Transport across Graphene - understanding electron optics

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Graphene is perhaps the most explored materials in the current day and age and has been making big waves in various directions of research including applications in quantum devices and even medicine[1,2]. In this report, I will explore the electron transport in Graphene using the NEGF method[3]. This will include exploring the conductance quantization, quantum hall effect in Graphene[4], and the phenomena of Klein tunneling[5].

I. INTRODUCTION

Graphene is made of carbon atoms arranged in an infinite regular hexagonal lattice on a plane. As a material it possesses various interesting properties beginning from the fact that it has a sub-lattice structure where two adjacent lattice sites are distinguishable.
Using the tight binding model, we would arrive at the following dispersion relation

$$E(\mathbf{k}) = \pm t\sqrt{\left(1 + 4\cos^2(k_y a) + 4\cos(k_y a)\cos\left(k_x\sqrt{3}a\right)\right)}$$

Here we have taken t as the hopping constant for the Hamiltonian and the energy at any site is set to zero. The interesting nature of this dispersion is that near the regions where $E = 0$, the dispersion is conical in shape. Due to this interesting linear dispersion at low energies,

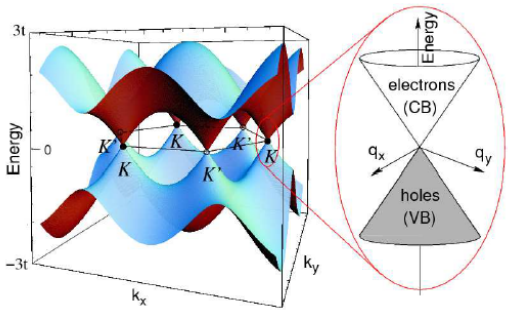

Figure 1. Figure taken from[5]. Dispersion relation for Graphene which becomes approximately conical near the points where $E = 0$.

one can see that it follows the Dirac equation in this regime with a psuedospin based on the sublattice structure. This leads to interesting consequences such as Klein tunneling which was discovered in the case for relativistic electrons following the Dirac equation[6]. The consequence of this is that an electron can tunnel through a barrier regardless of its height and width when it is travelling along a certain angle. This is known as the Klein paradox.
A similar effect has also been both predicted and observed in Graphene. We explore this along with other behaviors of barriers in Graphene which have optical like behaviors in section III.

II. NEGF AND CONDUCTANCE QUANTIZATION

For this section, the NEGF method has been used. We list out the relevant equations used in the NEGF method

$$E\boldsymbol{\psi} = [\mathbf{H} + \mathbf{\Sigma_1} + \mathbf{\Sigma_2}]\,\boldsymbol{\psi} + \mathbf{s_1}, \quad \mathbf{\Gamma_i} = \iota[\mathbf{\Sigma_i} - \mathbf{\Sigma_i^\dagger}]$$

We define $\mathbf{G^R} = [\mathbf{EI} - \mathbf{H} - \mathbf{\Sigma}]^{-1}$ and $\mathbf{G^A} = [\mathbf{G^R}]^\dagger$ and so we write $\boldsymbol{\psi} = \mathbf{G^R s_1}$
We know that for one level $2\pi s_1 s_1^* = \gamma_1$ and similarly the matrix relation obtained is $2\pi \mathbf{s_1 s_1^\dagger} = \mathbf{\Gamma_1}$. We declare $\mathbf{G^n} = \mathbf{2\pi\psi\psi^\dagger}$ hence $\mathbf{G^n} = \mathbf{G^R\Gamma_1 G^A}$

$$\mathbf{G^n} = \mathbf{G^R\Sigma^{in}G^A}, \quad \mathbf{\Sigma^{in}} = \mathbf{\Gamma_1 f_1(E)} + \mathbf{\Gamma_2 f_2(E)}$$

$$\tilde{T}(E) = \mathrm{Tr}(\mathbf{\Gamma_1 G^R \Gamma_2 G^A})$$

The interpretation of the equations can be seen as treating any general contact on the device as a source term in the Schrödinger's equation. This leads to a self-energy term related to every contact and the whole problem often boils down to finding this very term. In 1D it is rather easy, however in 2D there are a few non-trivial modifications that must be made[7].
For a square 2D lattice we can reduce the system to a 1D system where the energy and interaction terms itself are written as a matrices α and β.
Here we have

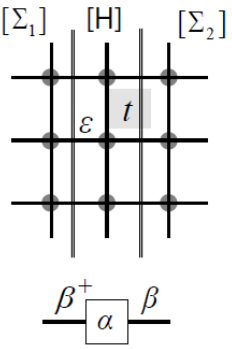

Figure 2.

$$\alpha = \begin{bmatrix} \varepsilon & t & 0 \\ t & \varepsilon & 0 \\ 0 & t & \varepsilon \end{bmatrix}, \quad \beta = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

We can simultaneously diagonalize these two and the basis where they are diagonalized gives three 1D channels of energies $\varepsilon_1, \varepsilon_2$ and ε_3 that are the eigenvalues of α.
However Graphene is not a square lattice and if we do redifine our lattice basis to convert it into a square lattice, the matrices α and β will not be simultaneously diagonlizable. The method here is known as a surface Green's function. We consider the device to be connected to an infinite contact described as $H_i - \iota\eta$. The coupling to the

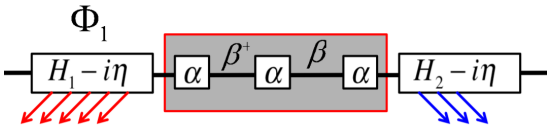

Figure 3. Modelling the contacts in a 2D device.

contact is described as τ_i. On solving the source term Schrödinger's equations and applying appropriate conditions we get

$$\Sigma_i = \tau_i g_i \tau_i^\dagger, \quad g_i = [E + \iota\eta - H_i]^{-1}$$

The equation $\Sigma_i = \tau_i g_i \tau_i^\dagger$ will hold for any number of contacts. The τ connects to only the surface of the contact and so we need a way to get the surface Green's function.
Take the contact to be N columns with g_N and treat the surface as a device, then for the $N-1$ column contact we have a green's function g_{N-1}. This gives us

$$g_N = [E + \iota\eta - \alpha - \beta^\dagger g_{N-1} \beta]^{-1}$$

This is a recursive map and for an infinite contact should converge to g such that

$$\beta^\dagger g \beta - (E + \iota\eta - \alpha) + g^{-1} = 0$$

This equation can be solved iteratively (see code for more details on this). Using this we obtain the conductance quantization for Graphene in its two arrangements (Armchair and Zigzag).

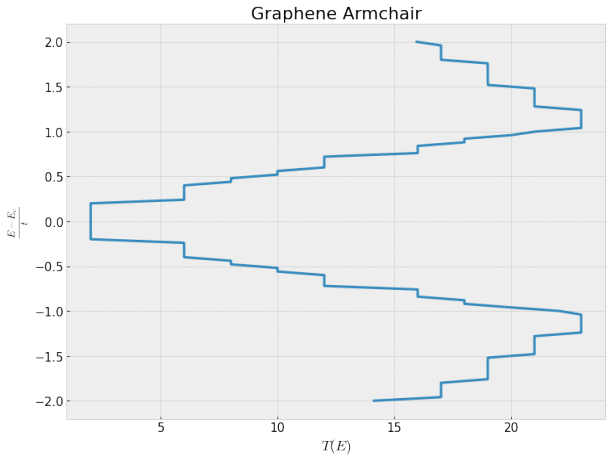

Figure 4. Conductance quantization for Graphene (armchair)

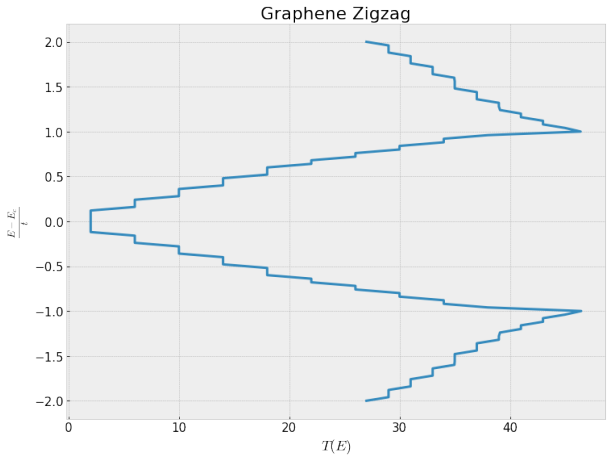

Figure 5. Conductance quantization for Graphene (zigzag)

III. ELECTRON OPTICS IN GRAPHENE

A. 2D massless Dirac equation

The 2D massless Dirac eigenvalue equation is written as

$$-\iota\hbar v_F \hat{\boldsymbol{\sigma}} \cdot \nabla\psi(\mathbf{r}) = \mathbf{E}\psi(\mathbf{r})$$

To derive this from the tight-binding model[8] we just need to expand the dispersion relation around $\mathbf{k} = \left(0, \pm\frac{2\pi}{3}\right)$ and we will arrive at a relation that energy is linear in $\mathbf{k}$, a characteristic of the Dirac equation. The fermi velocity comes out to be $v_F = \sqrt{3}ta/(2\hbar)$ which plays the role of an effective velocity of light. Here $\psi(\mathbf{r}) = (\psi_{\mathbf{A}}(\mathbf{r}), \psi_{\mathbf{B}}(\mathbf{r}))$ where A and B are the two types of lattice sites, and so these are the complex amplitudes of the contribution of these lattice sites to the wavefunction. The kinetic energy part of the Hamiltonian can be written as follows

$$\hat{H}_{\text{kin}} = \hbar v_F \begin{pmatrix} 0 & k_x - \iota k_y \\ k_x + \iota k_y & 0 \end{pmatrix}$$

An eigenstate here would correspond to a plane wave which we would write as

$$\psi(\mathbf{r}) = \mathbf{e}^{\iota \mathbf{k}\cdot\mathbf{r}} \begin{pmatrix} u \\ v \end{pmatrix} = \langle \mathbf{r} | \psi \rangle$$

For an oscillating wave, we have $u = 1$ and $v = \alpha e^{\iota\phi}$ where $\alpha = \pm 1$ based on whether it is the conduction band ($\alpha = 1$) or valence band ($\alpha = -1$). In case it is oscillating, $k_x^2 > 0$ and $k_y^2 > 0$ will always be true due to it being the direction of propogation.
There can also be evanescent waves in which case k_x is, imaginary. Let $k_x = -\iota\kappa$, then $u = 1$ and $v = \alpha\iota\sqrt{\frac{k_y - \kappa}{k_y + \kappa}}$.

B. Conservation laws

From the Heisenberg equation of motion, the velocity operator would be

$$\hat{v} = \dot{\mathbf{r}} = \frac{1}{\iota}[\mathbf{r}, \hat{\mathbf{H}}] = \hat{\boldsymbol{\sigma}}$$

From conservation of probability, the probability current must satisfy the following

$$\nabla \cdot \mathbf{j} = -\frac{\partial}{\partial \mathbf{t}} |\psi|^{\mathbf{2}}$$

For an eigenstate $|\mathbf{k}, \alpha\rangle$ this gives us the following for a unit system area.

$$\mathbf{j} = \alpha \frac{\mathbf{k}}{\mathbf{k}}$$

Note that due to translational invariance along y, $\mathbf{j}(\mathbf{x}, \mathbf{y}) = \mathbf{j}(\mathbf{x})$ and momentum projection along y must be conserved. Along with the probability conservation law this gives us $j_x(x) =$ constant.
Here we also define a chirality as follows, the chirality (or helicity) operator is the projection of the sublattice psuedo-spin operator on the momentum direction

$$\hat{C} = \frac{\mathbf{k} \cdot \hat{\boldsymbol{\sigma}}}{k}$$

The eigenvalues of this operator are $C = \pm 1$. In the absence of an external potential, $\hat{C}$ commutes with the Hamiltonian and hence is diagonalized by the same eigenvectors so $\hat{C}] |\mathbf{k}, \alpha\rangle = \alpha |\mathbf{k}, \alpha\rangle$.
The chirality factor has an interesting consequence for backscattering as observed in carbon nanotubes[9]. If we assume some impurity present inside the material giving a potential of $U(\mathbf{r})$, we can make use of the first order Born approximation to write the following

$$P(\theta) \propto |\langle \mathbf{k}', \alpha' | U(\mathbf{r}) | \mathbf{k}, \alpha \rangle|^{\mathbf{2}} = |\tilde{\mathbf{U}}(\mathbf{q})|^{\mathbf{2}} \times \cos^{\mathbf{2}}(\theta/\mathbf{2})$$

Here $\tilde{U}(\mathbf{q})$ is the Fourier transform of the potential $U(\mathbf{r})$ and θ is the angle between $\mathbf{k}'$ and $\mathbf{k}$. The importance of this is that there is no back-scattering when $k' = -k$ hence the Chirality factor kills off all back-scattering for the -1 eigenvalue. This can be explained by seeing that for the electron to back-scatter, it must also reverse the direction off the psuedospin but the potential is incapable of doing this since it does not act on the psuedospin space. Hence there will be no back-scattering at all.
The very interesting consequence of this is that a normally incident photon cannot be back-scattered hence has perfect transmission.
More concretely we would express the Heisenberg equation of motion for the velocity along x as follows

$$\dot{\hat{v}}_x = -\iota[\hat{\sigma}_x, \hat{H}] = 2\hat{\sigma}_z k_y$$

We have $\langle \psi(0) | \dot{\hat{v}}_x(t) | \psi(0) \rangle = 2 \langle \psi(0) | \hat{\sigma}) z(t) k_y(0) | \psi(0) \rangle = 0$ We can set this to zero if the initial state of the electron was having zero momentum along y. Hence this conserves the psuedo-spin along x for normal incidence which is the main explanation of why back-scattering is absent.

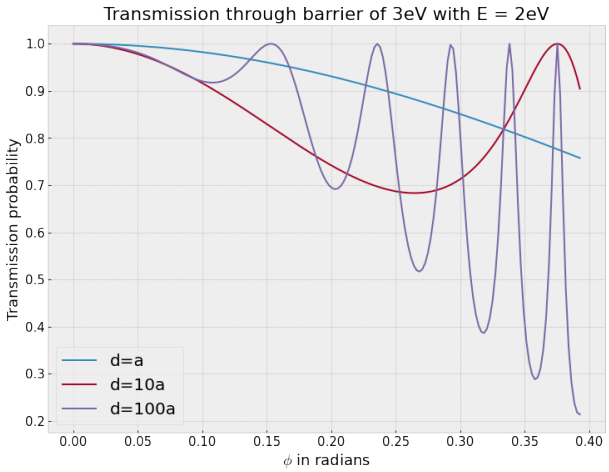

Figure 6. Transmission probability through a barrier in Graphene for different values of d in the case of $E < V_0$. The angle ϕ does not exceed the critical angle. It can be noted that at normal incidence, all the cases have full transmission and as we increase the value of d, we get the expected Fabry-Pérot resonances

C. Potential barriers

Once we introduce a potential barrier we can solve for transmission probability by observing the ansatz coefficient values similar to a 1D scattering problem with some boundary conditions. We must note that reflection caues the psuedospin to flip since the direction has been reversed and once inside the barrier the value of k_x will inevitably change.
Let us suppose it is incident on the barrier at an angle of ϕ, the angle of refraction is θ_A and finally it exits at the same angle ϕ, the wavefunction in these regions is as follows

$$\psi_1 = e^{\iota k_y y}\left[e^{\iota k_x x}\begin{pmatrix}1\\ e^{\iota\phi}\end{pmatrix} + re^{-\iota k_x x}\begin{pmatrix}1\\ -e^{-\iota\phi}\end{pmatrix}\right]$$

$$\psi_2 = e^{\iota k_y y}\left[Ae^{\iota k'_x x}\begin{pmatrix}1\\ e^{-\iota\theta_A}\end{pmatrix} + Be^{-\iota k'_x x}\begin{pmatrix}1\\ e^{-\iota\theta_A}\end{pmatrix}\right]$$

$$\psi_3 = te^{\iota k_y y}e^{\iota k_x x}\begin{pmatrix}1\\ e^{\iota\phi}\end{pmatrix}$$

By ensuring continuity at the boundaries we can see that the following expression comes for the transmission[10].

$$T = \frac{\cos^2(\phi)\cos^2(\theta_A)}{\cos^2(\phi)\cos^2(\theta_A)\cos^2(k'_x d) + \sin^2(k'_x d)[1 + \sin(\theta_A)\sin(\phi)]^2}$$

Here d represents the width of the barrier of height V_0. On solving the boundary conditions we get that $k'_x d =$

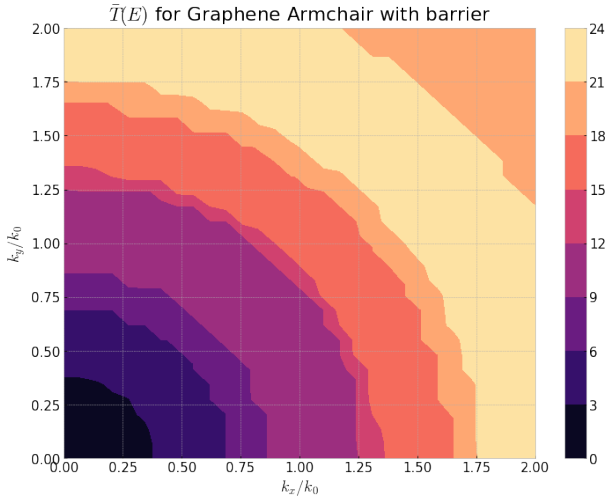

Figure 7. Value of $\bar{T}(E)$ for armchair graphene. This also depends on the density of states of the chosen material. Here the width of the barrier is $5a$ where a is the lattice constant.

$-\frac{V_0 d}{\hbar v_F}\sqrt{1-2\frac{E}{V_0}+\frac{E^2}{V_0^2}\cos^2(\phi)}$. Interestingly, snell's law will come as a consequence of momentum conservation along the barriers and the conseravtion of k_y.

$$E\sin(\phi) = (V_0 - E)\sin(\theta_A)$$

We can see that normal incidence has a full transmission regardless of the value of d which is a very strong consequence of the Chirality. Also there will be a value of energy where $\theta_A = \pi/2$ which is for $\phi = \phi_c$ the critical angle. This results in an evanescent wave and the value of $k_x'^2 < 0$.
Now if we think in a purely optical perspective, this barrier is very much like a Fabry-Pérot interferometer. This is due to the two interfaces of where the barrier begins and ends which gives it this behavior. Due to this there will be oblique incidences where the transmission would be equal to 1. This can be seen to occur for the case where $k_x' d = n\pi$ or rather

$$2l\sqrt{1-2\epsilon+\epsilon^2\cos^2(\phi)} = \text{integer}$$

Here $l = V_0 d/(\hbar v_F)$ and $\epsilon = E/V_0$. This is a very interesting consequence of the optical behavior since such a behavior is not possible for a device with a quadratic dispersion relation. One does achieve such resonances but that requires an actual double barrier setup hence making it interesting that these resonances are achieveable using just a single barrier.
Finally we combine this with the NEGF method to simulate for varying k_x and k_y how does the transmission $\bar{T}(E) = M(E)T(E)$ turn out to be. Note that this also includes the modes hence will look different from the expected transmission.

IV. CONCLUSION

In this report we have studied the optical behavior of graphene starting from the dispersion relation and treating it as the Dirac equation to unveil some very interesting properties of this. Along with this we have also used the NEGF method to verify certain properties of Graphene. These properties have found use in various places such as constructing a Klein tunneling transistor[11] and for p-n junctions for electron-optical applications[12]. The interesting property of this tunneling can be further explored for creating super-lattice type interference using a lesser barriers since a single barrier itself gives transmission resonances

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Motivation & Objective

- We will be exploring some of the interesting properties of electron transport in graphene that arise due to the linear dispersion relation.
- The linear dispersion relation causes the energy eigenvalue equation to become equivalent to the 2D massless dirac equation for low energies.
- Due to this nature it behaves like light at these energy levels travelling at the Fermi velocity.
- This leads to interesting consequences when we study the behavior when placed in barriers, the most interesting being Klein tunneling [6] which is a consequence of Chirality.

Linear dispersion leading to electron optics

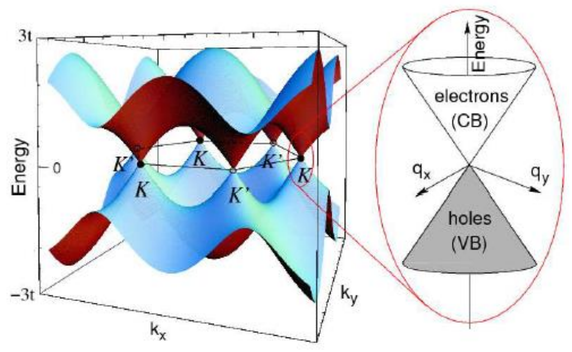
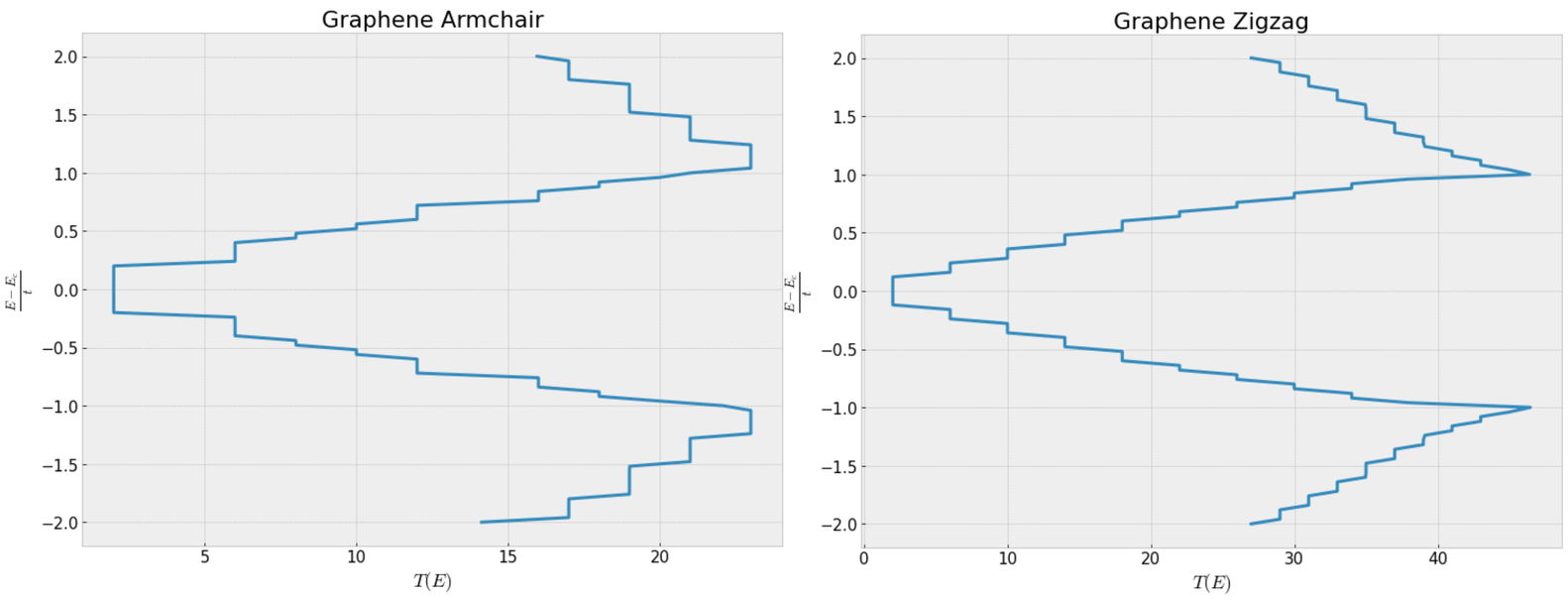


Figure taken from Allain and Fuchs 2011 [1]

- For low energies the dispersion is linear as can be seen by expanding the below expression around $(0, 2\pi/3)$

$$E(\mathbf{k}) = \pm t\sqrt{\left(1 + 4\cos^2(k_y a) + 4\cos(k_y a)\cos\left(k_x\sqrt{3}a\right)\right)}$$

Quantization of conductance



Transmission for Graphene solved using the surface green's functions method. We can observe the clear quantization which is the result of conductance having a quantum, This has been done for both arrangements of Graphene, armchair and zigzag.

$$E\boldsymbol{\psi} = [\mathbf{H} + \mathbf{\Sigma_1} + \mathbf{\Sigma_2}]\,\boldsymbol{\psi} + \mathbf{s_1}, \quad \mathbf{\Gamma_i} = \iota[\mathbf{\Sigma_i} - \mathbf{\Sigma_i^\dagger}]$$

We define $\mathbf{G^R} = [\mathbf{EI} - \mathbf{H} - \mathbf{\Sigma}]^{-1}$ and $\mathbf{G^A} = [\mathbf{G^R}]^\dagger$ and so we write $\boldsymbol{\psi} = \mathbf{G^R s_1}$

We know that for one level $2\pi s_1 s_1^* = \gamma_1$ and similarly the matrix relation obtained is $2\pi \mathbf{s_1 s_1^\dagger} = \mathbf{\Gamma_1}$. We declare $\mathbf{G^n} = \mathbf{2}\pi\boldsymbol{\psi}\boldsymbol{\psi}^\dagger$ hence $\mathbf{G^n} = \mathbf{G^R \Gamma_1 G^A}$

$$\mathbf{G^n} = \mathbf{G^R \Sigma^{in} G^A}, \quad \mathbf{\Sigma^{in}} = \mathbf{\Gamma_1 f_1(E)} + \mathbf{\Gamma_2 f_2(E)}$$

$$\tilde{T}(E) = \mathrm{Tr}(\mathbf{\Gamma}_1 \mathbf{G^R \Gamma_2 G^A})$$

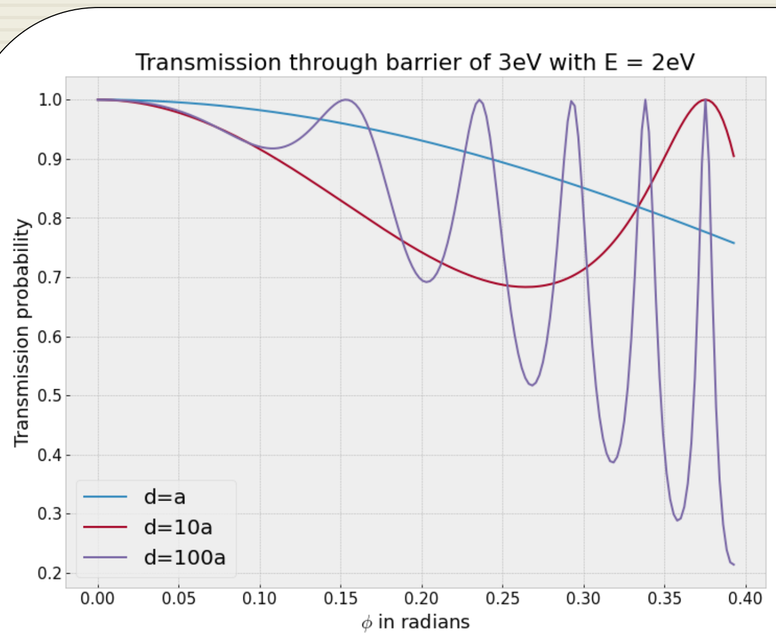
Take the contact to be N columns with g_N and treat the surface as a device, then for the $N-1$ column contact we have a green's function g_{N-1}. This gives us

$$g_N = [E + \iota\eta - \alpha - \beta^\dagger g_{N-1}\beta]^{-1}$$

This is a recursive map and for an infinite contact should converge to g such that

$$\beta^\dagger g \beta - (E + \iota\eta - \alpha) + g^{-1} = 0$$

Electron optics



Transmission through a single barrier of varying width d. We can see that normal incidence has T=1 and there are Fabry-Perot resonances

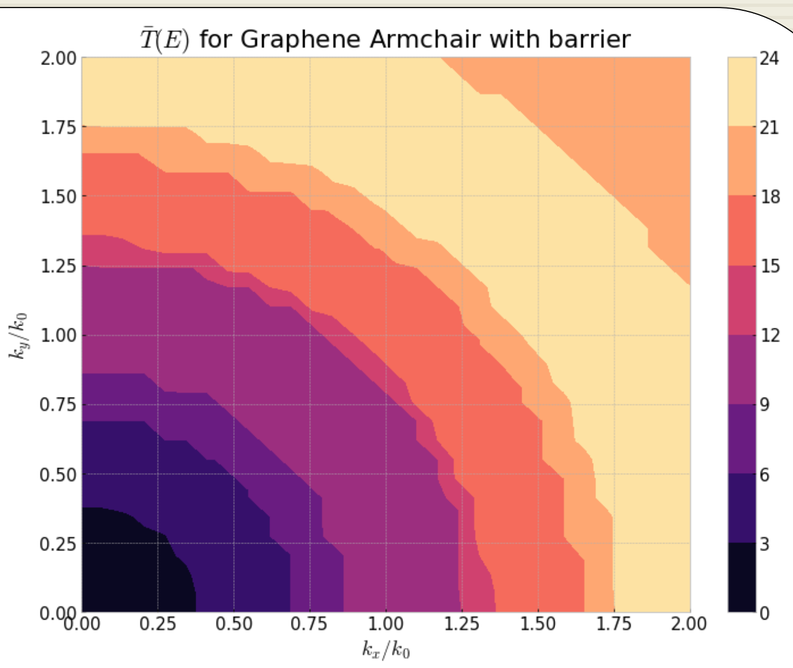
Transmission through potential barriers

$$T = \frac{\cos^2(\phi)\cos^2(\theta_A)}{\cos^2(\phi)\cos^2(\theta_A)\cos^2(k_x' d) + \sin^2(k_x' d)[1 + \sin(\theta_A)\sin(\phi)]^2}$$

Here d represents the width of the barrier of height V_0. On solving the boundary conditions we get that $k_x' d = -\frac{V_0 d}{\hbar v_F}\sqrt{1 - 2\frac{E}{V_0} + \frac{E^2}{V_0^2}\cos^2(\phi)}$. Interestingly, snell's law will come as a consequence of momentum conservation along the barriers and the conseravtion of k_y.

$$E\sin(\phi) = (V_0 - E)\sin(\theta_A)$$

- Along with normal incidence being guaranteed to have full transmission, for long enough barriers we will also have interference effects result in Fabry-Perot resonances.



$\bar{T}(E)$ obtained using the NEGF method. This also includes information on the density of states along with transmission.

Discussion & conclusion

- These properties have found use in various places such as constructing a Klein tunneling transistor [7] and for p-n junctions for electron-optical applications [5].
- The interesting property of this tunneling can be further explored for creating super-lattice type interference using a lesser barriers since a single barrier itself gives transmission resonances

Chirality and the consequences of it

- The sublattice structure results in a pseudospin being part of the state.
- Chirality is simply defined as the projection of the pseudospin operator along the momentum
- In the absence of a potential this has eigenvectors along the states of $|\boldsymbol{k}, \alpha\rangle$ with eigenvalue as α
- Due to conservation of pseudo-spin there will be no backscattering in the case of $\phi = 0$

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