

Here is a simple graphical explanation (no formulas!) of the perfect conductance of 120 degrees turn in Z-GNR vs. poor conductance of the 60 degrees turn. Nearest-neighbor π -orbital tight binding is used to obtain the band structures of graphene and graphene nanoribbons.

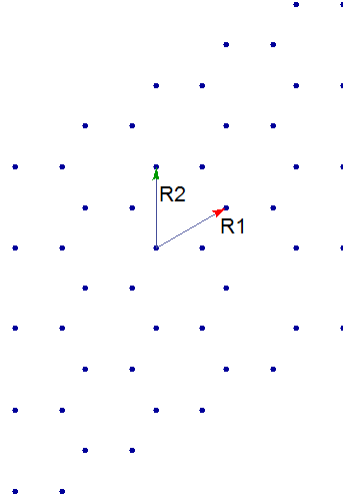


Figure 1. The graphene lattice and unit vectors R1 and R2. The axis of armchair graphene nano-ribbon (A-GNR) is in horizontal direction; the axis of zigzag nano-ribbon (Z-GNR) is vertical direction.

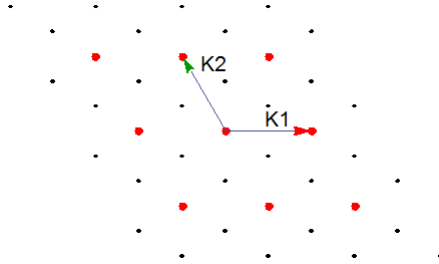


Figure 2. The reciprocal lattice (red dots) and reciprocal unit vectors K1 and K2 such that $R1 \cdot K1 = R2 \cdot K2 = 2\pi$; $R1 \cdot K2 = R2 \cdot K1 = 0$. Black dots are the Dirac points in which $E[K] = 0$. The orientation of the reciprocal lattice corresponds to the orientation of the real space lattice in Fig. 1.

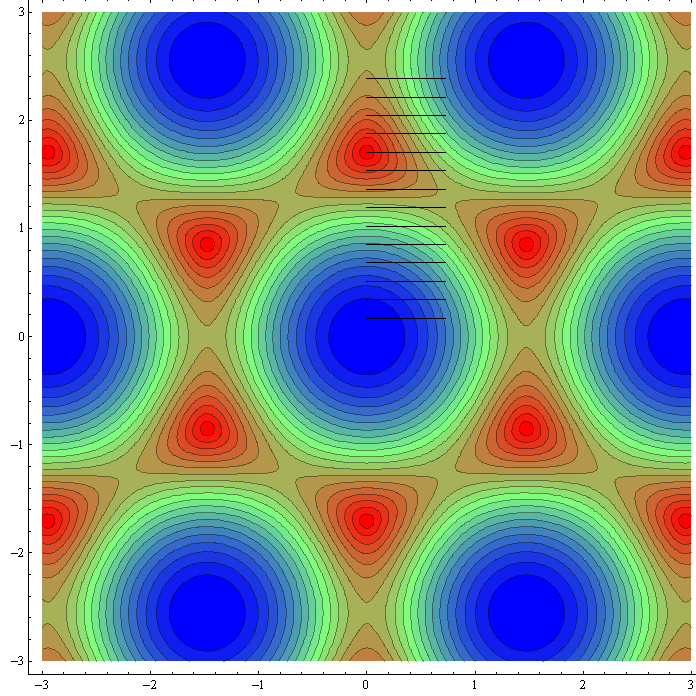


Figure 3. Contour plot of the graphene energy surface $E[\mathbf{K}]$ in the nearest neighbor approximation lying below the Fermi level. Orientation in \mathbf{K} -space corresponds to the Figs. 1-2. Red areas are the highest regions of $E[\mathbf{K}]$ located near the Dirac points. The band-structure of the A-GNR can be obtained from the $E[\mathbf{K}]$ as follows. Suppose the direction of A-GNR is along the horizontal axis and it is 14-dimers wide. In the vertical direction the \mathbf{k} -vector is allowed to take only 14 discrete values corresponding to the integer number of half-wavelength across the 14-dimers-wide A-GNR. These discrete values correspond to horizontal line segments on the plot. The length of the segments corresponds to the maximum length of the \mathbf{k} -vector in A-GNR.

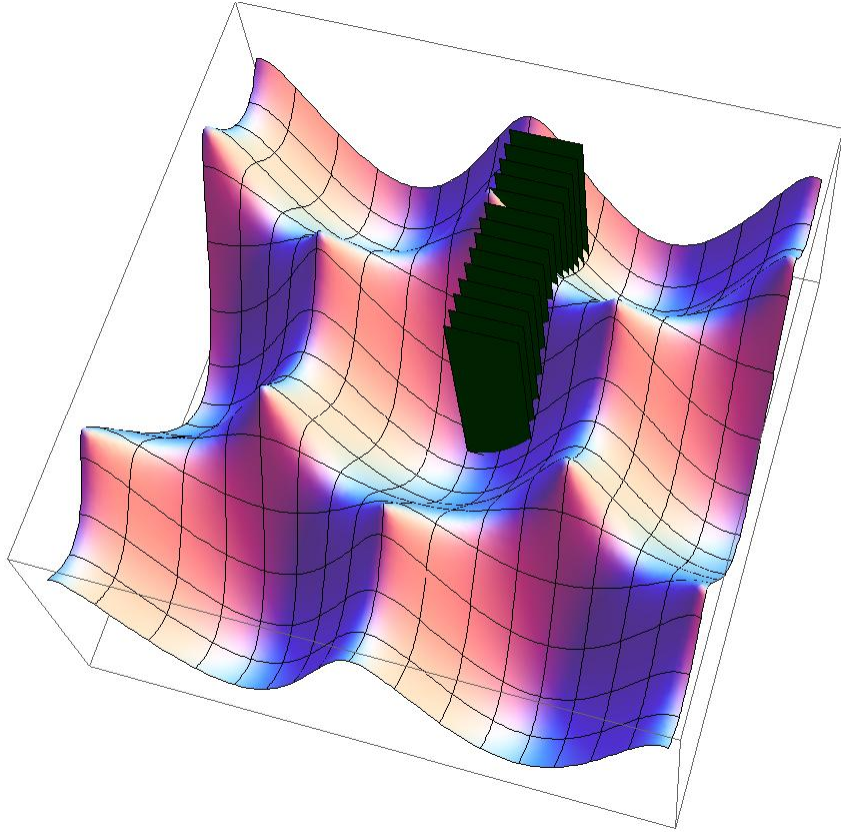


Figure 4. Same as Fig. 3 but in 3D. The band-structure of 2D graphene sheet with only one energy surface out of two shown for clarity. The band-structure of A-GNR is expected to correspond to the projections of the 3D $E[\mathbf{K}]$ surface on the 14 rectangles matching 14 line segments in Fig. 3.

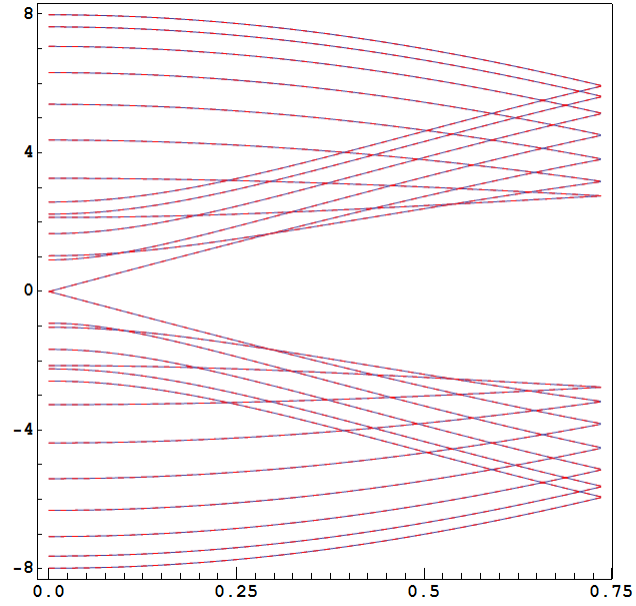


Figure 5. It appears that projections of $E[K]$ surface on the rectangles in Fig. 4 are identical to the 14 lower bands of A-GNR 14 dimers wide. The same is true for A-GNR of any width. The projections of the second $E[K]$ surface lying above the Fermi level will give the upper portion of the A-GNR band-structure. Red dashed lines are obtained from A-GNR one-dimensional Hamiltonian, blue lines (perfectly coinciding with the red ones) are the projections of $E[K]$ surface for infinite graphene sheet.

Now, let's project the graphene band structure on the Z(igzag)-GNR axis

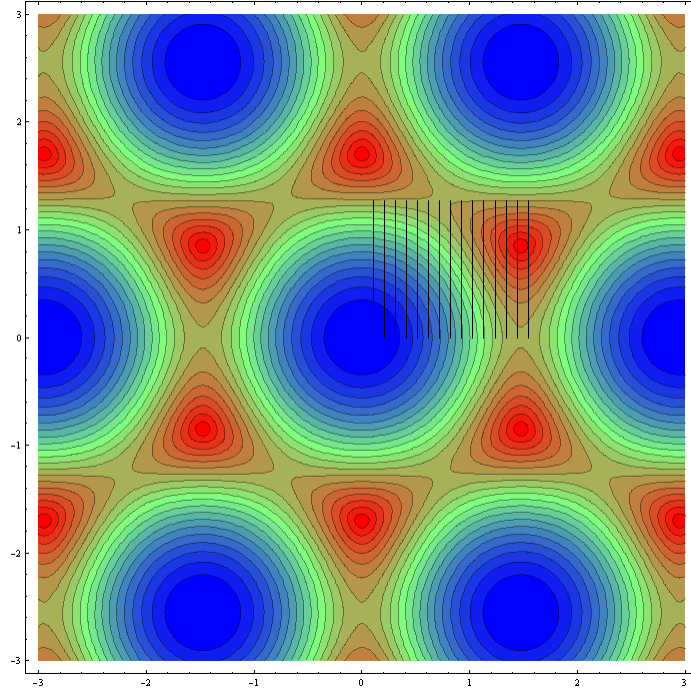


Figure 6. Contour plot of the graphene energy surface $E[\mathbf{K}]$ lying below the Fermi level (same as in Fig. 3). Our sample Z-GNR 15 dimers wide is aligned vertically, and analogously to the A-GNR case considered above, one can expect that the approximate Z-GNR band-structure can be obtained by sampling $E[\mathbf{K}]$ along the 15 line segments defined similarly to A-GNR case.

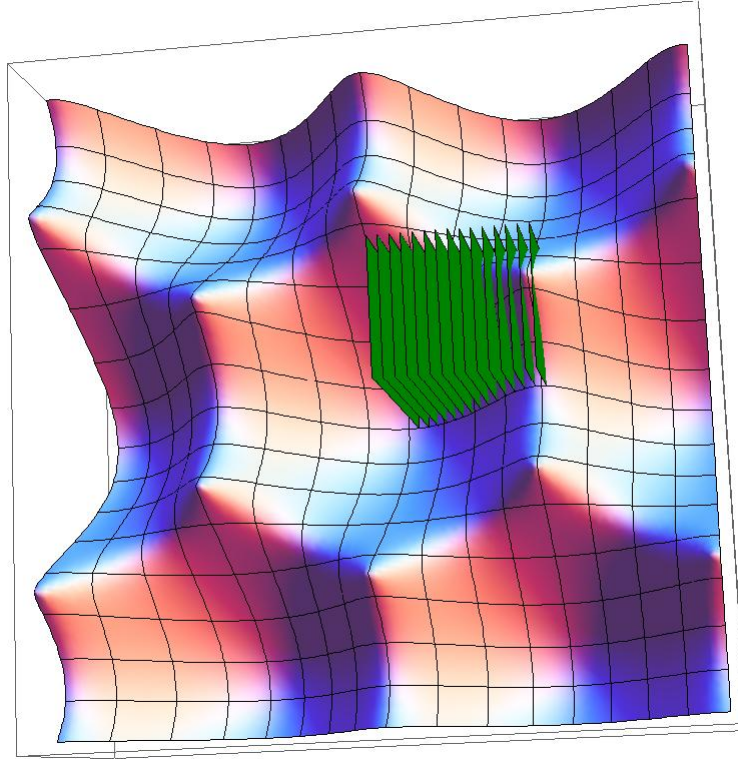


Figure 7. Same as in Fig 6 in 3D. The band-structure of 2D graphene sheet; only one energy surface out of two is shown for clarity. The band-structure of Z-GNR is expected to correspond to the projections of the 3D $E[\mathbf{K}]$ surface on the 15 rectangles matching 15 line segments in Fig. 6.

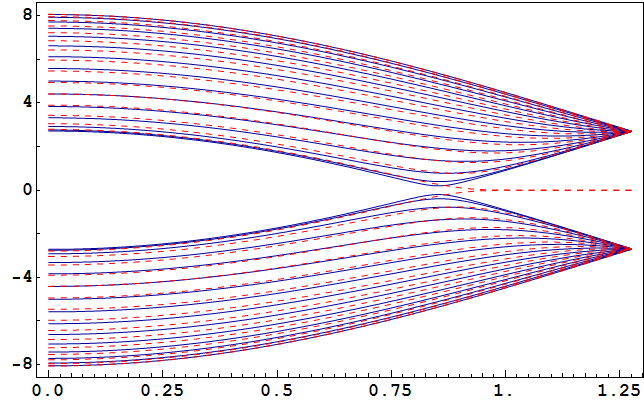


Figure 8. Unlike A-GNR, for Z-GNR the match between the Z-GNR band-structure and projections of the 3D $E[K]$ surface on the corresponding rectangles is only approximate. However, this approximate match indicates that the electronic states in the band nearest to the Fermi energy ($E_F = 0$), which form a single channel window near E_F , correspond to the states near the Dirac point for 2D graphene.

That were the prerequisites

Here is the explanation:

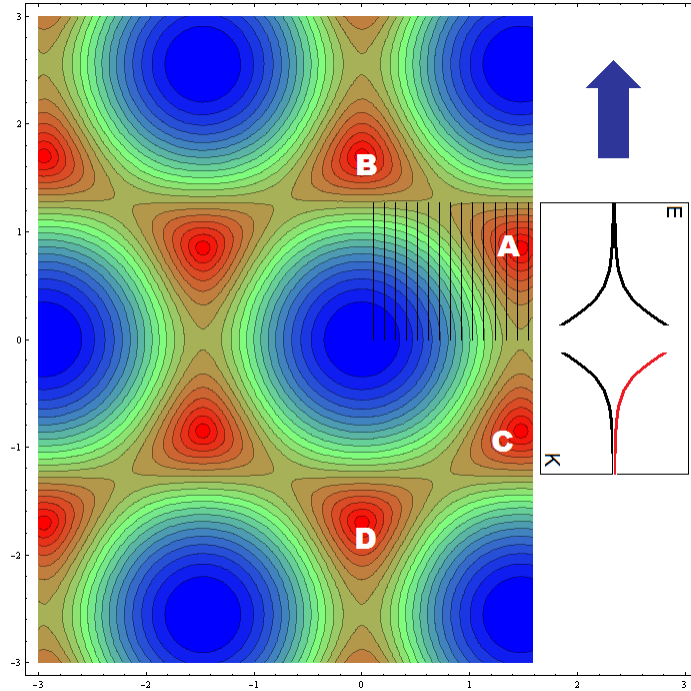


Figure 9. Suppose that the Z-GNR is aligned vertically, and the electron flux runs in the direction of the blue arrow. The insert to the right schematically shows the Z-GNR band-structure within the single channel conductance window. For definiteness, let us consider the electrons with the energy higher than the Fermi energy. For this energy range only the states corresponding to the red band contribute to the electron flux in the given direction. That means these electrons are associated with the states near the Dirac point at valley C.

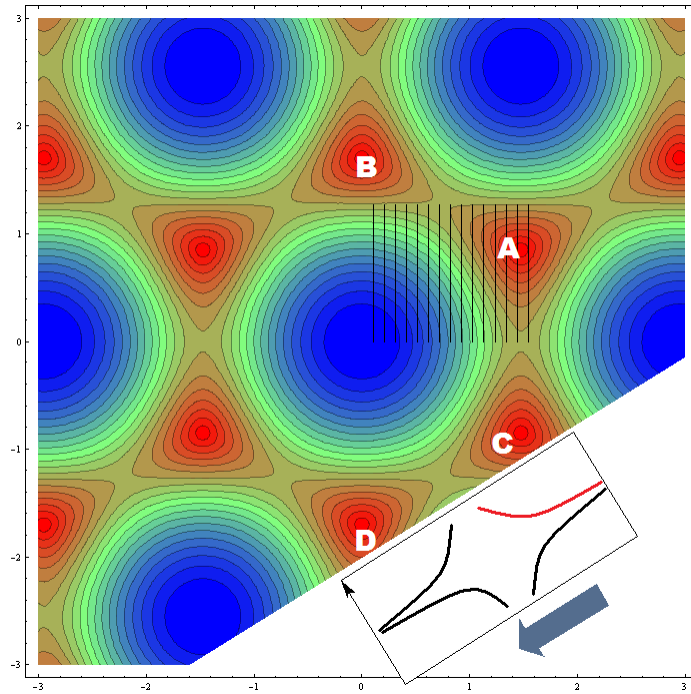


Figure 10. Now, let us consider the 120 turn with respect to the flux in Fig. 9. Again, the red band marks the electrons with positive energies participating in the flux. These electrons also belong to valley C.

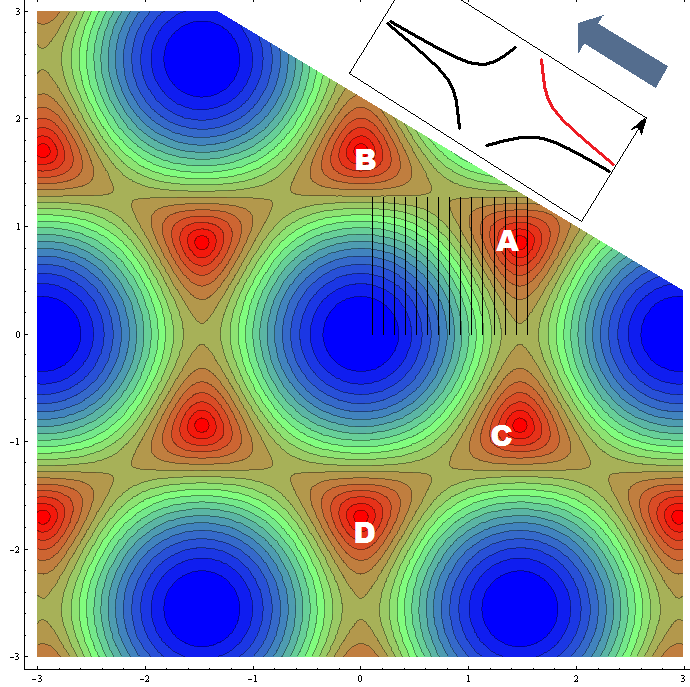


Figure 11. Unlike 120 degree turn, if the flux is turned into the Z-GNR, constituting 60 degrees angle with respect to the vertical strip, the participating electrons belong to valley A, which is of different type than valley C. That means the electrons, which were originally in the valley C, need to be scattered into valley A, before they can propagate in the strip turned by 60 degrees with respect to the original direction. Thus, good transmission in Fig. 10 corresponds to the in-valley scattering, while poor transmission - to the inter-valley scattering.

The explanation of 120 vs. 60 degrees transmission difference can be also done in real space, though it does not look that elegant. Rotating the graphene plane by 60 degrees swaps two principal valleys in k-space and two sub-lattices in real space. The outermost atoms at the opposite edges of zigzag strip belong to different sub-lattices regardless of the strip width. In the 120 degrees turn the outermost atoms always belong to the same sub-lattice even if the widths of the strips constituting the 120 turn are different. That results in the wave function continuity and nearly perfect transmission. On the contrary, in the 60 degrees turn the atoms along the same edge of the constituent strips belong to the different sub-lattices. Because of the very large contrast between the components of the wave function belonging to different sub-lattices at Z-GNR edges there is a strong mismatch between the wave functions in the two strips forming the 60 degrees turn. That results in a poor transmission.

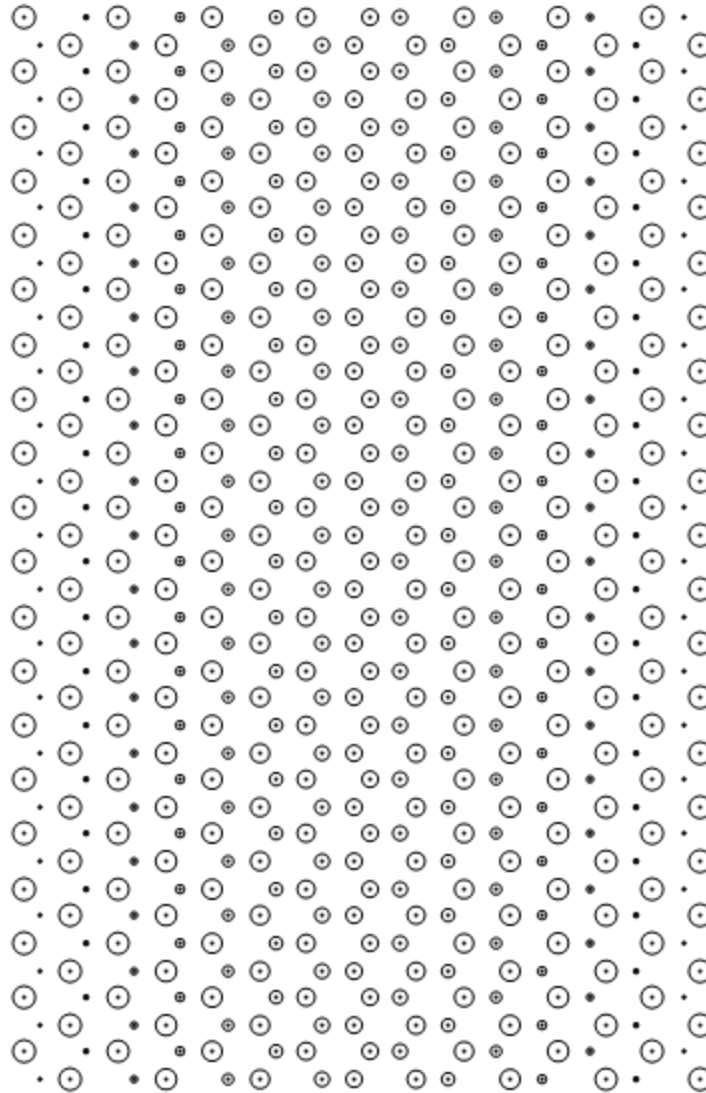


Figure 12. The absolute values of the wave function belonging to the single channel window. The radii of the circles are proportional to the wave-function component at the given site.