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Statistical magnitudes and the chiral tunneling in bilayer graphene: Influence of evanescent waves

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ABSTRACT

The problem of the chiral (Klein-like) tunneling across a potential barrier in bilayer graphene is addressed. The electron wave functions are treated as massive chiral particles. This treatment allows us to compute the statistical complexity and Fisher–Shannon information for each angle of incidence. The comparison of these magnitudes with the transmission coefficient through the barrier is performed. The role played by the evanescent waves on these magnitudes is disclosed. Due to the influence of these waves, it is found that the statistical measures take their minimum values not only in the situations of total transparency through the barrier, a phenomenon highly anisotropic for the chiral tunneling in bilayer graphene.

The calculation of information theory measures in quantum systems is nowadays a subject of increasing interest. The knowledge of the probability density is the basic ingredient [1–3] necessary to calculate these magnitudes, concretely the statistical complexity and the Fisher–Shannon information.

These indicators have been directly computed from the wave functions in different bound states such as for instance the H-atom [4]. In other cases, they have been numerically derived from a Hartree–Fock scheme [5,6]. These statistical quantifiers have revealed a connection with physical measures, such as the ionization potential and the static dipole polarizability in atomic physics [7,8]. Other relevant properties concerning the bound states of atoms and nuclei have been put in evidence when computing these indicators on these many-body systems. For instance, the extremal values of these measures on the closure of shells [9,10] and the trace of magic numbers [11,12] are some of these properties.

For no bound states, we have the particular case of the scattering process of quantum particles through potential barriers. It can be a first example to study the relationship of these entropy–information measures with some physical magnitude, such as the reflection coefficient. Thus, in the context of non-relativistic quantum mechanics (NRQM), it has been pointed out [13] that these statistical magnitudes present their minimum values just in the situations where the total transmission through the barrier is achieved. A similar result was obtained for the crossing of a barrier in a relativistic-like quantum mechanics context. This is the case of the so-called Klein tunneling [14] in single-layer graphene [15].

In this work, we are concerned with the calculation of these entropic magnitudes in another quantum scattering process through a potential barrier, specifically the Klein-like tunneling in bilayer graphene (BLG), a subject that can have interest in applied condensed matter [16–18].

Let us recall that the Klein tunneling (or paradox) is an exotic phenomenon with counterintuitive consequences in relativistic quantum mechanics (RQM) that has deserved a great interest in particle, nuclear and astrophysics [19–24]. Klein [14] showed that, in the frame of RQM, it is possible that all incident particles (electrons in the case of graphene) can cross a barrier, independently of how high and wide the potential barrier is. This is a paradoxical fact from the point of view of the NRQM, where we know that the higher and wider the potential barrier is, less number of particles can tunnel the barrier (exponential decay). The Klein paradox has never been realized in laboratory experiments. However, a possibility to observe this type of phenomenon has recently been proposed and tested by means of graphene [25–28]. In particular, the discussion of the Klein tunneling and related phenomena for Dirac fermions in monolayer and bilayer graphene was given in Ref. [25].

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It must be remarked at this point that although the Klein tunneling of an electron can occur in an AA-stacked BLG [29], it is more accurate to use the term "chiral tunneling" [16] for BLG instead of "Klein tunneling" since, as below displayed, at normal incidence the perfect reflection of electrons takes place.

From an electronic point of view, BLG is a 2D gapless semiconductor with chiral electrons and holes with a finite mass m [25]. The mass of these quasiparticles is a non-relativistic consequence of their parabolic energy spectrum. The chirality comes from the spinorial nature of their wavefunction, similar to the chirality of the carriers in single-layer graphene that can be viewed as relativistic fermions, in that case massless due to their linear energy dispersion at low Fermi energies. For the present case of the BLG, the quadratic energy dispersion implies four possible solutions for a given energy E,

$$E = \pm \frac{\hbar^2 k_F^2}{2m}, \tag{1}$$

where $\hbar$ is the Planck's constant divided by 2π, k_F is the Fermi wavevector of the quasiparticle, and $m \sim 0.035\, m_e$, with m_e the electron mass, is the effective mass of the carriers taken from Ref. [30], a value that is between the theoretical ($m = 0.054\, m_e$) and the experimental ($m = 0.028\, m_e$) values of this parameter reported in the Katsnelson monograph [16]. Two solutions correspond to propagating waves and the other two to exponentially growing and decaying waves (evanescent waves). The expression of these wavefunctions can be found by solving the off-diagonal Hamiltonian that describes the low-energy quasiparticles in BLG [25,31]:

$$H_0 = -\frac{\hbar^2}{2m} \begin{pmatrix} 0 & (\hat{k}_x - i\hat{k}_y)^2 \\ (\hat{k}_x + i\hat{k}_y)^2 & 0 \end{pmatrix}, \tag{2}$$

where $(\hat{k}_x, \hat{k}_y) = -i(\nabla_x, \nabla_y)$.

In order to study the chiral tunneling in BLG, an one-dimensional square potential barrier $V(x)$ is considered on the x–y plane:

$$V(x) = \begin{cases} 0, & x \le 0 \quad \text{(Region I)}, \\ V_0, & 0 < x < L \quad \text{(Region II)}, \\ 0, & x \ge L \quad \text{(Region III)}, \end{cases} \tag{3}$$

where V_0 and L are the height and width of the barrier, respectively, and the dimension along the Y axis is supposed to be infinite. This local potential barrier can be created by the electric field effect using local chemical doping or by means of a thin insulator [32,33]. The effect of this potential barrier has the chiral tunneling as the most intriguing effect for $V_0 > E$, where electrons outside the barrier transform into holes inside it, or vice versa, a phenomenon that allows to the charge carriers to pass through the barrier. In the case of BLG, this charge conjugation requires the appearance of evanescent waves (holes with wavevector ik) inside the barrier.

Now, we consider an electron wave that propagates under the action of the Hamiltonian $H = H_0 + V(x)$ at an incident angle ϕ respect to the x axis. The solutions for the two-component spinor representing these quasiparticles in the different regions are:

$$\Psi_I(x,y) = \left\{ a_1 \begin{pmatrix} 1 \\ se^{2i\phi} \end{pmatrix} e^{ik_x x} + b_1 \begin{pmatrix} 1 \\ se^{-2i\phi} \end{pmatrix} e^{-ik_x x} + c_1 \begin{pmatrix} 1 \\ -s \cdot h \end{pmatrix} e^{\kappa_x x} \right\} e^{ik_y y}, \tag{4}$$

$$\Psi_{II}(x,y) = \left\{ a_2 \begin{pmatrix} 1 \\ s' e^{2i\phi'} \end{pmatrix} e^{ik'_x x} + b_2 \begin{pmatrix} 1 \\ s' e^{-2i\phi'} \end{pmatrix} e^{-ik'_x x} + c_2 \begin{pmatrix} 1 \\ -s' \cdot h' \end{pmatrix} e^{\kappa'_x x} + d_2 \begin{pmatrix} 1 \\ -s'/h' \end{pmatrix} e^{-\kappa'_x x} \right\} e^{ik_y y}, \tag{5}$$

$$\Psi_{III}(x,y) = \left\{ a_3 \begin{pmatrix} 1 \\ se^{2i\phi} \end{pmatrix} e^{ik_x x} + d_3 \begin{pmatrix} 1 \\ -s/h \end{pmatrix} e^{-\kappa_x x} \right\} e^{ik_y y}, \tag{6}$$

where $k_x = k_F \cos\phi$, $k_y = k_F \sin\phi$ are the wavevector components of the propagative waves, $\kappa_x = k_F\sqrt{1+\sin^2\phi}$ is the decay rate of the evanescent wave, $k_F = \sqrt{2m|E|}/\hbar$ is the Fermi wavevector as given in expression (1), $s = \mathrm{sgn}(-E)$, $h = (\sqrt{1+\sin^2\phi} - \sin\phi)^2$, outside the barrier. The values of the correspondent parameters inside the barrier are: $k'_x = k'_F \cos\phi'$, $k'_y = k'_F \sin\phi'$, $\kappa'_x = k'_F\sqrt{1+\sin^2\phi'}$, $k'_F = \sqrt{2m|E-V_0|}/\hbar$, $s' = \mathrm{sgn}(V_0 - E)$, $h' = (\sqrt{1+\sin^2\phi'} - \sin\phi')^2$, $\phi' = \arcsin(\sqrt{|E|/|E-V_0|}\, \sin\phi)$.

The nine amplitudes $(a_1, b_1, c_1, a_2, b_2, c_2, d_2, a_3, d_3)$ are complex numbers determined, up to a global phase factor, by the normalization condition and the boundary constraints, namely the continuity of both components of the spinor and their derivatives, at $x = 0$ and $x = L$. All of them can be numerically calculated. Remark that divergent exponential waves only take place in Region II and the evanescent (exponentially decaying) waves appear in the three regions.

The scattering region (Region II) provokes a partial reflection of the incident electron wave. The reflection coefficient R gives account of the proportion of the incoming electron flux that is reflected by the barrier. The expression for R is:

$$R = \frac{Flux_{reflected}}{Flux_{incident}} = \frac{|b_1|^2}{|a_1|^2}. \tag{7}$$

In this process, there are no sources or sinks of flux, then the transmission coefficient T is given by $T = 1 - R$. This coefficient T is plotted in Fig. 1a (dashed line) for a given height V_0 of the potential barrier. The anisotropy of the behavior of T is evident in that figure but contrarily to the single-layer graphene case, where massless Dirac fermions in normal incidence ($\phi = 0$) are perfectly transmitted through the barrier [25], here in the BLG case the massive chiral fermions are always totally reflected for angles close to $\phi = 0$. The total transparency, $T = 1$, can be found for other angles of incidence. This is just the paradoxical chiral (Klein-like) tunneling in graphene consisting in the penetration of its charge carriers through a high and wide barrier, $E \ll V_0$ and $2\pi/k_F \ll L$. The calculation of T (and all other magnitudes plotted in the figures) has been performed by taking for the electron and hole concentration the typical values used in experiments with graphene (see Ref. [25]).

Now, the calculation of the statistical complexity C and the Fisher–Shannon entropy P is presented. These magnitudes are the result of a global calculation done on the probability density $\rho(x,y)$ given by $\rho(x,y) = \Psi^+(x,y)\Psi(x,y)$, taking into account that the region of integration must be adequate to impose the normalization condition in the two-component spinor. As a consequence of having a pure plane wave in the Y axis, the density is a constant in this direction. Then, without loss of generality, if we take a length of unity in the Y direction, the density does not depend on y variable, $\rho(x,y) \equiv \rho(x)$. The expressions for densities obtained for the different regions are cumbersome and are not explicitly given. To normalize these densities, the length of the integration interval in the X direction has been taken to be $[-2\pi/k_x, -\pi/k_x]$, $[0, L]$ and $[L + \pi/k_x, L + 3\pi/k_x]$, for Regions I, II and III, respectively. Observe that in Regions I and III the integration intervals are taken separated from the barrier walls at $x = 0, L$ in order to capture in the calculations the effect of the coupling between the evanescent and the plane waves. Evidently, when the intervals in these regions are taken close to the walls $x = 0, L$, the contribution of the evanescent waves influences in an important manner the value taken by the statistical indicators. Farther from