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Scattering in one-dimensional heterostructures described by the Dirac equation

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Abstract

We consider electronic transport across one-dimensional heterostructures described by the Dirac equation. We discuss the cases where both the velocity and the mass are position dependent. We show how to generalize the Dirac Hamiltonian in order to obtain a Hermitian problem for spatial dependent velocity. We solve exactly the case where the position dependence of both velocity and mass is linear. In the case of velocity profiles, it is shown that there is no backscattering of Dirac electrons. In the case of the mass profile, backscattering exists. In this case, it is shown that the linear mass profile induces less backscattering than the abrupt step-like profile. Our results are a first step towards the study of similar problems in graphene.

1. Introduction

Most of the accumulated knowledge about the physics of heterostructures assumes that the electrons in these materials are effectively described by the Schrödinger equation, with a position dependent mass. The common belief is that the Dirac equation is of no use in condensed matter physics (spin–orbit coupling can be treated using the Pauli version of the Schrödinger equation). The discovery of graphene [1, 2] changed this perspective drastically. Condensed matter physicists are now facing a condensed matter system where the effective low-energy model for the quasi-particles is that of an ultrarelativistic, i.e. massless, Dirac equation, albeit with an effective Fermi velocity that is much lower than the velocity of light. In graphene the Fermi velocity is $v_F = c/300$, with c the velocity of light. In fact, since the isolation of graphene crystallites [1–3] a renovated interest in the properties of the massless Dirac equation in $2 + 1$ dimensions has started to emerge [3, 4]. Although our interest in this paper is in the backscattering properties of electrons effectively described by the Dirac equation in $1+1$ dimensions, as an effective low-energy theory of the electronic properties of a quasi-one-dimensional solid, we shall revise some of the properties of Dirac electrons in the context of graphene, given the accumulated amount of evidence for Dirac fermions in graphene.

How can the low-energy description of a solid be given by an effective Dirac-like equation? In one-dimensional physics, this occurs due to the linearization of the spectrum close to the Fermi momentum, which introduces right- and left-movers with a linear energy–momentum relation. Another possibility, that we discuss in the bulk of the paper, is by having two atoms per unit cell with a special type of hopping. In two dimensions, this possibility has been realized by graphene. The electrons in graphene are confined to move within the π orbitals of the system, formed from the overlap of the $2p_z$ atomic orbitals of a single carbon atom. The transport and optical properties of graphene are determined essentially by the behavior of the π electrons. The electronic density is such that graphene has one π electron per carbon atom, and is therefore a half filled system. It turns out that the band structure of graphene around the *Fermi surface* is highly non-standard, since the relation between the momentum and the energy is linear, with a proportionality coefficient given by $v_F \simeq 1 \times 10^6$ m s^{-1} and termed the Fermi velocity. In fact, the *Fermi surface* is reduced to two points (the so called Dirac points $\boldsymbol{K}$ and $\boldsymbol{K}'$) in the Brillouin zone, with a zero density of states at the Fermi points. This fact gives graphene its non-conventional properties.

Starting from a $\boldsymbol{k}\cdot\boldsymbol{p}$ approach [5], adapted to degenerate bands off the Γ-point [6], we obtain an effective Hamiltonian in real space, valid around the $\boldsymbol{K}$ point, having the form

$$H = v_F \boldsymbol{\sigma}\cdot\boldsymbol{p}, \tag{1}$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y)$ is a vector using the Pauli matrices and $\boldsymbol{p} = -i\hbar(\partial_x, \partial_y)$. The Hamiltonian (1) is nothing but the

Dirac Hamiltonian for massless particles in $2+1$ dimensions, with an effective light velocity v_F. Clearly, one expects that the physical properties of such a system will be different from those where the Schrödinger equation is valid. Note that this situation is an example of complex emergent behavior [12], since the original problem was that of independent electrons (and therefore Schrödinger-like) in a periodic potential.

Those electrons in graphene lying close to the Fermi points ($\boldsymbol{K}$ and $\boldsymbol{K}'$) will have a different response to external potentials than those in other materials described by the Schrödinger equation. In fact, for Schrödinger electrons, if we consider that the potential varies at a given point in space from zero to a finite value V_0 (the so called step potential), there is always a finite fraction of impinging electrons that are reflected back. Moreover, if V_0 is greater than the energy of the impinging particles, there will be an exponential attenuated wavefunction in the region where the potential is finite.

For Dirac electrons the situation is different. It was shown by Klein [16] that Dirac particles can not be confined by an arbitrary large potential V_0. In fact, they pass through a strong repulsive potential without the exponential decay that characterizes Schrödinger particles. This is called Klein tunneling. If the particles are massless and moving in one dimension the situation is even more dramatic, since there is no backscattered probability flux, no matter how large the potential is [13, 14].

In addition to external potentials, a particle propagating in solid state systems can face a situation where its effective mass changes in space. This possibility occurs in heterostructures, where the mass of the particle is written as $m(\boldsymbol{r})$, $\boldsymbol{r}$ being the position of the particle. In this situation, the Schrödinger equation has to be modified, in order to comply with hermiticity and flux conservation.

If the particles are described by the Dirac equation, the information on the material properties is encoded both in the Fermi velocity [6] and in the mass. We can then imagine the possibility of producing a heterostructure where the Fermi velocity $v_F(\boldsymbol{r})$ and the mass change with the position of the particle. As we show below, even in this case, there will not be backscattering if the particle is massless and the velocity is allowed to vary from point to point. In the context of graphene physics, a position dependent Fermi velocity was already considered in the case of curved graphene [7]. Another possibility of producing both a Fermi velocity and a mass term that are position dependent is to subject the system to strain. It has already been shown using *ab initio* calculations, in the context of graphene physics, that strain leads to gap formation [8, 9]. It is to be expected that for general strain different parts of the material present local values of Fermi velocity and energy gap. Also in the case of graphene, it was shown that depositing the material on top of boron nitride leads to gap formation [10].

In this paper we discuss several possibilities for the scattering of Dirac particles through a region where both the velocity and the mass are position dependent. Although our motivation is to study graphene strips [15] in a later publication, we start by giving two exact solutions for one-dimensional systems. The generalization to a quasi-one-dimensional system, such as a narrow nano-wire, is easy to obtain and will be given in a follow-up publication. In order to see the differences between the Schrödinger and the Dirac problems, we start by revising the case of one-dimensional heterostructures described by the Schrödinger equations and later move to the study of the Dirac case.

2. Warming up: the Schrödinger electrons in 1D

In order to compare how the scattering of Schrödinger electrons differs from that of Dirac particles, we give a brief account of the scattering of electrons by the interface of a heterostructure.

Let us consider the case of 1D Schrödinger electrons with position dependent effective mass $m(x)$, such that $m(x) = m^-$ for $x < 0$ and $m(x) = m^+$ for $x > 0$. The boundary conditions in this case are (see final paragraph of this section; for more general boundary conditions see [11])

$$\psi^-(0) = \psi^+(0), \tag{2}$$

$$\frac{1}{m^-}\frac{\mathrm{d}}{\mathrm{d}x}\psi^-(0) = \frac{1}{m^+}\frac{\mathrm{d}}{\mathrm{d}x}\psi^+(0). \tag{3}$$

We consider that the particles are moving from the left to the right. Therefore the wavefunction is

$$\psi^-(x) = \mathrm{e}^{\mathrm{i}kx} + r\mathrm{e}^{-\mathrm{i}kx}, \tag{4}$$

$$\psi^+(x) = t\mathrm{e}^{\mathrm{i}px}, \tag{5}$$

where the values of k and p are fixed by energy conservation:

$$E = \frac{\hbar^2 k^2}{2m^-} = \frac{\hbar^2 p^2}{2m^+}. \tag{6}$$

The reflectance $|r|^2$ is determined from the boundary conditions as

$$|r|^2 = \frac{(m^+k - m^-p)^2}{(m^+k + m^-p)^2}, \tag{7}$$

which has the limiting value $|r|^2 \to 1$ for $m^+ \to \infty$. The transmittance coefficient $|t|^2$ is

$$|t|^2 = \frac{4(m^+k)^2}{(m^+k + m^-p)^2}. \tag{8}$$

We can check now that the boundary conditions used for the wavefunction are the correct ones, since they satisfy the flux current conservation. Using absolute values, we have indeed

$$j^{\mathrm{inc}} = j^{\mathrm{reft}} + j^{\mathrm{trans}}, \tag{9}$$

with $j^{\mathrm{inc}} = \hbar k/m^+$, $j^{\mathrm{reft}} = |r|^2\hbar k/m^+$, and $j^{\mathrm{trans}} = |t|^2\hbar p/m^-$.

The problem just described represents a heterostructure, where two materials are *glued* together (due to similar lattice constants), having different effective masses in the two materials. The used boundary conditions are obtained writing the Hamiltonian as

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}}{\mathrm{d}x}\frac{1}{m(x)}\frac{\mathrm{d}}{\mathrm{d}x}. \tag{10}$$

This choice defines a Hermitian problem[1] since $\int \mathrm{d}x\,(H\psi)^*\psi = \int \mathrm{d}x\,\psi^* H\psi$. The construction of (10) guarantees that the total probability flux is conserved. The boundary condition (3) follows immediately from writing the Hamiltonian in the Sturm–Liouville form.

3. Dirac electrons in 1D

Let us now study the case of the Dirac Hamiltonian. We are interested in cases where both the velocity and the mass of the particles depend on their position in space. We study first the case of massless Dirac particles, like those present in graphene. Later we add the mass term. The Hamiltonian for a massless quasi-particle described by an effective Dirac equation, with an effective velocity of light v_F, is given by

$$H = v_\mathrm{F}\sigma_x \frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}x}, \tag{11}$$

where σ_x is the x Pauli matrix. Let us now consider that we make a heterostructure of two different materials, both of them described by an effective Dirac equation, such as (11). An example could be a strip of the material where part of it is subjected to strain and other part is strain free; this leads to different velocities in the two parts of the material. This situation calls for a model where v_F is position dependent: $v_\mathrm{F} = v_\mathrm{F}(x)$. Although this situation does not make sense in high-energy physics, it is quite conceivable in condensed matter physics, since the value of v_F is determined by the material under consideration—different materials can have different Fermi velocities.

The trivial replacement $v_\mathrm{F} \to v_\mathrm{F}(x)$ renders the problem non-Hermitian, as can be seen by applying the definition given above, when we discussed the Schrödinger case. There is however a way out. It is a simple matter to show that the operator

$$H = \sqrt{v_\mathrm{F}(x)}\sigma_x \frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}x}\sqrt{v_\mathrm{F}(x)}, \tag{12}$$

is Hermitian and reduces to equation (11) in the particular case $v_\mathrm{F}(x) = v_\mathrm{F}$. Note that the derivative will act on the product $\sqrt{v_\mathrm{F}(x)}\psi(x)$. We stress that we are not studying the scattering of relativistic particles in condensed matter systems, but instead describing the scattering of particles represented by an effective low-energy model that is formally equivalent to the Dirac equation (a situation that occurs in graphene). It would be interesting to derive equation (12) from a microscopic Hamiltonian. In appendix A we give a tight-binding model whose effective low-energy theory is given by equation (12). Problem (12) has a spinorial wavefunction of the form $\psi^\dagger = (\psi_1^*, \psi_2^*)$ and the probability flux is computed as $S_x = v_\mathrm{F}(x)\psi^\dagger\sigma_x\psi$, as can be shown using the traditional derivation of computing the time change of the probability density [17].

[1] Equation (10) is a particular case of a Sturm–Liouville operator, which has the general form

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left(p(x)\frac{\mathrm{d}}{\mathrm{d}x}\right) + q(x)y = \lambda w(x)y,$$

where λ is to be determined from the boundary conditions, and $p(x)$, $q(x)$, and $w(x)$ are given functions. Sturm–Liouville problems are Hermitian.

The eigenproblem $H\psi = E\psi$, with H given by equation (12), corresponds to two coupled first-order differential equations of the form

$$\sqrt{v(x)}\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}[\sqrt{v(x)}\psi_2(x)]}{\mathrm{d}x} = E\psi_1(x), \tag{13}$$

$$\sqrt{v(x)}\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}[\sqrt{v(x)}\psi_1(x)]}{\mathrm{d}x} = E\psi_2(x). \tag{14}$$

It is straightforward to show that the two first-order differential equations given above can be put in Sturm–Liouville form:

$$-\frac{\mathrm{d}}{\mathrm{d}x}\left[v_\mathrm{F}(x)\frac{\mathrm{d}}{\mathrm{d}x}y_1(x)\right] = \frac{E^2}{v_\mathrm{F}(x)\hbar^2}y_1(x), \tag{15}$$

with $y_1(x) = \sqrt{v_\mathrm{F}(x)}\psi_1(x)$, $p(x) = v_\mathrm{F}(x)$, $\lambda = E^2/\hbar^2$, and $w(x) = 1/v_\mathrm{F}(x)$, and $\psi_2(x)$ obtained from

$$\psi_2(x) = \frac{\hbar}{\mathrm{i}E}\sqrt{v_\mathrm{F}(x)}\frac{\mathrm{d}}{\mathrm{d}x}[\sqrt{v_\mathrm{F}(x)}\psi_1(x)]. \tag{16}$$

If the velocity profile changes continuously, one expects that the continuity of the wavefunction should be valid. If the velocity profile changes abruptly at a given point in space, say at $x = 0$, from $v(x) = v_-$, for $x < 0$, to $v(x) = v_+$, for $x > 0$, one has to use equations (13) and (14) to derive the boundary conditions. Defining $y_2(x) = \sqrt{v_\mathrm{F}(x)}\psi_2(x)$ equations (13) and (14) can be written as

$$\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}[y_2(x)]}{\mathrm{d}x} = E\frac{y_1(x)}{v(x)}, \tag{17}$$

$$\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}[y_1(x)]}{\mathrm{d}x} = E\frac{y_2(x)}{v(x)}. \tag{18}$$

Integrating equations (17) and (18) using a symmetric infinitesimal interval around $x = 0$ one obtains the condition

$$y_i(0^-) = y_i(0^+), \tag{19}$$

with $i = 1, 2$. Note that condition (19) implies the discontinuity of the wavefunction. Let us now move to the solution of several particular cases.

3.1. The step-like velocity profile

Let us consider the case

$$v_\mathrm{F}(x) = v_\mathrm{F}^-\,\theta(-x) + v_\mathrm{F}^+\,\theta(x). \tag{20}$$

The solution of the Dirac equation reads

$$\psi_-(x) = \begin{pmatrix}1\\1\end{pmatrix}\mathrm{e}^{\mathrm{i}qx} + r\begin{pmatrix}1\\-1\end{pmatrix}\mathrm{e}^{-\mathrm{i}qx}, \tag{21}$$

and

$$\psi_+(x) = t\begin{pmatrix}1\\1\end{pmatrix}\mathrm{e}^{\mathrm{i}px}, \tag{22}$$

with $E = v_\mathrm{F}^- q\hbar$ and $E = v_\mathrm{F}^+ p\hbar$. The above wavefunctions were obtained by solving the Dirac equation for $x \gtrless 0$,

where the velocity is constant. Using these solutions and the boundary condition (19) one obtains

$$\sqrt{v_-}(1+r) = \sqrt{v_+}t, \qquad \sqrt{v_-}(1-r) = \sqrt{v_+}t, \tag{23}$$

which is satisfied only for $r = 0$. Had we considered the general case of both a velocity profile (20) and a potential profile of the form

$$V(x) = V_0\,\theta(x), \tag{24}$$

under the condition $E > V_0$, the boundary conditions would still give $r = 0$. This result is called Klein tunneling [16]. If we consider the same velocity and potential profiles, but now take the energy $E < V_0$, the boundary conditions still give the result (23), but the wavefunction of the propagating mode for $x > 0$ is now different and given by

$$\psi_+(x) = t\begin{pmatrix}1\\1\end{pmatrix}\mathrm{e}^{-\mathrm{i}px}. \tag{25}$$

In this case the result will also be $r = 0$. The conclusion is that it is not possible to backscatter massless Dirac electrons with a step-like velocity and potential profiles in 1D.

3.2. The linear velocity profile with massless particles

We have seen that an abrupt change of the velocity at the interface produces no reflected particles. Let us now study the case of a smooth change in the velocity from v_{F}^- to v_{F}^+. (The result can be guessed from the outset!) To this end, we choose the profile

$$v_{\mathrm{F}}(x) = v_{\mathrm{F}}^-\,\theta(-\delta - x) + (\bar{v} + x\Delta)\,\theta(\delta - |x|) + v_{\mathrm{F}}^+\,\theta(x - \delta), \tag{26}$$

where we have defined $\bar{v}$ and Δ as

$$\bar{v} = \frac{v_{\mathrm{F}}^- + v_{\mathrm{F}}^+}{2}, \tag{27}$$

$$\Delta = \frac{v_{\mathrm{F}}^+ - v_{\mathrm{F}}^-}{2\delta}. \tag{28}$$

For the cases $x < -\delta$ (region I) or $x > \delta$ (region III) the Fermi velocity is constant and the solution of the Dirac equation is elementary, as we have seen before. The interesting case is therefore the region $|x| < \delta$ (region II). In this case we have to use the Dirac equation in the form (12). Explicitly, we have to solve the problem $H\psi = E\psi$ with H given by

$$H = \sqrt{\bar{v} + x\Delta}\,\sigma_x\frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}}{\mathrm{d}x}\sqrt{\bar{v} + x\Delta}. \tag{29}$$

Writing the differential equations satisfied by the spinors, we obtain for the ψ_1 spinor (considering the substitution $y = \sqrt{\bar{v} + x\Delta}\psi_1$) the equation

$$-v_{\mathrm{F}}^2(x)\frac{\mathrm{d}^2y}{\mathrm{d}x^2} - \Delta v_{\mathrm{F}}(x)\frac{\mathrm{d}y}{\mathrm{d}x} = \epsilon^2 y, \tag{30}$$

with $\epsilon^2 = E^2/\hbar^2$. Making the replacement

$$z = \frac{\bar{v} + x\Delta}{\bar{v}} \equiv \theta(x), \tag{31}$$

we obtain the result

$$z^2\frac{\mathrm{d}^2y}{\mathrm{d}z^2} + z\frac{\mathrm{d}y}{\mathrm{d}z} + \nu^2 y = 0, \tag{32}$$

with $\nu^2 = \epsilon^2/\Delta^2$. Making the additional replacement $\omega = \ln z$, equation (32) is reduced to that of the harmonic oscillator[2]

$$\frac{\mathrm{d}^2y}{\mathrm{d}\omega^2} + \nu^2 y = 0. \tag{33}$$

The general solution of equation (33) is elementary and from it one obtains $y(x)$ given by

$$y(x) = A\sin[\nu L\theta(x)] + B\cos[\nu L\theta(x)], \tag{34}$$

with

$$L\theta(x) = \ln\frac{\bar{v} + x\Delta}{\bar{v}}. \tag{35}$$

The component ψ_1 of the spinor is obtained from $\psi_1(x) = y(x)/\sqrt{v_{\mathrm{F}}(x)}$, and ψ_2 is obtained using equation (16) and reads

$$\psi_2(x) = \frac{\hbar}{\mathrm{i}E}\sqrt{v_{\mathrm{F}}(x)}\frac{\mathrm{d}y\,(x)}{\mathrm{d}x}. \tag{36}$$

The boundary conditions are $\psi^{\mathrm{I}}(-\delta) = \psi^{\mathrm{II}}(-\delta)$ and $\psi^{\mathrm{II}}(\delta) = \psi^{\mathrm{III}}(\delta)$, and can be written as[3]

$$\begin{pmatrix} -\mathrm{e}^{\mathrm{i}k\delta} & S_-/\sqrt{v_{\mathrm{F}}^-} & C_-/\sqrt{v_{\mathrm{F}}^-} & 0\\ \mathrm{e}^{\mathrm{i}k\delta} & C_-\lambda^- & -S_-\lambda^+ & 0\\ 0 & S_+/\sqrt{v_{\mathrm{F}}^+} & C_+/\sqrt{v_{\mathrm{F}}^+} & -\mathrm{e}^{\mathrm{i}q\delta}\\ 0 & C_+\lambda^- & -S_+\lambda^+ & -\mathrm{e}^{\mathrm{i}q\delta}\end{pmatrix}\begin{pmatrix} r\\ A\\ B\\ t\end{pmatrix} = \begin{pmatrix}\mathrm{e}^{-\mathrm{i}k\delta}\\ \mathrm{e}^{-\mathrm{i}k\delta}\\ 0\\ 0\end{pmatrix} \tag{37}$$

with

$$S_\pm = \sin[\nu L\theta(\pm\delta)], \tag{38}$$

$$C_\pm = \sin[\nu L\theta(\pm\delta)], \tag{39}$$

$$\lambda_\pm = \frac{\hbar\sqrt{v_{\mathrm{F}}^\pm}}{\mathrm{i}E}\frac{\Delta}{\bar{v}}\frac{\nu}{\theta(\pm\delta)}. \tag{40}$$

The fraction of reflected flux is given by $|r|^2$ and the transmitted flux is $1 - |r|^2 = v_{\mathrm{F}}^+|t|^2/v_{\mathrm{F}}^-$. The explicit evaluation (which is somewhat lengthy) of the coefficients gives

$$|r|^2 = 0, \tag{41}$$

$$|t|^2 = \frac{v_{\mathrm{F}}^-}{v_{\mathrm{F}}^+}, \tag{42}$$

and therefore the electrons are totally transmitted across the heterojunction. Of course this result could have been anticipated from the conclusions of section 3.1, since it is always possible to represent a well behaved function by a sum of infinitesimal rectangles. (It is however elegant to have an exact solution to a given problem.)

[2] One should note that the solution of equation (32) can also be obtained by noticing that $y = z^m$ is a solution if $m^2 = -\nu^2$, leading to $y(z) = Az^{\mathrm{i}\nu} + Bz^{-\mathrm{i}\nu}$.

[3] Note that the dimensions of A and B are $\sqrt{L/T}$, and $\lambda^\pm$ has dimensions of $\sqrt{T/L}$.

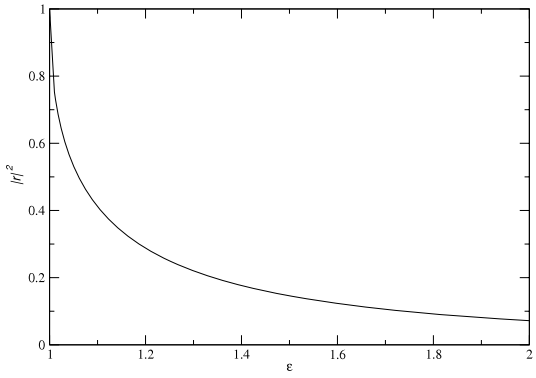

Figure 1. Plot of equation (45) as a function of the dimensionless energy.

3.3. The linear velocity profile with massive particles

We can now use what we have just learned to a deal with a more general situation where the electronic spectrum changes due to a change of the material. The simplest case is that where for $x = \delta$ the mass of the quasi-particles jumps from zero to a finite value. The connection between the two materials is represented by the linear profile of the velocity discussed in section 3.2. The mass profile is

$$m(x) = m\,\theta(x-\delta), \tag{43}$$

that is, the change is velocity takes place outside the region of finite mass. Since the particle has a finite mass the spectrum changes to $E = \pm\sqrt{v_+^2 q^2 + m^2 v_+^4}$, and the wavefunction in this region changes to

$$\psi^{\mathrm{III}}(x) = t\begin{pmatrix}\sqrt{E^2 - m^2 v_+^4}\\ E - m v_+^2\end{pmatrix} \mathrm{e}^{-\mathrm{i}qx}. \tag{44}$$

The overall modification is the replacement of $\mathrm{e}^{\mathrm{i}q}$ by $\sqrt{E^2 - m^2 v_+^4}\mathrm{e}^{\mathrm{i}q}$ in the third row, and of $\mathrm{e}^{\mathrm{i}q}$ by $(E - m v_+^2)\mathrm{e}^{\mathrm{i}q}$ in the fourth row. Working out the calculation of $|r|^2$ we obtain

$$|r|^2 = -[1 + 2\epsilon(-\epsilon + \sqrt{\epsilon^2 - 1})], \tag{45}$$

with $\epsilon = E/(m v_+^2)$. As expected, the result does not depend on δ and on $v_{\mathrm{F}}^{\pm}$, for the reasons discussed in section 3.2. A plot of equation (45) is given in figure 1. The situation is the same if the mass profile is chosen as

$$m(x) = m\,\theta(x+\delta), \tag{46}$$

that is, the linear profile rises inside the massive region.

3.4. The linear mass profile

We have seen above that the linear velocity profile does not contribute to the backscattering of Dirac fermions, even when it is combined with a region where fermions are massive. In fact, any velocity profile produces no backscattering in one dimension. All the backscattering comes from the change in the dispersion, due to the presence of the mass term. This fact motivates the question of what form of the wavefunction and of the coefficient $|r|^2$ is if the mass does not change abruptly but in a smooth way. A choice for the change of the mass profile, leading to an exact solution, is that described by

$$m(x) = m\,\theta(x-\delta) + m\frac{x}{\delta}\theta(x)\theta(\delta - x). \tag{47}$$

We approach the solution of the scattering problem by solving first the Dirac equation subjected to a mass profile $m(x) = m\frac{x}{\delta}$. The method of solution is inspired by that used for the 3+1 Dirac equation [18, 19]. In this case the Fermi velocity is constant, and therefore we have to solve equation (11) with the additional term $\sigma_z m v_{\mathrm{F}}^2 \frac{x}{\delta}\psi$:

$$v_{\mathrm{F}}\sigma_x \frac{\hbar}{\mathrm{i}}\frac{\mathrm{d}\psi}{\mathrm{d}x} + \sigma_z m v_{\mathrm{F}}^2 \frac{x}{\delta}\psi = E\psi. \tag{48}$$

The solution of this problem proceeds in several steps. The first is to operate on the left-hand side of equation (48) with the operator

$$\frac{\mathrm{d}}{\mathrm{d}x}\sigma_y\sigma_z. \tag{49}$$

After some algebra we obtain the following result:

$$\hbar^2 v_{\mathrm{F}}^2 \frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} = -[(E^2 - m^2 v_{\mathrm{F}}^4 x^2/\delta^2) + \sigma_y \hbar m v_{\mathrm{F}}^3/\delta]\psi. \tag{50}$$

The two components of the spinor are still coupled in equation (50). In order to decouple them we use the unitary transformation

$$\phi = U^{\dagger}\psi, \tag{51}$$

$$U = \begin{pmatrix}1 & 0\\ 0 & \mathrm{i}\end{pmatrix}. \tag{52}$$

The above transformation changes σ_y to $\tilde{\sigma}_y = U^{\dagger}\sigma_y U$, which, still mixing the spinors in equation (53) below, does it with the same sign (this is a crucial step). After applying the unitary transformation we obtain

$$\hbar^2 v_{\mathrm{F}}^2 \frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} = -[(E^2 - m^2 v_{\mathrm{F}}^4 x^2/\delta^2) + \tilde{\sigma}_y \hbar m v_{\mathrm{F}}^3/\delta]\phi. \tag{53}$$

We now introduce two new functions defined by $F_{\pm} = \phi_1 \pm \phi_2$, where ϕ_i (with $i = 1, 2$) are the components of the spinor ϕ. In terms of the functions $F_{\pm}$ the eigenproblem takes the form

$$-\hbar^2 v_{\mathrm{F}}^2 \frac{\mathrm{d}^2 F_{\pm}}{\mathrm{d}x^2} + [m^2 v_{\mathrm{F}}^4 x^2/\delta^2 - \epsilon_{\pm}^2]F_{\pm} = 0, \tag{54}$$

where $\epsilon_{\pm}^2 = E^2 \pm \hbar m v_{\mathrm{F}}^3/\delta$. The general solution of equation (54) is given in terms of parabolic cylinder functions $D_{\nu}(x)$ (see appendix B)

$$F_{\pm}(x) = A_{\pm} D_{\nu_1^{\pm}}(\sqrt{2}(b/a)^{1/4}x) + B_{\pm} D_{\nu_2^{\pm}}(\mathrm{i}\sqrt{2}(b/a)^{1/4}x), \tag{55}$$

with

$$\nu_1^{\pm} = -\frac{1}{2} + \frac{\epsilon_{\pm}^2}{2\sqrt{ab}} = \nu - (1 \mp 1)/2, \tag{56}$$

$$\nu_2^{\pm} = -\frac{1}{2} - \frac{\epsilon_{\pm}^2}{2\sqrt{ab}} = -\nu_1^{\pm} - 1 \tag{57}$$

$$\nu = \frac{E^2\delta}{2\hbar v_F^3 m}, \tag{58}$$

$$a = \hbar^2 v_F^2, \tag{59}$$

$$b = v_F^4 m^2/\delta^2. \tag{60}$$

As we were looking for the solution of the problem valid for all values of x, the functions $D_\nu(x)$ with imaginary argument, since they are not real and are not normalizable in the infinite volume, had to be excluded. Therefore, in the limit $x \to \pm\infty$ the normalizable solutions are those where $F_\pm(x)$ represents the one-dimensional harmonic oscillator wavefunctions (see appendix C). Therefore the solution in the interval $x \in [-\infty, \infty]$ is

$$F_\pm(x) = 2A_\pm D_{\nu_1^\pm}(\sqrt{2}(b/a)^{1/4}x). \tag{61}$$

This choice guarantees that the wavefunction is well behaved at $x \to \pm\infty$ when $\nu_1^\pm$ is equal to a positive integer (see appendix C). Therefore, in the infinite volume, the solution of equation (50) takes the form

$$\psi(x) = \begin{pmatrix} A_+ D_{\nu_1^+} + A_- D_{\nu_1^-} \\ \mathrm{i}A_+ D_{\nu_1^+} - \mathrm{i}A_- D_{\nu_1^-} \end{pmatrix}, \tag{62}$$

where the argument of the parabolic cylinder functions has been omitted for simplicity. We still have to check whether equation (62) is the solution of equation (48). Introducing the solution (62) in equation (48) we obtain that the wavefunction is a solution if

$$A_- = \frac{\Lambda\nu}{E} A_+, \tag{63}$$

$$\Lambda = v_F\hbar\sqrt{\frac{2v_F^2 m}{v_F\hbar\delta}} = v_F\hbar/\beta. \tag{64}$$

What we have discussed so far assumes that equation (48) holds for every x. Our interest, however, is in the scattering problem of electrons when equation (48) holds for $x \in]0, \delta[$. In this case, the general solution (55) with both real and complex wavefunctions must be used. The strategy is the same as used before. We know at the outset that the solution of equation (48) is obtained from solution (62) by fixing the value of a constant, as in equation (63). The final solution is

$$\psi(x) = A\begin{pmatrix} D_\nu(x/\beta) + \nu\Lambda/E D_{\nu-1}(x/\beta) \\ \mathrm{i}D_\nu(x/\beta) - \mathrm{i}\nu\Lambda/E D_{\nu-1}(x/\beta) \end{pmatrix} + B\begin{pmatrix} D_{-\nu}(\mathrm{i}x/\beta) + \mathrm{i}\nu\Lambda/E D_{-\nu-1}(\mathrm{i}x/\beta) \\ -\mathrm{i}D_{-\nu}(\mathrm{i}x/\beta) - \nu\Lambda/E D_{-\nu-1}(\mathrm{i}x/\beta) \end{pmatrix} \tag{65}$$

which is valid in the region $x \in]0, \delta[$. As in section 3.2, we have the incoming wavefunction given by equation (21), for $x < 0$, and the transmitted one given by equation (44), for $x > \delta$. The reflected and transmitted amplitudes r and t, respectively, are obtained by imposing the continuity of the wavefunction at $x = 0$ and δ. In figure 2 we give some numerical examples of our calculation. It is clear from figure 2 that the smoothness of the change of the mass profile leads to a larger transmittance, for a given energy, than when the mass profile changes abruptly. Also, when the change in the value of the mass takes place over a relatively large region, the transmittance shows the presence of resonances, as can be seen in panel (c) of figure 2.

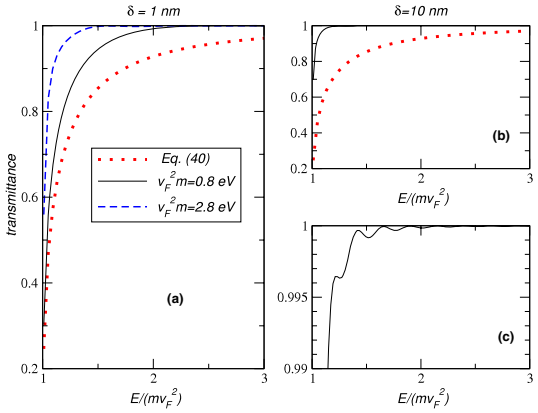

Figure 2. Transmittance of Dirac electrons across a region where the mass profile changes according to equation (47). The dotted line represents the transmittance in the case of an abrupt change of the mass profile, as given by equation (45). The energy gap is represented by the value of mv_F^2. In panel (a) we give the results for a value of δ of 1 nm. In panels (b) and (c) we plot the same but for $\delta = 10$ nm. In panel (c) we give a zoom-in of the solid curve of panel (b); the existence of resonances in the transmittance is clear. The Fermi velocity is 10^6 m s^{-1}, leading to $v_F\hbar = 0.66$ eV nm.

(This figure is in colour only in the electronic version)

4. Discussion and conclusions

We have studied several scattering problems using a modified version of the Dirac Hamiltonian which incorporates the possibility of a spatial dependent velocity and mass terms. Two exact solutions were given. We showed that in the case of a velocity profile the modification of the original Dirac Hamiltonian is necessary, in order to have a Hermitian problem. We have shown that Klein tunneling is not suppressed by a change in the velocity profile, with a transmittance always equal to unity. This was understood by studying the case of an abrupt change in the velocity profile and also by solving exactly the case where the velocity changes linearly across a given region.

We have also studied the case where the mass term depends on position. For this situation, we solved the cases of an abrupt change of the mass value and of a linear change of the mass profile. In both cases we see the presence of backscattering, with values of the transmittance smaller than unity. The smoother mass profile induces less backscattering.

It is interesting to consider next the case of Dirac electrons in a strip of finite width W, a situation relevant for graphene strips, and see if in this case a position dependent velocity profile does produce backscattering. This will be considered in a follow-up publication.

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Appendix A. A derivation of the Dirac equation with a position dependent velocity

Consider a one-dimensional tight-binding Hamiltonian with two atoms per unit cell such that the hopping parameter within a unit cell n is $-t_n$ and among nearest unit cells is t_n. The Hamiltonian in second quantization reads

$$H = \sum_n [-t_n(a_n^\dagger b_n + b_n^\dagger a_n) + t_n(a_n^\dagger b_{n-1} + b_{n-1}^\dagger a_n)]. \quad \text{(A.1)}$$

Then in the case $t_n = t$ (the hopping is independent of the unit cell) the spectrum of the electrons is

$$E_{\alpha=\pm} = \alpha 2t|\sin(kc/2)|, \quad \text{(A.2)}$$

with c is the length of the unit cell vector. Close to $k = 0$ (zero energy) the spectrum is linear in momentum and a massless Dirac spectrum is generated with a Fermi velocity given by v_F. Let us now assume the general case of a t_n dependent on the unit cell position, and obtain from the Hamiltonian (A.1) the effective field-theoretical model that describes the system at low energy ($E \simeq 0$). Since the momentum close to which the Dirac spectrum develops is $k = 0$, we can write immediately the effective field-theoretical model as

$$H = -\frac{1}{c}\int \mathrm{d}y\, t(y)\left[a^\dagger(y)c\frac{\mathrm{d}b(y)}{\mathrm{d}y} + c\frac{\mathrm{d}b^\dagger(y)}{\mathrm{d}y}a(y)\right], \quad \text{(A.3)}$$

where we have used the expansion $b^\dagger(y - c) \simeq b^\dagger(y) + cd[b^\dagger(y)]/\mathrm{d}y$. Integrating by parts the second term of equation (A.3) and using the Pauli matrices to help condensing the results we obtain

$$H = \frac{1}{c}\int \mathrm{d}y \left[\Psi^\dagger\sqrt{v_y(y)}\sigma_y p_y\sqrt{v_y(y)}\Psi + \Psi^\dagger\frac{c\sigma_x}{2}\frac{\mathrm{d}t(y)}{\mathrm{d}y}\Psi\right] \quad \text{(A.4)}$$

with $v(y) = ct(y)/\hbar$ and $\Psi^\dagger = [a^\dagger(y)b^\dagger(y)]$. The first term in equation (A.4) is our proposed Hamiltonian (12).

Appendix B. Weber's differential equation

We give here some basic information on the Weber's differential equation, aiming to give the text a self-contained nature and to fix notation and definitions. Weber's differential equation is defined as

$$y''(z) + (\nu + 1/2 - z^2/4)y(z) = 0, \quad \text{(B.1)}$$

and its two independent solutions are the parabolic cylinder functions $y(z) = D_\nu(z)$ and $y(z) = D_{-\nu-1}(\mathrm{i}z)$. Equation (54) is of the general form

$$y''(x) + (-ax^2 + c)y(x) = 0. \quad \text{(B.2)}$$

Making the transformation $x = \beta z$, with β given by $\beta = (4a)^{-1/4}$ and $\nu = -1/2 + c\beta^2$, we reduce equation (B.2) to Weber's equation (B.1). Using for a and c the particular values of our problem we obtain

$$\beta = \sqrt{\frac{\hbar v_F\delta}{2v_F^2 m}}, \quad \text{(B.3)}$$

and

$$\nu = -\frac{1}{2} + \frac{\epsilon_\pm^2\delta}{2\hbar v_F^3 m}. \quad \text{(B.4)}$$

The derivative of the parabolic cylinder functions obeys

$$D_\nu'(z) + zD_\nu(z)/2 - \nu D_{\nu-1}(z) = 0, \quad \text{(B.5)}$$

$$D_{\nu+1}(z) - zD_\nu(z) + \nu D_{\nu-1}(z) = 0. \quad \text{(B.6)}$$

Using the results of [20], the solution of $D_\nu(z)$ can be written in terms of the Kummer confluent hypergeometric function, $U(a, b, x)$, as

$$D_\nu(z) = 2^{\nu/2}\mathrm{e}^{-z^2/4}U(-\nu/2, 1/2, z^2/2). \quad \text{(B.7)}$$

The Kummer function $U(a, 1/2, z)$ is computed using the Kummer confluent hypergeometric function, $M(a, b, x)$, as

$$U(a, 1/2, z) = \sqrt{\pi}\,\frac{M(a, 1/2, z)}{\Gamma(a + 1/2)} - 2\sqrt{z\pi}\,\frac{M(a + 1/2, 3/2, z)}{\Gamma(a)}. \quad \text{(B.8)}$$

Appendix C. Eigenvalues of the scalar potential $V(x) = \sigma_z m v_F^2 x/\delta$

The problem we introduced in section 3.4 was that of a particle that moves in a heterostructure with a mass dependent position. We can, however, think of this problem as that of a Schrödinger particle moving in the scalar potential $V(x) = m^2 v_F^4 (x/\delta)^2$. Since equation (54) is that of an one-dimensional harmonic oscillator, the normalizable solutions have the well known form

$$z_n(u) = \frac{\pi^{-1/4}}{\sqrt{2^n n!}}\mathrm{e}^{-u^2/2}H_n(u), \quad \text{(C.1)}$$

where

$$u = x\left(\frac{V_F^2 m}{\delta V_F \hbar}\right)^{1/2} \quad \text{(C.2)}$$

upon the identification

$$\frac{1}{m_0} \leftrightarrow 2v_F^2, \quad \text{(C.3)}$$

$$\omega_0^2 \leftrightarrow 4v_F^6 m^2/\delta^2, \quad \text{(C.4)}$$

with m_0 and ω_0 the mass and the frequency of the oscillator, respectively. The spectrum is obtained from $\epsilon_\pm^2 = 2\hbar v_F^3 m(n + 1/2)/\delta$, with $n = 0, 1, 2, \ldots$, leading to

$$E_+^2 = 2\hbar v_F^3 mn\delta^{-1}, \quad \text{(C.5)}$$

$$E_-^2 = 2\hbar v_F^3 m(n + 1)\delta^{-1}. \quad \text{(C.6)}$$

Since the energy has to be the same for both F_+ and F_-, we choose the solutions[4] $F_+^n = z_n$ and $F_-^n = z_{n-1}$, with $z_{-1} = 0$. Finally, from the definition $F_\pm = \phi_1 \pm \phi_2$, we obtain (properly normalized)

$$\phi_1(x) = [z_n(x) + z_{n-1}(x)]/\sqrt{2}, \quad \text{(C.7)}$$

$$\phi_2(x) = [z_n(x) - z_{n-1}(x)]/\sqrt{2}. \quad \text{(C.8)}$$

The above equations are the solution of equation (50).

[4] It is interesting to note that the system supports a zero-energy mode: $F_+^{n=0} = z_0$ and $F_-^{-1} = 0$.

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