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Two-Dimensional Schrödinger Scattering and Electron Transport in Graphene

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Abstract

Two-dimensional Born scattering for the non-relativistic case is considered, the purpose being to investigate electron transport properties in mono-layer Graphene subject to an applied parallel electric field. Solutions for the Probability Density Current (PDC) are obtained in the Fresnel zone which provides a model for simulating the PDC subject to membrane crumpling. In this context a Random Fractal Defect Model is considered which is used to assess the effect of (Fractal) crumpling on the PDC.

Mathematics Subject Classification:
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Electron Transport, Two-dimensional Point Scattering, Schrödinger Scattering, Born Approximation, Fresnel Zone Analysis, Mono-layer Graphene, Random Fractal Defect Model.

1 Introduction

Modelling electron transport is important in understanding the properties of conductors and semi-conductors. In most cases, three-dimensional models are considered in keeping with the dimensional properties of the majority of crystalline structures. However, since the discovery of mono-layer Graphene in 2004 [1], a two-dimensional crystalline material, two-dimensional electron transport models have become important in attempting to determine the properties of this material, [2] and [3].

Graphene is a single layer of carbon atoms arranged into a two-dimensional hexagonal-based honeycomb lattice and can be considered as a basic building

block for graphitic materials of other dimensions. It is currently the only known one-atom-thick crystalline form of matter, but, on a theoretical basis at least, two-dimensional graphite has been studied since the late 1940s and is widely used for describing properties of various carbon-based materials.

An interesting property of Graphene is that the charge carriers are relativistic. Even though they are not actually travelling at relativistic speeds, their structural interaction causes them to act like two-dimensional Dirac Fermions with zero rest mass at the Dirac points on the six comers of the hexagon although this pseudo-relativistic description is restricted to the chiral limit. Thus, the charge carriers in Graphene have a unique property in that they mimic relativistic particles as described by the Dirac equation rather than the Schrödinger equation [4], [5]. The relativistic-like description of electron waves on honeycomb lattices has been considered on a theoretical basis for many years and is now being applied in an attempt to understand the electronic properties of Graphene since the experimental discovery of the material, e.g. [6], [7], [8] and [9].

Graphene is the strongest and most conductive room temperature material known and is a semi-metal (a zero-gap semi-conductor) with a wide range of potential applications including ballistic transistors, nano-ribbons, ultra-sensitive molecular sensing, super capacitance and Spintronics. Electron transport measurements show that Graphene has a remarkably high electron mobility at room temperature, with reported experimental values in excess of $200,000$ $\mathrm{cm}^2\mathrm{V}^{-1}\mathrm{s}^{-1}$ at electron densities of $2 \times 10^{11}\mathrm{cm}^2$ [10].

While the theoretical 'relativistic properties' of Graphene remains to be fully correlated with experimental evidence, the non-relativistic properties of the material remain a subject of research in terms of (non-relativistic) incident electrons scattering from a two-dimensional electrostatic lattice potential. This potential derives from the de-localised electrons associated with the hexagonal nature of the primary structure of Graphene as replicated throughout the lattice. In this sense, each primary element of Graphene is analogous to the structure of Benzene from which the concept of de-localised electrons was first derived. The de-localised electrons represent a repulsive electrostatic potential with respect to incident electrons propagating through the material through the application of an electric field and it is in this context that the results reported in this paper are derived.

In this paper, the two-dimensional properties of non-relativistic scattered wave functions are considered from which a quasi-one-dimensional model is derived under the Born approximation. By evaluating the PDC it is shown that when a uniform Electric Field $\mathcal{E}_x$ is applied, ballistic electron transport occurs when $\mathcal{E}_x >> 1$. The paper also introduces a Random Scaling Fractal based defect model for the material and provides example simulations of the two-dimensional PDC. The systematic analysis of non-realistic electron

scattering within the Born approximation coupled with the Random Fractal Defect Model and the results derived thereof are considered to be the principal original components associated with the material reported herein.

2 Electron Transport Model

Using natural units where the Dirac constant $\hbar = 1$ and the mass of an electron $m = 1$, for a real two-dimensional potential $\mathbf{r} \in \mathbb{R}^2 \mapsto V(\mathbf{r})$, the non-relativistic probability complex amplitude $\mathbf{r} \in \mathbb{R}^2 \mapsto \Psi(\mathbf{r}, t)$ for an electron is given by the (two-dimensional) Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi(\mathbf{r}, t) = -\frac{1}{2}\nabla^2\Psi(\mathbf{r}, t) + V(\mathbf{r})\Psi(\mathbf{r}, t) \tag{1}$$

Since

$$-i\frac{\partial}{\partial t}\Psi^*(\mathbf{r}, t) = -\frac{1}{2}\nabla^2\Psi^*(\mathbf{r}, t) + V(\mathbf{r})\Psi^*(\mathbf{r}, t)$$

we can construct the equation

$$\frac{\partial}{\partial t} \mid \Psi(\mathbf{r}, t) \mid^2 = \frac{i}{2}\nabla \cdot [\Psi(\mathbf{r}, t)\nabla\Psi^*(\mathbf{r}, t) - \Psi^*(\mathbf{r}, t)\nabla\Psi(\mathbf{r}, t)]$$

where it is noted that the term $V(\mathbf{r}) \mid \Psi(\mathbf{r}, t) \mid^2$ is cancelled. The PDC or Particle Flux is then defines as

$$\mathbf{j} = \frac{i}{2}[\Psi(\mathbf{r}, t)\nabla\Psi^*(\mathbf{r}, t) - \Psi^*(\mathbf{r}, t)\nabla\Psi(\mathbf{r}, t)]$$

by analogy with the continuity equation

$$\frac{\partial}{\partial t}\rho(\mathbf{r}, t) + \nabla \cdot \mathbf{j}(\mathbf{r}, t) = 0$$

for Particle Flux $\mathbf{j}$ and Particle Density ρ.

For $\mathbf{r} = \hat{\mathbf{x}}x + \hat{\mathbf{y}}y$, we assume the presence of a uniform electric field $\mathcal{E}_x$ which is applied over a region of compact support $x \in [-1, 1]$ and is uniform over $y \in [-1, 1]$, the area of the mono-layer Graphene sheet being taken to be 4. The potential is then given by $V(\mathbf{r}) := V(x, y) - x\mathcal{E}_x$ (where the charge of an electron is taken to be 1) [11].

A principal theme of the model developed in this paper is the evaluation of a relationship between the electric field $\mathcal{E}_x$ and the Particle Flux $\hat{\mathbf{n}} \cdot \mathbf{j}$ where $\hat{\mathbf{n}}$ is a unit vector pointing in the direction of the current flow. In respect of this, we consider the time-independent wave function $\psi(\mathbf{r}, \omega) = \Psi(\mathbf{r}, t)\exp(-i\omega t)$, where $\omega = \sqrt{2E}$ for electron energy E, and, from equation (1), the corresponding time-independent equation is

$$(\nabla^2 + k^2)\psi(\mathbf{r}, \omega) = V(\mathbf{r})\psi(\mathbf{r}, \omega) \tag{2}$$

where $k^2 = 2\omega$, $V(\mathbf{r}) := 2V(\mathbf{r})$ and the PDC becomes

$$\mathbf{j} = \frac{i}{2}[\psi(\mathbf{r},\omega)\nabla\psi^*(\mathbf{r},\omega) - \psi^*(\mathbf{r},\omega)\nabla\psi(\mathbf{r},\omega)] \tag{3}$$

In the context of equations (2) and (3), the problem is to establish a relationship between E and $\hat{\mathbf{n}}\cdot\mathbf{j}$ given a model for $V(\mathbf{r})$ and a solution for $\psi(\mathbf{r},\omega)$. This requires a solution for $\psi(\mathbf{r})$ given $V(\mathbf{r})$ which can then be used to compute $\mathbf{j}$ via equation (3).

3 Fundamental Solution

The fundamental solution to equation (2) is given by the Green's function transformation [12]

$$\psi(\mathbf{r},\omega) = \psi_i(\mathbf{r},\omega) + \psi_s(\mathbf{r},\omega) \;\text{ where }\; \psi_s(\mathbf{r},\omega) = g(r,k) \otimes_{\mathbf{r}} V(\mathbf{r})\psi(\mathbf{r},\omega) \tag{4}$$

and ψ_i is the incident wave-field which is the solution of $(\nabla^2 + k^2)\psi_i(\mathbf{r},\omega) = 0$, $g(r,\omega)$ is the free space Green's function which is the solution of

$$(\nabla^2 + k^2)g(r,\omega) = -\delta^2(\mathbf{r}), \quad r \equiv \mid \mathbf{r} \mid$$

and $\otimes_{\mathbf{r}}$ denotes the (two-dimensional) convolution integral over $\mathbf{r} \in \mathbb{R}^2$. We note that [12]

$$g(r,\omega) = \frac{\exp(i\pi/4)\exp(ikr)}{\sqrt{8\pi kr}}, \quad kr >> 1 \tag{5}$$

3.1 Point Scattering Analysis

For a single point scattering potential model when $V(\mathbf{r}) = \delta^2(\mathbf{r})$, $\psi_s(\mathbf{r},\omega) = g(r,\omega)$ and $\mid \psi_s(\mathbf{r},\omega) \mid^2 = 1/8\pi kr = 1/8\pi r\sqrt{2\omega}$. Given that $\mid \psi_s \mid^2$ is a measure of the differential scattering cross section, it is clear that as the energy of an electron increases the cross-section decreases according to a $1/\sqrt{\omega}$ scaling law. This is significant only in the sense of the single point scattering model considered although the scaling law holds for an assemble of N randomised point scatterers when

$$V(\mathbf{r}) = \sum_{j=1}^{N} \delta^2(\mathbf{r} - \mathbf{r}_j)$$

given that

$$\mid \psi_s(\mathbf{r},\omega) \mid^2 = \frac{1}{8\pi\sqrt{2\omega}} \left| \sum_{j=1}^{N} \frac{\exp(ik \mid \mathbf{r} - \mathbf{r}_j \mid)}{\sqrt{\mid \mathbf{r} - \mathbf{r}_j \mid}} \right|^2$$

$$= \frac{1}{8\pi\sqrt{2\omega}} \sum_{j=1}^{N} \frac{\exp(ik \mid \mathbf{r} - \mathbf{r}_j \mid)}{\sqrt{\mid \mathbf{r} - \mathbf{r}_j \mid}} \sum_{\ell=1}^{N} \frac{\exp(-ik \mid \mathbf{r} - \mathbf{r}_\ell \mid)}{\sqrt{\mid \mathbf{r} - \mathbf{r}_\ell \mid}}$$

$$= \frac{1}{8\pi\sqrt{2\omega}} \left(N \sum_{j=1}^{N} \frac{1}{\mid \mathbf{r} - \mathbf{r}_j \mid} + \sum_{j=1, j\neq\ell}^{N} \frac{\exp(ik \mid \mathbf{r} - \mathbf{r}_j \mid)}{\sqrt{\mid \mathbf{r} - \mathbf{r}_j \mid}} \sum_{\ell=1}^{N} \frac{\exp(-ik \mid \mathbf{r} - \mathbf{r}_\ell \mid)}{\sqrt{\mid \mathbf{r} - \mathbf{r}_\ell \mid}} \right)$$

$$= \frac{N}{8\pi\sqrt{2\omega}} \sum_{j=1}^{N} \frac{1}{\mid \mathbf{r} - \mathbf{r}_j \mid}, \quad N \to \infty$$

Note that $1/\sqrt{\omega}$ scaling is not exhibited in three-dimensions where the (point) scattering cross-section is energy independent, the Green's function being given by $\exp(ikr)/4\pi r$. Also note that the time dependence of the two-dimensional (point) scattering cross section scales as $1/\sqrt{t}$ given that

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{\exp(i\omega t)}{(i\omega)^q} d\omega = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} \frac{\exp(st)}{s^q} ds = \frac{1}{\Gamma(q) t^{1-q}}; \quad t > 0, \quad q > 0$$

This scaling law is the same as that associated with a one-dimensional classical diffusion processes. The scattering amplitude $\mid \psi_s \mid$ scales according to the power law $1/\omega^{1/4}$ with a time dependent characteristic determined by $1/t^{3/4}$.

If we define the transmission coefficient in terms of the ratio of the scattering amplitude to the incident amplitude, then the electrical conductance associated with a 'quantum conductor' due to the scattering properties of the conductor may be defined in terms of a measure of this transmission coefficient (analogous to the Landauer definition of the quantum conductivity). On this basis, taking the incident wave-field to be a unit plane wave, the (quantum) conductance associated with a two-dimensional Schrödinger (point) scattering process is determined by a $1/t^{3/4}$ scaling law. Consequently, it is clear that in regard to the time evolution associated with a point scattering processes (at least for $t \to 0$), the (quantum) conductivity of a two-dimensional scatterer is significantly greater than that of a three dimensional equivalent (which is independent of time).

The correlation between the electron energy scaling of the scattering amplitude and the dimension of the scattering process is quantified in the following:

Theorem 3.1
For $\mathbf{r} \in \mathbb{R}^n$, $n = 1, 2, 3$, the point-scattering amplitude scales according to $1/\omega^{(3-n)/4}$.

Proof of Thereom 3.1
The out-going Green's functions are given by equation (5) for $n = 2$ and by

[12]

$$g(r,\omega)=\frac{\exp(ikr)}{4\pi r},\quad n=3\ \text{ and }\ g(x,\omega)=i\frac{\exp(ikx)}{2k},\quad n=1$$

Application of point scattering analysis for each case yields (for $N\rightarrow\infty$):

$$n=1:\ \mid\psi_s(x,\omega)\mid^2=\frac{N}{8\omega}$$

and

$$n=3:\ \mid\psi_s(\mathbf{r},\omega)\mid^2=\frac{N}{16\pi^2}\sum_{j=1}^{N}\frac{1}{\mid\mathbf{r}-\mathbf{r}_j\mid^2}$$

Thus, given that

$$n=2:\ \mid\psi_s(\mathbf{r},\omega)\mid^2=\frac{N}{8\pi\sqrt{2\omega}}\sum_{j=1}^{N}\frac{1}{\mid\mathbf{r}-\mathbf{r}_j\mid},\quad N\rightarrow\infty$$

it is clear that we can construct the following scaling relationship for the scattering amplitude:

$$\mid\psi_s(\mathbf{r},\omega)\mid\propto\frac{1}{\omega^{(3-n)/4}},\quad n=1,2,3$$

3.2 Scattering Amplitude in the Fresnel Zone

Application of an asymptotic solution to equation (4) is not appropriate for the determination of the scattering amplitude generated by the lattice of monolayer Graphene. For this reason, we consider an 'intermediate field' solution under the Fresnel approximation with the aim of generating a convolution integral based model for the scattering amplitude.

In the Fresnel zone, the Green's function given by equation (5) can be approximated thus (for a δ-source function located at $\mathbf{s}$ where $s\equiv\mid\mathbf{s}\mid$):

$$g(\mathbf{r},\mathbf{s},\omega)=\frac{\exp(i\pi/4)\exp(iks)}{\sqrt{8\pi ks}}\exp(-ik\hat{\mathbf{n}}\cdot\mathbf{r})\exp(i\alpha r^2),\quad\hat{\mathbf{n}}=\frac{\mathbf{s}}{s}$$

where

$$\alpha=\frac{k}{2s}=\frac{1}{s}\sqrt{\frac{\omega}{2}}$$

which is based on relaxing the condition $r/s<<1$ and ignoring all terms with higher order powers greater than 2 in the binomial expansion of $\mid\mathbf{r}-\mathbf{s}\mid$. Noting that

$$\frac{ik}{2s}\mid\mathbf{s}-\mathbf{r}\mid^2=\frac{ik}{2s}(s^2+r^2-2\mathbf{s}\cdot\mathbf{r})=\frac{iks}{2}+\frac{ikr^2}{2s}-ik\hat{\mathbf{n}}\cdot\mathbf{r}$$

we can then write equation (4) in the form

$$\psi_s(\mathbf{r},\omega) = \frac{\exp(i\pi/4)\exp(iks/2)}{\sqrt{8\sqrt{2}\pi s}} A_s(\mathbf{r},\omega)$$

where

$$A_s(\mathbf{r},\omega) = \frac{1}{\omega^{1/4}} \exp(i\alpha r^2) \otimes_{\mathbf{r}} V(\mathbf{r})\psi(\mathbf{r},\omega) \tag{6}$$

is the (Fresnel zone) scattering amplitude. Equation (6) expresses the scattering amplitude in terms of the convolution of the function $V(\mathbf{r})\psi(\mathbf{r},\omega)$ with a 'Fresnel Kernel'.

3.3 Born Field Analysis

Under the Born approximation, equation (6) reduces to the form

$$A_s(\mathbf{r},\omega) = \frac{1}{\omega^{1/4}} \exp(i\alpha r^2) \otimes_{\mathbf{r}} V(\mathbf{r})\psi_i(\mathbf{r},\omega)$$

where we assume a simple unit plane wave model for the incident field of the form $\psi_i(\mathbf{r},\omega) = \exp(i\mathbf{k}\cdot\mathbf{r})$. For a crystalline lattice consisting of a regularly spaced replica structure such as in a monolayer Graphene lattice, $V(\mathbf{r}) = V(\mathbf{r}+\mathbf{R})$, where $\mathbf{R}$ is a **constant** two-dimensional vector taken to describe the distance in the plane between each scattering potential $V(\mathbf{r})$. It is trivial to show that in this case,

$$A_s(\mathbf{r},\omega) = \frac{\exp(-i\mathbf{k}\cdot\mathbf{R})}{\omega^{1/4}} \exp(i\alpha r^2) \otimes_{\mathbf{r}} V(\mathbf{r}) \exp(i\mathbf{k}\cdot\mathbf{r})$$

which is a manifestation of Bloch's Theorem under the Born approximation, [13] and [14].

Let the plane wave be taken to propagate along the direction of the electric field $\mathcal{E}_x$. Then, $\mathbf{k} = \hat{\mathbf{x}}k$ and

$$A_s(x,y,\omega) = \frac{\exp(-ikR_x)}{\omega^{1/4}} \exp[i\alpha(x^2+y^2)] \otimes_x \otimes_y V(x,y)\exp(ikx)$$

$$-\frac{\exp(-ikR_x)}{\omega^{1/4}} \mathcal{E}(y,\omega)\exp(i\alpha x^2) \otimes_x x\exp(ikx)$$

where

$$\mathcal{E}(y,\omega) = \mathcal{E}_x \exp(i\alpha y^2) \otimes_y H(y) \equiv \mathcal{E}_x \int_{-1}^{1} \exp[i\alpha(y'-y)^2]dy' \tag{7}$$

and $\otimes_x$ and $\otimes_y$ denote the convolution integrals over x and y, respectively. From equation (3), differentiation with respect to the Fresnel Kernel, for the scattered field gives

$$\nabla A_s(x,y,\omega) = 2i\alpha(\hat{\mathbf{x}}x+\hat{\mathbf{y}}y)\frac{\exp(-ikR_x)}{\omega^{1/4}}\exp[i\alpha(x^2+y^2)]\otimes_x\otimes_y V(x,y)\exp(ikx)$$

$$-2i\alpha\hat{\mathbf{x}}x\frac{\exp(-ikR_x)}{\omega^{1/4}}\mathcal{E}(y,\omega)\exp(i\alpha x^2)\otimes_x x\exp(ikx)$$

$$-\hat{\mathbf{y}}\frac{\exp(-ikR_x)}{\omega^{1/4}}\left[\frac{\partial}{\partial y}\mathcal{E}(y,\omega)\right]\exp(i\alpha x^2)\otimes_x x\exp(ikx)$$

from which it follows that

$$j_x(x,y,\omega)\equiv\hat{\mathbf{x}}\cdot\mathbf{j}(x,y,\omega)=2\alpha x\mid A_s(x,y,\omega)\mid^2$$

This result demonstrates that the PDC is scale invariant with regard to the electron energy. This is a consequence of the scaling by $1/\omega^{1/4}$ associated with the Green's function for $\mathbf{r}\in\mathbb{R}^2$ whereas for $\mathbf{r}\in\mathbb{R}^3$, and, using the same analysis, the PDC is proportional to $\sqrt{\omega}$.

Introducing the functions

$$\phi(x,y,\omega)=\frac{\exp(-ikR_x)}{\omega^{1/4}}\exp[i\alpha(x^2+y^2)]\otimes_x\otimes_y V(x,y)\exp(ikx)$$

and

$$\chi(x,\omega)=\frac{\exp(-ikR_x)}{\omega^{1/4}}\exp(i\alpha x^2)\otimes_x x\exp(ikx)$$

the PDC j_x is related to the modified electric field $\mathcal{E}$ - equation (7) - via the quadratic equation

$$j_x(x,y,\omega)=2\alpha x[\mid\mathcal{E}(y,\omega)\mid^2\mid\chi(x,\omega)\mid^2-\mathcal{E}^*(y,\omega)\phi(x,y,\omega)\chi^*(x,\omega)$$

$$-\mathcal{E}(y,\omega)\phi^*(x,y,\omega)\chi(x,\omega)+\mid\phi(x,y,\omega)\mid^2] \tag{8}$$

We now focus on an analysis of the first term in equation (8) which is dominant in the case when $\mathcal{E}_x >> 1$ and consider the y-integrated PDC defined by

$$J_x(x,\omega)=2\alpha x\mathcal{E}_y(\omega)\mid\chi(x,\omega)\mid^2 \tag{9}$$

where

$$J_x(x,\omega)=\frac{1}{2}\int_{-1}^{1}j_x(x,y,\omega)dy\ \text{ and }\ \mathcal{E}_y(\omega)=\frac{1}{2}\int_{-1}^{1}\mid\mathcal{E}(y,\omega)\mid^2 dy$$

In this case, the PDC is proportional to $\mathcal{E}_x^2$ and becomes independent of the scattering processes that takes place within the lattice of the material due to

scattering potential $V(x, y)$. The electrons can therefore be taken to flow unimpeded, without being slowed down by collisions as they are in a conventional transistor, for example. The condition $\mathcal{E}_x >> 1$ is therefore a qualification for ballistic behaviour under the Born approximation.

Figure 1 shows examples of the PDC defined by equation (9) for a range of values of ω using a 1000 element array with $\alpha = \sqrt{\omega/2}$; ranges that avoid aliasing particularly with regard to the computation of the Fresnel Kernel $\exp(i\alpha x^2)$, the convolution operation being evaluated using the MATLAB *conv* function (with option 'same'). From Figure 1, it is clear that the PDC increases in amplitude as ω decreases.

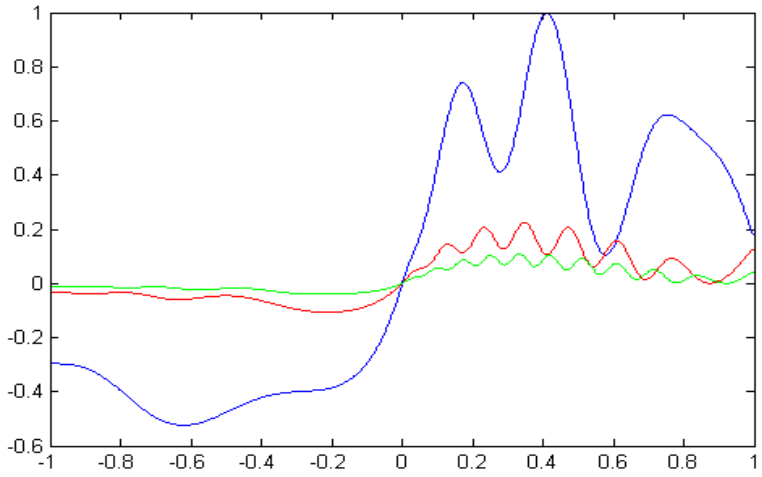

Figure 1: Comparison of the function $J_x(x, \omega)$ for $\omega = 100$ (Blue), $\omega = 500$ (Red) and $\omega = 1000$ (Green). The plots are normalised with regard to the maximum absolute value for the case when $\omega = 100$.

4 Fractal Defected Graphene

A freely suspended Graphene membrane is partially crumpled [15]. This is because two-dimensional crystals in a three-dimensional space can not be flat due to bending instabilities and thermally induced perturbations. According to the Mermin-Wagner Theorem (which states that 'in one- and two-dimensions, continuous symmetries cannot be spontaneously broken at finite temperature in systems with sufficiently short-range interactions' ([16], [17] and [18]), long-wavelength fluctuations destroy the long-range order of two-dimensional crystals. Thus, two-dimensional membranes embedded in a three-dimensional

space have a tendency to be crumpled. Consequently the spatial characteristics of Graphene include intrinsic defects (warping, crumpling and rippling) as, under harmonic approximation theory, a membrane cannot be flat although anharmonic coupling (bending-stretching) may also be present [19].

Graphene ripples have various sizes, have a broad distribution and power-law correlation functions of normals together with some typical scale lengths due to te intrinsic tendency of carbon to be bonded. Consequently, there have been a variety of attempts to model the Graphene defects and the defect dynamics of the material, [20], [21] and [22]. Moreover, the deformation of Graphene effects the electron transport properties of the material [23] and it is therefore important to incorporate this phenomenon in a model for electron transport [24]. In this paper, we consider a Random Fractal surface model for the defect potential as given by the solution to the Fraction Poison Equation [24]

$$\nabla^{\gamma} W(\mathbf{r}) = N(\mathbf{r}), \quad \mathbf{r} \in \mathbb{R}^2, \quad \gamma = 4 - D, \quad D \in [2,3] \tag{10}$$

where $N(\mathbf{r})$ is a stochastic field with an arbitrary Probability Density Function but a Uniform Power Spectral Density Function and D is the Fractal Dimension of a surface. We consider a generic perturbation of the form $V(\mathbf{r}) := V(\mathbf{r}+\mathbf{R})+ W(\mathbf{r})$. This expression for $V(\mathbf{r})$ takes into account both scalar (electrostatic) potential and the potential created by defects (Fractal Defects) in the material, the solution of equation (10) being givn by (ignoring scaling) [24]

$$W(\mathbf{r}) = \frac{1}{r^{2-\gamma}} \otimes_r N(\mathbf{r})$$

The basis for equation (10) comes from an analysis of the evolution equation

$$W(\mathbf{r}, t+\tau) = W(\mathbf{r}, t) \otimes_{\mathbf{r}} P(\mathbf{r}) + N(\mathbf{r}, t)$$

where W is the Density Function and P is the Probability Density Function (PDF) that is a characteristic of the system statistics in which the evolution of the Density Function occurs. For a Lévy PDF with a Characteristic Function $\exp(-a \mid \mathbf{k} \mid^{\gamma})$, $\gamma \in (0,2]$ where a is a constant and γ is the Lévy index, application of the Taylor series for $\tau << 1$ and the convolution theorem yields the result

$$\tau \frac{\partial}{\partial t} \widetilde{W}(\mathbf{k}, t) = a \mid \mathbf{k} \mid^{\gamma} \widetilde{W}(\mathbf{k}.t) + \widetilde{N}(\mathbf{k}, t), \quad a << 1$$

where, for any function F, $\widetilde{F}$ denotes the (two-dimensional) Fourier transform. Application of the Reisz definition for a Fractional Laplacian then yield the result

$$\tau \frac{\partial}{\partial t} W(\mathbf{r}, t) = -a \nabla^{\gamma} W(\mathbf{r}.t) + N(\mathbf{r}, t)$$

so that for $\tau \to 0$ (ignoring scaling by a), equation (10) is obtained with $\gamma \in [1,2]$ given that $D \in [2,3]$. Equation (10) can thus be taken to be a

Fractal surface representation of a Graphene sheet at a fixed point in time t, and, for this case, the PDC becomes

$$j_x(x, y, \omega) = x \mid A_s(x, y, \omega) \mid^2$$

where

$$A_s(x, y, \omega) = \exp[i\alpha(x^2 + y^2)] \otimes_x \otimes_y [\exp(-ikR_x)V(x, y) + W(x, y)] \exp(ikx)$$
$$- \exp(-ikR_x)\mathcal{E}(y, \omega) \exp(i\alpha x^2) \otimes_x x \exp(ikx)$$

We consider a 'Mexican Hat' function of the form (for constant σ)

$$V(x, y) = (x^2 + y^2) \exp[-\sigma(x^2 + y^2)]$$

to represent the electrostatic potential associated with the delocalised electrons. Figure 2 shows an example of the effect of Random Fractal Defects on the PDC which changes the periodicity of the PDC in the positive half-space (for a 100^2 array). In this simulation the one- and two-dimensional convolutions are implemented using the MATLAB *conv* and *conv2* functions, respectively (with the option 'same'), the computation of the Graphene Defect Function $W(x, y)$ being undertaken using a Fourier transform with the MATLAB function *FFT2*, Gaussian Random Number Generator *randn* and noting that (ignoring scaling)

$$\frac{1}{r^{2-\gamma}} \otimes_r N(\mathbf{r}) \leftrightarrow \frac{\widetilde{N}(\mathbf{k})}{\mid \mathbf{k} \mid^{4-D}}$$

5 Conclusions

The purpose of this paper has been to investigate non-relativistic electron transport in a two-dimensional regular lattice such as Graphene subject to a applied parallel electric field. In particular, the PDC has been evaluated under the Born approximation in the Fresnel zone. For the case when the electric field is large, scattering effects become less significant and the material behaves as a ballistic conductor. The Fractal defect model considered in Section 4 reveals that the presence of (Fractal) defects has a relatively weak effect on the amplitude but a pronounced effect on the periodicity of the PDC, at least according to the model developed. The 'key' to understanding the electron transport properties of a two-dimensional material such as Graphene is that (non-relativistic) electrons 'propagate' according to an Energy$^{-1/4}$ scaling law as discussed in Section 3.1. This is not a feature of three-dimensional electron transport which is (point scattering) energy invariant. Consequently, the dimensionality of mono-layer materials implies high conductivity, low energy electrons yielding a larger differential scattering cross-section (within the context of the point scattering analysis given in Section 3.1).

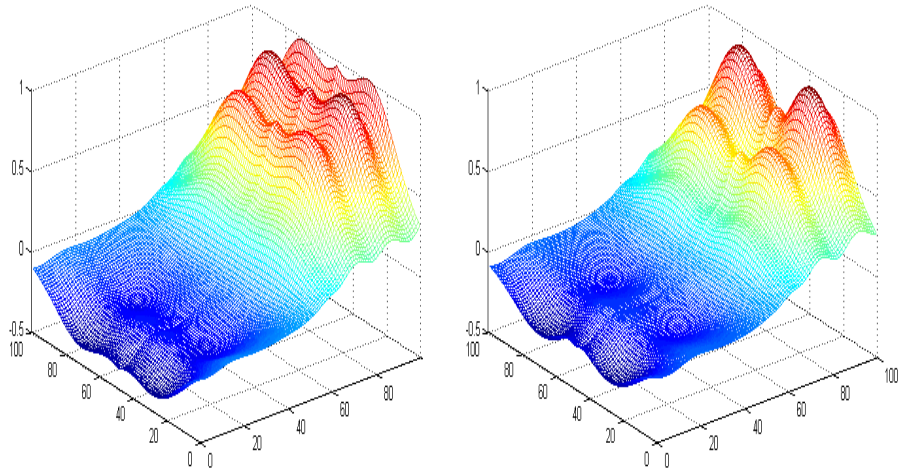

Figure 2: Comparison of normalised two-dimensional PDC for $\omega = 10^3$, $\sigma = 5$, $D = 2.5$, $R_x = 1$ with $\|W(x,y)\| = 0$ (Left) and $\|W(x,y)\|/\|V(x,y)\| = 1$ (Right).

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References

[1] *This Month in Physics History: October 22, 2004: Discovery of Graphene*, APS News, The American Physical Society, Series II Vol. 18, No. 9, Page 2, October 2009.

[2] M. I. Katsnelson, *Graphene: Carbon in Two Dimensions*, Cambridge University Press, 2012, ISBN-10: 0521195403.

[3] E. L. Wolf, *Graphene: A New Paradigm in Condensed Matter and Device Physics*, Oxford University Press, 2013, ISBN-10: 0199645868.

[4] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, *The Electronic Properties of Graphene*, Rev. Mod. Phys., Vol. 81, 109, 2009.

[5] D. S. L. Abergela, V. Apalkovb, J. Berashevicha, K. Zieglerc and T. Chakraborty, *Properties of Graphene: A Theoretical Perspective*, Vol. 59, Issue 4, 261-482, 2010.

[6] L. Brey and H. A. Fertig, *Electronic States of Graphene Nano-ribbons Studied with the Dirac Equation*, Phys. Rev. B 73, 235-411, 2006.

[7] M. I. Katsnelson1, K. S. Novoselov and A. K. Geim, *Chiral Tunnelling and the Klein Paradox in Graphene*, Nature Physics 2, 620 - 625, 2006.

[8] J. H. Bardarson, J. Tworzydlo, P. W. Brouwer, and C. W. J. Beenakker, *One-Parameter Scaling at the Dirac Point in Graphene*, Phys. Rev. Lett. 99, 106-801, 2007.

[9] , N. Gi, *Relativistic Dynamics and Dirac Particles in Graphene*, PhD Thesis, Massachusetts Institute of Technology, 2011.

[10] K. J. Sikesb, K. J. Sikes, Z. Jianga, M. Klimac, G. Fudenberga, J. Hone, P. Kim and H. L. Stormera, *Ultrahigh Electron Mobility in Suspended Graphene*, Solid State Communications, Elsevier, Vol. 146, Issue 910, 351355, 2008

[11] K. Beauchard, *Local Controllability of a 1D Schrödinger Equation*, Journal de Mathématiques Pures et Appliquées, Vol. 84, 851-956, 2005.

[12] G. Evans, J. M. Blackledge and P. Yardley, *Analytic Solutions to Partial Differential Equations*, Springer, 1999, ISBN: 2540761241.

[13] F. Bloch, *Über die Quantenmechanik der Elektronen in Kristallgittern*, Z. Physik, Vol. 52, 555600, 1928.

[14] M. S. P. Eastham, *The Spectral Theory of Periodic Differential Equations*, Texts in Mathematics, Edinburgh: Scottish Academic Press, 1973.

[15] J. C. Meyer, A. K. Geim, M. I. Katsnelson, K. S. Novoselov, T. J. Booth and S. Roth, *The Structure of Suspended Graphene Sheets*, Nature, Vol. 446, 60-63, 2007.

[16] A. Werner, *The Mermin-Wagner Theorem*, 24 June, 2010, `http://itp.uni-frankfurt.de/~valenti/TALKS_BACHELOR/mermin-wagner.pdf`

[17] P. C. Hohenberg, *Existence of Long-range Order in One- and Two-Dimensions*, Phys. Rev. Vol. 158, No. 2, 383-386,1967.

[18] S. Coleman, *There are no Goldstone Bosons in Two-Dimensions*, Comm. Math. Phys., 31, 259-264, 1973.

[19] D. R. Nelson, T. Piran and S. Weinberg, *Statistical Mechanics of Membranes and Surfaces*, World Scientific Publishing, 2004, ISBN-10: 9812387722.

[20] C. C. Chen, W. Bao, J. Theiss, C. Dames, C. N. Lau and S. B. Cronin, *Raman Spectroscopy of Ripple Formation in Suspended Graphene*, Nano Lett., Vol. 9, No. 12, 41724176, 2009.

[21] K.V. Zakharchenko, J.H. Los, M.I. Katsnelson, A. Fasolino, *Atomistic Simulations of Structural and Thermodynamic Properties of Bilayer Graphene*, 2010, `http://arxiv.org/pdf/1004.0126.pdf`.

[22] L.L. Bonilla, C. Rodrguez and A. Maria *Theory of Defect Dynamics in Graphene: Defect Groupings and their Stability*, Continuum Mechanics and Thermodynamics, Vol. 23, No. 4, 337-346, 2011, ISSN 0935-1175.

[23] M. Zwierzycki, *Transport Properties of Rippled Graphene*, ACTA PHYSICA POLONICA A, Vol. 121, 1246-1249, 2012.

[24] C. H. Lui, L. Liu, K. F. Mak, G. W. Flynn and T. F. Heinz, *Ultraflat Graphene*, Nature (Letters), Vol. 462, 339-341, 2009.

[25] M. J. Turner, J. M. Blackledge and P. R. Andrews, *Fractal Geometry in Digital Imaging*, Academic Press, 1998, ISBN: 0127039708.