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On Klein tunneling in graphene

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The essential features of Klein tunneling of massless fermions in graphene may be treated in one dimension without the need for Dirac spinors. Two dimensions needs a spinor treatment and is investigated numerically, which lets us compare tunneling through smooth potential barriers with that through idealized step potentials.
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I. INTRODUCTION

There has been a massive explosion of interest in graphene since its discovery just a few years ago.[1] There are several reasons for the interest in graphene. Foremost is its remarkable quantum properties, which will be exploited in new scientific and technical applications. In addition, the electrodynamic properties of graphene exhibit some remarkable characteristics that allow it to serve as an analogue for a number of exotic processes, which, although known theoretically, has not been observed previously. Graphene may prove to be a key test bed for a number of fundamental physical processes, just as superconductors lead Nambu[2] to a deeper understanding of spontaneous symmetry breaking in fundamental particle physics in the 1950s.

One of the phenomena on which graphene appears to shed some light is Klein tunneling,[3] which is a form of potential scattering that was originally associated with the Dirac equation. It has not been observed in that context due to the unrealizably high potentials required. Graphene allows Klein tunneling to be studied experimentally for the first time, and also provides important insights into the nature of the Dirac equation and more generally, into quantum field theory.[4] For this reason a knowledge of graphene is important to physicists other than specialists in materials science and technology. Graphene is also a potentially attractive example for students of quantum mechanics. However, the current literature on the quantum mechanics of graphene is beyond the scope of the usual undergraduate courses and outside the experience of most non-specialist physicists. One reason for the difficulty is that graphene is usually treated by the use of Dirac's relativistic theory adapted to massless fermions, including multiple component spinors.[3] It is not immediately obvious how the Dirac spinor formalism arises in the Hamiltonian for graphene, because the speed of electrons in graphene is well below the speed of light in a vacuum. Also, electrons are normally considered as massive particles, at least when they are free, and the spin of the electron, whose presence usually becomes known in the company of magnetic fields, does not have any obvious physical role in the dynamics of the electrons in graphene.

A key goal of this paper is to make Klein tunneling in graphene more accessible to non-specialists and, in particular, to encourage its inclusion in undergraduate courses, which usually are over reliant on the Schrödinger equation. One aspect of the approach adopted here is to show that the use of spinors is not essential in certain cases if we focus on the dispersion relation of electrons in graphene.[5] The reason for the formal appearance of Dirac spinors in the dynamical properties of electrons in grapheme is explained in terms of the requirements for representing the original form of the graphene dispersion relation, which depends on the modulus of the wavevector. The appearance of spinors is demystified somewhat by discussing the role they play in an alternative representation of the modulus from the usual Pythagorean one. Also the role of wave mode coupling in inhomogeneous media is emphasized in dealing with reflection processes.

An important aspect of potential scattering is the role of boundary conditions in determining the reflection and transmission coefficients. Most physicists have encountered these issues in the context of potential scattering problems with the Schrödinger equation, where idealized discontinuous steps and square barriers are commonly treated by considering the continuity conditions for the wavefunctions. Such idealized potentials and their associated boundary conditions will be examined for massless fermions. It is useful and instructive to investigate the effects of more realistic smooth potentials. To this end a numerical method is employed to compare the effects of smooth and sharp edged potential barriers.

The paper is organized as follows. The nature of Klein tunneling is outlined in Sec. II. The dispersion properties of electrons in graphene are introduced in Sec. III, and in Sec. IV the calculations of the reflection and transmission coefficients of electrons in graphene, in one and two dimensions, are presented. The results are briefly discussed in Sec. V.

II. A BRIEF DESCRIPTION OF KLEIN TUNNELING

Klein's original analysis was on the transmission of relativistic electrons across a potential step. Dirac's full relativistic spinor theory of the electron is required to properly calculate the reflection and transmission coefficients in massive particles. This calculation is beyond the scope of the present paper, but the essential features of Klein tunneling can most easily be understood with reference to the energy-wavenumber dispersion relation. The energy eigenvalues of the Dirac equation for a single relativistic electron of mass m take the form

$$E = \pm\sqrt{\hbar^2 k^2 c^2 + m^2 c^4}, \tag{1}$$

where E is the energy, k is the wavenumber, c is the speed of light in vacuum, and $\hbar$ is Planck's constant divided by 2π. One of the main issues arising from Eq. (1) that interested Dirac was that there is one positive and one negative root, which famously lead to Dirac's idea of anti-particles. In the E-k diagram in Fig. 1 the A branch represents the positive energy states and the B branch represents the negative ones. The straight lines labeled L and R are asymptotes, the relevance of which we will discuss later. For real k, we must have $E > mc^2$ for the positive energy states or $E < -mc^2$ for

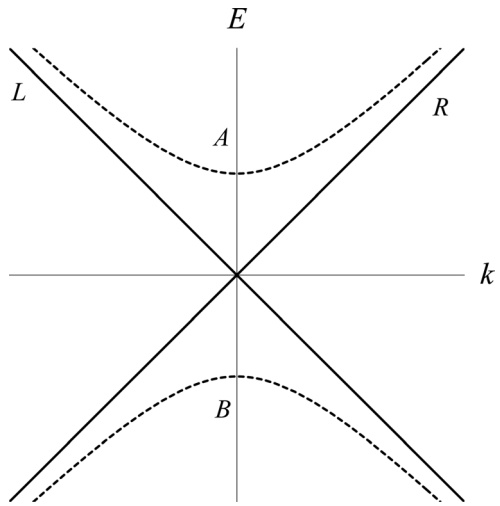

Fig. 1. Dispersion curves A and B for massive relativistic particles (dashes) and asymptotes L and R (solid lines) representing massless particles.

negative ones. It is important to keep in mind that the states in the A and B branches may both be occupied by electrons. The connection to anti-electrons, that is, positrons, is not relevant here.

Imagine an electron in a positive energy state from the A branch, traveling along the x-axis in the direction of increasing x, with positive momentum in the absence of a potential. At some point it encounters a potential step, $V=V_0$. If $E-V_0>mc^2$, the electron will continue to propagate to the right with the new positive wavenumber, k, such that $E-V_0=\sqrt{\hbar^2k^2c^2+m^2c^4}$. If $E-V_0<mc^2$, the dispersion relation can be satisfied only if $k^2<0$. Hence, the momentum $\hbar k$ inside the potential becomes imaginary, the wave function decays exponentially, and there is have total reflection. If the potential is increased further, so that $E-V_0<-mc^2$, then we can have $E-V_0=-\sqrt{\hbar^2k^2c^2+m^2c^4}$ and once again $k^2>0$, so that propagation inside the potential is possible. However, propagation is possible only for states from the B branch. Pauli pointed out that if the particles are to continue propagating to the right, they need a positive group speed. For the A branch, the group velocity (the gradient of the E-k curve) is positive for positive k, but for the B branch a positive group speed requires negative k. Hence, the electron continues to propagate to the right with a positive group speed, but with a negative momentum in a B state. In principle, transmission through the potential becomes perfect as its value approaches infinity. This puzzling result was originally called the Klein paradox.[4]

In the limit as the mass goes to zero, the two dashed curves in Fig. 1 become equal to the two solid curves. We remark that there is now no gap between the A and B branches because they coalesce at the apices. In the massless limit the dispersion relation becomes, $E=\pm\hbar c|k|$, which, in one dimension, is a pair of "Vs" in E-k space, one upright in the upper half plane and one inverted in the lower half plane. We see that the upper curve in Fig. 1 becomes $E=+\hbar c|k|$ and the lower curve becomes $E=-\hbar c|k|$. This result can be seen as the natural limit of the massive case because it maintains the distinction between the positive and negative energy states.

For graphene the characteristic speed c is replace by the Fermi velocity V_F (see Sec. III). In this sense graphene can be seen as an analogue to the relativistic massless case of the Dirac equation. Klein tunneling still occurs in this massless situation, but there is no imaginary k phase, because there is no energy gap between the positive and negative energy states.

Although the previous analysis points to an important physical connection between Klein tunneling in graphene and relativistic electrodynamics, it gives rise to mathematical difficulties, in the same way as they arise in the Dirac's relativistic equation. This difficulty leads to the need for spinors. The reason is that it is necessary to find the square root of the Laplacian differential operator. In the one-dimensional massless case considerable simplification is possible, because in one dimension, the Laplacian is a perfect square, and we can take its square root, as we will explain in Sec. III.

III. ELECTRON WAVE MODES IN GRAPHENE

The dispersion relation for electrons in graphene is derived from the tight-binding approximation for the band theory of graphite, which was developed long before graphene existed. According to Wallace,[5] the dispersion relation for electrons with energy E and wave vector $\mathbf{k}$, near the corners of the Brillouin zone, in a single hexagonal layer, can be written as

$$|E-E_C|=\hbar V_F|\mathbf{k}-\mathbf{k}_C|, \tag{2}$$

where the subscript C refers to the location of the corner in $\mathbf{k}$-space and V_F is a characteristic velocity. For graphene, V_F is the Fermi velocity. If we redefine the energy and momentum relative to E_C and $\mathbf{k}_C$, respectively, we have

$$E=\pm\hbar V_F|\mathbf{k}|. \tag{3}$$

It is important to realize that Eq. (3) represents a dispersion relation that depends on the wavevector through its magnitude only. Thus, it represents a set of modes forming the surfaces of a pair of cones in energy-momentum space. The upper cone represents positive energy modes (with respect to E_C) and the lower cone represents negative energy modes. Because the cones touch at their apices, the electrons are gapless.

Equation (3) is not as simple as it might first appear. It is sometimes referred to as a linear relation between E and $\mathbf{k}$, but, the magnitude of a vector is not strictly a linear function, because the Cartesian vector (k_x,k_y,k_z) has magnitude $\sqrt{k_x^2+k_y^2+k_z^2}$, which is not linear in the components. The difficulty associated with the nonlinearity of the magnitude can be seen when we try to replace $\mathbf{k}$, or rather the momentum, by the usual operator involving spatial derivatives of a wave function ψ. Then Eq. (3) becomes

$$E\psi=\pm\hbar V_F\sqrt{-\partial^2/\partial x^2-\partial^2/\partial y^2-\partial^2/\partial z^2}\psi. \tag{4}$$

We now have the problem of taking the square root of the Laplacian operator, a problem similar to the one that faced Dirac in finding a wave equation for a single relativistic electron with a first-order time derivative. Dirac's reasons for wanting to do so are not relevant here, but his brilliant solution is. Because of these difficulties, it is worth looking at the problem in more detail.

The problem is to find a form for the magnitude of a vector. We are all familiar with the Pythagorean definition of the magnitude squared as $k^2=k_x^2+k_y^2+k_z^2$. It is advantageous,

particularly when it is desired to substitute differential operators for the components of **k**, to write the magnitude of **k** as a linear function of its components. We can do so by first writing[6]

$$|\mathbf{k}| = k = \sigma_x k_x + \sigma_y k_y + \sigma_z k_z. \tag{5}$$

If we square both sides of Eq. (5) and equate the coefficients of the terms of the resulting expression with those in the equivalent Pythagorean expression, we obtain the requirement that $\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1$ and $\sigma_x\sigma_y + \sigma_y\sigma_x = 0$, together with cyclic permutations in the indices of the latter relation. These conditions are satisfied by the well-known Pauli spin matrices. The Pauli matrices are inextricably linked to electron spin, and because Dirac found them by factoring the relativistic single particle equation, spin is often considered a relativistic effect, despite the fact that there is nothing particularly relativistic about spin.[6,7] The Pauli matrices are really about rotational symmetry rather than specific dynamical effects of the electron. The properties of the components of σ imply that the right-hand side of Eq. (5) is isotropic, despite being linear in the components of the vector. Hestenes has argued that this complication is necessary only because of the shortcomings of vector algebra as it is currently used. Hestenes' view is not surprising when we recall that what we call vector algebra, unlike matrix algebra, contains neither universal unit element nor multiplicative inverse. The lack of these features by vector algebra means it is much more limited than matrix algebra in what it can represent. These considerations are beyond the scope of this paper and the reader is advised to consult Ref. 8 and the references therein for further discussions of this issue.

If we replace the right-hand side of Eq. (3) by the spinor form as indicated in Eq. (5), we find the form of the graphene Hamiltonian, $H = -i\hbar V_F \sigma.\nabla$, commonly used in the research literature. The resulting equation is used in Sec. IV as the basis of a wave equation for analyzing Klein tunneling in graphene. A useful simplification of these equations is possible in one dimension, which allows us to explore the essential features of Klein tunneling without the need for Dirac spinors. The basis for this simplification is as follows.

There is an important but subtle point in one dimension, which is that neither $E = +\hbar V_F|k|$ nor $E = -\hbar V_F|k|$ separately constitute linear relations, because both have discontinuities in their gradients at the origin. However, the pair $E = \pm\hbar V_F|k|$ taken together is identical to the pair of relations $E = \pm\hbar V_F k$, which is a pair of straight lines of positive or negative slope that have been labeled *L* (left propagating) and *R* (right propagating) in Fig. 1. That is, we can split an "X" symbolically into two "Vs" (*V* and V^{-1}) or into two straight lines (/ and \). Thus, in quantum mechanical terms we can replace a positive-negative energy pair of states by an equivalent left-right propagation pair of states. This exchange of state labels is not possible in the massive case, even in one dimension.

The nature of left and right propagation needs some clarification, because the sign of *k* changes, which corresponds to a reversal of momentum as the straight lines cross the *k*-axis. Because the direction of propagation is connected to the sign of the group velocity rather than that of *k*, the line labeled *R* always has a positive gradient, regardless of the sign of *E* or *k*. Thus, the dispersion relation represented by the line *R* always gives rise to a positive group velocity, which indicates right propagation. Similarly, the negative gradient

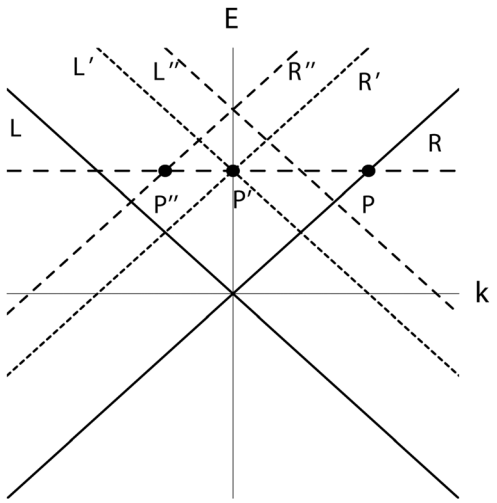

Fig. 2. Effect of potentials on the massless particle dispersion curves. Solid lines, *L* and *R* represent the case with zero potential, with the effects of increasing potential indicated by the lengthening of the dashes. *P*, *P*′, and *P*″ indicate the position in *E*-*k* space of a particle in a region of increasing potential.

of line *L* always gives rise to a negative group speed and represents left propagating particles. This situation is unaffected by the potential as can be seen in Fig. 2. As the particle enters the region of increasing potential, *E* is replaced by $E - V$ in the *E*-*k* relation, so the lines *L* and *R* shift to new positions *L*′ and *R*′, but their respective slopes and hence group speeds are unaffected. This insensitivity of the group speed to the potential has important consequences for potential scattering of electrons in grapheme, which we consider in Sec. IV.

The one-dimensional case may be treated with the aid of a pair of first-order wave equations, which are obtained by setting the partial derivatives with respect to *y* and *z* in Eq. (4) to zero and by writing the square root of the second order derivative with respect to *x* as a pair of first-order derivatives, in analogy with the two linear functions, $\pm k$. Then, Eq. (4) becomes

$$E\psi = \pm i\hbar V_F \sqrt{\partial^2/\partial x^2}\psi = \pm i\hbar V_F \partial\psi/\partial x. \tag{6}$$

The result is a pair of well-behaved, first-order differential equations with scalar wavefunctions. There is no need for spinors in this case.

This simple option was not available to Dirac, because there is an extra term for electrons proportional to the square of the electron mass inside the square root in Eq. (6) which does not constitute a perfect square, even in one dimension. We will show more formally that Eq. (6) is the limit of the more general two-dimensional case which does require multi-component wave functions.

Given the problems involved in dealing with the difficulties of the modulus function, it is worth considering why we did not square both sides of Eq. (3) before operating on the wavefunction. The result would be a single second-order differential equation which eliminates the need for taking the square root of the differential operators. In the massless case, we obtain the wave equation, which is ubiquitous in classical physics as well as accounting for photons, among other things, in quantum theory. For massive particles the result is the Klein-Gordon equation, which was Dirac's starting point.

In the absence of a potential the single second-order equation is equivalent to the pair of first-order equations in Eq. (6). This equivalence is most easily understood by writing

$$(E^2 + \hbar^2 V_F{}^2 \partial^2/\partial x^2)\psi = (E - i\hbar V_F \partial/\partial x)(E + i\hbar V_F \partial/\partial x)\psi = 0. \quad (7)$$

Note that the two bracketed operators after the first equals sign in Eq. (7) commute, and thus can be written in reverse order without changing the result. With the order as written in Eq. (7), the solution is obtained by setting the wave function operated on by the last bracketed factor equal to zero. This procedure is equivalent to choosing the minus sign in Eq. (6). With the order reversed, we obtain the positive form in Eq. (6). We can see that the two solutions in Eq. (6) are identical to those of Eq. (7) and its reversed form. In the massive case without a potential, Dirac's relativistic equation for a single electron is equivalent to the Klein-Gordon equation in that the equations have the same eigenvalues. It is only when potentials are included that there are differences in the solutions; for example, the appearance of electron spin when a magnetic field is added. Without the potentials, spin effects remain hidden.

There is a simple interpretation of the solutions of the two equations in Eq. (6). We designate the solution with the plus sign on the right-hand side of Eq. (6) as ψ_R, and the one with the minus sign as ψ_L, where the subscripts indicate propagation to the right and to the left, respectively. Equation (7) shows that left and right propagating waves are uncoupled. The equivalence of Eqs. (6) and (7) disappears in the presence of inhomogeneous potentials. To see this difference, we note that if there exists a one-dimensional potential, $V(x)$, which is inhomogeneous in the direction of motion of the electrons, that is, along the x-axis, then Eq. (6) can be generalized to

$$(E - V(x))\psi = \pm i\hbar V_F \partial\psi/\partial x. \quad (8)$$

In this case, equipotentials are planes with normals parallel to the electron motion. If we choose a one-dimensional potential with equipotential planes that are not normal to the electron motion, the problem is two-dimensional. For the one-dimensional case with an inhomogeneous potential, Eq. (7) becomes

$$((E - V(x))^2 + \hbar^2 V_F^2 \partial^2/\partial x^2)\psi = 0, \quad (9)$$

and Eq. (9) can no longer be factored into the two parts of Eq. (8). Equation (9) can be written as

$$(E - V(x) - i\hbar V_F \partial/\partial x)(E - V(x) + i\hbar V_F \partial/\partial x)\psi = i\hbar V_F \partial V(x)/\partial x)\psi. \quad (10)$$

Equation (9) shows that left and right propagating waves are coupled if the right-hand side is non-zero, that is, where there is a potential gradient. In the presence of inhomogeneous potentials Eqs. (8) and (9) are not equivalent. They are in a sense opposite sides of the same coin because they both represent massless particles, with Eq. (8) representing fermions and Eq. (9) representing bosons. The latter case is beyond the scope of this paper.

IV. KLEIN TUNNELING IN GRAPHENE

A. One dimension

We first examine the solutions of Eq. (8). As long as Eq. (8) holds rather than Eqs. (9) and (10), we still have two independent waves, ψ_R, and ψ_L. ψ_R satisfies

$$(E - V(x) - i\hbar V_F \partial/\partial x)\psi_R = 0. \quad (11)$$

Equation (11) can be integrated to give $\psi_R = \psi_R(0)e^{i\alpha}$, where

$$\alpha(x) = \int_0^x (E - V(x))dx/\hbar V_F. \quad (12)$$

The result for the left propagating wave is $\psi_L = \psi_L(0)e^{-i\alpha}$. This result looks trivial. It implies that if we start out with a right propagating wave, there is a right propagating wave of the same amplitude, irrespective of the shape and size of the potential. If there were a potential step, the boundary condition would also be trivial and we would only need one, that is, ψ is continuous. There is no need for a second because no other wave is excited, unlike the second-order case. There is no reflection, although there is refraction, in the sense that the wavenumber k ($=\partial\alpha/\partial x$) varies. This complete lack of a reflected wave constitutes perfect Klein tunneling. However, although it implies the continuity of the wave function, it also implies that the gradient of the wave function continually changes. If there were a step in the potential, there would be a corresponding step in the gradient of the wavefunction, which is in contrast to what is found with the Schrödinger equation.

This result is not as trivial as it first appears, because it is possible that a particle of given energy E can, in principle, enter a region where the potential energy V exceeds it. As we saw in Sec. III, the wave number changes sign and the momentum of the particle reverses, while the group velocity, $d\omega/dk$, which always equals V_F in this case, is independent of the potential. Thus, the energy flux is undisturbed by the potential. Note also that the particle remains on the right propagating branch even though it is now in the lower branch, B (see Figs. 1 and 2). Thus, a right propagating particle does not excite a left propagating mode when it enters the potential, which re-emphasizes the point that there is no mode coupling. The point in E-k space just slides along the same linear branch of the dispersion curve as the value of the potential changes (see Fig. 2). Here the sequence of pairs of lines (R, L), (R', L'), and (R'', L'') represents the state of the system on the E-k diagram as the particle enters increasing values of the potential. The particle starts in a zero potential at point P and moves to points P' and P'' in E-k space. If it starts in the upper V as an electron, it moves through the apex when the energy and potential are equal, and then continues onto the lower inverted V state as an electron. All that happens as far as the wavefunction is concerned is that as the particle approaches the potential, its phase winds forward until $E = V$, at which point phase progression stops. If V continues to increase, the phase begins to unwind. There is no dramatic physical change implied.

B. Two dimensions

In two dimensions there is no simple way of avoiding Dirac's brilliant maneuver of taking the square root of the

Laplacian operator. Substituting the spinor form for the magnitude of the wave vector in Eq. (5) into the dispersion relation leads to the two-dimensional wave equation

$$E\psi = \hbar V_F \sqrt{-\partial^2/\partial x^2 - \partial^2/\partial y^2}\psi = -i\hbar V_F(\sigma_x \partial/\partial x + \sigma_y \partial/\partial y)\psi. \quad (13)$$

As is well known, the appearance of the Pauli matrices in Eq. (13) implies that the wave function needs two components to describe it. If we represent it by a column vector with components X and Y, then, with the addition of a potential that depends only on x, Eq. (13) becomes

$$(E - V(x))X = -i\hbar V_F(\partial/\partial x + q)Y \quad (14)$$

and

$$(E - V(x))Y = -i\hbar V_F(\partial/\partial x - q)X, \quad (15)$$

where we have assumed that the y-dependence of both components of the wave function is proportional to $\exp(iqy)$ for all x. In a uniform potential with plane wave solutions, the two eigensolutions to Eqs. (14) and (15) are $Y = \pm X\exp(i\phi)$, where $\tan\phi = q/k$ and $k^2 = (E-V)^2 - q^2$. In the one-dimensional limit when q is zero, Eqs. (14) and (15) can be written in terms of the phase angle α in Eq. (12) as $Y = -i\partial X/\partial\alpha$ and $X = -i\partial Y/\partial\alpha$. These two relations may be combined to give

$$(\partial^2/\partial\alpha^2 + 1)X = (\partial/\partial\alpha - i)(\partial/\partial\alpha + i)X = 0, \quad (16)$$

with an identical equation for Y. This result reduces to the pair of uncoupled left and right propagating waves found in Sec. IV A and justifies the simplified, non-spinor analysis in one dimension.

In the same spirit it is instructive to note that combining Eqs. (14) and (15) leads to

$$(\partial/\partial\alpha - i)(\partial/\partial\alpha + i)X = (\partial\beta/\partial\alpha + \beta^2)X, \quad (17)$$

where $\beta = \hbar q V_F/(E - V(x))$, which indicates the coupling between left and right propagating solutions so that reflection occurs in inhomogeneous potentials in two dimensions, and therefore perfect Klein tunneling does not usually occur. However, partial Klein tunneling does occur. It is straightforward to calculate the reflection coefficient for a potential step that is zero for $x<0$ and a constant $V = V_0$, for $x \geq 0$. Then assuming that for $x<0$, there is an incident wave with wavenumber k and a reflected wave with wave number $-k$, and that for $x>0$, there is a transmitted wave with wavenumber, l, then the condition for the continuity of X is

$$1 + r = t, \quad (18)$$

where r and t are the relative amplitudes of the reflected and transmitted waves, respectively. The corresponding relation for the continuity of Y is

$$\exp(i\phi) - r\exp(-i\phi) = t\exp(i\theta), \quad (19)$$

where $\tan\theta = q/l$.

We note that ϕ is essentially the particle's angle of incidence on the potential step. Hence, the reflection coefficient $R = |r|^2$ is

$$R = \frac{1 - \cos(\phi - \theta)}{1 + \cos(\phi + \theta)}, \quad (20)$$

as long as $\theta < \pi/2$. For $\phi = 0$, $\theta = 0$, and the one-dimensional result is recovered and $R = 0$, whatever the value of V_0. As ϕ increases from zero, R increases until ϕ reaches $\pi/2$. For $V_0 < E$, this occurs when $\sin\phi$ equals $1 - V_0/E$, at which point R reaches unity. For larger angles of incidence than this critical one, R remains at unity and the transmitted wave decays exponentially. For values of V_0 between E and $2E$, the critical angle occurs when $\sin\phi = V_0/E - 1$. For $V_0 > 2E$, there is no critical angle, so that there is always some transmission. For $V_0 \gg E$, Eq. (20) reduces to

$$R = \frac{1 - \cos\phi}{1 + \cos\phi}. \quad (21)$$

Hence, even in infinite potentials Eq. (21) implies that reflection is only partial and there is Klein tunneling.

There is now a considerable literature on Klein tunneling, both in the massless case[3] as in graphene, as well as the massive relativistic case.[4,9] Much of this literature is on step potentials or square barriers. Quantum mechanical transmission and reflection of particles at potential steps and barriers is a standard problem in introductory quantum mechanics textbooks.[10] However, step potentials are highly idealized and have limited applications, and it is worthwhile to consider more general inhomogeneous potentials. Smooth potentials are more realistic than discontinuous steps and allow us to explore the inhomogeneous potential problem without being troubled by boundary conditions at discontinuities that can sometimes lead to ambiguity and pathological results. In the following, we investigate Klein tunneling in graphene in smooth inhomogeneous potentials using numerical methods to integrate the resulting differential equations. Hyperbolic tangent functions provide suitable adjustable analytical potentials of sufficient generality for this purpose.

Katsnelson *et al.*[3] have recently studied Klein tunneling in graphene using analytical methods with square potential barriers of finite width. Their results provide a useful comparison for our smooth potential results. An appropriate hyperbolic tangent form of a smooth potential takes the form

$$V(x) = V_0(\tanh((x + L/2)/W_1) - \tanh((x - L/2)/W_2)))/2, \quad (22)$$

where V_0 is a constant that corresponds roughly to the barrier maximum, L is the width of the barrier, and W_1 and W_2 the respective rise and fall distance of the leading and trailing edges of the barrier. L, W_1, and W_2 are scaled to the incident electron wavelength. An example of this potential barrier is illustrated in Fig. 3, for $L = 2$, $W_1 = 0.2$, and $W_2 = 0.3$. $V(x)$ from Eq. (22) is substituted into Eqs. (14) and (15), which are then integrated numerically. It is assumed that a plane wave propagates obliquely in the x-y plane, in the direction of increasing x and y, from x equal to negative infinity toward the potential barrier. This right propagating incident wave excites a left propagating reflected wave as well as continuing as a right propagating transmitted mode. Far from the barrier, we assume there is a pair of left and right propagating plane waves to the left of the barrier and a right propagating plane wave to the right of it. All that is needed for the input data for the integration of Eqs. (14) and (15) is concerned is the choice of energy and the angle of incidence of the electron. Integration is begun far enough to the right of the barrier so that it can be assumed that the wave amplitude

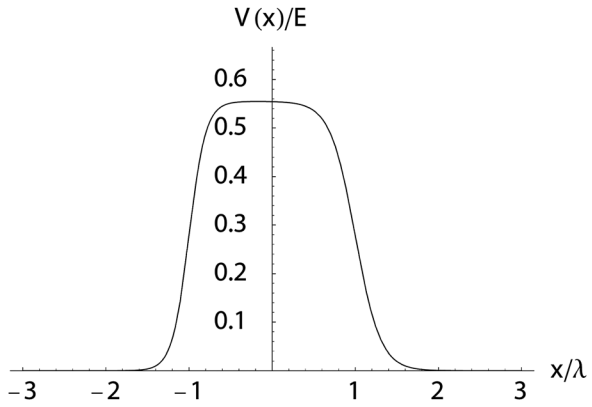

Fig. 3. An example of a smooth potential profile of the form in Eq. (22), with $L=2$, $W_1=0.2$ and $W_2=0.3$.

components X and Y are plane waves. At this distant point, we assume $X=1$, because the transmitted wave amplitude is arbitrary at this stage. The plane wave assumption means that Y is $\exp(i\phi)$, where ϕ is the angle of incidence and is given by $\tan\phi=q/k$. The numerical integration of Eqs. (14) and (15) is then straightforward. Once the amplitudes of X and Y have been determined in this manner for x from $-x_0$ to $+x_0$, where x_0 is chosen to be many free electron wavelengths, the reflection and transmission coefficients may be determined from $X(-x_0)$, $X(-x_0+2\pi/k)$, and $X(+x_0)$. For details of the method, see the Appendix.

Figure 4 shows an example of a solution for the transmission coefficient as a function of the angle of incidence for $V_0/E=225/80$, $L=2$, $W_1=0.05$, and $W_2=0.06$ (solid curve). Also displayed in Fig. 4 is the analytical solution from Ref. 3 (dashed curve) for the square potential with the same values of L and V_0/E. It is clear from Fig. 4 that, despite the fact that the smooth potential deviates only slightly from a square potential, with the rise and fall distances of the edges only small fractions of the electron wavelength, there is a noticeable difference between the two results. The numerical integration was also run with the values of both W_1 and W_2 reduced by a factor of ten. In this case the smooth and square results were almost indistinguishable. This result is a good test for the validity of the numerical solution.

The result in Fig. 4 is significant, because it implies that unless the values of W_1 and W_2 are smaller than a few percent of the free electron wavelength, the results of experiments on

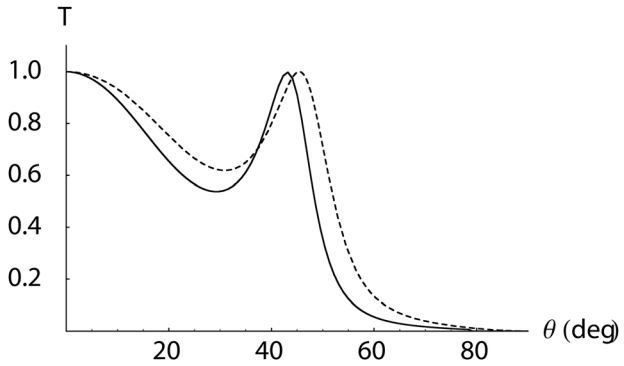

Fig. 4. Transmission coefficients, T, as a function of the incidence angle for two-dimensional scattering in graphene. The dashed curve represents the square potential with $V_0/E=225/80$ and $L=2$. The solid curve is a smooth barrier with the same amplitude and width, with $W_1=0.05$ and $W_2=0.06$.

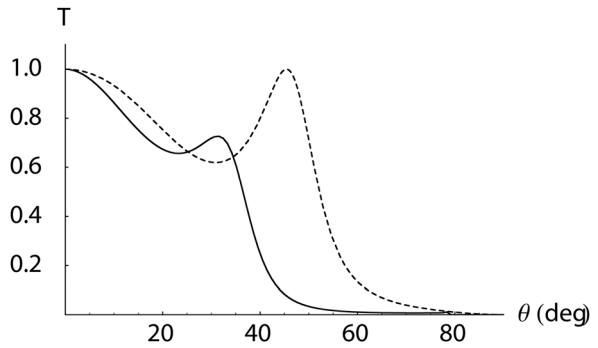

Fig. 5. Similar to Fig. 4, but with $W_1=0.005$ and $W_2=0.2$. There is a larger difference between the dashed and continuous curves than in Fig. 4, showing the effect of the weaker potential gradient (indicated by the larger W_2) at the trailing edge of the barrier, despite the sharper leading edge. In this case there is extreme asymmetry between the leading and trailing edges of the barrier.

Klein tunneling in graphene will depart significantly from what is expected from the analytic calculations for idealized square potentials.

Figure 5 shows another example with the potential and width the same as in Fig. 4, but with an extremely asymmetric barrier with $W_1=0.005$ and $W_2=0.2$. The result is an even bigger discrepancy between the ideal square and the smooth barriers.

V. COMMENTS

By representing the dependence of the electron dispersion relation on the magnitude of the wavevector, we emphasized the geometrical aspect of spinors rather than associating them immediately with electron spin. Spinors and non-commuting and non-anticommuting algebras arise in a simpler way in the graphene context than in the way they were originally introduced in the relativistic theory of the electron. It is possible that spinor physics may be brought more easily into the core physics curriculum graphene route from this point of view.

Graphene sits at the crossroads of a number of important phenomena and methodologies in quantum physics that in some cases also have counterparts in classical physics. A strong case has already been made for its role as an analogue of relativistic dynamics and field theory. We speculate that it might be possible for some other analogue for massive relativistic dynamics to be found. If graphene, with its gapless characteristic can mimic massless fermions, can a situation such as is found in the ground state of a superconductor, where there exists an energy gap, be manipulated to mimic massive particles? Mass is one of the most mysterious properties in nature and its origin remains the subject of much speculation. We know that photons acquire mass in a plasma[11] and in waveguides,[12] where they obey the massive Klein-Gordon equation rather than the massless wave equation. It would be interesting to find a corresponding analogue for massive fermions.

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APPENDIX: CALCULATION OF REFLECTION AND TRANSMISSION COEFFICIENTS

The reflection and transmission coefficients can be obtained from numerical integration as follows. Having integrated the appropriate wave equation, the field amplitude, $X(x)$, is known between $x = \pm x_0$, where x_0 is many wavelengths away from the location of the inhomogeneities in the potential. We now assume that far from the barrier along the negative x-axis, there is field an incident wave $U\exp(ikx)$ and a reflected wave, $rU\exp(-ikx + i\gamma)$, where γ is an arbitrary phase angle. We choose two points, $x = x_1$ and x_2, far from the potential barrier. Then

$$\rho = X(x_1)/X(x_2) = \frac{\exp(ikx_1) + r\exp(i\gamma - ikx_1)}{\exp(ikx_2) + r\exp(i\gamma - ikx_2)}. \quad \text{(A1)}$$

Having ensured that $k(x_1 - x_2) = \pi/2$, rearranging Eq. (A1) gives

$$r\exp(i\gamma) = -\frac{1 - i\rho}{1 + i\rho}\exp(2ikx_1). \quad \text{(A2)}$$

The reflection coefficient, $R = r^*r$ is thus

$$R = \frac{(1 - i\rho)(1 + i\rho*)}{(1 + i\rho)(1 - i\rho*)}, \quad \text{(A3)}$$

which depends only on the known complex ratio, $\rho = X(x_1)/X(x_2)$.

The transmission coefficient, $T = t^*t$ can be found in a similar way, if we recall that $X(x_0)$ was set to 1 as a boundary condition, we have

$$t = \exp(ikx_0 + i\delta)/U, \quad \text{(A4)}$$

where δ is another arbitrary phase angle. Because $X(x_1) = U(\exp ikx_1 + r\exp(-ikx_1 + i\gamma))$, we have

$$T = \frac{4\rho * \rho}{(1 + i\rho)(1 - i\rho*)}(X * (x_1)X(x_1))^{-1} = \frac{4(X * (x_2)X(x_2))^{-1}}{(1 + i\rho)(1 - i\rho*)}. \quad \text{(A5)}$$

[1] A. K. Geim and K. S. Novoselov, "The rise of graphene," Nat. Matter **6**, 183–191 (2007).
[2] Y. Nambu, "Nobel lecture: Spontaneous symmetry breaking in particle physics: A case of cross fertilization," Rev. Mod. Phys. **81**, 1015–1017 (2009).
[3] M. I. Katsnelson, K. S. Novselov, and A. K. Geim, "Chiral tunneling and the Klein paradox in graphene," Nature Phys. **2**, 820–825 (2006).
[4] N. Dombey and A. Calogeracos, "Seventy years of the Klein paradox," Phys. Rep. **315**, 41–58 (1999).
[5] P. R. Wallace, "The band theory of graphite," Phys. Rev. **71**, 622–634 (1947).
[6] A. Halprin, "Pedagogy of spin in nonrelativistic quantum mechanics," Am. J. Phys. **46**, 768 (1978).
[7] B. Williams and T. Robinson, "Pedagogy of spin in nonrelativistic quantum mechanics," Am. J. Phys. **49**, 645–647 (1981).
[8] D. Hestenes, "Oersted medal lecture 2002: Reforming the mathematical language of physics," Am. J. Phys. **71**, 104–121 (2003).
[9] A. Calogeracos and N. Dombey, "History and physics of the Klein paradox," Contemp. Phys. **40**, 313–321 (1999).
[10] A. I. M. Rae, *Quantum Mechanics*, 5th ed. (Taylor and Francis, New York, 2008).
[11] J. T. Mendonca, A. M. Martins, and A. Guerreiro, "Field quantization in plasma: Photon mass and charge," Phys. Rev. E **62**, 2989–2991 (2000).
[12] N. Marinescu, "The use of quantum mechanics in the treatment of waveguides," Prog. Quantum Electron **16**, 183–247 (1992).