Theory of Quantum Hall Effect in Graphene Sheets

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PH354 PROJECT

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Contents

In this project, we will go through the detailed implementation of the injection model that has been developed throughout the paper.

The Necessity of a new Model

What are the assumptions and limitations of the previous models?

The two main state-of-the-art systems, **the disorder model and the edge state model assume translational invariance** which is a strong assumption.

The disorder model models the electrons as distributed in **quantized levels around the Landau levels**. It models the splitting of energy levels between **continuous energy levels near Landau levels surrounded by discredited energy levels**.

The edge state model states that due to a **strong magnetic field, the charge carriers are pushed to the corners** of the graphene flake giving rise to two opposite flowing currents.

Moreover, a model effectively taking into account the **inter-electron interaction which is the main reason for the formation of the Hall Potential** is required. Something more than Fermi Gas Models…

Here we describe the **injection model** for two terminal measurements.

METHODOLOGY

The potential at the corner is given by

$$V_{\text{corner}}(x,y) = \frac{2}{\pi} V_{SD} \arctan\left(\frac{y}{x}\right)$$

From the 4x4 Dirac type Hamiltonian , it is guessed that the the wavefunctions consists of 4 components.

$$c\begin{pmatrix} V(x,y)/c & \Pi_x - i\Pi_y & 0 & 0 \\ \Pi_x + i\Pi_y & V(x,y)/c & 0 & 0 \\ 0 & 0 & V(x,y)/c & \Pi_x + i\Pi_y \\ 0 & 0 & \Pi_x - i\Pi_y & V(x,y)/c \end{pmatrix}$$

Calculate the Eigen energies of the Landau levels

$$c\,\mathrm{sgn}(n)\sqrt{2|n|e\hbar\mathcal{B}}\left[1-\frac{\mathcal{E}^2}{(c\mathcal{B})^2}\right]^{3/4} + \frac{\mathcal{E}}{\mathcal{B}}p_x$$

Calculate the appropriate Landau coordinates

$$\xi = \sqrt{\frac{e\beta}{\hbar c}}\left(y + \frac{c^2 p_x \mathcal{B} - \mathcal{E}E_{n,p_x}}{e\beta^2}\right), \quad \beta = \sqrt{(c\mathcal{B})^2 - \mathcal{E}^2}$$

Calculate the spinor oscillator functions

$$u_n(\xi) = \frac{\mathrm{e}^{-\xi^2/2}\mathrm{H}_n(\xi)}{\sqrt{2^n n!\sqrt{\pi}}}$$

Calculate the wave function

$$a = -\frac{\sqrt{c\mathcal{B}+\beta}}{\sqrt{2c\mathcal{B}}}, \quad b = \frac{\mathcal{E}}{\sqrt{2c\mathcal{B}}}\frac{1}{\sqrt{c\mathcal{B}+\beta}}$$

with the plane-wave solution in the x-direction, $\phi_{p_x}(x) = \mathrm{e}^{\mathrm{i}p_x x/\hbar}/\sqrt{2\pi}$, we obtain:

$$\psi_{1,n,p_x}(\mathbf{r}) = \phi_{p_x}(x)\left(\frac{e\beta}{\hbar c}\right)^{1/4}\left(\mathrm{sgn}(n)au_{|n|}(\xi) - bu_{|n|-1}(\xi)\right)$$

$$\psi_{2,n,p_x}(\mathbf{r}) = \phi_{p_x}(x)\left(\frac{e\beta}{\hbar c}\right)^{1/4}\left(au_{|n|-1}(\xi) - \mathrm{sgn}(n)bu_{|n|}(\xi)\right)$$

$$\psi_{3,n,p_x}(\mathbf{r}) = \psi_{2,n,p_x}(\mathbf{r}), \quad \psi_{4,n,p_x}(\mathbf{r}) = \psi_{1,n,p_x}(\mathbf{r}).$$

Calculate LDOS and then incorporate spin.

$$n_{\mathcal{E}\times\mathcal{B}}(\mathbf{r};E) = \sum_{i=1}^{4}\sum_{n=-\infty}^{\infty}\int \mathrm{d}p_x \left|\psi_{i,n,p_x}(\mathbf{r})\right|^2 \delta\left(E - E_{n,p_x}\right)$$

$$= \sum_{i=1}^{4}\sum_{n=-\infty}^{\infty}\left|\frac{\partial E_{n,p_x}}{\partial p_x}\right|^{-1}_{p_x=p_\delta}\left|\psi_{i,n,p_\delta}(\mathbf{r})\right|^2$$

$$p_\delta = \frac{\mathcal{B}}{\mathcal{E}}E - \mathrm{sgn}(n)\frac{c\mathcal{B}}{\mathcal{E}}\sqrt{2|n|e\hbar\mathcal{B}}\left[1-\frac{\mathcal{E}^2}{(c\mathcal{B})^2}\right]^{3/4}$$

Incorporating spin we get :

$$n^{\uparrow,A,B}_{\mathcal{E}\times\mathcal{B}}(\mathbf{r};E) = n_{\mathcal{E}\times\mathcal{B}}\left(\mathbf{r};E - \frac{g^*\mu_B}{2}\right) + n_{\mathcal{E}\times\mathcal{B}}\left(\mathbf{r};E + \frac{g^*\mu_B}{2}\right)$$

Calculate the current convolution integral over the Fermi distribution.

$$I_{\mathrm{SD}} = e\int_0^\infty \mathrm{d}E \int \mathrm{d}\mathbf{r_c} f\left(E,E_F\right)\frac{\mathcal{E}\left(\mathbf{r}_c\right)}{\mathcal{B}} n^{\uparrow\downarrow,,B}_{\mathcal{E}\times\mathcal{B}}\left(\mathbf{r}_c;E\right)$$

Our Objective

What do want to achieve here?

OBJECTIVE # 1

Calculate LDOS and plot it. Analyzing the modulations with the peaks and right-left shift due to 2 different spins.

OBJECTIVE # 2

Calculate the convolution Integral to plot constant curve resistivity characters.

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Computational Challenges

The fundamental constants are too many in number and too different in dimensions. This gives rise to **terms having radically different orders** which makes the calculation more prone to round-off errors.

The summation in the case of calculating LDOS in from **-infinity to +infinity**, we need to handle this integral.

The LDOS plot has **sharp peaks which means integrating over it should be done with care**, otherwise, peaks may be missed giving erroneous results.

The convolutional integral can not be done from r=0, **because the integrand diverges**. Choosing an appropriate critical lower bound is crucial for getting consistent values. We need to handle another infinite integral on Energy here.

The constant current characteristic for varying Fermi Energy is tricky business to obtain, it involves **iterating over potential values to get an appropriate current for a given Fermi Energy**, this is basically a root-finding problem.

How to Tackle

What are the assumptions and limitations of the previous models?

Grouping the fundamental constant in such a way that ensures homogeneity in order needs to be maint. It is done in the paper in quite a good way.

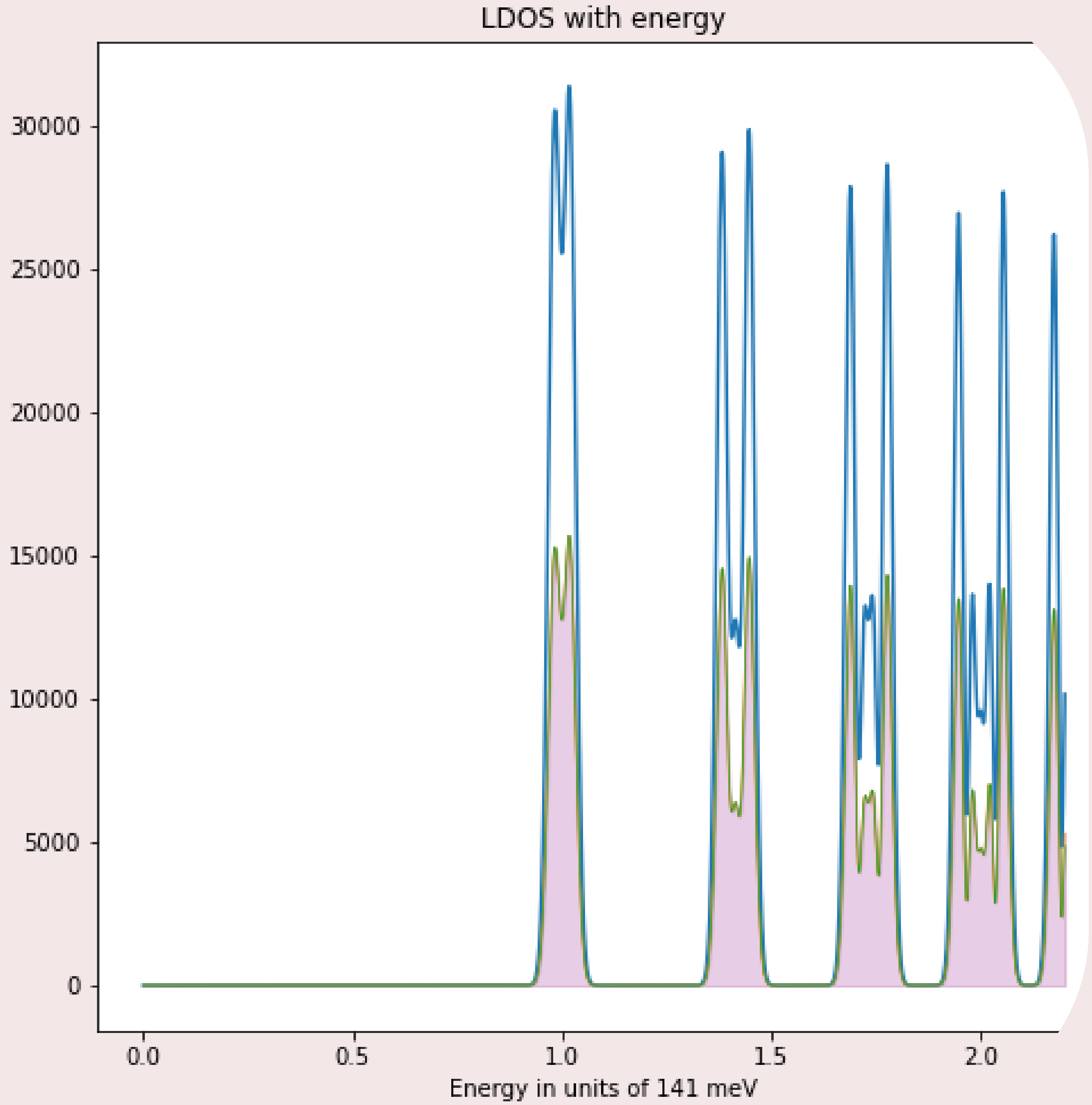
When we analyze the dependence on the wave function on the spinor function, we can clearly conclude that contributions from higher 'n' tends to be 0. This makes the integral easily obtainable by imposing upper and lower bounds

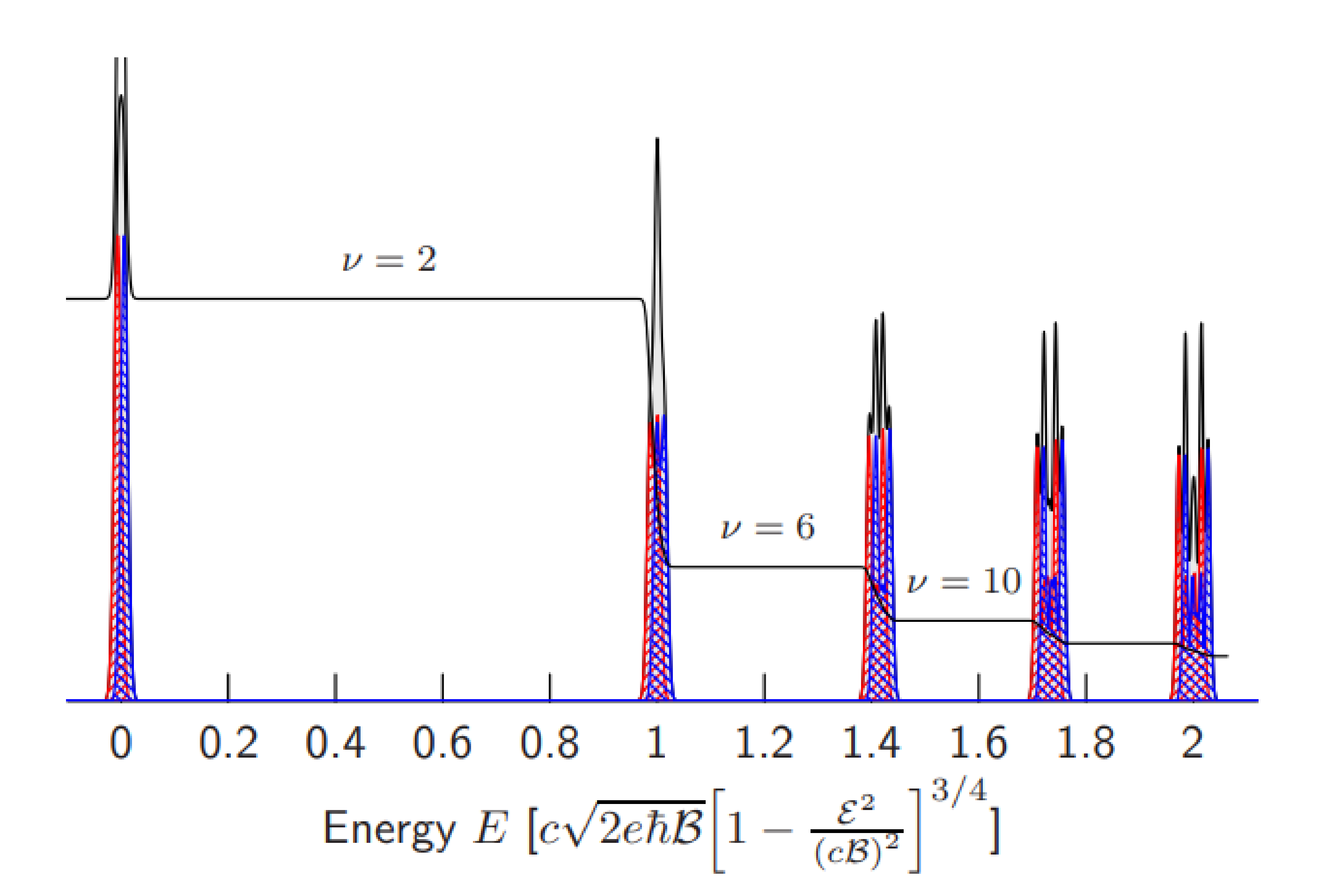
Using Scipy libraries takes care of the problem of sharp peaks, because of better design than hand-written trapezoidal or Simpson method.

We have chosen r_critical to be a very small value so that we can get the maximum contribution from the corner. It is chosen to be 1e-72. The infinite integral in energy has been resolved by noting that contribution from energies higher than the Fermi Energy is really small and T=5K in this case, which imposes this condition more thoroughly.

I have devised an iterative method which from an assumed value of potential iterates and finds when the potential cross the optimum value.. I have failed to reproduce the final result completely because of dimension mismatch and long run-time. I belive the algorithm is really inefficient.

Results–LDOS Graph



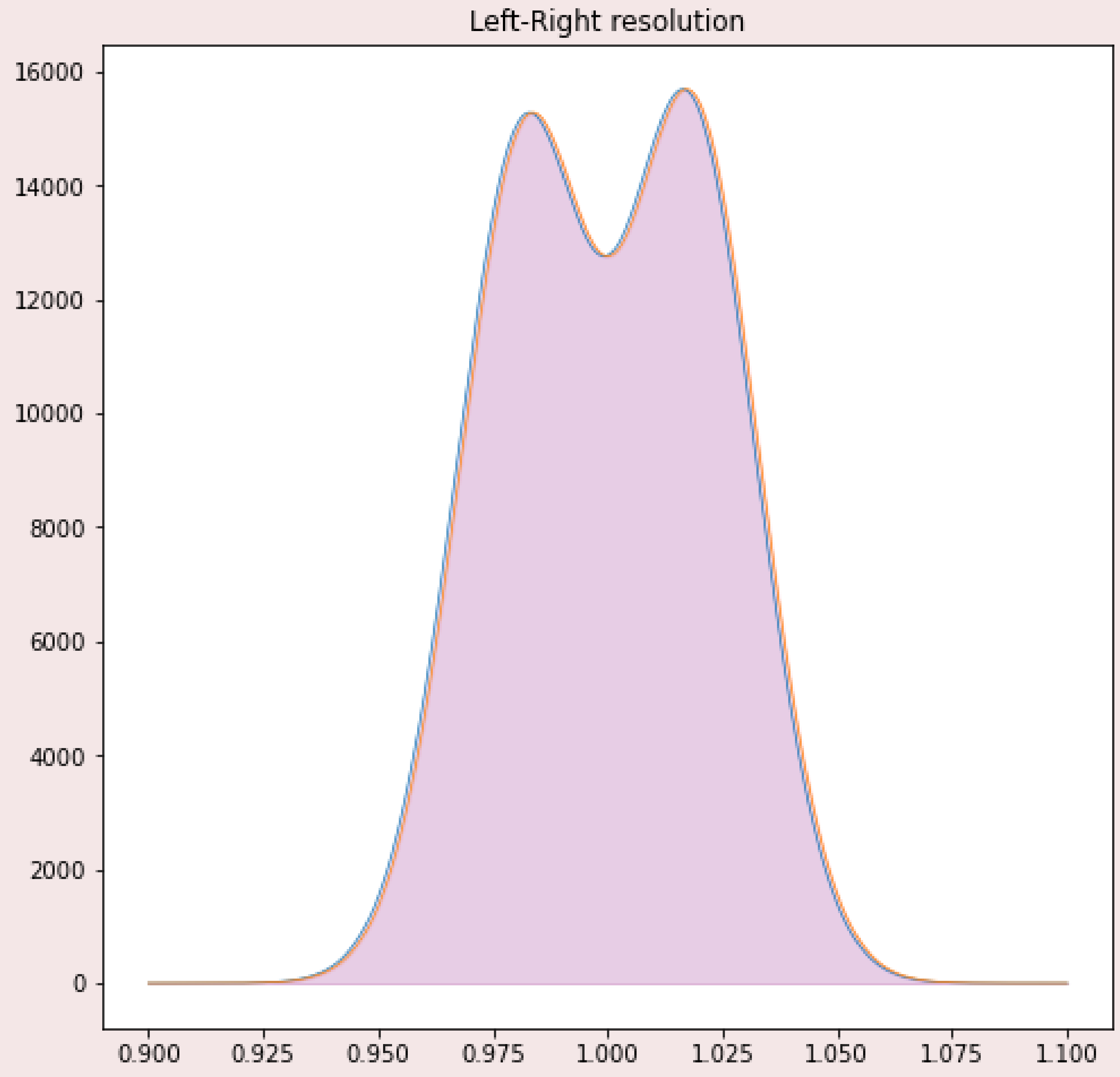


Here, the unit mentioned in the graph of the paper is approximately 141 mEV

Comments: Here we have missed the peak at zero energy but otherwise the scaling is consistent

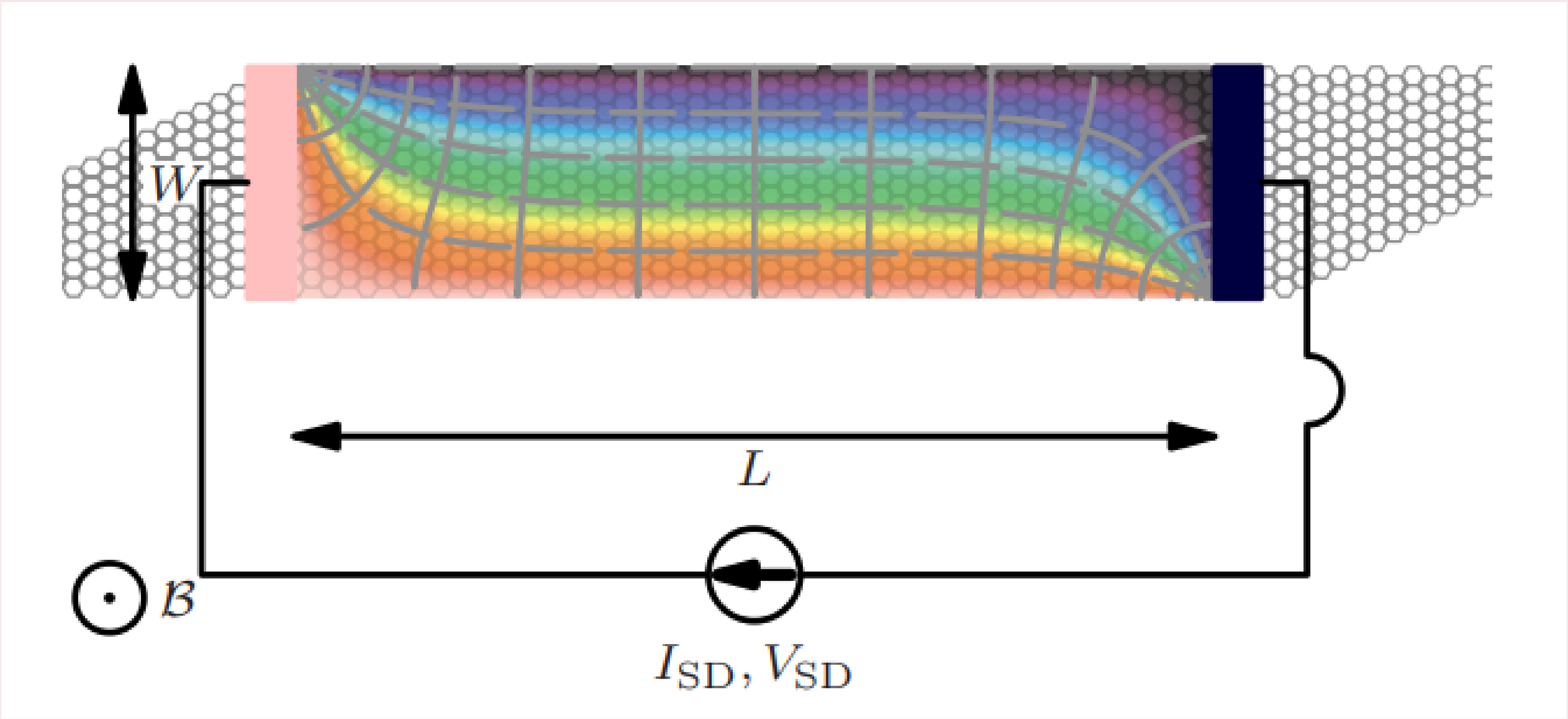
Carefully seeing we can observe left-right hatching and the peaks occur at roots of integers.

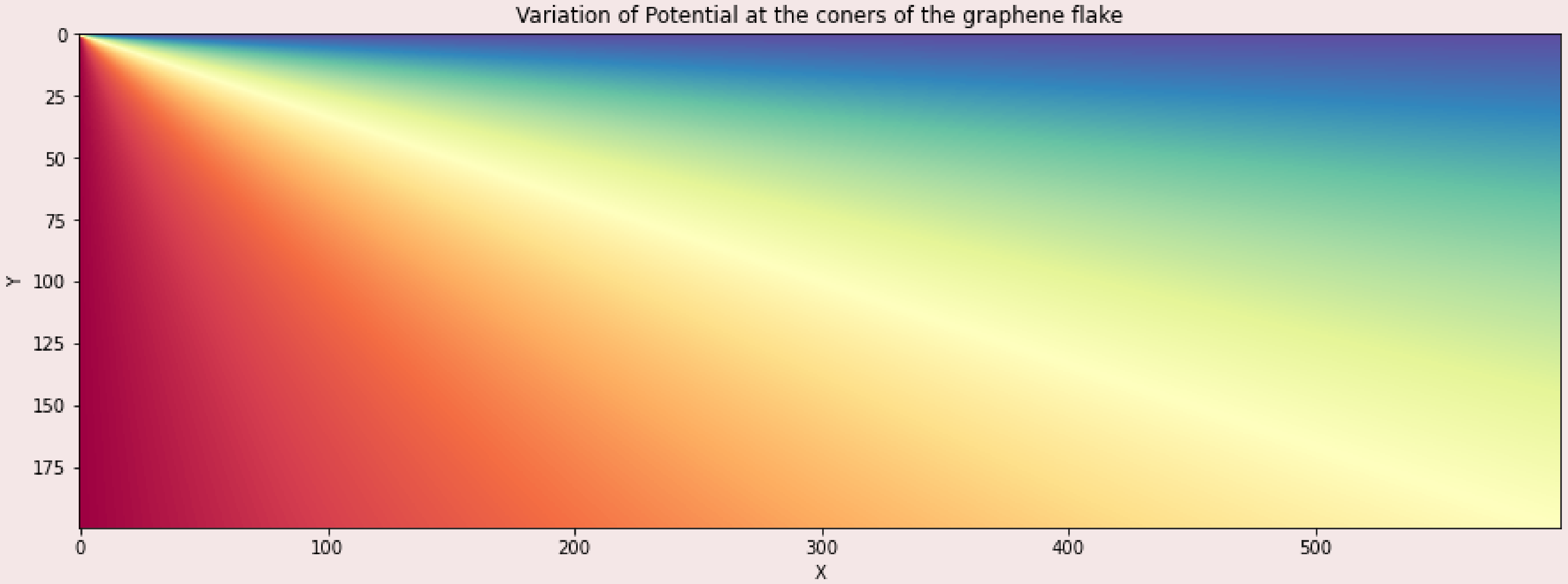
Results–Left Right Hatching



Separate graph to show left-right hatching.

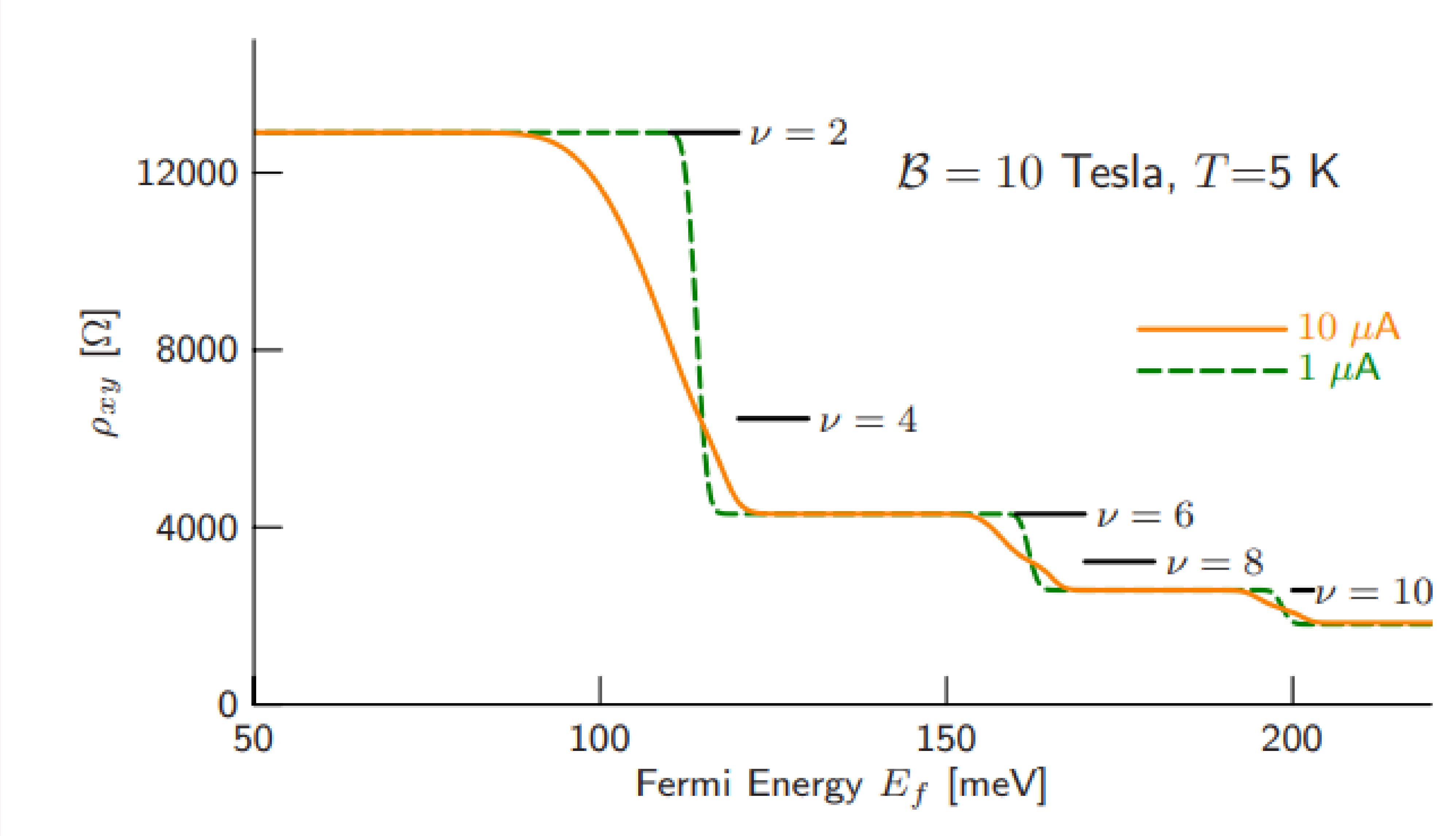
Results–Corner potential form

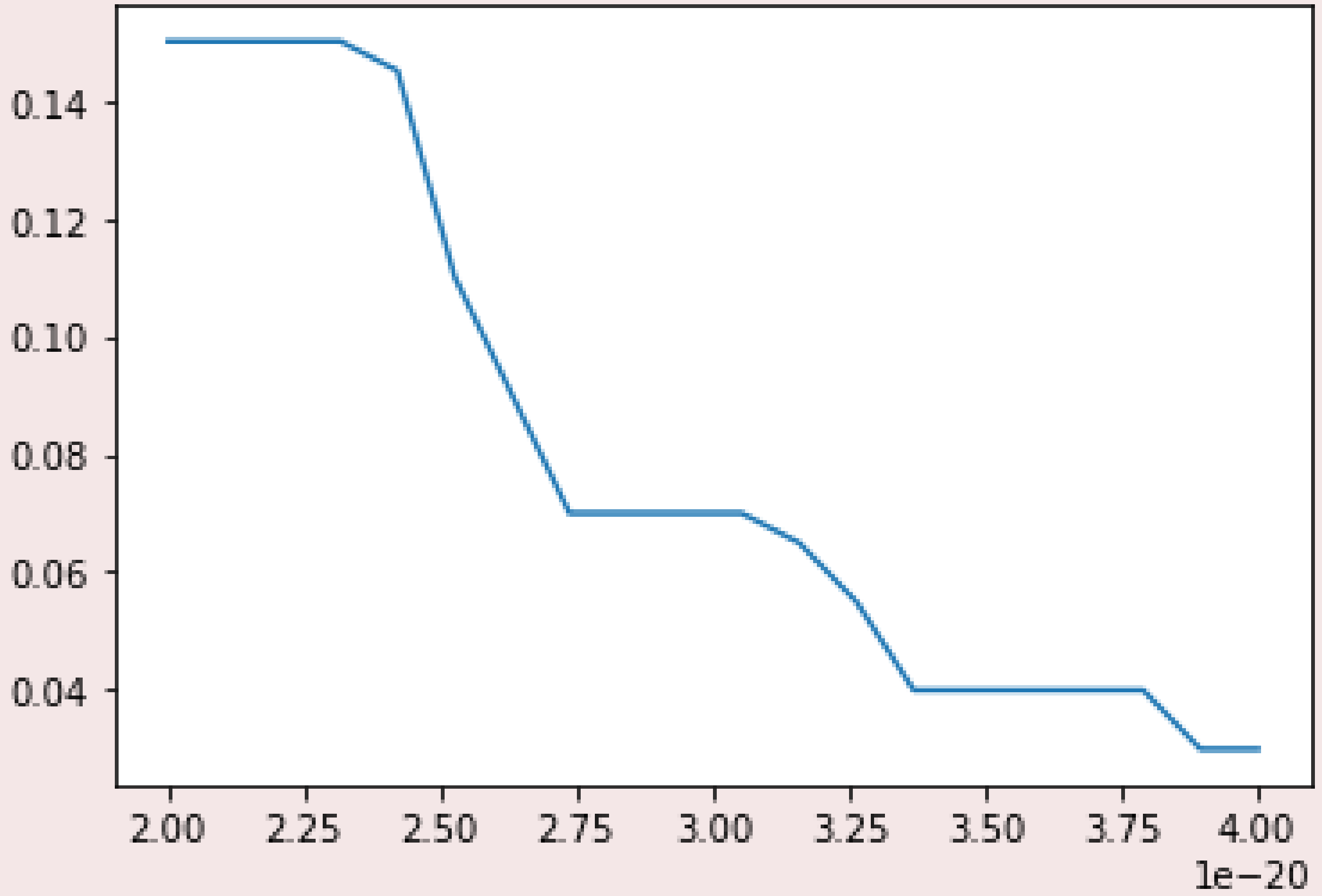


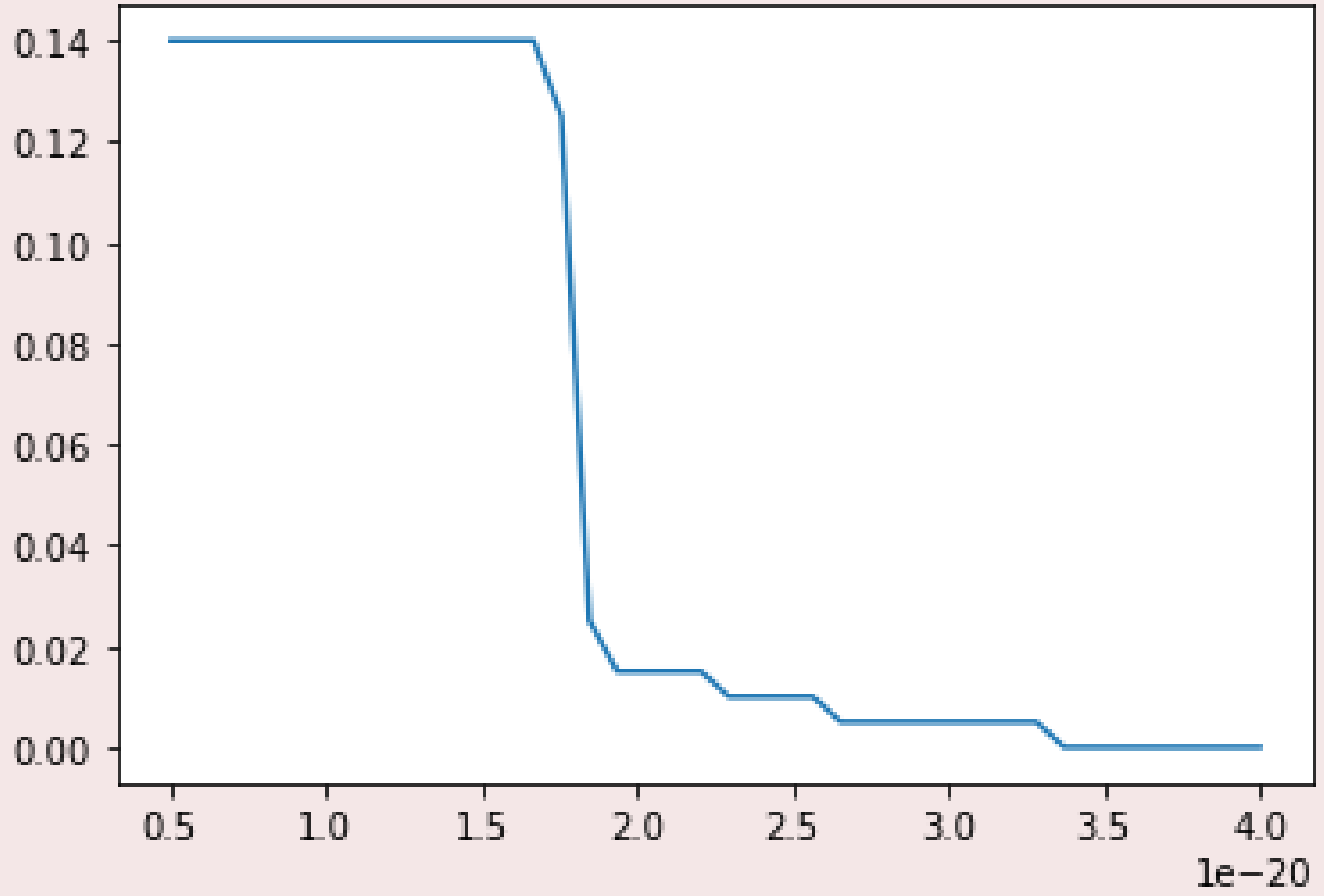


At teh top left corner
we can see the similitude
between the figure in the paper and the
picture plotted.

Results–Resistivity Quantisation







Clearly, this result has not been reproduced completely, due to the inefficiency of the algorithm used and the extended run-time.

The upper graph is for 10 microAmps and the down is for 1 MicroAmp. So, We can see that the 10 micro amp graph is dying down in a smoother fashion as seen in the paper. The quantization is apparent although the Chern numbers and the intersections are not shown.

What Improvements are possible

After this endeavor,
my main priority would be
to devise a better algorithm
to reproduce the potential plot.

GENERALIZATION OF THE MODEL

We have seen the extrapolation of corner potential characteristics to the whole sample. It is argued that the propagation of the corner solution of hall potential governs the whole sample. But it is imperative to look and see the general case scenario where the potential can be defined over the flake and worked with.

INTRA PEAK MODULATION

It was interesting to see the LDOS peaks had modulations within each peak. It is fascinating to further investigate what is happening in the peaks.

Acknowledgment

I thank Professor Manish Jain for this wonderful course and this opportunity of reproducing an entire paper which regretfully, I failed to completely execute.

I thank Professor Vibhor Singh for choosing the pa per which was appropriate with respect to my depth of conceptual knowledge and computational capabilities, and for guiding me when I faced some problems