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The Foldy-Wouthuysen and scattering matrix method for calculating the transmission of electrons through two dimensional graphene

Relativistic Electron Optics

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Abstract This paper provides a novel approach to solving the transmission of electrons through large graphene nano-structures, which is shown to be accurate both at high and low speeds. The model for graphene being solved is the continuum model governed by an analogue to the Dirac equation. For a solution, the Dirac equation is scalarised using the Foldy-Wouthuysen expansion approximation, to reduce the problem of calculating the electron wave propagation to a scalar differential equation. Also transformed is the exact solution of the Dirac equation in homogeneous space for the calculation of the propagation of electron waves. By analytically calculating the boundary conditions of the transformed wave functions, we have been able to generate transfer matrices for the scalar propagation equations. Furthermore, we have implemented the scattering matrix method upon these transfer matrices. Implementing the scattering matrix method makes a numerical stable propagation of the waves through the graphene. Finally we test the convergence and accuracy of the new method against analytic solutions. Also included is a rich appendix detailing the results of our research into relativistic Green's functions.

Keywords Quantum Electrodynamics · Special Relativity · Relativistic effects · Foldy-Wouthuysen Transformation · Transfer matrix · Quantum Tunneling · Electron Transport · Continuum model · Dirac equation · Graphene

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Mathematics Subject Classification (2000) 26B12 · 34A25 · 26A33

1 Introduction

There has been much attention paid recently to the electronic transport properties of graphene. However accurately solving the transmission problem for arbitrary boundaries is challenging, since electrons propagating through graphene’s honeycomb lattice effectively lose their mass, producing quasi-particles which can be described by a two dimensional analogue of the Dirac equation for spin half particles. This appearance of the Dirac equation motivates further study since it was the reason for interesting graphene properties to be predicted [1].

The possibility of device applications has motivated the theoretical and experimental study of electronic transport through various graphene nano-structures [2–13]. Examples of application of these previous works are the use of graphene as a semiconductor, with graphene layers used to create NAND flash memory and other logic gates, in the process exploiting the fantastic conductivity of graphene.

So far two types of theoretical approach, the tight binding method and the continuum model, have been employed to study the electron transport properties of graphene nano-structures [14–17]. However which of
these two models is numerically appropriate depends on the size of the graphene nano-structures under consideration.

The tight binding model for graphene is impractical for large structures due to the need to treat large matrices. To circumvent these numerical issues it is typical to switch to the continuum model, where the quantum mechanical bonding of the carbon structure is taken into account by an effective electron mass, potential, and importantly the Dirac equation [18,19]. Hence the solution of the Dirac equation for structures constructed from layers of potential and effective mass will be the subject of this paper.

An accurate method is required to predict transmission through graphene, particularly since Dirac equation electrons are regarded as useful for verifying quantum electrodynamic results [1]. Since Dirac equation electrons poses spin, relations between spin and graphene have also been studied [20].

In this paper we provide a novel approach to solving the transmission of electrons through graphene, which is accurate both at high and low speeds. we have scalarised the Dirac equation using the Foldy-Wouthuysen expansion approximation [21], to reduce the problem of calculating the electron wave propagation to a scalar differential equation. we have also transformed the exact solutions of the Dirac equation in order to calculate the propagation of the electron waves by this transformed equation. By analytically calculating the boundary conditions of the transformed wave functions, we have been able to generate transfer matrices for the scalar equation. Furthermore, we have implemented the scattering matrix method upon these transfer matrices [22]. Implementing the scattering matrix method makes a numerical stable propagation of the waves through the graphene [22].

Essentially my work has led me to develop a new type of perturbation theory for the boundary conditions of Quantum-Mechanical plane waves that allows for relativistic effects to be taken into account by way of a series of corrections in powers of \((v/c)\). The new method is currently limited to spin half particles, which require a four-component wave function for their full description. we used scalar wave functions for a numerical solution, this was made possible by a set of equations that we derived to translate back and forth between the numerical solutions and the four-component wave function.

In some ways this manuscript is similar to an earlier article [23] which transforms the Dirac equation into the telegrapher’s equation. However in that article, the approach did not make use of the Foldy-Wouthuysen transformation and so importantly was not perturbative. Also in contrast to Ref.[23] my approach differs by always reducing propagation to a scalar problem.

By formulating Relativistic Quantum Mechanics of plane waves as an optical problem it will in the future be possible to make use of Ref.[24] in order to calculate electronic transmission of translational invariant 1-dimensional chains to which defects such as ruptures are then introduced. Such works have relevance to polymeric systems.

The paper is organized as follows, Sec. 2 outlines the derivation of the Foldy-Wouthuysen scalarised Dirac equation from the Dirac equation. Sec. 3 gives the transformations of the solution back and forth between the two equations and derives the relationship between the transmission of the Foldy-Wouthuysen scalarised wave function and the Dirac wave function. Sec. 4 derives the boundary conditions of the Foldy-Wouthuysen equation. Sec. 5 derives the scattering matrix solution of the Foldy-Wouthuysen equation. Sec. 6 gives the transfer matrices in the special case of the delta potential barrier. Sec. 7 calculates parameters appearing in the scattering matrix solution of the Foldy-Wouthuysen equation. Sec. 8 calculates parameters appearing in the scattering matrix solution of the Foldy-Wouthuysen equation in the special case of the zero mass limit. Sec. 9 A, B, C and D gives the numerical validation of the new method using an example with an exact solution as well as studying the convergence of the new method. Importantly in Sec. 9 E the current-voltage (I-V) characteristics of a Graphene device are investigated.

The appendices are organized as follows, Appendix A gives the derivation of the homogeneous slab Green’s function. Appendix B gives the calculation of the free space Green’s function, Higher order Born approximation and transmission via a new Green’s function method. Appendix C gives a detailed analysis of the calculation method of the two probe Landauer conductance, orignally provided in Ref.[31]. Appendix D gives an approach to use our methods to calculate the band-gap of a one-dimensional Graphene super-lattice.

Green’s functions approaches for Relativistic Quantum Mechanics have proven fruitful in the past for previous authors when developing mathematical methods for analyzing the multi-channel coherent transport in Graphene [25].

2 The Dirac equation and its scalarisation in 2-dimensions

In this section I develop the scalarisation of the Dirac equation in 2D using the Foldy-Wouthuysen transformation [21] in the Newton-Wigner representation [26].
This is in order to recast the vector Dirac equation into a scalar equivalent. This recast equation will be developed for the purposes of the scattering matrix method in Sec. 5.

The well-known Dirac equation with scalar potential \( V \) is given in Hamiltonian form as

\[
[\alpha \cdot \hat{p} + \beta mc^2 - iV] \Psi = H \Psi = E \Psi
\]  

(1)

where

\[
\hat{p} = -ih \nabla = -ih \left( \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z} \right)
\]

(2)

from now on take \( \hbar = 1 \)

\[
\beta = \begin{pmatrix} +1 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & +1 \end{pmatrix}, \quad \hat{i} = \begin{pmatrix} +1 & 0 & 0 & 0 \\ 0 & +1 & 0 & 0 \\ 0 & 0 & +1 & 0 \\ 0 & 0 & 0 & +1 \end{pmatrix}
\]

(3)

\[
\alpha_{x,y,z} = \gamma_i \gamma_{x,y,z}
\]

(4)

\[
\alpha_x^2 = \alpha_y^2 = \alpha_z^2 = \beta^2 = 1
\]

(5)

\[
\gamma_i = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}
\]

(6)

\[
\gamma_{x,y,z} = \begin{pmatrix} 0 & +\sigma_{x,y,z} \\ -\sigma_{x,y,z} & 0 \end{pmatrix}
\]

(7)

\[
I = \begin{pmatrix} +1 & 0 \\ 0 & +1 \end{pmatrix}, \quad \sigma_x = \begin{pmatrix} 0 & +1 \\ +1 & 0 \end{pmatrix}
\]

(8)

\[
\sigma_y = \begin{pmatrix} 0 & -i \\ +i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} +1 & 0 \\ 0 & -1 \end{pmatrix}
\]

(9)

It will be noted that \( \alpha \) and \( \beta \) are Hermitian matrices in our special representation, so that in this representation \( H \) is Hermitian.

The Hermitian property of \( \alpha \) and \( \beta \) is necessary in order to obtain

\[
\rho = \Psi^* \Psi
\]

(10)

\[
j = \Psi^* \alpha \Psi
\]

(11)

as the expressions for charge and current density.

It can be shown by simple calculus and the de Broglie principle that for our Hamiltonian, solved for plane waves,

\[
E + V = \sqrt{p^2c^2 + m^2c^4}
\]

(12)

where \( p \) is the expectation value of momentum for the particle of mass \( m \). \( E \) is the energy eigenvalue.

There are two linearly independent solutions of the free particle Dirac equation. It is convenient to choose

the independent solutions so that each has two components which are zero. The two linearly independent solutions can be taken as

\[
\psi = \begin{pmatrix} E + V + mc^2 \\ 0 \\ 0 \\ \hbar c(p_x + ip_y) \end{pmatrix} e^{(p_x + ip_y)/\hbar}
\]

(13)

\[
\psi = \begin{pmatrix} 0 \\ E + V + mc^2 \\ \hbar c(p_x - ip_y) \\ 0 \end{pmatrix} e^{(p_x + ip_y)/\hbar}
\]

(14)

The idea upon which this manuscript is based is that by making use of the Foldy-Wouthuysen transformation the four coupled differential equations of the Dirac equation in Hamiltonian form can be decoupled to give four independent and importantly identical scalar equations. We only require to calculate the propagation of the single electron for one of these equations to get the full Green’s function and transmission. This considerably reduces the numerical complexity and yields great benefits in numerical accuracy and stability as we will see in the results section.

Let us now briefly outline the derivation of this transformation to arrive at the important results upon which the principle findings of this manuscript will be based.

\[
H \Psi = E \Psi \implies e^{+iS} H e^{-iS} e^{+iS} \Psi = E e^{+iS} \Psi
\]

(15)

Since we know

\[
e^{+iS} V e^{-iS} = V
\]

(16)

due to the scalarity of the potential and because \( e^{+iS} \) is unitary, let us only be concerned with

\[
e^{+iS} (\alpha \cdot \hat{p} + \beta mc^2) e^{-iS}
\]

(17)

We choose just as was done by Foldy and Wouthuysen

\[
e^{+iS} = \cos(\theta) + \beta \alpha \cdot \frac{\hat{p}}{|p|} \sin(\theta)
\]

(18)

\[
e^{-iS} = \cos(\theta) - \beta \alpha \cdot \frac{\hat{p}}{|p|} \sin(\theta)
\]

(19)

where

\[
is = \beta \alpha \cdot \frac{\hat{p}}{|p|} \theta
\]

(20)
Therefore it was shown by Foldy and Wouthuysen that
\[
e^{i S} \left( \alpha \cdot \hat{p} + \beta mc^2 \right) e^{-i S} = \left( \alpha \cdot \hat{p} + \beta mc^2 \right) \left( \cos(\theta) - \beta \alpha \cdot \frac{\hat{p}}{|p|} \sin(\theta) \right)^2 \]
\[
= \left( \alpha \cdot \hat{p} + \beta mc^2 \right) \left( e^{-2\alpha \cdot \hat{p} \theta / |\hat{p}|} \right)
\]
\[
= \alpha \cdot \hat{p} \left( \cos(2\theta) - \frac{mc}{|p|} \sin(2\theta) \right) + \beta \left( mc^2 \cos(2\theta) + c|p| \sin(2\theta) \right)
\]

We have arrived at the results of Foldy-Wouthuysen by exactly following their derivation.

The Foldy-Wouthuysen transformation gave us a choice for \( \theta \). However we required that \( H \) be transformed into diagonal form. Hence we had to follow the work of Newton and Wigner [26] and choose
\[
\frac{\sin(2\theta)}{\cos(2\theta)} = \tan(\theta) = \frac{|p|}{mc}
\]

Further following [26], we had to make another choice according to Eq. (22)
\[
\cos(2\theta) = \frac{mc^2}{\sqrt{c^2 p^2 + m^2 c^4}}
\]
\[
\sin(2\theta) = \frac{c|p|}{\sqrt{c^2 p^2 + m^2 c^4}}
\]

By direct substitution of Eq. (153) to Eq. (145) into Eq. (21) we arrive just as Newton and Wigner did, at the Newton-Wigner representation of the Dirac equation,
\[
\left[ \beta \sqrt{p^2 c^2 + m^2 c^4} - \hat{1} (V + E) \right] \Psi^{(FW)} = 0
\]

Eq. (25) is the Newton-Wigner representation of Foldy-Wouthuysen transformed equation.

We exploit the freedom of the sign associated with the square-root in Eq. (25) to ensure that the following decoupled equations are completely identical:
\[
\left[ \sqrt{p^2 c^2 + m^2 c^4} - (V + E) \right] \Psi_j^{(FW)} = 0
\]

where \( j = 1, 2, 3 \) or \( 4 \).

The solutions \( \Psi^{(FW)} \) in homogeneous space are given by rotation of Eq. (13) and Eq. (14) as
\[
e^{i S} \Psi = \Psi^{(FW)} = \begin{bmatrix} \psi_1^{(FW)} \\ \psi_2^{(FW)} \\ \psi_3^{(FW)} \\ \psi_4^{(FW)} \end{bmatrix}
\]

We will show in the subsequent sections of this manuscript that it is always possible to use these equations to formulate the problem of calculating the solution of electron wave propagation through a layered structure in such a way as the mathematics becomes identical to that of electromagnetic wave propagation through stacks of layered dielectric material.

By formulating electron propagation at relativistic speeds analogously to wave optics, we are able to make use of the powerfully accurate and numerically stable scattering matrix method of Ref. [22].

Furthermore we open the gates for a great deal more Optical theory to be transferred to the subject of Quantum Electrodynamics, especially with regards to photonic crystals [27].

3 The relationship between transmission of the Foldy-Wouthuysen transformed equation and the Dirac equation for inclined geometry

In this section we transform back and forth between the solution of the Dirac equation and the Foldy-Wouthuysen transformed wave equation. Furthermore we derived the relationship between the transmission calculated using the Foldy-Wouthuysen scalarised Dirac equation and the Dirac equation. This is necessary in order to translate the results from the propagation of \( \Psi^{(FW)} \) to the transmission of the full Dirac equation.

Firstly, let us denote \( d = p/|p| \), so that
\[
\frac{p_x}{|p|} = d_x, \quad \frac{p_y}{|p|} = d_y
\]

In order to make the necessary transformations we must evaluate \( \beta \alpha \cdot d \) which is,
\[
\beta \alpha \cdot d = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & + (d_x + id_y) & 0 \\ 0 & -(d_x - id_y) & 0 & 0 \\ -d_x & 0 & 0 & 0 \end{pmatrix}
\]

We now evaluate the transformed Foldy-Wouthuysen wave function. Since
\[
e^{+ \beta \alpha \cdot d \theta} \Psi = [\cos(\theta) + \beta \alpha \cdot d \sin(\theta)] \Psi = \Psi^{(FW)}
\]

where \( \Psi \) is given by Eq. (13) and Eq. (14) as,
\[
\Psi = A \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \end{pmatrix} e^{i(p_x x + p_y y)}
\]

we know by application of Eq. (29), Eq. (30) and Eq. (31) that
\[
\Psi_1^{(FW)} = [u_1 \cos(\theta) + (d_x - id_y) u_4 \sin(\theta)] A e^{i(p_x x + p_y y)}
\]
Hence we see that $\Psi$ by, the Dirac equation description is, a homogeneous space, please see Eq. (60) for more details.

Here we see the exponential wave form of $\Psi$ which is useful for calculating the electron propagation through homogeneous space, please see Eq. (60) for more details.

Conversely since we have seen that $\Psi^{(FW)}$ is given by,

$$\Psi^{(FW)} = \begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ F_4 \end{bmatrix} e^{i(p_x x + p_y y)}$$

we can construct the inverse transformation to be

$$u_1 A = [F_1 \cos(\theta) - (d_x - i d_y) F_4 \sin(\theta)]$$

$$u_2 A = [F_2 \cos(\theta) - (d_x + i d_y) F_3 \sin(\theta)]$$

$$u_3 A = [F_3 \cos(\theta) + (d_x - i d_y) F_2 \sin(\theta)]$$

$$u_4 A = [F_4 \cos(\theta) + (d_x + i d_y) F_1 \sin(\theta)]$$

Hence we see that $\Psi^{(FW)}$ combined with the Foldy-Wouthuysen transformation carries all the information needed to calculate the full solution of the Dirac equation in an infinitely homogeneous space.

Taking into account Eq. (10), Eq. (13) and Eq. (14), the incident wave upon the layered structure for the Dirac equation description is,

$$\Psi = A^{\text{incident}} \begin{bmatrix} u_1^{(i)} \\ u_2^{(i)} \\ u_3^{(i)} \\ u_4^{(i)} \end{bmatrix} e^{i(p_x x + p_y y)}$$

The transmitted wave for the Dirac equation is (please see Eq. (10), Eq. (13) and Eq. (14)),

$$\Psi = A^{\text{transmitted}} \begin{bmatrix} u_1^{(t)} \\ u_2^{(t)} \\ u_3^{(t)} \\ u_4^{(t)} \end{bmatrix} e^{i(p_x x + p_y y)}$$

The transmission to and from a vacuum and through the layered structure is given by,

$$t = \frac{A^{(\text{transmitted})}}{A^{(\text{incident})}}$$

However from Eq. (37) to Eq. (40) we see

$$t = \frac{F_1^{(t)} \cos(\theta^{(i)}) - (d_x^{(t)} - i d_y^{(t)}) F_4^{(t)} \sin(\theta^{(i)})}{F_1^{(i)} \cos(\theta^{(i)}) - (d_x^{(i)} - i d_y^{(i)}) F_4^{(i)} \sin(\theta^{(i)})} \frac{u_1^{(i)}}{u_1^{(t)}}$$

$$t = \frac{F_2^{(t)} \cos(\theta^{(i)}) - (d_x^{(t)} + i d_y^{(t)}) F_3^{(t)} \sin(\theta^{(i)})}{F_2^{(i)} \cos(\theta^{(i)}) - (d_x^{(i)} + i d_y^{(i)}) F_3^{(i)} \sin(\theta^{(i)})} \frac{u_2^{(i)}}{u_2^{(t)}}$$

$$t = \frac{F_3^{(t)} \cos(\theta^{(i)}) + (d_x^{(t)} - i d_y^{(t)}) F_1^{(t)} \sin(\theta^{(i)})}{F_3^{(i)} \cos(\theta^{(i)}) + (d_x^{(i)} - i d_y^{(i)}) F_1^{(i)} \sin(\theta^{(i)})} \frac{u_3^{(i)}}{u_3^{(t)}}$$

$$t = \frac{F_4^{(t)} \cos(\theta^{(i)}) + (d_x^{(t)} + i d_y^{(t)}) F_2^{(t)} \sin(\theta^{(i)})}{F_4^{(i)} \cos(\theta^{(i)}) + (d_x^{(i)} + i d_y^{(i)}) F_2^{(i)} \sin(\theta^{(i)})} \frac{u_4^{(i)}}{u_4^{(t)}}$$

Hence we have arrived at the general set of formula which converts the transmission of $\Psi^{(FW)}$ to transmission of $\Psi$.

Next, for the special case we are assuming that the potential is the same on both sides of the slab so that $u_1, u_2, u_3$ and $u_4$ are the same on both sides of the structure, so that also $\theta^{(i)} = \theta^{(t)}$. $F^{(i)}$ and $F^{(t)}$ are the incident and transmitted wave amplitudes of the Foldy-Wouthuysen transformed equation.

Furthermore I note that for each Foldy-Wouthuysen equation $CF_1^{(i)} = F_1^{(i)}$, $CF_2^{(i)} = F_2^{(i)}$, $CF_3^{(i)} = F_3^{(i)}$, and $CF_4^{(i)} = F_4^{(i)}$. This is because all four Foldy-Wouthuysen transformed equations are identical up to some proportionality factor, calculated from Eq. (13) and Eq. (14).

Hence substituting these assumptions and observations into Eq. (44) to Eq. (47), we have

$$t = \frac{F_j^{(t)}}{F_j^{(i)}} = C$$

where $j = 1, 2, 3$ or $4$.

In the general case of varying potential from one side to the barrier to the other, the Dirac vectors $u_j$ used in Eq. (44) to Eq. (47) must be normalized to the same value either side of the barrier using Eq. (10). This is so that the transmission squared can be calculated according to its usual definition, which is the ratio of charge incident to charge transmitted.

Thus transmission calculated from the Foldy-Wouthuysen equation can easily be used to calculate the transmission for the Dirac equation, with these derived relationships.
4 Boundary Conditions of the Foldy-Wouthuysen equation

Whilst we can find the solution of the homogeneous space Foldy-Wouthuysen equation relatively easily from the analytics of Sec. 2 and Sec. 3, in order to calculate the propagation of the single electron through several layers of Graphene and barrier stacks we require to know how the $\Psi^{(FW)}$ wave function propagates from layer to layer.

To this end I derive the boundary conditions of the scalarised Foldy-Wouthuysen equation by integrating across boundaries and taking advantage of the order, scalarity and linearity of the differential operator occurring in the Foldy-Wouthuysen equation.

Since
\[
\left[ \sqrt{p^2c^2 + m^2c^4} - (V + E) \right] \Psi^{(FW)} = 0 \tag{49}
\]
let us write $E = mc^2 + W$, then Eq. (49) becomes
\[
[L - (V + W)] \Psi^{(FW)} = 0 \tag{50}
\]
where
\[
L = mc^2 \left[ \frac{1}{2} \left( \frac{\hat{p}}{mc} \right)^2 - \frac{1}{8} \left( \frac{\hat{p}}{mc} \right)^4 + \frac{1}{16} \left( \frac{\hat{p}}{mc} \right)^6 - ... \right] \tag{51}
\]
due to the Taylor expansion of $\sqrt{p^2c^2 + m^2c^4}$

Next consider a boundary at $x = a$, a boundary between two homogeneous layers of material in a layered structure, such as a Bragg Mirror. If we integrate the scalarised Dirac equation through the boundary, normal to the boundary
\[
\lim_{|x+| \to \infty} \int_{a-}^{a+} [L - (V + W)] \Psi^{(FW)} dx = 0 \tag{52}
\]
But from Eq. (51) we can see that the following operators $\hat{L}$ and $\hat{p}_x$ commute,
\[
\hat{L} \Psi^{(FW)} = -\hat{L} \hat{p}_x \Psi^{(FW)} = -\hat{p}_x \hat{L} \Psi^{(FW)} \tag{53}
\]
We give a discussion of Eq. (53) in Appendix E.

Hence since by continuity of the quantum mechanical wave function,
\[
\lim_{|x+| \to \infty} \int_{a-}^{a+} (V + W) \Psi^{(FW)} dx = 0 \tag{54}
\]
due to the function integrated being finite but the integration range tending to zero, we have
\[
[i\hat{L} \Psi^{(FW)}]_{a+} = \lim_{|x+| \to \infty} \int_{a-}^{a+} L \Psi^{(FW)} dx = 0 \tag{55}
\]
We can understand Eq. (55) more clearly when we consider that
\[
\lim_{|x+| \to \infty} \int_{a-}^{a+} L \Psi^{(FW)} dx = \lim_{|x+| \to \infty} i \int_{a-}^{a+} \frac{d \Psi^{(FW)}}{dx} dx \tag{56}
\]
due to
\[
L \equiv -\hat{p}_x \hat{L} \equiv i \frac{d \hat{L}}{dx} \tag{57}
\]

Therefore, by Eq. (55) the Foldy-Wouthuysen wave function is continuous with respect to the operation of $\hat{L}$ in addition to the continuity of the $\Psi^{(FW)}$.

In order to evaluate $\hat{L} \Psi^{(FW)}$ and hence the boundary conditions note,
\[
\hat{L} \Psi^{(FW)} = (W + V) \Psi^{(FW)} = -\hat{L} \hat{p}_x \Psi^{(FW)} = -\hat{p}_x \hat{L} \Psi^{(FW)} \tag{58}
\]
hence
\[
\hat{L} \Psi^{(FW)} = -\frac{W + V}{\hat{p}_x} \Psi^{(FW)} = \alpha \Psi^{(FW)} \tag{59}
\]

Furthermore we note that $\hat{p} \Psi^{(FW)}$, the momentum operation, always gives a finite observed value, therefore $\Psi^{(FW)}$ is continuous everywhere. This follows simply by noting that the momentum is a gradient operator and that if the gradient is everywhere finite, then the function is by definition continuous. Furthermore conservation of energy demands that the energy and therefore the momentum of the particle is everywhere finite.

Hence we have developed a pair of boundary conditions for the scalarised Dirac Equation, which we can use to calculate the propagation of an electron through layered structures.

5 Scattering Matrix method for the Foldy-Wouthuysen Dirac equation

The continuity conditions derived in the last section for the relativistic electron wave at the interface adjoining layers will be expressed as matrix equations in this section. These matrix equations define the transfer matrices. By multiply successive transfer matrices an overall solution propagating waves through the whole structure is obtained. For more details of the origin of this technique in optics, see Ref.[29] and Ref.[30].

There are some problems with the transfer matrix. In the presence of beyond-critical-angle incidence wave modes of the system become a set of exponentially decaying and growing waves. Thus the problem arises that
the transfer matrix becomes dominated by exponentially growing waves that are several orders of magnitude larger in amplitude than the decaying waves. The consequences of combining such large and small numerical values together is that overall the transfer matrix become highly numerically unstable and inaccurate. In optics these points were first noted and addressed in Ref. [22].

Fortunately in the field of Optics a method to counter these numerical problems just mentioned has already been developed in Ref. [22]. In brief, the method of Ref. [22] explicitly separates the exponentially growing terms and the exponentially decaying terms.

In light of these considerations we will now formulate a set of equations describing propagation at the boundary which are mathematically identical to those governing propagation of electromagnetic waves through layered dielectric mediums so that the scattering matrix method of Ref. [22] can be applied.

Let \( a_0 \) and \( a_1 \) denote forward traveling Foldy-Wouthuysen scalarised wave parts and \( b_0 \) and \( b_1 \) denote backward travelling Foldy-Wouthuysen scalarised wave parts, 0 denotes on the left, 1 denotes on the right, then inside a layer thickness \( D \)

\[
\begin{pmatrix}
  e^{-ipD\cos(\phi)} & 0 \\
  0 & e^{+ipD\cos(\phi)}
\end{pmatrix}
\begin{bmatrix}
  a_1 \\
  b_1
\end{bmatrix}
= \begin{bmatrix}
  a_0 \\
  b_0
\end{bmatrix}
\tag{60}
\]

Eq. (60) is just the well-known transfer matrix, propagating wave functions of momentum \( p \) in the layer, through the layer, only now recast for the purposes of Quantum Electrodynamics. The electron is travelling at a transformed angle \( \phi \) to the layer boundary normal, where we see that

\[
P_x = p \cos(\phi)
\tag{61}
\]

For the boundary case, applying the two conditions derived in the last section gives

\[
a_0 + b_0 = a_1 + b_1
\tag{62}
\]

which is the continuity of the electron wave function through the boundary.

Secondly,

\[
\tilde{L}a_0 + \tilde{L}b_0 = \tilde{L}a_1 + \tilde{L}b_1
\tag{63}
\]

implies

\[
a_0a_0 - b_0a_0 = a_1a_1 - b_1a_1
\tag{64}
\]

Eq. (64) is a statement of the continuity of the wave function with respect to the \( \tilde{L} \) operator.

Eq. (62) and Eq. (64) can be written in matrix form as

\[
\begin{pmatrix}
  (1 + \alpha_1/\alpha_0)/2 & (1 - \alpha_1/\alpha_0)/2 \\
  (1 - \alpha_1/\alpha_0)/2 & (1 + \alpha_1/\alpha_0)/2
\end{pmatrix}
\begin{bmatrix}
  a_1 \\
  b_1
\end{bmatrix}
= \begin{bmatrix}
  a_0 \\
  b_0
\end{bmatrix}
\tag{65}
\]

This is just the well-known transfer matrix method at a boundary from the theory of Optics, recast now for the purposes of Quantum Electrodynamics.

The transfer matrix in the special case of the delta potential barrier is given in Sec. 6.

We are now in a position to apply the scattering matrix method of [22]. We let

\[
\begin{bmatrix}
  a_N \\
  b_N
\end{bmatrix}
= S(0, N) \begin{bmatrix}
  a_0 \\
  b_0
\end{bmatrix}
\tag{66}
\]

starting with

\[
S(0, 0) = \begin{pmatrix}
  1 & 0 \\
  0 & 1
\end{pmatrix}
\tag{67}
\]

and

\[
\begin{bmatrix}
  a_n \\
  b_n
\end{bmatrix}
= I(n + 1) \begin{bmatrix}
  a_{n+1} \\
  b_{n+1}
\end{bmatrix}
\tag{68}
\]

Now let us denote

\[
S(0, n) = \begin{pmatrix}
  S_{11} & S_{12} \\
  S_{21} & S_{22}
\end{pmatrix}
\tag{69}
\]

and

\[
I(n + 1) = \begin{pmatrix}
  I_{11} & I_{12} \\
  I_{21} & I_{22}
\end{pmatrix}
\tag{70}
\]

We can now write as was first done in Ref. [22] for optical systems,

\[
S_{11}(0, n + 1) = (1 - I_{11}^{-1}S_{12}I_{21})^{-1}I_{11}^{-1}S_{11}
\tag{71}
\]

\[
S_{12}(0, n + 1) = (1 - I_{11}^{-1}S_{12}I_{21})^{-1}I_{11}^{-1}(S_{12}I_{22} - I_{12})
\tag{72}
\]

\[
S_{21}(0, n + 1) = S_{22}I_{21}S_{11}(0, n + 1) + S_{21}
\tag{73}
\]

\[
S_{22}(0, n + 1) = S_{22}I_{21}S_{12}(0, n + 1) + S_{22}I_{22}
\tag{74}
\]

The scattering matrix method for the Dirac equation is hence formulated. Transmission can be derived from the numerically calculated propagation using the results in Sec. 3.

6 Quantum Electrodynamic transfer matrix for the delta potential barrier

In this Section we calculate the transfer matrix for the delta potential barrier.

The scalarised Foldy-Wouthuysen equation for the delta potential barrier in this case is given by

\[
[L - (W + g\delta(x))]\Psi^{(FW)} = 0
\tag{75}
\]

Integrating Eq. (75) across the delta function \([0_-, 0_+]\) where \(0_-, 0_+ \to 0\) gives

\[
[i\tilde{L}\Psi^{(FW)}]^{0_+}_{0_-} = g\Psi^{(FW)}\bigg|_{x=0}
\tag{76}
\]
Let \( a_0 \) and \( a_1 \) denote forward travelling Foldy-Wouthuysen scalarised wave parts and \( b_0 \) and \( b_1 \) denote backward travelling Foldy-Wouthuysen scalarised wave parts, 0 denotes on the left of the barrier, 1 denotes on the right of the barrier, then applying the continuity conditions upon the wave functions gives
\[
a_0 + b_0 = a_1 + b_1
\]  
which is the continuity of the electron wave function through the barrier.

Secondly,
\[
[i \bar{L} (a + b)]_{0-}^0 = g (a + b) \bigg|_{x=0}
\]  
implies
\[
i \alpha_k (a_1 - b_1) - i \alpha_k (a_0 - b_0) = g (a_1 + b_1)
\]  
Eq. (79) is a statement of discontinuity of \( \bar{L} \psi(FW) \) at \( x = 0 \).

Eq. (77) and Eq. (79) can be written in the following matrix form
\[
\begin{pmatrix}
(1 - ig/2\alpha_k) & (-ig/2\alpha_k) \\
(+ig/2\alpha_k) & (1 + ig/2\alpha_k)
\end{pmatrix}
\begin{bmatrix}
a_1 \\
b_1
\end{bmatrix} = \begin{bmatrix} a_0 \\ b_0 \end{bmatrix}
\]  
(80)

Hence we have derived the transfer matrix in the special case of the delta potential barrier.

7 The calculation of scattering matrix parameters for the case of varying effective mass and effective speed of light

An accurate method for calculating the \( \alpha \) parameters in the scattering matrix method formulated in the previous section is developed in this section. The method is based on a Taylor series of increasing powers of \((v/c)\), where \( v \) is the velocity of the electron travelling through the Graphene.

In this appendix we calculate the parameters appearing in the scattering matrix method for the important case of the effective mass and corresponding light speed, of the electron, varying from layer to layer.

In free space, by the Theory of Special Relativity, 
\[
W = E - mc^2 = \sqrt{p^2c^2 + m^2c^4} - mc^2
\]  
Let \( mk \) replace \( p \) as the momentum
\[
W = mc^2 \left[ \sqrt{1 + \left( \frac{k}{c} \right)^2} - 1 \right]
\]  
(82)

Inside a layer, again by Special Relativity,
\[
(E + V)^2 = m^2c^4 \left[ 1 + \left( \frac{q}{c} \right)^2 \right]
\]  
(83)

where \( m^* \) is the effective mass of the electron in the layer and \( c^* \) is the corresponding effective speed of light.

Comparing Eq. (81), Eq. (82) and Eq. (83), we find
\[
\frac{g^2}{k^2} = \left( \frac{mc}{m^*c^*} \right)^2 + \frac{mc^2}{m^*c^*} \frac{2V}{mk^2} + \frac{mc^2}{m^*c^*} \frac{2g(k/c)V}{mk^2}
\]
\[
+ \left( \frac{V}{m^*c^*k} \right)^2 + \frac{(mc^2 - m^*c^2)(mc^2 + m^*c^2)}{(m^*c^*)^2} \frac{1}{k^2}
\]
(84)

and in the last term we used the well-known analytic formula for the difference of two squares so as to greatly improve numerical accuracy. The analogue to velocity \( k \) becomes \( q \) inside the layer.

The function \( g(k/c) \) is given by,
\[
g(k/c) = \sqrt{1 + \left( \frac{k}{c} \right)^2 - 1} = \frac{(k/c)^2}{2} + \frac{(k/c)^4}{8} + \frac{(k/c)^6}{16} - ...
\]  
(85)

which can be expanded up to any order with Taylor series (see numerical results). Provided \((k/c)^2 \leq 1\) we are guaranteed convergence of \( g(x_k) \) in series form. Computationally we add smallest terms together first for improved numerical accuracy.

Interestingly Eq. (84) is analogous to
\[
(m^*q) = (mk)n_k
\]  
(86)

where \( n_k \) plays the role of the refractive index, in the Foldy-Wouthuysen transformed space. Assuming that the electron waves takes the route with the shortest time of flight in the transformed space, where \( mk \) plays the role of wave number, we arrive at the analogue of Snell’s law by following the derivation of Fermat (using Fermat’s principal of least time)
\[
\frac{\sin(\phi_i)}{\sin(\phi_t)} = \frac{m^*_t q_t}{m^*_i q_i}
\]  
(87)

where \( m^*_t q_t \) is the momentum of the electron in the transmitted layer, \( m^*_i q_i \) is the momentum of the electron in the incident layer. Also \( \phi \) is the transformed angle to the boundary normal in the incident layer made by the electrons trajectory. Furthermore \( \phi_t \) is the transformed angle to the boundary normal in the transmitted layer made by the electrons trajectory.

We have been able to apply Snell’s law because of the mathematical similarities between wave optics and our solutions to the scalarised Dirac equation. Also to do this I had to make analogies with wave number of planar electromagnetic waves and refractive index of the medium of propagation. Furthermore the concept of time of flight has changed, it is no longer ordinary time, but an analogy to time, consistent with the analogous
wave number. In brief, we have identified the quantities in the scalar wave function that are playing a role consistent with the various parameters in a Transverse Electric planar electromagnetic mode and then applied Snell’s law.

By Eq. (87) we can calculate the \( p_x \) component to be \( p \cos(\phi) \), which is useful when calculating \( \alpha \). Furthermore we calculate the \( p_y \) component to be \( p \sin(\phi) \).

To calculate \( \alpha_i \)

\[
\alpha_i = -\frac{W + V}{p_e} = -\frac{m^*c^2\left[\sqrt{1 + \left(\frac{q}{c}\right)^2} - 1\right]}{m^*q_x} \tag{88}
\]

In Eq. (88) we made use of Eq. (83),

\[
W + V = (E + V) - m^*c^2 = m^*c^2\sqrt{1 + \left(\frac{q}{c}\right)^2} - m^*c^2 \tag{89}
\]

Eq. (88) becomes with simple rearrangement,

\[
\alpha_i = -q\left(\frac{m^*\sqrt{1 + \left(\frac{q}{c}\right)^2}}{(q/c)^2} - \frac{m^*}{(q/c)^2}\right) \frac{q}{m^*q_x} \tag{90}
\]

\[
\alpha_i = -q\left(1 - \frac{(q/c)^2}{4} + \frac{(q/c)^4}{8} - \frac{5(q/c)^6}{64} + ...\right) \frac{q}{2q_x} \tag{91}
\]

which can be expanded to any order by considering the Taylor expansion of

\[
\sqrt{1 + \left(\frac{q}{c}\right)^2} \tag{92}
\]

Please note, that it is very important not to Taylor expand when \( (q/c)^2 > 1 \) since the expansion will diverge in this case. This condition puts limits on the numerical results possible (see results section). Again it should be noted that for reduced machine rounding error, smallest terms should be added together first to produce the most accurate simulated results.

Hence we see the case of application of the new theory to the important case of varying effective mass and corresponding light speed, of the electron, from layer to layer. Therefore we are able to take into account band structure and dispersion effects in various semiconductors.

8 Special case of zero mass limit

In this section we see the calculation of the various parameters required to apply the new scattering matrix method to the spin half particles with zero mass. An interesting question remains to be answered and may be the topic of future work, what are the boundary conditions between a region where the particle has zero mass and the region where the particle has an effective mass with regards to propagation.

Let us now consider the zero mass limit. When in the limit of \( m = 0 \), the neutrino or single photon limit, we see from Eq. (18) that,

\[
e^{iS} = \cos(\theta) + \beta \alpha \frac{\hat{p}}{|p|} \sin(\theta) \tag{93}
\]

\[
e^{iS} \Psi = \psi^{(FW)} \tag{94}
\]

and \( \theta = \pm \pi/4 \) by Eq. (153).

Furthermore Eq. (26), in the case of \( m = 0 \) limit, crosses over to becomes

\[\hat{p}c - (E + V)\] \( \psi^{(FW)} = 0 \tag{95}\]

However, equivalently we can write

\[\hat{p}c + (E + V)\] \[\hat{p}c - (E + V)\] \( \psi^{(FW)} = 0 \tag{96}\]

If we are only interested in the wave solution in infinitely homogeneous space, which for the present moment is the case, \( V \) and \( E \) are not dependent on position. Therefore we can commute \( E, V \) and \( \hat{p}, \) whilst also making use of the well-known formula for the difference of two squares and hence forth arrive at

\[\frac{\hat{p}c}{2} - (E + V)^2\] \( \psi^{(FW)} = 0 \tag{97}\]

or

\[M - (E + V)^2\] \( \psi^{(FW)} = 0 \tag{98}\]

We see again the same trick but this time for a different set of operators,

\[M = \hat{p}_z M = -\hat{M}\hat{p}_z \tag{99}\]

Therefore we can integrate across Eq. (98) at the boundary, as we did for Eq. (50) in Sec. 4 to find that in this special case of \( m = 0 \) \( \psi^{(FW)} \) is continuous with respect to \( M \).

In order to evaluate \( \hat{M}\psi^{(FW)} \) and hence the second boundary condition we note

\[M\psi^{(FW)} = (E + V)^2\psi^{(FW)} = -\hat{M}\hat{p}_z\psi^{(FW)} = -p_z M\psi^{(FW)} \tag{100}\]
hence

\[ \hat{M} \Psi^{(FW)} = -\frac{(E + V)^2}{p_x} \Psi^{(FW)} = -\frac{\gamma^2}{q_x} \Psi^{(FW)} = \alpha \Psi^{(FW)} \]  

(101)

In free space by Eq. (81), with \( m = 0 \) and momentum \( p = k \)

\[ E = kc \]  

(102)

so that from this dispersion it is clear that the spin half particle travels through the vacuum at the speed of light.

Furthermore in a potential \( V \), when \( m = 0 \) and momentum \( p = q \) by Eq. (81) again, we have

\[ q = k + V/c \]  

(103)

Again we note that \( \hat{p} \Psi^{(FW)} \), the momentum operation, always gives a finite observed value, therefore \( \Psi^{(FW)} \) is continuous everywhere.

9 Numerical Validation

In this section we run through a series of demonstrations and validations of the new numerical method which I have developed.

Throughout this numerical demonstration \( m = 2 \), also we use mixed notation of \( \gamma = c \) to make figures clearer. The motivation for using \( \gamma \) instead of \( c \) is that in Graphene the effective speed limit \( \gamma \) on the electrons is much less than \( c \). Importantly \( c = 50c \). The Graphene electrons are obeying an equation analogous to the Dirac equation, actually the typical speed of an electron in a Graphene device is 0.03c.

All arithmetic is carried out with 15 decimal digits of precision allocated for every variable.

9.1 Validation of the new method with an analytic Green’s function

In this sub-section is presented the validation of the Foldy-Wouthuysen scattering matrix method by comparison with the analytic Green’s function for the scalarised Dirac equation which we have derived in Appendix A.

The analytic Green’s function \( G(x, x') \) is used to generate the transmission via,

\[ T(k) = |2\alpha k G(x, x')|^2 \]  

(104)

which I have derived in Appendix B.

The system under consideration is described by the simple potential slab of Graphene with \( a = 1 \)

\[ V(x) = \begin{cases} \frac{mc^2}{\alpha} & \text{for } |x| < a/2, \\ 0 & \text{elsewhere}. \end{cases} \]  

(105)

Furthermore due to the limitations upon the analytic solution, this section is restricted to the treatment of the 1-dimensional problems, i.e. \( p_y = 0 \) at all points on the electron journey, and furthermore the layer boundaries are parallel to the \( y \)-axis.

The absolute error in transmission for the structure in Eq. (105) over a range of momentums is shown in Fig. 1. In Fig. 1 the absolute error is calculated using the exact Green’s function solution for the slab. The exact solution is calculated using 160 relativistic corrections in the calculation of each momentum and \( \alpha \) parameter.

In Fig. 1 we see a power law convergence with number of Taylor series corrections to the new scattering matrix method towards the exact solution. For \( N = 80 \) corrections we see that the absolute error in transmission is less than \( 10^{-15} \) for all speeds less than \( v = \gamma/2 \).
9.2 Convergence of the new method for Bragg Mirror Microcavities

Again this sub-section is restricted to the momentum of 1-dimensional problems, i.e. $p_y = 0$ at all points in the electron journey, and furthermore the layer boundaries are parallel to the $y$-axis. In this sub-section, we test the new scattering matrix method further we move on to a non-trivial example which has no known analytic solution. The potential profile is shown in Fig. 2.

The estimated absolute error in transmission for the structure in Fig. 2 over a range of momentums is shown in Fig. 3. In Fig. 3 the absolute error is estimated using the scattering matrix having $N = 160$ relativistic corrections in place of an exact solution. In Fig. 3 we see a power law convergence with the number of Taylor series corrections, towards the exact transmission. For $N = 80$ corrections we see that the estimated absolute error in the transmission is less than $10^{-15}$ for all speed less than $v = 2\gamma/3$.

9.3 Convergence of the new method for inclined geometry

This sub-section is restricted to the treatment of the 2-dimensional problems, i.e. $k_y/\gamma = 0.2$ for the incident momentum parallel to the $y$-axis, and furthermore the layer boundaries are parallel to the $y$-axis.

The absolute error in transmission for the structure in Fig. 2 over a range of momentums is shown in Fig. 4. In Fig. 4 the absolute error is estimated using a Foldy-Wouthuysen scattering matrix method expansion and $N = 160$ relativistic corrections.

In Fig. 4 we see a power law convergence with the number of Taylor series corrections of the new method towards the estimated exact solution. For $N = 80$ corrections we see again the estimated error in transmission is less than $10^{-15}$ for all speed less than $v = 2\gamma/3$.

9.4 Comparison of the new method with analytic results from the literature

This sub-section is restricted to the treatment of 1-dimensional problems, i.e. $p_y = 0$ at all points in the electron journey, and furthermore the layer boundaries are parallel to the $y$-axis.

In this sub-section we test the new method against the analytic solution provided by Ref.[28] in order to compare the new method to existing techniques. We find the new relativistic scattering matrix method is in agreement with the method of Ref.[28].

The simple structure for this test is given by Eq. (105). The new scattering matrix method has already been validated for this structure in Sec. 9 A.

For the simple example with analytic solutions we consider a potential slab of Graphene, taking $a = 1$. The analytic solution I use for this simple structure Eq. (105) was developed in [28] and is given in simplified

---

Fig. 2 (Color online) Cross-section of the non-trivial nano-structure used to test the new method of calculating the transmission, potential $V$ is given as a function of coordinate $2x/a$, where $a$ is the slab width. Importantly, I set the parameter $a = 1$.

Fig. 3 (Color online)(a) Electron transmission through Graphene nano-structure in Fig. 2, both relativistic (blue) and non-relativistic (black) (b) Estimated absolute error in the transmission for the numerical values from the Foldy-Wouthuysen scattering matrix method. A Foldy-Wouthuysen scattering matrix method expansion with $N = 160$ relativistic corrections is used as an estimate for the exact transmission. The number of relativistic corrections is $N = 20, 40, 80$ as labelled. For further comparison the solution without relativistic corrections is included.
The treatment of 2-dimensional problems, i.e. $k_s/\gamma = 0.2$. (a) Electron transmission through the structure in Fig. 2 over a range of momentums, both relativistic (blue) and non-relativistic (black) (b) Estimated absolute error in the transmission for the numerical values from the Foldy-Wouthuysen scattering matrix method. A Foldy-Wouthuysen scattering matrix method expansion with $N = 160$ relativistic corrections is used as an estimate for the exact transmission. The number of relativistic corrections is $N = 20, 40, 80$ as labelled. For further comparison the solution without relativistic corrections is included.

\[
T(k) = |t|^2 = \frac{4k^2}{4k^2 + (1 - k^2)^2 \sin^2(mqa)} \quad (106)
\]

\[
k = \frac{q (-kma + 2me^2)}{kt(-kma + 2me^2 + V)} \quad (107)
\]

In Fig. 5 we can see as we increase the number of relativistic corrections, the absolute error in the Foldy-Wouthuysen scattering matrix method converges to the analytic solution of Ref.[28]. As the exact solution we used the analytic solution of Ref.[28] with 160 relativistic corrections to the energy and wave number.

We can see from the results of the previous four subsections that the Foldy-Wouthuysen scattering matrix method is in complete agreement with analytic solutions and has a power law convergence with the number of relativistic corrections.

**9.5 Demonstration of the calculation of current-voltage characteristics of a device**

This subsection demonstrates the calculation of useful quantities for Graphene devices. Furthermore the convergence of the calculated quantities with number of Relativistic corrections is also studied. We consider transmission through a slab geometry for the more general case where the Graphene leads are doped. This is achieved by using our numerical transmission to evaluate the two-probe Landauer conductance which was first done in Ref.[31] and is justified with more detail in Appendix C where we re-derive (from Ref.[31]) the following useful relations, however with increased mathematical detail,

\[
I(V) = \frac{e^2}{\pi h} \langle T(E_F) \rangle (4\pi gn)^{1/2} L_y V \quad (108)
\]

\[
V = \frac{\mu_L - \mu_R}{e} \quad (109)
\]

\[
\langle T(E_F) \rangle = \int_0^{+\pi/2} \frac{d\theta}{2\pi} T(E_F, \theta) \cos(\theta) \quad (110)
\]

In Eq. (108) we see a power law convergence with the number of relativistic corrections. For an exact solution we use a simulation with $N = 160$ relativistic corrections. Importantly in Eq. (108) we take $aK_F/\gamma = 0.8$ as the Fermi wavenumber. To make the integration in Eq. (110) we use the adaptive Symson method.

The geometry we consider is given in Fig. 6 where we see that the potential of the cavity is varied from $V_{cav}/\gamma^2 = 0.0590$ and $V_{cav}/\gamma^2 = 0.0610$. Fig. 6 corresponds to a Bragg-mirror microcavity.
We can see from Fig. 7 that as the number of Relativistic corrections increases the absolute error in \( \langle T(E_F) \rangle \) reduces like a power law. When we have more than \( N = 80 \) relativistic corrections we typically have absolute error less than \( 10^{-10} \).

In light of the results and convergence shown in this subsection, it is clear that the theory developed in this manuscript is well suited to the modeling and prediction of practical Graphene electronic devices.

### 10 Summary

In this work we see developed a new scattering matrix method for Graphene in 2D, we have studied the convergence and seen that the error in calculated transmission converges like a power law with respect to the number of relativistic corrections included in the Foldy-Wouthuysen scalarisation transformation, for both 1-dimensional and 2-dimensional geometries. It is hoped that in the future this new mathematical method will be further numerically validated and benchmarked against other methods for its numerical stability and accuracy.

Future developments will involve the inclusion of dispersive RSE perturbation theory [32–40]. Specifically we plan to extend the derivation of the normalization which Doost made in Ref.[35] to relativistic open systems. As always, we note that as a subsequences to my rigorous normalization derivations of Ref.[35] E. A. Muljarov incorporated his zero frequency mode discovery into my now generalized normalization. Furthermore we note that the first of the series of RSE waveguide papers, which we reference, was predominantly the work of E. A. Muljarov.

#### A Analytic Green’s function for the 1-dimensional homogeneous slab

This appendix is restricted to the treatment of 1-dimensional problems, i.e. \( p_y = 0 \) at all points in the electrons journey, and furthermore the layer boundaries are parallel to the \( y \)-axis.

In this appendix we will derive an analytic Green’s function for the homogeneous Graphene slab.

For convenience and mathematical compactness the slab half width is taken to be \( a = 1 \). Consider

\[
[L - (V + W)] G(x, x') = \delta(x - x')
\]

(111)

Let \( \Psi_L(x) \) and \( \Psi_R(x) \) be the left and right homogeneous solutions, which each separately satisfy the boundary conditions at \( x = -a \) and \( x = +a \) respectively. Then I will show that the Green’s function of Eq. (111) for the case of a homogeneous 1-dimensional slab can be written as

\[
G(x, x') = \frac{\Psi_L(x)}{W} \Psi_R(x')
\]

(112)
where \( x_- = \min(x, x') \) and \( x_+ = \max(x, x') \) and
\[
W = iW_R(x)\Psi_L(x) - \Psi_R(x)iW_L(x)
\] (113)
is the Wronskian, which does not depend on \( x \) and therefore can be calculated for any value of \( x \) producing the same result.

To prove these points note that from Eq. (111)
\[
\lim_{s \to 0} \int_{x'_-}^{x'_+} LG(x', x) dx = \int_{x'_-}^{x'_+} \delta(x - x') dx = 1
\] (114)
which implies
\[
iLG(x, x') - iLG(x, x') = 1
\] (115)
We write out Eq. (112) explicitly to find
\[
G(x, x') = \frac{1}{W} \int \frac{\Psi_L(x)\Psi_R(x')}{x < x'}, \quad \frac{1}{W} \int \frac{\Psi_L(x')\Psi_R(x)}{x > x'},
\] (116)
applying \( L \)
\[
iLG(x, x') = \frac{1}{W} \int \frac{i\Psi_L(x)\Psi_R(x')}{x < x'}, \quad \frac{1}{\Psi_L(x')}\Psi_R(x')\frac{1}{W} \int \Psi_L(x)\Psi_R(x)
\] (117)
and substituting into Eq. (115) gives
\[
\frac{1}{W} \int \frac{\Psi_L(x')}\Psi_R(x')\frac{1}{W} \int \frac{\Psi_L(x)\Psi_R(x)}{x > x'} = 1
\] (118)
which is the definition of the Wronskian. Hence our proof is complete.

Let us now make use of these results to calculate the Green’s function.

\[
\Psi_1(x) = \begin{cases} 
C_{e^{imkx}} + De^{-imkx}, & x > a, \\
0, & x < a.
\end{cases}
\] (119)

Boundary conditions at \( x = +a \) (continuity of \( \Psi_1(x) \)) give
\[
C_{e^{imkx}} + De^{-imkx} = e^{imkx}
\] (120)
and (continuity of \( \Psi_1(x) \) with respect to \( L \))
\[
C_{e^{imkx}} - De^{-imkx} = \frac{\alpha_k}{\alpha_q} e^{imkx}
\] (121)
Therefore
\[
C = \frac{\omega_q + \alpha_k}{2\alpha_q} e^{imkx} \quad D = \frac{\alpha_q - \alpha_k}{2\alpha_q} e^{imkx}
\] (122)
\[
\Psi_2 \text{ the left hand solution is given by } \Psi_2(+x) = \Psi_1(-x). \quad \text{Hence the Wronskian is given by}
\]
\[
W = 2i\alpha_q(C^2 - D^2)
\] (123)
as can be seen easily by evaluating the Wronskian at \( x = 0 \). Hence when \( x = +a \) and \( x' = -a \), Eq. (112) simplifies to
\[
G(a, -a) = \frac{1}{2\alpha_q} \left( \frac{4\alpha_q^2}{(\alpha_q + \alpha_k)^2e^{-2imkx} - (\alpha_q - \alpha_k)^2e^{2imkx}} \right)
\] (124)
or for improved numerical performance
\[
G(a, -a) = \frac{i\alpha_q}{t(\alpha_q + \alpha_k)^2(2m^2\alpha_q) - (\alpha_q - \alpha_k)^2e^{2imkx}}
\] (125)
Hence we derive a new analytic Greens function which can be used in Eq. (131) of Appendix B to formulate a new and highly accurate mathematical expression for the transmission of electrons through a homogeneous slab of potential \( V \) embedded in a vacuum, which is valid for relativistic and non-relativistic tunneling.

**B Analytic Green’s function for the 1-dimensional free space**

This appendix is restricted to the treatment of 1-dimensional problems, i.e. \( p_y = 0 \) at all points in the electrons journey, and furthermore the layer boundaries are parallel to the \( y \)-axis.

For convenience and mathematical compactness the slab half width is taken to be \( a \) in this section.

Here we develop the free space Green’s function of the scalarised Dirac equation in 1-dimensional free space. Also developed in this appendix is a Green’s function expression for the transmission through a nano-structure.

The free space Green’s function in this case can be written as
\[
[L - W]G^{fs}(x, x') = \delta(x - x')
\] (127)
when \( x' = 0 \)
\[
G^{fs}(x, 0) = \begin{cases} 
A e^{-imkx}, & x < 0, \\
A e^{imkx}, & x > 0.
\end{cases}
\] (128)

Integrating Eq. (127) across the delta source \( [0, 0] \) gives
\[
\frac{i}{A L e^{imk0} - A L e^{-imk0}]} = 1
\] (129)
But since \( L e^{imk0} = +\alpha_k \) as \( 0_+ \to 0, L e^{-imk0} = -\alpha_k \) as \( 0_- \to 0, \) we find
\[
A = \frac{1}{2i\alpha_q}
\] (130)
Hence the transmission for a homogeneous slab, embedded in a vacuum free space, with scalarised wave function described by \( G(x, x') \) follows simply by comparing \( G^{fs}(x, x') \) and \( G(x, x') \) as
\[
T(k) = \frac{2\alpha_k G(x, x')}{G^{fs}(+a, -a)}
\] (131)
since
\[
t(k) = T(k) = \frac{G(+a, -a)}{G^{fs}(+a, -a)}
\] (132)

The Eq. (132) is simply a mathematical expression of \( t(k) \) being the ratio of incident to transmitted probability density for the electron through the structure. The incident wave is given by \( G^{fs}(+a, -a) \) and the transmitted wave is given by \( G(+a, -a) \). The source of the waves is at \( x = -a \) and the point of observation is at \( x = +a \), the boundaries of the effectively 1-dimensional structure. The structure of width \( 2a \) is of homogeneous potential \( V \), embedded in free space. The momentum of the incident and transmitted electrons is \( mk \).

In principal \( G(+a, -a) \) could be the Green’s function of any 1-dimensional slab embedded in free space, we are not restricted to homogeneous slabs, an arbitrary potential profile for the slab, within the boundaries, is allowed by Eq. (132).

A potential application of Eq. (128) in the Higher order Born approximation arises if we take the effective speed of light and electron mass to be constant throughout its journey. In this case the Dyson equation follows naturally from the properties of \( L \) and is given in its usual form as:
\[
G_k(x, x'') = G^{fs}_k(x, x') + \int G^{fs}_k(x, x') V(x') G_k(x', x'') dx'
\] (133)
Title Suppressed Due to Excessive Length

C Derivation of the two probe Landauer conductance

For completeness of our manuscript, this appendix repeats the mathematical derivation of Ref.[31], however in this case with much more detailed mathematical analysis.

I will now re-introduce the notation of Ref.[31]. In this section, we consider transmission through a slab geometry for the more general case where the Graphene leads are doped. At first, we define a vertical (y directed) surface $\Sigma$ somewhere to the right of the $N^{th}$ slab. The current across that surface will be a sum of three contributions. First, there will be carriers injected from the left side, with chemical potential $\mu_L$, moving at angle $\theta$, which make it past the slabs with probability $T(E, \theta)$. These are all right-movers. Second, there will be carriers from the right lead, with chemical potential $\mu_R$, moving at angle $\theta$. Because of this range of $\theta$, all these are left-movers. Finally, with probability $R(E, \theta)$, each of these left-moving carriers reflects off the barrier region, scattering into a state with $\theta' = \pi - \theta$. Putting this all together, we get

$$I_\Sigma = L_\Sigma \hat{n}_\Sigma \int_{-\infty}^{+\infty} dE N(E) \int_{-\pi/2}^{+\pi/2} d\theta$$

$$\times \left[ T(E, \theta) J(E, \theta) f(E - \mu_L) + [J(E, \pi + \theta) + R(E, \pi + \theta) J(E, -\theta)] f(E - \mu_R) \right]$$

$$= \frac{g |E|}{2\pi \hbar^2 v_F}$$

Due to the Pauli Exclusion Principal, not all the electrons can occupy the ground state. Infact only two electrons (Spin up and Spin down) can occupy each Quantum-state, hence states become occupied up to the very high Fermi energy $E_F$.

This high $E_F$ is very important. Since electrons can only tunnel from occupied to unoccupied states, we expect only significant tunneling to occur near the Fermi surface.

Let us check the comments just made. At $T = 0$ we can see that when $E$ is less than the chemical potential

$$\exp \left( \frac{E - \mu}{k_B T} \right) \approx 1 \implies f(E, 0) = \frac{1}{2}$$

otherwise $f = 0$.

From Eq. (141), substituting in Eq. (145) we find

$$I_\Sigma = L_\Sigma \hat{n}_\Sigma \int_{-\infty}^{+\infty} dE N(E) \int_{-\pi/2}^{+\pi/2} d\theta$$

$$\times \left[ T(E, \theta) J(E, \theta) f(E - \mu_L) + [J(E, \pi + \theta) + R(E, \pi + \theta) J(E, -\theta)] f(E - \mu_R) \right]$$

Since $T(E, \theta) + R(E, \pi + \theta) = 1$ due to the S-matrix $I_\Sigma = 0$ in this case.
Therefore we must consider $T \neq 0$ whilst at the same time $T \approx 0$. In this case we can make the following Taylor expansion about $T = 0$,

$$f(E, T) \approx f(E, 0) + T \cdot \frac{df(E, 0)}{dT} = \left( \frac{1}{2} + T \cdot \frac{df(E, 0)}{dT} \right)$$

(147)

From detailed analytics it can be shown that

$$\frac{df(E, 0)}{dT} = \frac{(E - \mu) \exp \left( \frac{E - \mu}{k_B T} \right)}{k_B T^2 \left[ \exp \left( \frac{E - \mu}{k_B T} \right) + 1 \right]^2}$$

(148)

Hence

$$\frac{df(E, 0)}{dT} = \frac{(E - \mu)}{k_B T^2}$$

(149)

and so

$$f(E, T) \approx f(E, 0) + T \cdot \frac{df(E, 0)}{dT} = \frac{1}{2} + \frac{(E - \mu)}{k_B T^4}$$

(150)

Due to the high $E_F$, only very few electrons are excited, those very close to the Fermi-Surface. This region close to the surface, therefore contains unoccupied states, states that can be tunneled into. It is well-known that this range is given to good approximation by

$$E_F - 2k_BT < E < E_F + 2k_BT$$

(151)

These effects just described are a direct consequence of the Pauli exclusion Principle.

These results regarding the Fermi-Dirac distribution and the Fermi-surface, particular the derived Taylor expansion allow us to evaluate the following integral,

$$\int f(E, T) dE \approx \int_{E_F - 2k_BT}^{E_F + 2k_BT} f(E_F) dE = 2k_BT + (E_F - \mu) + ...$$

(152)

This is important information necessary to understand Eq.47 of Ref.[31]. In fact, substituting Eq. (150) into Eq. (141), over range Eq. (151), taking account that as we have shown $I_{\Sigma} = 0$ when $T = 0$, we arrive at,

$$I_{\Sigma} = L_{\Sigma} \left\{ \frac{g(E_F)}{\pi \hbar^2 v_F^2} \int_{-\pi/4}^{\pi/4} d\theta \frac{(2\pi gn)^{1/2}}{2\pi} \right\} \int_{-\pi/4}^{\pi/4} T(E_F, \theta) \cos(\theta) \right\}(\mu_L - \mu_R)$$

(153)

which gives us Eq.47 from Ref.[31]

$$I(V) = \frac{e^2}{\pi \hbar} \left\{ (T(E_F)) \right\} (4\pi gn)^{1/2} L_y V$$

(154)

$$V = \frac{\mu_L - \mu_R}{\epsilon}$$

(155)

$$N_c = \frac{g}{\pi} k_F L_y = \left( \frac{4\pi gn}{\pi} \right)^{1/2} L_y$$

(156)

$$\langle T(E_F) \rangle = \int_0^{\pi/2} \frac{d\theta}{2\pi} T(E_F, \theta) \cos(\theta)$$

(157)

D Derivation of Band Gap in one dimensional Graphene super-lattices

In infinitely periodic Graphene structures, of spacial period $D$, we see that the wav-function also has the same periodicity. This is the well-known Blocha Theorem, which can be stated as,

$$\psi(FW)(x + D) = e^{iKD}\psi(FW)(x)$$

(158)

which in terms of transfer matrices this can be written alternatively as

$$M\hat{\psi}(FW)(x) = e^{-iKD}\hat{\psi}(FW)(x)$$

(159)

where

$$M = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix}$$

(160)

Hence from Eq. (159)

$$(M_{11} - \lambda)(M_{22} - \lambda) - M_{12}M_{21} = 0$$

(161)

Also we have, since $M$ is unitary,

$$M^2 = I$$

(162)

From Eq. (161), we have,

$$\lambda = \frac{M_{11} + M_{22} \pm \sqrt{(M_{11} + M_{22})^2 - 4(M_{11}M_{22} - M_{12}M_{21})}}{2}$$

(163)

If we make use of Eq. (162) then Eq. (163) simplifies to,

$$\lambda = \frac{M_{11} + M_{22}}{2} = e^{iKD}$$

(164)

Since $M$ is real and $K$ is real, we know that,

$$-1 \leq \cos(KD) = \frac{M_{11} + M_{22}}{2} \leq 1$$

(165)

We know that $M_{11}$ and $M_{22}$ are dependent on $k$. Hence we see the conditions for a band gap to arise, a range of electron momentums at which electrons cannot propagate and at which the periodic structure acts like a filter. Band-gaps arise in the one dimensional super-lattice if the condition of Eq. (165) is not met.

E Proof of commutation

In this appendix we will provide a proof of the important relation

$$L = -\hat{\rho}_x \hat{L} = -\hat{L}\hat{\rho}_x \equiv i\frac{d\hat{L}}{dx}$$

(166)

In order to make our proof of this section we must consider the form of the form of the operator $L$

$$L = mc^2 \left[ \frac{1}{2} \left( \frac{\hat{p}}{mc} \right)^2 - \frac{1}{8} \left( \frac{\hat{p}}{mc} \right)^4 + \frac{1}{16} \left( \frac{\hat{p}}{mc} \right)^6 - ... \right]$$

(167)

where

$$\frac{1}{2} \left( \frac{\hat{p}}{mc} \right)^2 = -\frac{1}{2m^2c^2} \left( \frac{d^2}{dx^2} + \frac{d^2}{dy^2} \right)$$

(168)
We can see this from the mathematical form of $L$ and Eq. (171) that we can extract this is our assumption in our proof. We see from Eq. (170) when every term in $f$ is a function of not just $y$ but also $x$, this is our assumption in our proof. We see from Eq. (170) and Eq. (171) that we can extract $d/dx$ from either side of the operator $d^n/dy^n$, in this case.

When our assumption is not met, i.e. $f(x,y) = f(y)$, then in general
\[
\frac{d^n}{dy^n}f(x,y) \neq 0
\] (172)
but
\[
\frac{d}{dx}f(y) = 0
\] (173)
therefore in general
\[
0 \neq \frac{d^n}{dy^n}f(y) \neq \frac{d^{n-1}}{dy^{n-1}} \cdot \frac{dx}{dy} \cdot \frac{d}{dx}f(y) = 0
\] (174)

In this case, when our assumption is not met, in general we cannot extract $d/dx$ from either side of the operator $d^n/dy^n$, as is shown by Eq. (174).

In conclusion, we can see that Eq. (166) is true when we assume that $L$ acts on a function of not just $y$ but also $x$. We can see this from the mathematical form of $L$ and the mathematical relations in this appendix.

### F Future work

We plan to develop a time dependent Born approximation, based on Fold-Wouthuysen transformation, as part of a general software package. Also we will use Monte Carlo techniques for electron thermal transport in Graphene. Moreover, we predict the application of new generation of Graphene to make and design new quantum computers and a new way for describing quantum tunelling.

### G Conflict of interest statement

The corresponding author states that there is no conflict of interest.

### References

31. arXiv:1002.3655v2