Klein Paradox and Graphene

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This paper is intended to be a self-contained textbook-type review on Klein paradox and its realization in graphene. The Klein paradox are first explained in single-particle picture. Properties of electronic carriers in graphene, whose equation of motion is described by massless Dirac equation, are briefly introduced. Then the phenomenon of Klein tunneling based on the solution of 2+1D massless Dirac equation is studied.

Keywords: Klein paradox, Klein tunneling, graphene

I. INTRODUCTION

Klein paradox refers to the counterintuitive phenomenon that when a Dirac particle is incident to a step potential with its height larger than twice the particle's rest mass, the transmitted current is nonzero. What's more, the transmitted current will not vanish when the potential barrier approaches to infinity. Though this problem has been thoroughly studied in theory, it has never been directly observed in experiments. This is partly because the required step like potential, meaning a $\sim m$ jump within a distance of the order of the electron's Compton length $1/m$, or in other words an electric field larger than 10^{16}V/cm, is extremely hard to realize in experiments.

Recently, graphene, a carbon based material, is found to mimic a QED system. The low energy charge carriers in graphene obey massless 2+1D Dirac equation, with a 2-fold degeneracy resembles the spin degrees of freedom of spin-$\frac{1}{2}$ particles. The realization of Klein tunneling is then much easier to achieve in this system, since the pseudoparticles are massless and there is no theoretical requirement of the minimal electric field.

This paper is organized as follows: In Sec. II the original problem by Klein is given and is discussed in single-particle approach. In Sec. III the equation of motion of charge carriers in graphene is given, which is just the 2+1D massless Dirac equation. Klein tunneling in this case is studied. Conclusive remarks will be given in the final section.

II. KLEIN PARADOX AND ITS SINGLE-PARTICLE EXPLANATION

A. The problem

Consider a step potential in 1D:

$$V(z) = \begin{cases} 0 & z < 0 \\ V_0 & z \geq 0 \end{cases}. \tag{1}$$

Then assuming a Dirac particle, which is represented by a plane wave solution of Dirac equation, comes from $z = -\infty$, one is asked the penetration and reflection coefficient of the charge current.

B. Solution and paradox: single particle

First, in the case of 1D, Dirac equation

$$(i\gamma^\mu \partial_\mu + m)\psi = 0 \tag{2}$$

can be rewritten as

$$(i\gamma^0 \partial_t + i\gamma^3 \partial_z + m)\psi = 0 \tag{3}$$

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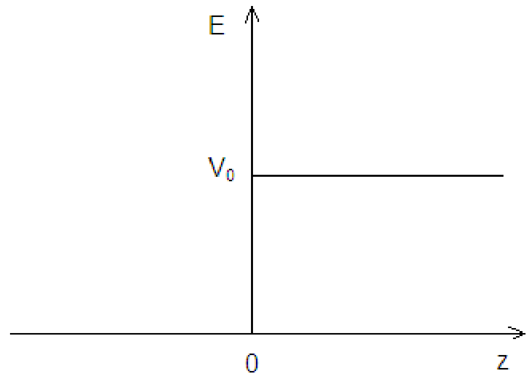

FIG. 1: The step potential V.

since the degrees of freedom in x and y directions are completely decoupled.

Assuming plane wave solution $\psi = ue^{-ipx}$ ($p^\mu = (E\ 0\ 0\ p_z)$), we can get rid of the time dependence of Dirac equation and arrive at:

$$(E - V)\gamma^0 u = \gamma^3 p_z u + mu, \tag{4}$$

which implies (we set $pz \equiv p$ from now on)

$$(E - V)^2 = p^2 + m^2. \tag{5}$$

Choose the representation of γ^μ to be:

$$\gamma^\mu = (\begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}) \tag{6}$$

and assume

$$u = \begin{pmatrix} \alpha \\ 0 \\ \beta \\ 0 \end{pmatrix}, \tag{7}$$

we get

$$\frac{\alpha}{\beta} = \frac{E - V - p}{m}. \tag{8}$$

Thus we have

$$u = N \begin{pmatrix} 1 \\ 0 \\ \frac{m}{E-V-p} \\ 0 \end{pmatrix}. \tag{9}$$

Considering $E - V$ may be positive or negative, we use different normalization relations to determine N for positive and negative energy solution, respectively. We finally get the complete positive and negative energy solutions:

$$\psi^{(+)}(z,t) = \sqrt{\frac{(E-V)-p}{2m}} \begin{pmatrix} 1 \\ 0 \\ \frac{m}{E-V-p} \\ 0 \end{pmatrix} e^{-ipx} \equiv u(E-V,p)e^{-ipx},\ \ E - V > 0 \tag{10}$$

$$\psi^{(-)}(z,t) = \sqrt{\frac{p-(E-V)}{2m}} \begin{pmatrix} 1 \\ 0 \\ \frac{m}{E-V-p} \\ 0 \end{pmatrix} e^{-ipx} \equiv v(E-V,p)e^{-ipx},\ \ E - V < 0 \tag{11}$$

Now return to the problem in Sec. II A, the solution of Dirac equation in region I ($z < 0$) should include incident and reflected wave, i. e.

$$\psi_I = a\psi_i + b\psi_r = au(E,p)e^{ipz} + bu(E,-p)e^{-ipz} \tag{12}$$

in which $p = \sqrt{E^2 - m^2}$, and we have ignored the time dependence.

In region II, we have the energy momentum relation

$$p^2 = (E - V)^2 - m^2. \tag{13}$$

Our interest is in the case of $E - V < 0$, and it is easy to see that when $V < E + m$, $p^2 < 0$ and we have only a decaying wave. In this case the transmitted current is equal to zero and the reflection coefficient R is equal to 1, same as that in the 1D scattering problem of a Schrödinger particle. However, when $V > E + m$, which is the case considered by Klein, p^2 becomes positive again. So we will have a plane wave in region II, which must be a negative energy solution of Dirac equation since $E - V < 0$. Then in region II the solution is (we change p to q in region II to avoid confusion)

$$\psi_{II} = cv(E - V_0, q)e^{iqz}. \tag{14}$$

Then at $z = 0$, the condition of continuity is written as

$$\psi_I|_{z=-0} = \psi_{II}|_{z=+0}, \tag{15}$$

or

$$a\begin{pmatrix} 1 \\ 0 \\ \frac{m}{E-p} \\ 0 \end{pmatrix} + b\begin{pmatrix} 1 \\ 0 \\ \frac{m}{E+p} \\ 0 \end{pmatrix} = c\begin{pmatrix} 1 \\ 0 \\ \frac{m}{E-V_0-q} \\ 0 \end{pmatrix}. \tag{16}$$

Thus we have two equations of a, b and c

$$a + b = c \tag{17}$$

$$a\frac{m}{E-p} + b\frac{m}{E+p} = c\frac{m}{E - V_0 - q}, \tag{18}$$

and the solutions are

$$\frac{b}{a} = \frac{(E+p)(p - V_0 - q)}{(E-p)(p + V_0 + q)}, \tag{19}$$

$$\frac{c}{a} = \frac{2p(E - V_0 - q)}{(E-p)(p + V_0 + q)}. \tag{20}$$

It is well known that the current density of Dirac particles is

$$j^i = \psi^\dagger \gamma^0 \gamma^i \psi. \tag{21}$$

Then the incident, reflected and transmitted currents can be easily written down:

$$j_i = \psi_i^\dagger \gamma^0 \gamma^3 \psi_i = a^* a \frac{m^2 - (E-p)^2}{(E-p)^2} \tag{22}$$

$$j_r = \psi_r^\dagger \gamma^0 \gamma^3 \psi_r = b^* b \frac{m^2 - (E+p)^2}{(E+p)^2} \tag{23}$$

$$j_t = \psi_{II}^\dagger \gamma^0 \gamma^3 \psi_{II} = c^* c \frac{m^2 - (E - V_0 - q)^2}{(E - V_0 - q)^2} \tag{24}$$

Finally we find the coefficients of reflection and transmission:

$$R = \frac{|j_t|}{|j_i|} = \frac{E+p}{E-p} \cdot \frac{(p - V_0 - q)^2}{(p + V_0 + q)^2}, \tag{25}$$

$$T = \frac{|j_r|}{|j_i|} = \frac{2p}{E-p} \cdot \frac{(E - V_0 - q)^2 - m^2}{(p + V_0 + q)^2} \tag{26}$$

And it can be checked that $1 - R = -T$, or in other words $j_i + j_r = j_t$, since the signs of j_r and j_t are opposite to that of j_i.

This is the original version of Klein paradox [1–3], namely, the reflection coefficient is larger than 1. However, Klein noted that Pauli had pointed out to him the group velocity of the wave in region II, which can be calculated from Eq. 5 as

$$v_g = \frac{dE}{dq} = \frac{q}{E - V_0} \tag{27}$$

is negative if q is positive. This means one must assume there is a source of particles at $z = +\infty$, which is in contradiction with the boundary condition given in the original problem, i.e., there is only one particle source at $z = -\infty$. On the other hand, we note that left going ($v_g < 0$,$q > 0$) and right going ($v_g > 0$, $q < 0$) waves are all solutions of the Dirac equation in region II. To choose which one of them to be ψ_{II} in Eq. 15 must be determined by boundary conditions. Then it's clear that we need to change q to $-q$ in above calculations (in this way $q = \sqrt{(E-V)^2 - m^2}$ is a positive quantity, just like the use of $-p$ in the expression of the reflected wave). The correct results of R and T now are

$$R = \frac{E+p}{E-p} \cdot \frac{(p - V_0 + q)^2}{(p + V_0 - q)^2}, \tag{28}$$

$$T = \frac{2p}{E-p} \cdot \frac{m^2 - (E - V_0 + q)^2}{(p + V_0 - q)^2}. \tag{29}$$

Then we have $R + T = 1$ and both R and T are smaller than 1. We also note that the transmitted current:

$$j_t = c^* c \frac{m^2 - (E - V_0 + q)^2}{(E - V_0 + q)^2} \tag{30}$$

is now positive.

So far, so good. However, if we go to the limit that $V_0 \to \infty$, then

$$R = \frac{E-p}{E+p}, \tag{31}$$

$$T = \frac{2p}{E+p}, \tag{32}$$

which means even in an infinitely high barrier there is still a nonzero transmitted current. This is what people call Klein paradox today. Though this is just the consequence of the existence of negative energy solution of Dirac equation, for which an infinite barrier becomes an infinite well. Hence it is not a real paradox. The proper use of negative energy solution in the barrier region is also key to the introduction of Klein tunneling in graphene.

III. KLEIN TUNNELING IN GRAPHENE

Graphene is a single layer graphite. In graphene carbon atoms are sp^2 bonded to their nearest neighbors, and thus form a honeycomb lattice made of hexagons(Fig. 2). The honeycomb lattice is actually made of two interpenetrating triangular lattices, and the Brillouin zone is also a hexagon(Fig. 3), and the points at the corners of the hexagon are called Dirac points. The reason for this name will be seen later.

Considering only nearest neighbor and next nearest neighbor hopping in the lattice sites for electrons in graphene, a tight-binding Hamiltonian can be written as:

$$H = -t \sum_{\langle i,j \rangle, \sigma} (a^\dagger_{\sigma,i} b_{\sigma,j} + \text{h.c.}) - t' \sum_{\langle\langle i,j \rangle\rangle, \sigma} (a^\dagger_{\sigma,i} a_{\sigma,j} + b^\dagger_{\sigma,i} b_{\sigma,j} + \text{h.c.}), \tag{33}$$

where $a_{\sigma,i}(b_{\sigma,i})$ annihilates an electron with spin $\sigma(\sigma = \uparrow, \downarrow)$ on site $\mathbf{R}_i$ on sublattice A (B). The energy spectrum derived from this Hamiltonian is visualized in Fig. 4 And it can be seen that the dispersion of energy bands around the Dirac points, where the Fermi level lies, is linear, rather than parabolic in normal materials.

To get a better idea of the dynamics of the charge carriers in graphene, let's derive the equation of motion from the Hamiltonian (33). We set $t' = 0$ as an approximation. Since we are only interested in the portion of carriers near the Fermi level, we can expand the field operators around the Dirac points. And we only need to consider two Dirac

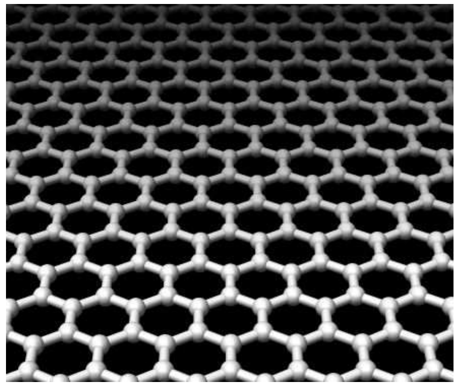

FIG. 2: The structure of graphene.

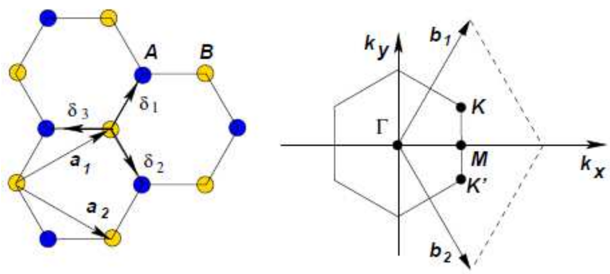

FIG. 3: Left: The honeycomb lattice is composed of two triangular lattices. Right: Brillouin zone.[4]

points, i. e., K and K' in Fig. 3 since all the other ones only differ from K and K' by a reciprocal lattice vector. Thus we have

$$\begin{aligned} a_i &\simeq e^{-i\mathbf{K}\cdot\mathbf{R}_i} a_{1,i} + e^{-i\mathbf{K}'\cdot\mathbf{R}_i} a_{2,i}, \\ b_i &\simeq e^{-i\mathbf{K}\cdot\mathbf{R}_i} b_{1,i} + e^{-i\mathbf{K}'\cdot\mathbf{R}_i} b_{2,i}. \end{aligned} \tag{34}$$

And we assume the new fields, $a_{n,i}$ and $b_{n,i}$, $n = 1, 2$, vary slowly over the unit cell, since their Fourier components are all close to $k = 0$.

Then we substitute the expansion of a and b into the Hamiltonian (33) without the next nearest term. Considering the vectors connecting nearest neighbors:

$$\delta_1 = \frac{a}{2}(1, \sqrt{3}), \qquad \delta_2 = \frac{a}{2}(1, -\sqrt{3}), \qquad \delta_3 = -a(1, 0), \tag{35}$$

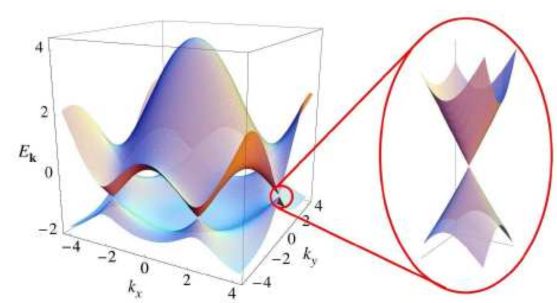

FIG. 4: Left: Energy spectrum of graphene. Right: zoom-in of the energy bands close to one of the Dirac points.[4]

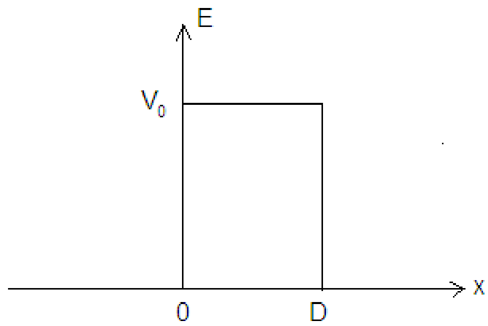

FIG. 5: An energy barrier with width D in x direction, infinite in y direction, and height V_0.

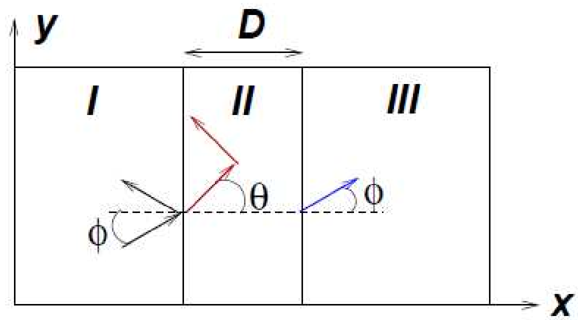

FIG. 6: Three regions in this problem.

and going to the continuum limit, we can finally write down

$$H = -iv_F \int dxdy(\hat{\Psi}_1^\dagger(\mathbf{r})\sigma \cdot \nabla\hat{\Psi}_1(\mathbf{r}) + \hat{\Psi}_2^\dagger(\mathbf{r})\sigma^* \cdot \nabla\hat{\Psi}_2(\mathbf{r})), \tag{36}$$

with $\sigma = (\sigma_x, \sigma_y)$, $\sigma^* = (\sigma_x, -\sigma_y)$, and $\hat{\Psi}_i = (a_i^\dagger, b_i)$. It is then straightforward to derive the equation of motion:

$$-iv_F\sigma \cdot \nabla\psi(\mathbf{r}) = E\psi(\mathbf{r}), \tag{37}$$

which is just the massless Dirac equation or Weyl equation.

The solution of Eq. 37, neglecting normalization factor, can be easily found to be

$$\psi^{(\pm)}(\mathbf{r}) = \begin{pmatrix} 1 \\ \pm e^{i\phi} \end{pmatrix} e^{i(k_x x + k_y y)}, \tag{38}$$

with $\pm$ denoting positive and negative energy solutions, and $\phi = \arctan(\frac{k_x}{k_y})$.

We now consider an energy barrier in 2D, as depicted in Fig. 5 Assuming a plane wave described by Eq. 38 is incident from left ($x < 0$), we are going to find out the tunneling coefficient through the barrier when $E < V_0$.

We first write down the wave functions in three different regions (Fig. 6):

$$\psi_I(\mathbf{r}) = \begin{pmatrix} 1 \\ e^{i\phi} \end{pmatrix} e^{i(k_x x + k_y y)} + r \begin{pmatrix} 1 \\ e^{i(\pi-\phi)} \end{pmatrix} e^{i(-k_x x + k_y y)}, \tag{39}$$

$$\psi_{II}(\mathbf{r}) = a \begin{pmatrix} 1 \\ -e^{i\theta} \end{pmatrix} e^{i(q_x x + q_y y)} + r \begin{pmatrix} 1 \\ -e^{i(\pi-\theta)} \end{pmatrix} e^{i(-q_x x + q_y y)}, \tag{40}$$

$$\psi_{III}(\mathbf{r}) = t \begin{pmatrix} 1 \\ e^{i\phi} \end{pmatrix} e^{i(k_x x + k_y y)}, \tag{41}$$

in which $\theta = \arctan(k_y/q_x)$ and $q_x = \sqrt{(V_0 - E)^2/v_F^2 - k_y^2}$.

Similar as before we enforce conditions of continuity to ψ_I, $\psi_{II}$and ψ_{III}:

$$\psi_I(0,y) = \psi_{II}(0,y), \qquad \psi_{II}(D,y) = \psi III(D,y). \tag{42}$$

Then after some algebra we can get the transmission coefficient

$$T = t^* t = \frac{\cos^2\theta\cos^2\phi}{\cos^2(Dq_x)\cos^2\phi\cos^2\theta + \sin^2(Dq_x)(1+\sin\phi\sin\theta)^2}. \tag{43}$$

And if we go to the $V_0 \to \infty$ limit,

$$T = \frac{\cos^2\phi}{1-\cos^2(Dq_x)\sin^2\phi}. \tag{44}$$

From Eq. 43 or Eq. 44 we can see that when $Dq_x = n\pi$, n is an integer, $T = 1$. This is the normal resonant tunneling. However, when $\phi = 0$ (thus $\theta = 0$), T is always equal to 1, whatever the value of Dq_x is. This behavior is solely due to the negative energy solution in region II, and we can call it Klein tunneling since it has the same origin as Klein paradox. This phenomenon has already been studied 20 years ago by T. Ando, et al.[6], and is related to the absence of backscattering in carbon nanotube.

IV. DISCUSSION

As mentioned in Sec. II B, the choice of the sign of q in region II cannot be determined from the Dirac equation. But the original incorrect solution by Klein was later picked up by some researchers and is related to the phenomenon of particle-antiparticle pair production in strong fields[2, 7]. This explanation is first questioned by Dombey and Calogeracos [2], who find that being a time-dependent process, the pair production cannot serve as a suitable explanation of Klein paradox. Then Dragoman [7] argued that if the sign of q is correctly chosen, there is no particle-antiparticle pair current at all.

On the other hand, as proposed in [5], a graphene p-n junction is realized in experiment [8] and the result does not indicate a larger than unity reflection coefficient [7].

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