphene by applying a bias is another way of tuning the band structure. In this review, we classify these SLs into four types. Another interesting result of applying a bias locally is that sign flips of the bias introduce bound states along the interfaces (Martin et al. 2008; Martinez et al. 2009). These bound states break the time-reversal symmetry and are distinct for the two $K$ and $K'$ valleys; this opens up perspectives for valley-filter devices (San-Jose et al. 2009).

In this review, we will use the following methods to describe our findings. For both single-layer and bilayer graphene we will use the nearest neighbour, tight-binding Hamiltonian in the continuum approximation, and restrict ourselves to the electronic structure in the neighbourhood of the $K$ point. We then apply the transfer-matrix method to study the spectrum of and transmission through various potential barrier structures, which we approximate by piecewise constant potentials. We consider structures with a finite number of barriers and SLs.

We will study ballistic transport in systems with a finite number of barriers using the two-probe Landauer conductance, while in an SL (infinite number of barriers) we will evaluate the spectrum and the diffusive conductivity, i.e. we will study non-ballistic transport.
The work is organized as follows. In §2, we investigate various aspects of ballistic transport through a finite number of barriers on single-layer graphene as well as the spectrum of SLs, with emphasis on collimation and extra Dirac points and their influence on non-ballistic transport. In §3, we carry on the same studies, whenever possible, for bilayer graphene. In addition, we consider various types of band alignments in the presence of a bias that can lead to different types of heterostructures and SLs. We present a summary and concluding remarks in §4.

2. Single-layer graphene

We describe the electronic structure of an infinitely large, flat graphene flake by the nearest-neighbour tight-binding model and consider wave vectors close to the $K$ point. The relevant Hamiltonian in the continuum approximation is

$$
\mathcal{H} = v_F \sigma \cdot \hat{p} + V \mathbb{1} + m v_F^2 \sigma_z,
$$

with $\hat{p}$ the momentum operator, $V$ the potential, $\mathbb{1}$ the $2 \times 2$ unit matrix, $\sigma = (\sigma_x, \sigma_y)$, $\sigma_z$ the Pauli matrices and $v_F \approx 10^6 \text{ m s}^{-1}$ the Fermi velocity. Explicitly, $\mathcal{H}$ is given by

$$
\mathcal{H} = \begin{pmatrix}
V + m v_F^2 & -i v_F \hbar (\partial_x - i \partial_y) \\
-i v_F \hbar (\partial_x + i \partial_y) & V - m v_F^2
\end{pmatrix}.
$$

(2.1)

The mass term is in principle zero in the nearest-neighbour, tight-binding model but owing to interaction with a substrate (Giovannetti et al. 2007), an effective mass term can be induced and results in the opening of an energy gap. Recently, there have been proposals to induce an energy gap in single-layer graphene, and it is appropriate that we consider this mass term where relevant.

In the presence of a one-dimensional rectangular potential $V(x)$, such as the one shown in figure 1, the equation $(\mathcal{H} - E)\psi = 0$ admits (right- and left-travelling) plane wave solutions of the form $\psi_{l,r}(x) e^{ik_y y}$ with

$$
\psi_r(x) = \left( \begin{array}{c} \epsilon + \mu \\ \lambda + i k_y \end{array} \right) e^{i k x} \quad \text{and} \quad \psi_l(x) = \left( \begin{array}{c} \epsilon + \mu \\ -\lambda + i k_y \end{array} \right) e^{-i k x},
$$

(2.2)

where $\lambda = [(\epsilon - u(x))^2 - k_y^2 - \mu^2]^{1/2}$ is the $x$ component of the wave vector, $\epsilon = EL/\hbar v_F$, $u(x) = V(x)L/\hbar v_F$ and $\mu = mv_F L/\hbar$. The dimensionless parameters $\epsilon$, $u(x)$ and $\mu$ scale with the characteristic length $L$ of the potential barrier structure. For the single or double barrier system, this $L$ will be equal to the barrier width while for an SL it will be its period. Neglecting the mass term, one rewrites equation (2.2) in the simpler form

$$
\psi_r(x) = \left( \begin{array}{c} 1 \\ s e^{i \phi} \end{array} \right) e^{i k x} \quad \text{and} \quad \psi_l(x) = \left( \begin{array}{c} 1 \\ -s e^{-i \phi} \end{array} \right) e^{-i k x},
$$

(2.3)

with $\lambda = [(\epsilon - u(x))^2 - k_y^2]^{1/2}$, $\tan \phi = k_y/\lambda$ and $s = \text{sgn}(\epsilon - u(x))$.

(a) A single or double barrier

The model barriers and wells we consider are shown in figure 1. It is interesting to look at the tunnelling through such barriers, which was previously studied by Katsnelson et al. (2006) for a single barrier. This was later extended to massive electrons with spatially varying mass (Gomes & Peres 2008).
Transmission. To find the transmission $T$ through a square-barrier structure, one first observes that the wave function in the $j$th region $\psi_j(x)$ of the constant potential $V_j$ is given by a superposition of the eigenstates given by equation (2.2),

$$\psi_j(x) = A_j \psi_{r,j} + B_j \psi_{l,j}. \quad (2.4)$$

The wave function should be continuous at the interfaces. This boundary condition gives the transfer matrix $\mathcal{N}_j$ relating the coefficients $A_j$ and $B_j$ of region $j$ with those of the region $j + 1$ in the manner

$$\begin{pmatrix} A_j \\ B_j \end{pmatrix} = \mathcal{N}_{j+1} \begin{pmatrix} A_{j+1} \\ B_{j+1} \end{pmatrix}. \quad (2.5)$$

By employing the transfer matrix at each potential step, we obtain, after $n$ steps, the relation

$$\begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = \prod_{j=1}^{n} \mathcal{N}_j \begin{pmatrix} A_n \\ B_n \end{pmatrix}. \quad (2.6)$$

In the region to the left of the barrier, we assume $A_0 = 1$ and denote by $B_0 = r$ the reflection amplitude. Likewise, to the right of the $n$th barrier, we have $B_n = 0$ and denote by $A_n = t$ the transmission amplitude.

The transmission probability $T$ can be expressed as the ratio of the transmitted current density $j_x$ over the incident one, where $j_x = v_F \psi \sigma_x \psi$. This results in $T = (\lambda'/\lambda)|t|^2$, with $\lambda'/\lambda$ the ratio between the wave vector $\lambda'$ to the right and $\lambda$ to the left of the barrier. If the potential to the right and left of the barrier is the same, we have $\lambda' = \lambda$. For a single barrier, the transmission amplitude is given by $T = |t|^2 = |N_{11}|^{-1}$, with $N_{ij}$ the elements of the transfer matrix $\mathcal{N}$. Explicitly, $t$ can be written as

$$\frac{1}{t} = \cos(\lambda_b W_b) - iQ \sin(\lambda_b W_b) \right\} \quad (2.7)$$

where the indices 0 and b refer, respectively, to the region outside and inside the barrier and $\epsilon_b = \epsilon - u$. A contour plot of the transmission is shown in figure 2a. We clearly see: (i) $T = 1$ for $\phi = 0$, which is the well-known Klein tunnelling and (ii) strong resonances, in particular for $E < 0$, when $\lambda_b W_b = n\pi$, which describe hole-scattering above a potential well.

Figure 1. (a) A one-dimensional potential barrier of height $V_b$ and width $W_b$. (b) A single unit of a potential well next to a potential barrier.
Figure 2. (a) Contour plot of the transmission through a single barrier with $\mu = 0$, $W_b = L$ and $v_b = 10$. (b) As in (a), for a single $\delta$-function barrier with $\mu = 0$ and $u(x) = P\delta(x)$; the transmission is independent of the energy. (c) As in (a) for two barriers with $\mu = 0$, $v_b = 10$, $v_w = 0$, $W_b = 0.5L$ and $W_w = L$. (d) Spectrum of the bound states versus $k_y$ for a single ($L = 1$, solid black line), two parallel (dashed curves) and two anti-parallel (dashed-dotted curves) $\delta$-function barriers ($L$ is the inter-barrier distance).

In the limit of a very thin and high barrier, one can model it by a $\delta$-function barrier, $V(x)/\hbar v_F = P\delta(x)$. Using equation (2.7) for $t$ gives (Barbier et al. 2009a)

$$T = \frac{1}{1 + \sin^2 P \tan^2 \phi},$$

(2.8)

with $\tan \phi = k_y/\lambda_0$ the angle of incidence. Notice that this transmission is independent of the energy and is a periodic function of $P$. The latter is very different from the non-relativistic case where $T$ is a decreasing function of $P$. A contour plot of the transmission is shown in figure 2b and $T = 1$ for $\phi \approx 0$, which is nothing else than Klein tunnelling. Notice also the symmetry $T(\pi - P) = T(P)$.

For two barriers, the system becomes a resonant structure, for which it was found that the resonances in the transmission depend mostly on the width $W_w$ of the well between the barriers (Pereira et al. 2007a). A plot of the transmission is shown in figure 2c. In the limit of two parallel $\delta$-function barriers of equal strength $P$, we obtain the transmission

$$T = \left[1 + \tan^2 \phi \left(\cos \lambda_0 \sin 2P - \frac{2s \sin \lambda_0 \sin^2 P}{\cos \phi}\right)^2\right]^{-1}.$$ (2.9)
Figure 3. (a) Conductance $G$ versus strength $P$ of a $\delta$-function barrier in single-layer graphene; the conductance is independent of the energy. (b) Conductance $G$ versus energy for the single (solid black curve) and double (dashed grey curve) square barrier of figure 2a,c.

The case of two anti-parallel $\delta$-function barriers of equal strength is also interesting. The relevant transmission is

$$T = \left[ \cos^2 \lambda_0 + \frac{\sin^2 \lambda_0 (1 - \sin^2 \phi \cos 2P)^2}{\cos^4 \phi} \right]^{-1}. \quad (2.10)$$

*Conductance.* The two-terminal conductance is given by

$$G(E_F) = G_0 \int_{-\pi/2}^{\pi/2} T(E_F, \phi) \cos \phi \, d\phi, \quad (2.11)$$

with $G_0 = 2E_F L_y e^2/(v_F h^2)$ for single-layer graphene, and $L_y$ the width of the system. For a single and double barrier, the transmission through which is plotted in figure 2a,c, the conductance $G$ is shown in figure 3b and exhibits multiple resonances despite the integration over the angle $\phi$.

Taking the limit of a $\delta$-function barrier leads to $G$ periodic in $P$ and given by

$$\frac{G}{G_0} = \frac{2[1 - \text{arctanh}(\cos P) \sin P \tan P]}{\cos^2 P}. \quad (2.12)$$

For one period, $G$ is shown in figure 3a.

*Bound states.* For $k_y^2 + \mu_0^2 > \varepsilon^2$, the wave function outside the barrier (well) becomes an exponentially decaying function of $x$, $\psi(x) \propto \exp(\pm |\lambda_0| x)$ with $|\lambda_0| = [k_y^2 + \mu_0^2 - \varepsilon^2]^{1/2}$. Localized states form near the barrier boundaries (Pereira et al. 2006); however, they are propagating freely along the $y$-direction. The spectrum of these bound states can be found by setting the determinant of the transfer matrix equal to zero. For a single potential barrier (well), it is given by the solution of the transcendental equation

$$|\lambda_0| q_x \cos(q_x W_b) + (k_y^2 + \mu_0 \mu_b - \varepsilon (\varepsilon - u)) \sin(\lambda_b W_b) = 0. \quad (2.13)$$

In figure 4b these bound states are shown, as a function of $k_y$, by the dashed grey (dashed dark grey) curves.

An interesting structure to study is that of a potential barrier next to a well, but with average potential equal to zero, considered by Arovas et al. (2010). This is the unit cell (shown in figure 1b) of the SL we will use in §2c, where extra Dirac
points will be found. In figure 4a the Dirac cone outside the barrier is shown as a grey area, inside this region there are no bound states. Superimposed are grey lines corresponding to the edges of the Dirac cones inside the well and barrier that divide the \((E, k_y)\) plane into four regions. Region I corresponds to propagating states inside both the barrier and well, while region II (III) corresponds to propagating states only inside the well (barrier). In region IV no propagating modes are possible, neither in the barrier nor in the well. For high thin barriers, region I will become a thin area adjacent to the upper cone, converging to the dark grey line in the limit of a \(\delta\)-function barrier. Figure 4b shows that the bound states of this structure are composed of those of a single barrier and those of a single well. Anti-crossings take place where the bands otherwise would cross. The resulting spectrum is clearly a starter of the spectrum of an SL shown in figure 4d.

In the limit of \(\delta\)-function barriers and wells, the expressions for the dispersion relation are strongly simplified by setting \(\mu = 0\) in all regions. For a single \(\delta\)-function barrier, the bound state is given by

\[
\varepsilon = \text{sgn}(\sin P)|k_y| \cos P, \tag{2.14}
\]
which is a straight line with a reduced group velocity $v_y$; the result is shown in figure 2d by the dark grey curve. Comparing with the single-barrier case, we notice that owing to the periodicity in $P$, the $\delta$-function barrier can act as a barrier or as a well depending on the value of $P$.

For two $\delta$-function barriers, there are two important cases: the parallel and the anti-parallel case. For parallel barriers one finds an implicit equation for the energy

$$|\lambda' \cos P + \epsilon \sin P| = |e^{-\lambda' k_y} \sin P|,$$

where $\lambda' = |\lambda_0|$, while for anti-parallel barriers one obtains

$$k_y^2 \sin^2 P = \frac{\lambda'^2}{(1 - e^{-2\lambda'})}.$$

For two (anti-)parallel $\delta$-function barriers we have, for each fixed $k_y$ and $P$, two energy values $\pm 3$, and therefore two bound states. In both cases, for $P = n\pi$, the spectrum is simplified to the one in the absence of any potential $\epsilon = \pm |k_y|$. In figure 2d, the bound states for double (anti-)parallel $\delta$-function barriers are shown, as a function of $k_yL$, by the dashed (dashed-dotted) curves. For anti-parallel barriers, we see that there is a symmetry around $E = 0$, which is absent when the barriers are parallel.

\(b\) Superlattice

Now, we consider a square-barrier SL with the corresponding one-dimensional periodic potential given by

$$V(x) = V_0 \sum_{j=-\infty}^{\infty} [\Theta(x - jL) - \Theta(x - jL - W_b)],$$

with $\Theta(x)$ the step function. The corresponding wave function is a Bloch function and satisfies the periodicity condition $\psi(L) = \psi(0) \exp(ik_x)$, with $k_x$ now the Bloch phase. Using this relation together with the transfer matrix for a single unit, $\psi(L) = \mathcal{M}\psi(0)$, leads to the condition

$$\det[\mathcal{M} - \exp(ik_x)] = 0.$$

This gives the transcendental equation

$$\cos k_x = \cos \lambda_w W_w \cos \lambda_b W_b - Q \sin \lambda_w W_w \sin \lambda_b W_b,$$

from which we obtain the energy spectrum of the system. In equation (2.19), we used the following notation:

$$\epsilon_w = \epsilon + uW_b, \quad \epsilon_b = \epsilon - uW_w, \quad u = \frac{V_0L}{\hbar v_F}, \quad W_{b,w} \rightarrow \frac{W_{b,w}}{L},$$

$$\lambda_w = [\epsilon_w^2 - k_y^2 - \mu_w^2]^{1/2}, \quad \lambda_b = [\epsilon_b^2 - k_y^2 - \mu_b^2]^{1/2} \quad \text{and} \quad Q = \frac{\epsilon_w \epsilon_b - k_y^2 - \mu_b \mu_w}{\lambda_w \lambda_b}.$$

Numerical results for the dispersion relation $E(k_y)$ are shown in figure 4d. We see the appearance of bands (grey areas) which for large $k_y$ values collapse into the bound states (where the grey and dark grey curves meet) while the charge carriers move freely along the $y$ direction.
(c) Collimation and extra Dirac points

As shown by various studies, carriers in graphene SLs exhibit several interesting peculiarities that result from the particular electronic SL band structure. In a one-dimensional SL, it was found that the spectrum can be altered anisotropically (Park et al. 2008a; Bliokh et al. 2009). Moreover, this anisotropy can be made very large such that for a broad region in \( k \) space, the spectrum is dispersionless in one direction, and thus electrons are collimated along the other direction (Park et al. 2009a). Even more intriguing was the ability to split off extra Dirac points (Ho et al. 2009) with accompanying zero modes (Brey & Fertig 2009), which move away from the \( K \) point along the \( k_y \) direction with increasing potential strength. Here, we will describe these phenomena for an SL of square potential barriers.

We start by describing the collimation as done by Park et al. (2009a); subsequently, we will find the conditions on the parameters of the SL for which a collimation appears. It turns out that they are the same as those needed to create a pair of extra Dirac points.

Following Park et al. (2009a), we find that the condition for collimation to occur is

\[
\int_{BZ} e^{i\mathbf{s} \mathbf{a}(x)} = 0,
\]

where the function \( \mathbf{a}(x) = 2 \int_0^x u(x') \, dx' \) embodies the influence of the potential, \( s = \text{sign}(\varepsilon) \) and \( \mathbf{s} = \text{sign}(k_x) \). For a symmetric rectangular lattice, this corresponds to \( u/4 = n\pi \). The spectrum for the lowest energy bands is then given by (Park et al. 2008b)

\[
\varepsilon \approx \pm \left[ k_x^2 + |f_l|^2 k_y^2 \right]^{1/2} + \frac{\pi l}{L},
\]

with \( f_l \) being the coefficients of the Fourier expansion \( e^{i\alpha(x)} = \sum_{l=-\infty}^{\infty} f_l e^{i2\pi lx/L} \). The coefficients \( f_l \) depend on the potential profile \( V(x) \), with \( |f_l| < 1 \). For a symmetric SL of square barriers, we have \( f_l = u \sin(l\pi/2 - u/2)/(l^2 u^2 - u^2/4) \). The inequality \( |f_l| < 1 \) implies a group velocity in the \( y \) direction \( v_y < v_F \), which can be seen from equation (2.20).

In figure 5b,d we show the dispersion relation \( E \) versus \( k_x \) for \( u = 0, 4\pi \) at constant \( k_y \). As can be seen, when an SL is present in most of the Brillouin zone, the spectrum, partially shown in figure 5c, is nearly independent of \( k_y \). That is, we have collimation of an electron beam along the SL axis. The condition \( u = V_0 L/\hbar v_F = 4n\pi \) shows that altering the period of the SL or the potential height of the barriers is sufficient to produce collimation. This makes an SL a versatile tool for tuning the spectrum. Comparing with figure 5a,b, we see that the cone-shaped spectrum for \( u = 0 \) is transformed into a wedge-shaped spectrum (Park et al. 2009a).

We now compare this result with another approximate result for the spectrum, where we suppose \( \varepsilon \) small instead of \( k_y \) small. We start with the transcendental equation (2.19). As we are interested in an analytical approximate expression for the spectrum, we choose to expand the dispersion relation around \( \varepsilon = 0 \) up to second order in \( \varepsilon \). The resulting spectrum is

\[
\varepsilon_{\pm} = \pm \left[ \frac{4|a^2|^2 k_y^2 \sin^2(a/2) + a^2 \sin^2(k_x/2)}{k_y^4 a \sin a + a^2 u^4/16 - 2k_y^2 u^2 \sin^2(a/2)} \right]^{1/2},
\]
Figure 5. The lowest conduction band of the spectrum of graphene near the $K$ point $(a,b)$ in the absence of SL potential and $(c,d)$ in its presence with $u = 4\pi$. $(a,c)$ Contour plots of the conduction band with a contour step of $0.5 \hbar v_F / L$. $(b,d)$ Slices along constant $k_y L = 0$ (dark grey), 0.2 (grey), 0.4 (black).

with $a = [u^2/4 - k_y^2]^{1/2}$. In order to compare this spectrum with that of Park et al. (2009a), we expand equation (2.19) for small $k$ and $\varepsilon$; this leads to

$$\varepsilon \approx \pm \left[ k_x^2 + \frac{k_y^2 \sin^2(u/4)}{(u/4)^2} \right]^{1/2}.$$  

(2.22)

This spectrum has the form of an anisotropic cone and corresponds to that of equation (2.20) for $l = 0$ (higher $l$ corresponds to higher energy bands). In figure 6a,b, we see that the cone-shaped spectrum in figure 6a, for $u = 0$, is transformed into an anisotropic one in figure 6b, for $u = 4.5\pi$, that has peculiar extra Dirac points. These extra Dirac points cannot be described by a spectrum having an anisotropic cone shape, therefore we compare the two approximate spectra. In figure 6c,d we show how equations (2.21) and (2.22) differ from the ‘exact’ numerically obtained spectrum. From this figure one can see that equation (2.21) describes the lowest bands rather well for $\varepsilon < 1$, while equation (2.22) is sufficient to describe the spectrum near the Dirac point. The former equation will be useful when describing the spectrum near the extra Dirac points and we will use it to obtain the velocity.

We now move on to another important feature of the spectrum, the extra Dirac points first obtained by Ho et al. (2009) using tight-binding calculations. These extra Dirac points are found as the zero-energy solutions of the dispersion relation in equation (2.19) for zero energy (Barbier et al. 2010).
Figure 6. The spectrum of graphene near the $K$ point (a) in the absence of an SL and (b) in its presence with $u = 4.5\pi$. (c,d) The SL spectrum with $u = 10\pi$. The lowest conduction bands are coloured in light grey, black and grey for, respectively, the exact, and the approximations given by (c) equation (2.21) and (d) equation (2.22). The approximate spectra are delimited by the dashed curves.

In order to find the location of the Dirac points, we assume $k_x = 0$, $\epsilon = 0$, $\mu_b = \mu_w = 0$ and consider the special case of $W_b = W_w = 1/2$ in equation (2.19). The resulting equation

\[
1 = \cos^2 \frac{\lambda}{2} + \left[ \frac{u^2/4 + k_y^2}{(u^2/4 - k_y^2)} \right] \sin^2 \frac{\lambda}{2}
\]

has solutions for $u^2/4 - k_y^2 = u^2/4 + k_y^2$ or $\sin^2 \lambda/2 = 0$. This determines the values of $k_y = 0$ (at the Dirac points) and

\[
k_{y,j} = \pm \sqrt{\frac{u^2}{4} - 4j^2\pi^2};
\]

the extra Dirac points occur for $j \neq 0$. For an SL spectrum symmetric around zero energy, the extra Dirac points are at $\epsilon = 0$. We expect from the considerations of §2b (and figure 4b) that for unequal barrier and well widths this will no longer be true. Indeed, in such a case, the extra Dirac points shift in energy.
as seen in figure 4d, and their position in the spectrum is given, for \( k_x = 0 \), by

\[
\varepsilon_{j,m} = \frac{u}{2} (1 - 2 W_b) + \frac{\pi^2}{2u} \left( \frac{j^2}{W_w^2} - \frac{(j + 2m)^2}{W_w^2} \right)
\]

and

\[
k_{y,j,m} = \pm \left[ (\varepsilon_{j,m} + u W_b)^2 - \left( \frac{j\pi}{W_w} \right)^2 \right]^{1/2},
\]

where \( j \) and \( m \) are integers, and \( m \neq 0 \) corresponds to higher and lower crossing points. Also, perturbing the potential with an asymmetric term, as done by Park et al. (2009b), leads to qualitatively similar results.

An investigation of the group velocity near the (extra) Dirac points is appropriate for understanding the transport of carriers in the energy bands close to zero energy. Near the extra Dirac points, the group velocity tends to renormalize differently when compared with the original Dirac point. Near them \( \mathbf{v} \) is oriented along the \( y \) direction, while near the latter one \( \mathbf{v} \) is oriented along the \( x \) direction (Ho et al. 2009). The group velocity near the extra Dirac points can be calculated from equation (2.21). At the \( j \)th extra Dirac point, the magnitude of the velocity \( \mathbf{v}/v_F = (\partial \varepsilon/\partial k_x, \partial \varepsilon/\partial k_y) \) is given by

\[
\frac{v_x}{v_F} = \frac{16\pi^2 j^2 \cos(k_x/2)}{u^2},
\]

and

\[
\frac{v_y}{v_F} = \frac{u^2/4 - 4j^2\pi^2}{u^2},
\]

while at the main Dirac point, it is given by \( v_x/v_F = 1 \) and \( v_y/v_F = 4\sin(u/4)/u \). The dependence of the velocity components on the strength of the potential barriers is shown in figure 7. From this figure we observe that new extra Dirac points emerge upon increasing \( u = V_0 L/hv_F \) (consistent with equation (2.24)) and \( v_x \) decreases while \( v_y \) increases. The Dirac point itself, however, shows a different behaviour upon increasing \( u \), namely \( v_x = v_F \) constant, and \( v_y \) is here a globally decaying function showing \( v_y = 0 \) for periodic values of \( u, u = 4n\pi \), with \( n \) a non-zero positive integer.

**Conductivity.** We now turn to the transport properties of an SL and look at the influence of these extra Dirac points on the conductivity. The diffusive DC conductivity \( \sigma_{\mu\nu} \) for the SL system can be readily calculated from the spectrum if we assume a nearly constant relaxation time \( \tau(E_F) \equiv \tau_F \). It is given by (Charbonneau et al. 1982)

\[
\sigma_{\mu\nu}(E_F) = \frac{e^2 \beta\tau_F}{A} \sum_{n,k} v_{n\mu} v_{n\nu} f_{nk} (1 - f_{nk}), \quad (2.27)
\]

with \( A \) the area of the system, \( n \) the energy band index, \( \mu, \nu = x, y \) and \( f_{nk} = 1/\exp(\beta(E_F - E_{nk})) + 1 \) the equilibrium Fermi–Dirac distribution function; \( \beta = 1/k_B T \) and the temperature enters the results through the dimensionless value for \( \beta \), which is \( \beta = hv_F/k_B TL = 20 \).
Figure 7. The group velocity components $v_y$ and $v_x$ at the Dirac point $j = 0$ (shown, respectively, by the solid and the double dotted-dashed curve), and at the extra Dirac points $j = 1, 2, 3$ (shown, respectively, by the dotted-dashed and the dashed curves) as a function of the barrier parameter $u = V_0 L / h v_F$.

Figure 8. Conductivities (a) $\sigma_{xx}$ and (b) $\sigma_{yy}$, versus Fermi energy for an SL on single-layer graphene with $u = 4\pi$ and $6\pi$ shown by, respectively, the dashed and solid curves. In both cases, $W_h = W_w = 0.5$. The dash-dotted black curves show the conductivities in the absence of the SL potential, $\sigma_{xx} = \sigma_{yy} = \epsilon_F \sigma_0 / 4\pi$.

For comparison, we first look at the conductivity tensor at zero temperature and in the absence of an SL. For single-layer graphene, the conductivity is given by

$$\frac{\sigma_{\mu\nu}(\epsilon_F)}{\sigma_0} = \frac{\epsilon_F}{4\pi},$$

(2.28)

with $\sigma_0 = e^2 / \hbar$. In figure 8a, b the conductivities $\sigma_{xx}$ and $\sigma_{yy}$ are shown for an SL as functions of the energy. Notice that for small energies, the slope of the conductivity $\sigma_{yy}$ is tunable to a large extent by altering the parameter $u$ of the SL. The dashed curves correspond to $u = 4\pi$ and the rather flat dispersion in the $y$ direction for the lowest conduction band (figure 5c, d) translates to a small $\sigma_{yy}$ (for energies $EL / h v_F < 1$) compared with the conductivity in the absence of an SL. The solid curves, on the other hand, correspond to $u = 6\pi$ and owing to the extra Dirac points, which have a rather flat dispersion in the $x$ direction (Ho et al. 2009), the conductivity $\sigma_{yy}$ is large.
(d) Dirac lines

In an effort to simplify the expressions for the dispersion relation we replace, as we did for the few-barrier structures, the SL barriers by δ-function barriers. The square SL potential is then approximated by

$$V(x) = P \sum_{j=-\infty}^{\infty} \delta(x - jL).$$

(2.29)

This potential leads to the dispersion relation

$$\cos k_x = \cos \lambda \cos P + \left(\frac{\xi \lambda}{\lambda}\right) \sin \lambda \sin P,$$

(2.30)

which is periodic in \(P\). This is in sharp contrast with that for standard electrons, which is not periodic in \(P\) and which in our notation reads

$$\cos k_x = \cos \lambda' + \left(\frac{\mu P}{\lambda'}\right) \sin \lambda',$$

(2.31)

where \(\mu = m v_F L/\hbar\) and \(\lambda' = [2\mu \epsilon - k_y^2]^{1/2}\). As can be seen from figure 10a, the energy band near the Dirac point has an interesting property in that it becomes nearly flat in \(k_x\), forming a plane, for large \(k_y\). The angle which the asymptotic plane makes with the zero-energy plane depends on \(P\) and the group velocity \(v_y\) corresponding to this asymptotic plane varies from \(-v_F\) to \(v_F\) in each period \(n\pi < P < (n + 1)\pi\). Notice that no extra Dirac points are found and the reason is the same as that for the asymmetric SL potential, i.e. the extra Dirac points shift away from zero energy. Alternatively, we can try to shed some light by comparing with §2b, where it is explained that the bound states for a single unit of the SL potential are similar to those of the combined single barrier and well. In the region where the bound states cross (denoted by I in figure 4a), anti-crossings occur and corresponding crossings in the SL spectrum (extra Dirac points) are expected. In the limit of a δ-function barrier, this region is reduced to a line (the dark grey line in figure 4a). This prevents anti-crossings from occurring. Also, in this way no extra Dirac points are expected.

**Extended Kronig–Penney (KP) model.** To re-establish the symmetry between electrons and holes, as in the case of square barriers with \(W_b = W_w\), we can use alternating-in-sign δ-function barriers. The unit cell of the periodic potential contains one such barrier up, at \(x = 0\), followed by a barrier down, at \(x = L/2\) (figure 9b). The potential is given by

$$V(x) = P \sum_{j=-\infty}^{\infty} \left[ \delta(x - jL) - \delta \left(x - jL - \frac{L}{2}\right) \right],$$

(2.32)

and is the asymptotic limit of the potential shown in figure 1b. The resulting transfer matrix leads to the dispersion relation

$$\cos k_x = \cos \lambda - \left(\frac{2k_y^2}{\lambda^2}\right) \sin^2 \left(\frac{\lambda}{2}\right) \sin^2 P.$$

(2.33)
This dispersion relation is periodic in $P$. As shown in figure 10b, no extra Dirac points occur, but for the particular case of $P = (n + 1/2)\pi$, $n$ an integer, the spectrum shows an interesting feature: for all $k_y$ we see that equation (2.33) has a solution with $\varepsilon = k_x = 0$, which means the Dirac point at $k_x = k_y = 0$ turned into a Dirac line along the $k_y$ axis. If we take $k_y$ not too large (of the order of $k_x$), this spectrum has a wedge structure as was also found for rectangular SLs. For $k_y \to \infty$, though, the spectrum becomes a horizontal plane situated at $\varepsilon = 0$. We can generalize this model by taking the distance $W$ between the two barriers of the unit cell not equal to $L/2$. This was done by M. Ramezani Masir, P. Vasilopoulos & F. M. Peeters (2010, unpublished work). They found an approximate analytical expression for the dispersion given by

$$\varepsilon \approx [k_x^2 + Fk_y^2]^{1/2} \quad \text{with} \quad F = W^2 + (L - W)^2 + 2W(L - W)\cos(2P). \quad (2.34)$$

This dispersion has the shape of an anisotropic cone with a renormalized velocity in the $y$ direction. Comparing with equations (2.20) and (2.22), we observe that the condition for collimation and the velocity renormalization in the $y$ direction is very different for square barriers. For instance, in the extended KP model, with $W = L/2$, we find $v_y/v_F = |\cos P|$, while for square barriers the result is
\[ v_y/v_F = \sin(u/4)/(u/4). \] The latter means that if we consider \( P \equiv u/4 \), the velocity in the \( y \) direction is maximum \( v_y = v_F \) for \( P = (1/2 + n)\pi \) in the extended KP model while for square barriers \( v_y = 0 \) at these points.

### 3. Bilayer graphene

We now turn to bilayer graphene and use again the nearest-neighbour, tight-binding Hamiltonian in the continuum approximation with \( k \) close to the \( K \) point. If we include a potential difference between the two layers, the Hamiltonian is given by

\[
\mathcal{H} = \begin{pmatrix}
U_1 & v_F \pi & t_\perp & 0 \\
v_F \pi^\dagger & U_1 & 0 & 0 \\
t_\perp & 0 & U_2 & v_F \pi^\dagger \\
0 & 0 & v_F \pi & U_2
\end{pmatrix}.
\] (3.1)

Here \( U_1 \) and \( U_2 \) are the potentials on layers 1 and 2, respectively, \( 2\Delta = U_1 - U_2 \) is the potential difference and \( t_\perp \) describes the coupling between the layers. The energy spectrum for free electrons is given by (McCann 2006; Barbier et al. 2009b)

\[
\varepsilon = u_0 \pm \sqrt{\Delta^2 + k^2 + \frac{t_\perp^2}{2} + \left(4\Delta^2 k^2 + k^2 t_\perp^2 + \frac{t_\perp^2}{4}\right)^{1/2}} \right)^{1/2}
\] (3.2)

with \( u_1 = u_0 + \Delta \) and \( u_2 = u_0 - \Delta \). Contrary to §2, we use units in inverse distance, namely, \( \varepsilon = E/\hbar v_F, \ u_j = U_j/\hbar v_F \) and \( k = [\lambda^2 + k_y^2]^{1/2} \). This spectrum exhibits an energy gap that for \( 2\Delta \ll t_\perp \) equals the difference \( 2\Delta \) between the conduction and the valence band at the \( K \) point (McCann 2006).

Solutions for this Hamiltonian are four-vectors \( \psi \) and for one-dimensional potentials we can write \( \psi(x, y) = \psi(x) \exp(i k_y y) \). If the potentials \( U_1 \) and \( U_2 \) do not vary in space, these solutions are of the form

\[
\psi_{\pm}(x) = \begin{pmatrix} 1 \\ f_{\pm} \\ h_{\pm} \\ g_{\pm} \end{pmatrix} e^{\pm i \lambda x + i k_y y}, \] (3.3)

with \( f_{\pm} = [-ik_y \pm \lambda]/[e' - \delta], \ h_{\pm} = [(e' - \delta)^2 - k_y^2 - \lambda^2]/[t_\perp (e' - \delta)] \) and \( g_{\pm} = [ik_y \pm \lambda]/[e' + \delta] \); the wave vector \( \lambda \) is given by

\[
\lambda_{\pm} = \left[ e'^2 + \delta^2 - k_y^2 \pm \sqrt{4e'^2\delta^2 + t_\perp^2 (e'^2 - \delta^2)} \right]^{1/2}.
\] (3.4)

We will write \( \lambda_+ = \alpha \) and \( \lambda_- = \beta \).

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Figure 11. Four different types of band alignments in bilayer graphene. $E_{c,b}, E_{c,w}, E_{v,c}$ and $E_{v,b}$ denote the energies of the conduction ($c$) and valence ($v$) bands in the barrier ($b$) and well ($w$) regions. The corresponding gap is, respectively, $2\Delta_b$ and $2\Delta_w$.

(a) Tuning of the band offsets

It was shown before that using a one-dimensional biasing, indicated in figure 11a–c by $2\Delta$, one can create three types of heterostructures in graphene (Dragoman et al. 2010). A fourth type, where the energy gap is spatially kept constant but the bias periodically changes sign along the interfaces, can be introduced (figure 11d). We characterize these heterostructures as follows.

— Type I: the gate bias applied in the barrier regions is larger than in the well regions.
— Type II: the gaps, not necessarily equal, are shifted in energy but they have an overlap as shown.
— Type III: the gaps, not necessarily equal, are shifted in energy and have no overlap.
— Type IV: the bias changes sign between successive barriers and wells but its magnitude remains constant.

Type IV structures have been shown to localize the wave function at the interfaces (Martin et al. 2008; Martinez et al. 2009). To understand the influence of such interfaces in this section, we will separately investigate structures with such a single interface embedded by an antisymmetric potential.

To describe the transmission and bound states of some simple structures, we notice that in the energy region of interest, i.e. for $|E| < t_\perp$, the eigenstates that are propagating are the ones with $\lambda = \alpha$. Accordingly, from now on we will assume
that $\beta$ is complex. In this way, we can simply use the transfer-matrix approach of §2 in the transmission calculations. This leads to the relation
\[ \begin{pmatrix} t \\ 0 \\ e_d \\ 0 \end{pmatrix} = N \begin{pmatrix} 1 \\ r \\ 0 \\ e_g \end{pmatrix}, \]
(3.5)
Again the transmission is given by $T = |t|^2$.

For a single barrier, the transmission in bilayer graphene is given by a complicated expression. Therefore, we will first look at a few limiting cases. First we assume a zero bias $\Delta = 0$ that corresponds to a particular case of type III heterostructures. In this case, we slightly change the definition of the wave vectors: for $\Delta = 0$, we assume $\alpha(\beta) = [\epsilon^2 + (-)\epsilon t_\perp - k_y^2]^{1/2}$. If we restrict the motion along the $x$-axis, by taking $k_y = 0$, and assume a bias $\Delta = 0$, then the transmission is $T = |t|^2$ with $t$ given by
\[ \frac{1}{t} = e^{i\alpha_0 D}[\cos(\alpha_0 D) - i Q \sin(\alpha_0 D)] \]
(3.6)
with
\[ Q = \frac{1}{2} \left( \frac{\alpha_0 \epsilon_0 + \alpha_0 \epsilon_b}{\alpha_0 \epsilon_b} \right). \]
This expression depends only on the propagating wave vector $\alpha$ ($\beta$ for $E < 0$) as propagating and localized states are decoupled in this approximation. This also means that one does not find any resonances in the transmission for energies in the barrier region, i.e. for $0 < \epsilon < u$. Owing to the coupling for non-zero $k_y$ with the localized states, resonances in the transmission will occur (figure 12). We can easily generalize this expression to account for the double barrier case.
under the same assumptions. With an inter-barrier distance \( W_w \), one obtains the transmission (Barbier et al. 2009b) \( T_d = |t_d|^2 \) from

\[
t_d = \frac{e^{i2\alpha_0(W_w+2W_b)|t|^2} e^{i2\phi_t}}{1 - |r|^2 e^{i2\phi_r} e^{i2\alpha_0 W_w}}, \tag{3.7}
\]

with \( r = |r|e^{i\phi_r} \) and \( t = |t|e^{i\phi_t} \) being, respectively, the single barrier transmission and reflection amplitudes. In this case, we do have resonances owing to the well states; they occur for \( e^{i2\phi_r} e^{i2\alpha_0 W_w} = 1 \). As \( \phi_r \) is independent of \( W_w \), one obtains more resonances by increasing \( W_w \).

For a single \( \delta \)-function barrier with potential \( V(x)/\hbar v_F = P\delta(x) \) under zero bias, we find the transmission amplitude

\[
\frac{1}{t} = \cos P + i\mu \sin P + \frac{(\alpha - \beta)^2 k_y^2}{4\alpha\beta e^2} \sin P \cot P + iv,
\]

where \( \mu = (\varepsilon + t_{\perp}/2)/\alpha \) and \( \nu = (\varepsilon - t_{\perp}/2)/\beta \). Notice that this formula is periodic in the strength of the barrier \( P \) as in the single-layer case.

For the general case, we obtained numerical results for the transmission through various types of single and double barrier structures, which are shown in figure 13. The different types of structures clearly lead to different behaviours of the tunnelling resonances.

An interesting structure to study is the fourth type of SLs shown in figure 11d. To investigate the influence of the localized states (Martin et al. 2008; Martinez et al. 2009) on the transport properties, we embed the antisymmetric potential profile in a structure with unbiased layers.

Conductance. At zero temperature, \( G \) can be calculated from the transmission using equation (2.11) with \( G_0 = (4e^2L_y/2\pi \hbar) (E_F^2 + t_{\perp} E_F)^{1/2}/\hbar v_F \) for bilayer graphene and \( L_y \) the width of the sample. The angle of incidence \( \phi \) is given by \( \tan \phi = k_y/\alpha \) with \( \alpha \) the wave vector outside the barrier. Figure 14 shows \( G \) for the four SL types. Notice the clear differences in (i) the onset of the conductance and (ii) the number and amplitude of the oscillations.

Bound states. To describe bound states, we assume that there are no propagating states, i.e. \( \alpha \) and \( \beta \) are imaginary or complex (the latter case can be solved separately), and only the eigenstates with exponentially decaying behaviour are non-zero leading to the relation

\[
\begin{pmatrix}
  f_d \\
  0 \\
  e_d
\end{pmatrix}
= N
\begin{pmatrix}
  0 \\
  f_g \\
  0
\end{pmatrix},
\tag{3.9}
\]

From this relation we can find the dispersion relation for the bound states.

To study the localized states for the antisymmetric potential profile (Martin et al. 2008; Martinez et al. 2009), we will use a sharp kink profile (step function). The spectrum found by the method above is shown in figure 15a. We see that there are two bound states, both with negative group velocity \( v_y \propto \partial \varepsilon/\partial k_y \), as found previously by Martin et al. (2008). No bound state near zero energy was
Figure 13. Contour plot of the transmission through a single barrier in (a,b), for width $W_b = 50\text{nm}$, and through double barriers in (c–f) of equal widths $W_b = 20\text{nm}$ that are separated by $W_w = 20\text{nm}$. Other parameters are as follows: (a) $\Delta_b = 100\text{meV}$, $V_b = 0\text{meV}$. (b) $\Delta_b = 20\text{meV}$, $V_b = 50\text{meV}$. (c) Type I: $V_b = V_w = 0\text{meV}$, $\Delta_w = 20\text{meV}$ and $\Delta_b = 100\text{meV}$. (d) Type II: $V_b = -V_w = 20\text{meV}$, $\Delta_w = \Delta = 50\text{meV}$. (e) Type III: $V_b = -V_w = 50\text{meV}$, $\Delta_w = \Delta_b = 20\text{meV}$. (f) Type IV: $V_b = V_w = 0\text{meV}$, $\Delta_b = -\Delta_w = 100\text{meV}$.

found for $k_y \to \infty$ in contradiction with the study of Martinez et al. (2009). For zero energy, we find the solution

\[
k_y = \pm \frac{1}{2} [\Delta^2 + (\Delta^4 + 2\Delta^2 t_{\perp}^2)^{1/2}]^{1/2}
\]

\[
\approx \pm \sqrt{\frac{\Delta t_{\perp}}{2^{3/4}}}, \quad \Delta \ll t_{\perp};
\]

the approximation on the second line leads to the expression found by Martin et al. (2008).
Figure 14. Two-terminal conductance of four equally spaced barriers versus energy for \(W_b = W_w = 10\,\text{nm}\) and different SL types I–IV. The solid curve (type I) is for \(\Delta_b = 50\,\text{meV}, \Delta_w = 20\,\text{meV}\) and \(V_w = V_b = 0\). The dashed curve (type II) is for \(\Delta_b = \Delta_w = 50\,\text{meV}\) and \(V_b = -V_w = 20\,\text{meV}\). The dotted curve (type III) is for \(\Delta_b = \Delta_w = 20\,\text{meV}\) and \(V_b = -V_w = 50\,\text{meV}\). The dashed-dotted curve (type IV) is for \(\Delta_b = -\Delta_w = 50\,\text{meV}\) and \(V_w = V_b = 0\).

Figure 15. (a) Bound states of the antisymmetric potential profile (type IV) with bias \(\Delta_w = -\Delta_b = 200\,\text{meV}\). (b) Contour plot of the transmission through a 20\,\text{nm}-wide barrier consisting of two regions with opposite biases \(\Delta = \pm 100\,\text{meV}\).

(b) Superlattices

The heterostructures discussed above (figure 11) can be used to create four different types of SLs (Dragoman et al. 2010). We will especially focus on type IV and type III SLs in certain limiting cases.

For a type I SL, we see in figure 16a that the conduction and valence band of the bilayer structure are qualitatively similar to those in the presence of a uniform bias. Type II structures maintain this gap (figure 16b), as there is a range in energy for which there is a gap in the SL potential in the barrier and well regions. In type III structures we have two interesting features that can close the gap. First we see from figure 12b that for zero bias, similar to single-layer graphene, extra Dirac points appear for \(k_x = 0\), likewise for figure 4d. For \(W_b = W_w = L/2 = W\), \(k_x = 0\) and \(E = 0\), the \(k_y\) values at which extra Dirac points occur are given by the transcendental equation

\[
[\cos(\alpha W) \cos(\beta W) - 1] + \frac{\alpha^2 + \beta^2 - 4k_y^2}{2\alpha\beta} \sin(\alpha W) \sin(\beta W) = 0.
\]
Figure 16. Lowest conduction and highest valence band of the spectrum for a square SL with period $L = 20\text{nm}$ and $W_b = W_w = 10\text{nm}$. (a) Type I: $\Delta_b = 100\text{meV}$ and $\Delta_w = 0$. (b) Type II: as in (a) for $\Delta_b = \Delta_w = 50\text{meV}$ and $V_b = -V_w = 25\text{meV}$. (c) Type III: $V_b = -V_w = 25\text{meV}$ and $\Delta_b = \Delta_w = 0$. (d) Type III: $V_b = -V_w = 50\text{meV}$ and $\Delta_b = \Delta_w = 0$. (e) Type IV: plot of the spectrum for a square SL with average potential $V_b = V_w = 0$ and $D_b = -D_w = 100\text{meV}$. The contours are for the conduction band and show that the dispersion is almost flat in the $x$ direction.

Comparing figure 12b with figure 4d we remark that, different from the single-layer case, for bilayer graphene the bands in the barrier region are not only flat in the $x$ direction for large $k_y$ values but also for small $k_y$. The latter corresponds to the zero transmission value inside the barrier region for tunnelling through a single unbiased barrier in the bilayer graphene. Secondly, if there are no extra Dirac points (small parameter $uL$) for certain SL parameters, the gap, at the Fermi-level for $k_y = 0$, closes at two points. We will investigate these points somewhat more in the extended KP model. Periodically changing the sign of the bias (type IV) introduces a splitting of the charge neutrality point along the $k_y$ axis; this agrees with what was found by Martin et al. (2008). We illustrate that in figure 13e for an SL with $\Delta_b = -\Delta_w = 100\text{meV}$. We also see that the two valleys in the spectrum are rather flat in the $x$ direction. Upon increasing the parameter $\Delta L$, the two touching points shift to larger $\pm k_y$ and the valleys become flatter in the $x$ direction. For all four types of SLs, the spectrum is anisotropic and results in very different velocities along the $x$ and $y$ directions.

Extended KP model. To understand which SL parameters lead to the creation of a gap, we look at the KP limit of type III SLs for zero bias (M. Barbier, P. Vasilopoulos & F. M. Peeters 2010, unpublished work). Also we choose the extended KP model to ensure spectra symmetric with respect to the zero-energy value, such that the zero-energy solutions can be traced down more easily. If the latter zero modes exist, there is no gap. To simplify the calculations, we restrict the spectrum to that for $k_y = 0$. This assumption is certainly not valid if the
parameter $uL$ is large because in that case we expect extra Dirac points (not in the KP limit) to appear that will close the gap. The spectrum for $k_y = 0$ is determined by the transcendental equations

$$\cos k_x L = \cos \alpha L \cos^2 P + D_\alpha \sin^2 P$$

(3.12a)

and

$$\cos k_x L = \cos \beta L \cos^2 P + D_\beta \sin^2 P,$$

(3.12b)

with $D_\lambda = [(\lambda^2 + \epsilon^2) \cos \lambda L - \lambda^2 + \epsilon^2]/4\lambda^2 \epsilon^2$, and $\lambda = \alpha, \beta$. To see whether there is a gap in the spectrum, we look for a solution with $\epsilon = 0$ in the dispersion relations. This gives two values for $k_x$ where zero energy solutions occur

$$k_{x,0} = \pm \arccos \frac{1 - (L^2/16) \sin^2 P}{L},$$

(3.13)

and the crossing points are at $(\epsilon, k_x, k_y) = (0, \pm k_{x,0}, 0)$. If the $k_{x,0}$ value is not real, then there is no solution at zero energy and a gap arises in the spectrum. From equation (3.12), we see that for $\sin^2 P > 16/L^2$ a band gap arises.

Conductivity. In bilayer graphene, the diffusive DC conductivity, given by equation (2.27), takes the form

$$\frac{\sigma_{\mu\mu}(\epsilon_F)}{\sigma_0} = \left(\frac{k_F^3}{4\pi^2 e_F^2}\right) \left[1 \pm \frac{\delta}{2} \left(\frac{k_F^2 \delta + 1}{4}\right)^{1/2}\right]^2,$$

(3.14)

with $k_F = [\epsilon_F^2 + \Delta^2 \mp (\epsilon_F^2 \delta - \Delta^2)^{1/2}]^{1/2}$, $\delta = 1 + 4\Delta^2$ and $\sigma_0 = e^2 \tau_F t_\perp / h^2$.

In figure 17a,b, the conductivities $\sigma_{xx}$ in figure 17a and $\sigma_{yy}$ in figure 17b for bilayer graphene are shown for the various types of SLs defined in §3b. Notice that for type IV SL, the conductivities $\sigma_{xx}$ and $\sigma_{yy}$ differ substantially owing to the anisotropy in the spectrum.

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4. Conclusions

We reviewed the electronic band structure of single-layer and bilayer graphene in the presence of one-dimensional periodic potentials. In addition, we investigated the conditions that lead to carrier collimation in single-layer graphene and determined when extra Dirac points appear in the spectrum and what their influence is on the conductivity. Furthermore, we investigated the tunnelling through, and bound states created by, simple barrier structures. In single-layer graphene, we found that the SL spectrum can be linked to the bound states of a combined barrier and a well.

In bilayer graphene, we considered transport through different types of heterostructures, where we distinguished between four types of band alignments. We also connected the bound states in an antisymmetric potential (type IV) with the transmission through such a potential barrier. Furthermore, we investigated the same four types of band alignments in SLs. The differences between the four types of SLs are reflected not only in the spectrum but also in the conductivities parallel and perpendicular to the SL direction. For type III SLs, which have a zero bias, we found a feature in the spectrum similar to the extra Dirac points found for single-layer graphene. Also, for not too large strengths of the SL barriers, we found that the valence and conduction bands touch at points in \( k \) space with \( k_y = 0 \) and non-zero \( k_y \). Type IV SLs tend to split the \( K \) \( (K’) \) valley into two valleys.

In the KP limit, in which the barriers are \( \delta \) functions, \( V(x)/\hbar v_F = P\delta(x) \), we saw that the SL spectra, the transmission, the conductance, and so on are periodic in the strength of the barriers. As is well known, this is not the case for standard electrons. An important qualitatively new feature is encountered in the extended KP limit for \( P = (n + 1/2)\pi \), see §2d: the Dirac point becomes a Dirac line.

We expect that these relatively recent findings, that we reviewed in this work, will be tested experimentally in the near future.

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