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Zener Tunnelling in Graphene Based Semiconductors - the k·p Method

William Vandenberghe1,2, Bart Sorée1, Wim Magnus1,3 and Guido Groeseneken1,2

1 IMEC, Kapeldreef 75, 3001 Leuven, Belgium
william.vandenberghe@imec.be
2 Dept. of Electrical Engineering, Katholieke Universiteit Leuven
Kasteelpark Arenberg 10, 3001 Leuven, Belgium
3 Department of Physics, Universiteit Antwerpen
Groenenborgerlaan 171, 2020 Antwerpen, Belgium

Abstract.
The carbon nanotube and graphene nanoribbon band structure is derived using the two-band k·p method and shown to have a similar band structure as a III-V semiconductor. Contrary to a previous claim, it is shown that the tunnelling probability is lower for a graphene based semiconductor than for a III-V semiconductor with the same bandgap. Considering the relation between the bandgap and the effective mass we conclude that a graphene based semiconductor is not well-suited for a classical device which suffers from Zener tunnelling, but is rather promising for a device which has its working principle based on Zener tunnelling.

1. Introduction
Graphene based materials such as carbon nanotubes and graphene nanoribbons provide an interesting research topic since they have a band structure which is different from traditional semiconductors. Graphene has a zero bandgap at the K-points in the Brillouin zone, but some carbon nanotubes or graphene nanoribbons exhibit a non-zero bandgap which, in principle, enables the fabrication of semiconductor devices. These semiconducting carbon nanotubes and graphene nanoribbons will be referred to as graphene based semiconductors throughout this paper.

Graphene based semiconductors generally have a small bandgap and hence Zener tunnelling, also called band-to-band tunnelling (BTBT), cannot be neglected in possible graphene based semiconductor devices. A recent publication [1] shows a calculation of the Zener tunnelling current using the WKB method and concludes that it exceeds the current of group IV and III-V semiconductors with identical bandgaps.

In this paper, we first develop the band structure within the k·p scheme for bulk graphene as well as for nanoribbons or nanotubes with a non-zero bandgap. Next, we consider the tunnelling probability and refute the claim that tunnelling is more efficient in a graphene based semiconductor compared to a III-V semiconductor with the same bandgap, and we explain the discrepancy with the previous publication [1].

2. Graphene based semiconductors: band structure
For the k·p expansion of the bulk graphene band structure around the K-point we use two bands: the π+ conduction band and the π valence band which are degenerate at the K-point due to symmetry [2]. Using these states to construct the k·p Hamiltonian, we need to determine the momentum matrix elements

\[
p_{11} = \int u_1^*(r,z)\mathbf{p} u_1(r,z) d^3r \quad , \quad p_{12} = \int u_1^*(r,z)\mathbf{p} u_2(r,z) d^3r \quad , \quad p_{22} = \int u_2^*(r,z)\mathbf{p} u_2(r,z) d^3r,\]

(1)
appearing as integrals over the 2D graphene unit cell in the plane and over the entire space in the \( z \)-direction perpendicular to the plane,

\[
\int d^3r = \int_{\text{unitcell}} d^2r \int_{-\infty}^{\infty} dz.
\]

(2)

Here, \( u_1(r, z) \) and \( u_2(r, z) \) are two Bloch functions which are orthogonal solutions to the Schrödinger equation with eigen energy equal to zero:

\[
\left[ -\frac{\hbar^2 \nabla^2}{2m} + U_{\text{lat}}(r, z) \right] u_{1,2}(r, z) = 0
\]

(3)

\( U_{\text{lat}}(r, z) \) is the potential due to the graphene lattice which is periodic with respect to \( r \), \( m \) is the free electron mass and \( \hbar \) is the reduced Planck constant.

As the \( z \)-axis stands perpendicular to the graphene plane, both the \( \pi \) and \( \pi^* \) bands are odd under a reflection in the \( xy \)-plane and as a result the 3 selected matrix elements have no \( z \) component. The \( y \) direction is chosen such that \( u_1 \) and \( u_2 \) are respectively odd and even under reflection in the \( yz \)-plane. This requires \( p_{11} \) and \( p_{22} \) to be in the \( y \) direction and \( p_{12} \) in the \( x \) direction. At the \( K \)-point the valence and conduction band are degenerate due to an additional rotational symmetry over 120°. This adds the requirement \( |p_{11}| = |p_{12}| = |p_{22}| = p \) and \( p_{11} = -p_{22} \).

According to the \( \mathbf{k} \cdot \mathbf{p} \) method a state with wavevector \( \mathbf{k} \) relative to a \( K \)-point can be written as

\[
\psi(r, z) = e^{i\mathbf{k} \cdot \mathbf{r}} (a_1 u_1(r, z) + a_2 u_2(r, z))
\]

(4)

and its energy eigenvalues \( E_{\pm}(\mathbf{k}) \) are determined by the 2-band \( \mathbf{k} \cdot \mathbf{p} \) Hamiltonian

\[
H = \left( \frac{\hbar^2}{2m} (k_x^2 + k_y^2) + \frac{\hbar p}{m} k_x \right) + \frac{\hbar p}{m} k_y
\]

(5)

yielding

\[
E_{\pm}(\mathbf{k}) = \frac{\hbar^2 |\mathbf{k}|^2}{2m} \pm \frac{\hbar p}{m} |\mathbf{k}|, \quad |\mathbf{k}| = \sqrt{k_x^2 + k_y^2}.
\]

(6)

To first order, this corresponds to the nearest neighbor tight binding expression

\[
E_{\pm}(\mathbf{k}) \approx \pm \hbar v_F |\mathbf{k}|
\]

(7)

and the matrix element \( p \) can be determined as \( p = m v_F \) with \( v_F \) the graphene Fermi velocity.

Note that an alternative choice of basis functions \( u_1 \) and \( u_2 \) and omission of the second derivative transforms Eq. (5) into a more familiar formulation of the Hamiltonian

\[
H = \frac{\hbar m}{p} \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix},
\]

(8)

the resulting Schrödinger equation being algebraically identical to the 2D Weyl equation [3].

Returning to Eq. (5) for the case of a semiconducting nanoribbon or nanotube we use the zone folding technique to determine the band structure. The \( \mathbf{k} \) vector is continuous in one direction and quantized in the perpendicular direction. For the sake of convenience we select a zig-zag nanoribbon or nanotube such that \( k_x \) is quantized and \( k_y \) is continuous. The following derivation of the band structure is valid however for an arbitrary orientation of the tube or ribbon since Eq. (6) is invariant under rotations.

Denoting \( k_0 \) by the smallest allowed value of \( k_x \) we obtain the bandgap of the graphene based semiconductor

\[
E_g = \frac{2\hbar p}{m} k_0
\]

(9)

where size quantization allows for \( k_0 \neq 0 \) in the case of a semiconducting nanotube or ribbon, while Eq. (5) turns into

\[
H = \left( E_0 + \frac{k_x^2}{2m} + \frac{k_y^2}{2m} \right) \begin{pmatrix} 0 & \frac{\hbar p}{m} k_x \\ \frac{\hbar p}{m} k_y & 0 \end{pmatrix} \begin{pmatrix} E_0 + \frac{\hbar p}{m} k_y \\ \frac{\hbar p}{m} k_x \end{pmatrix}
\]

(10)
with $E_0 = \hbar^2 k_0^2 / 2m$ and the energy dispersion relation for the lowest subband reads

$$E_k = E_0 + \frac{\hbar^2 k_y^2}{2m} \pm \sqrt{\frac{E_k^2}{4} + \frac{\hbar^2 p^2}{m^* k_y^2}}. \tag{11}$$

Within the 2 band approximation Eq. (10) is formally identical to the $k \cdot p$ Hamiltonian of a III-V semiconductor with a bandgap $E_g$, a matrix element $p$ and an energy offset $E_0$ [4, 5]. More specifically, in a III-V semiconductor, the two-band Hamiltonian describes the interaction between the light valence band and the conduction band. The energy dispersion relation of a graphene based semiconductor is therefore the same as that of a III-V semiconductor apart from the absence of a heavy and a split-off valence band.

3. Tunnelling probability

As a graphene based semiconductor and a III-V semiconductor share a similar band structure, the expression of the Zener tunnelling probability for an electron in a uniform field will also be the same:

$$T = \exp\left(-\frac{\pi E_p^2 m}{4 \hbar pqF}\right) \tag{12}$$

with $F$ the applied uniform electric field and $q$ the unit charge [5]. To compare different materials, we consider the matrix element $p$ which is generally expressed as the energy unit $E_p = 2p^2 / m$ taking the value $E_p = 2mv_F^2 = 11.4eV$ for graphene and $E_p \approx 20eV$ for III-V semiconductors, such as GaAs, InAs, InSb, ... [6].

For conventional devices, such as the metal-oxide-semiconductor field-effect transistor (MOSFET), BTBT is a detrimental effect since it increases the off-state current. To make a fair comparison concerning the amount of BTBT we must consider MOSFETs with a common figure of merit such as the transport effective mass. Making use of the relation between the effective mass and the bandgap, $m^* \approx mE_g/E_p$ and the definition of $E_p$, the transmission coefficient (12) can be written as

$$T \approx \exp\left(-\frac{\pi E_p^{3/2} m^{*2}}{2\sqrt{2m^{3/2}\hbar qF}}\right). \tag{13}$$

Since $E_{p, \text{graphene}} < E_{p, \text{III–V}}$, Eq. (13) shows that for the same effective mass, the tunnelling probability will be much greater for a graphene based MOSFET compared to a III-V based MOSFET as shown in Fig. 1. Or, in other words a graphene based MOSFET with the same on-current characteristics as a III-V based MOSFET will show a higher leakage current due to increased BTBT.

In the case of a III-V semiconductor, the effective mass ($m^*$) refers to the conduction band mass or the light hole mass. In the case of a graphene based semiconductor, there is only one direction with a continuous wavevector defining single valence and conduction bands. The absence of a heavy hole and a split-off band in graphene band structure could still allow graphene to outperform a similar III-V device but certainly for nMOS devices we do not expect an improvement over III-V MOSFETs.

For devices operating on the basis of BTBT such as the tunnel FET [7], large tunnelling probabilities are required. Since the matrix element $p \propto \sqrt{E_p}$ is smaller for graphene than for III-V semiconductors, graphene based semiconductors have a smaller tunnel probability for the same bandgap as shown in Fig. 1. To obtain the same performance as a III-V tunnel FET, a graphene based semiconductor tunnel FET must have a smaller bandgap. But since for graphene based semiconductors the bandgap can be made smaller by selecting a different size of nanoribbon or nanotube, this needs not be a disadvantage if graphene based semiconductors can be fabricated reliably.

Finally, we report on a discrepancy between our results and the work by Jena et al. [1] who came to the opposite conclusion concerning the tunnelling probability. To our opinion, the disagreement stems from the assumption by Jena et al. that traditional semiconductors have a “parabolic bandgap”. Obviously, the parabolic nature of the band structure in any semiconductor only holds in a limited energy range and does not cover the entire Brillouin zone.

As we have shown in our previous section, there is no formal difference in the band structure between a graphene based semiconductor and a III-V semiconductor except for the presence of an additional heavy hole and split-off band in the latter.
Figure 1. Comparison between the Zener tunnelling probability of InSb and a graphene based semiconductor with the InSb bandgap (Eq. 12) and a graphene based semiconductor with the InSb effective mass (Eq. 13).

The direct cause of the disagreement lies in the use of the transmission coefficient \[ T = \exp \left( -\frac{4\sqrt{2m^*E_g}}{3\hbar F} \right) \] (14)
by Jena et al. In the case of Zener tunnelling, the “parabolic bandgap” approximation is too crude, comparing Eq. (14) with Eq. (12) and using \( p = \frac{m}{\sqrt{2\sqrt{E_g/m^*}}} \) we observe a deviation of a factor \( 3\pi/16 = 0.59 \) in the exponential. Correcting for this factor the conclusion from the previous publication that graphene has a larger tunnel probability compared to a III-V with the same bandgap is reversed and agrees with our current publication, claiming that the III-V material will show the larger tunnel probability for the same bandgap.

4. Conclusions
The band structure of the valence and the conduction band in a graphene based semiconductor can be described in the same way as the light valence and the conduction band structure in a III-V semiconductor.

Graphene based semiconductors have a lower Zener tunnelling probability than III-V semiconductors for the same bandgap.

Semiconductor devices where the effective mass is a figure of merit and where leakage (off-current) due to Zener tunnelling is unwanted such as the MOSFET will show higher leakage for the same on-current in the case of graphene based semiconductors compared to III-V semiconductors. On the other hand, graphene based semiconductors are well suited for devices which operate on the basis of Zener tunnelling such as the tunnel FET.

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