Study of Electronic Properties of Finite Size Square and Hexagonal Lattices Using KPM Technique

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1 Density of state (DOS)

The second kind Chebychev polynomial (**CBP**) is defined

$$U_m(x) = \frac{\sin[(m+1)\arccos(x)]}{\sin[\arccos(x)]} \tag{1}$$

The global DOS can be expanded in terms of CBP as

$$n(E) = \mathrm{Tr}[\delta(E-\mathcal{H})] = \pi\sqrt{(1-E^2)}\sum_{m=0}^{\infty}\mu_n U_m(E) \tag{2}$$

By multiplying both sides of the equation with $U_n(E)$ and integrating over $[-1,1]$ interval we get

$$\mu_m = \frac{2}{\pi^2}\int_{-1}^{1}\mathrm{d}E\mathrm{Tr}[\delta(E-\mathcal{H})]U_m(E) = \frac{2}{\pi^2}\mathrm{Tr}[U_m(\mathcal{H})]. \tag{3}$$

The DOS can be written as

$$n(E) = \frac{2}{\pi}\sqrt{(1-E^2)}\sum_{m=0}^{M} g_m^M U_m(E)\mathrm{Tr}[U_m(\mathcal{H})] \tag{4}$$

where g_m^M is the Jackson kernel

$$g_m^M = \frac{1}{M+1}\left[(M-m+1)\cos\frac{m\pi}{M+1} + \sin\frac{m\pi}{M+1}\cot\frac{\pi}{M+1}\right] \tag{5}$$

to avoid the Gibbs oscillations in finite terms cut-off. In figure (1) the DOS of finite square and hexagonal lattice is presented. The results are compared with analytical approach for infinite lattice.

2 Kubo-Greenwood (KG) formula and longitudinal conductance

The dc conductance at zero temperature can be calculated using the Kubo-Greenwood formula

$$\sigma_{ab} = \frac{4\pi^2}{\Omega}\left(\frac{e^2}{h}\right)\Lambda_{ab}(E) \tag{6}$$

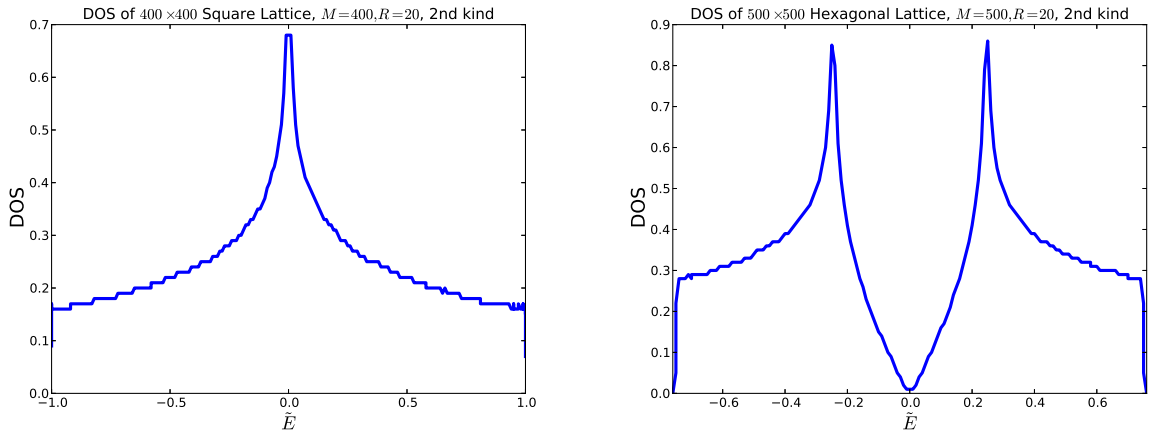

Figure 1: The DOS of pristine (a) 400×400 square and (b) 500×500 (b) hexagonal lattices. The number of CBP is $M = 500$ with $R = 20$ random vectors.

where

$$\Lambda_{ab}(E) = \mathrm{Tr}\left[\hbar v_a \delta(E - \mathcal{H}) \hbar v_b \delta(E - \mathcal{H})\right] \tag{7}$$

Since it depends on double δ-function, we prefer to write it as

$$\Lambda_{ab}(E) = \sum_{kk'} \langle k|\hbar v_a \delta(E - \mathcal{H})|k'\rangle\langle k'|\hbar v_b \delta(E - \mathcal{H})|k\rangle \tag{8}$$

$$= \sum_{kk'} \mathcal{M}_{kk'}(E)\mathcal{N}_{k'k}(E). \tag{9}$$

$\mathcal{M}$ and $\mathcal{N}$ is expanded separately

$$\mathcal{M}_{kk'}(E) = \pi\sqrt{1 - E^2} \sum_{m=0}^{M} \frac{2}{\pi^2} \langle k|\hbar v_a U_m(\mathcal{H})|k'\rangle U_m(E) g_m^M \tag{10}$$

Substitute $\mathcal{M}$ back to equation (7), the conductance will be

$$\sigma_{ab}(E) = \frac{16}{\Omega}\left(\frac{e^2}{h}\right)(1 - E^2) \sum_{mn}^{M} g_m^M g_n^M U_m(E) U_n(E) \Gamma_{mn} \tag{11}$$

where

$$\Gamma_{mn} = \mathrm{Tr}[\hbar v_a U_m(\mathcal{H}) \hbar v_b U_n(\mathcal{H})] \tag{12}$$

In figure (2), the longitudinal conductance vs. energy of a square lattice in the presence of applied magnetic field is shown. Compare the graph with the DOS for the same system.

3 Kubo-Bastin (KB) conductance formula

Let's start with the scaled[1] KB equation

$$\sigma_{ab}(\mu, T) = \frac{ie^2\hbar}{\Omega} \int_{-1}^{1} \mathrm{d}\epsilon f(\epsilon) \mathrm{Tr}\left[v_a \delta(\epsilon - \mathcal{H}) v_b \frac{\mathrm{d}G^+}{\mathrm{d}\epsilon} - v_a \frac{\mathrm{d}G^-}{\mathrm{d}\epsilon} v_b \delta(\epsilon - \mathcal{H})\right] \tag{13}$$

[1] All energy scales and the Hamiltonian must be transformed into the interval $[-1, 1]$ which CBPs are defined.

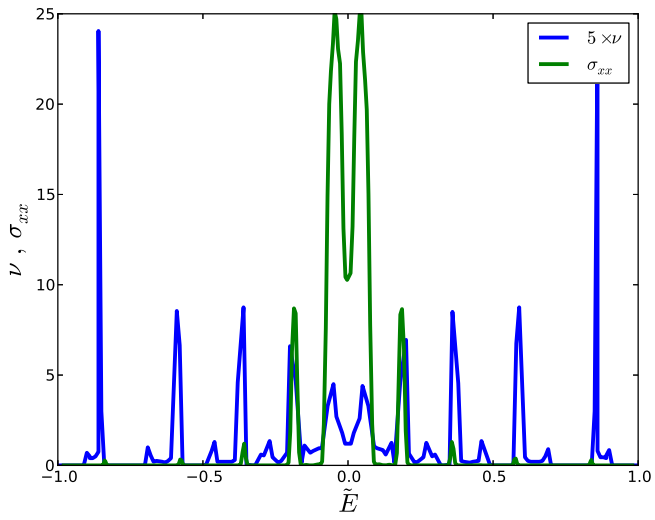

Figure 2: The longitudinal conductance of a 100×30 square lattice in the presence of $\phi/\phi_0 = 0.2$ applied magnetic field. Compare with the DOS of the same system.

At this point we assume that the system is enough large to be considered with continuous spectrum, so

$$G^+(\epsilon, \mathcal{H}) = \int G^+(\epsilon, \epsilon_k)|k\rangle\langle k|dk \tag{14}$$

is valid. The advanced and retarded Green's function are expanded in terms of second kind CBP as

$$G^{\pm}(\epsilon, \mathcal{H}) = \sum \mu_m U_m(\mathcal{H}). \tag{15}$$

Multiply both sides by $\pi\sqrt{1-\mathcal{H}^2}U_n(H)$ [2] an integrating over interval $[-1, 1]$, the moments will be

$$\mu_n^{\pm} = \frac{2}{\pi^2}\int_{-1}^{1} G^{\pm}(\epsilon, \mathcal{H})\pi\sqrt{1-\mathcal{H}^2}U_n(\mathcal{H})\mathrm{d}\mathcal{H} \tag{16}$$

$$= \frac{2}{\pi^2}\left[\Pr\int_{-1}^{1}\frac{\pi\sqrt{1-\mathcal{H}^2}}{E-\mathcal{H}}\mathrm{d}\mathcal{H} \mp i\pi\int_{-1}^{1}\delta(\epsilon-\mathcal{H})\pi\sqrt{1-\mathcal{H}^2}U_n(\mathcal{H})\mathrm{d}\mathcal{H}\right] \tag{17}$$

The first integral can be evaluated using the Hilbert transformation. So it will be

$$\mu^{\pm} = \frac{2}{\pi}\left[-\pi T_{n+1}(\epsilon) \mp i\pi\sqrt{1-\epsilon^2}U_n(\epsilon)\right] \tag{18}$$

$$= -2\exp[\pm i(n+1)\arccos(\epsilon)] \tag{19}$$

So the Green's function will be

$$G^{\pm}(\epsilon, \mathcal{H}) = -2\sum_{m=0}^{\infty} e^{\pm i(n+1)\arccos(\epsilon)}U_m(\mathcal{H}) \tag{20}$$

[2] By this notation we mean expanding in terms of eigenenergies then integrating over energy.

In the KB equation we need the derivative of the Green's function respect to energy

$$\frac{\mathrm{d}G^{\pm}(\epsilon,\mathcal{H})}{\mathrm{d}\epsilon} = \frac{\pm 2i}{\sqrt{1-\epsilon^2}} \sum_{m=0}^{\infty} (m+1) e^{\pm i(m+1)\arccos(\epsilon)} U_m(\mathcal{H}) \tag{21}$$

So the conductance in terms of CBP would be

$$\sigma_{ab} = \frac{-8}{\Omega}\left(\frac{e^2}{h}\right) \int_{-\infty}^{\infty} \mathrm{d}\epsilon f(\epsilon) \sum_{m,n=0}^{M} \Gamma_{mn}(\epsilon) \mathrm{Tr}\left[\hbar v_a U_m(\mathcal{H}) \hbar v_b U_n(\mathcal{H})\right] \tag{22}$$

where

$$\Gamma_{mn} = g_m^M g_n^M \left[U_m(\epsilon)(n+1)e^{i(n+1)\cos^{-1}(\epsilon)} + U_n(\epsilon)(m+1)e^{-i(m+1)\cos^{-1}(\epsilon)}\right] \tag{23}$$

In figure (3), the transverse conductivity σ_{xy} is shown. The quantum Hall effect can be seen through the plateaus which introduced to the system. Each plateau corresponds to a Landau's level and matches a peak in the DOS.

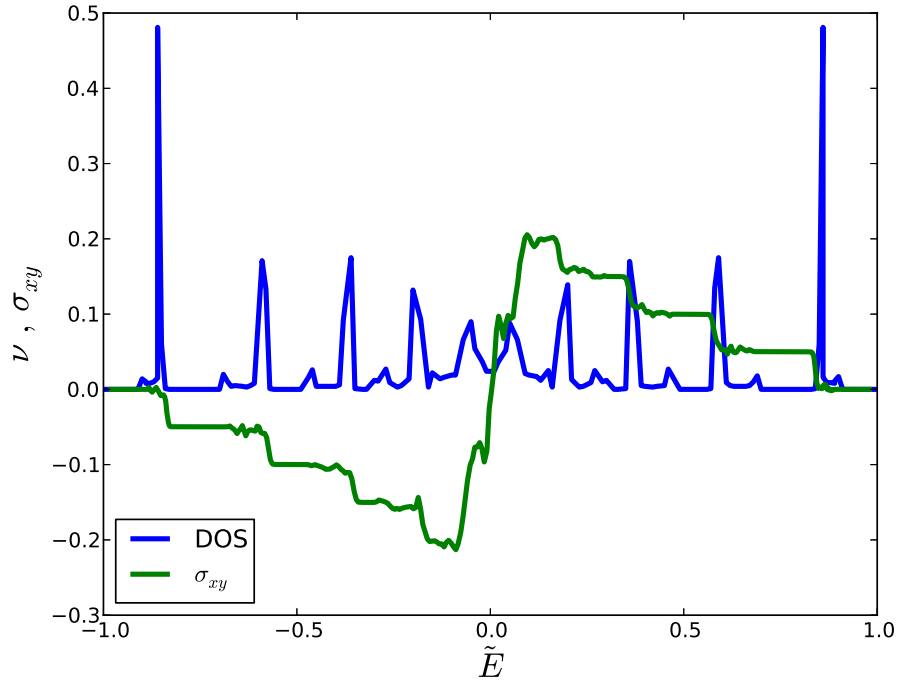

Figure 3: The transverse conductance σ_{xy} of a 100×30 square lattice

4 Trace Evaluation

After constructing R vectors as

$$|r\rangle = |\xi_1^r, \xi_2^r, \xi_3^r, \ldots, \xi_D^r\rangle \tag{24}$$

where $\xi_i^r = e^{i\phi}$, $\phi \in [0, 2\pi]$ is a random number and D is the dimension of the Hamiltonian matrix (total number of sites in the lattice.) The trace can be calculated stochastically as

$$\mathrm{Tr}[U_m(\mathcal{H})] \simeq \frac{1}{R}\sum_{r=1}^{R}\langle r|U_m(\mathcal{H})|r\rangle \tag{25}$$

The advantage of this technique is that instead of calculating $U_m(\mathcal{H})$ recursively

$$U_{m+1} = 2\mathcal{H}U_m - U_{m-1} \tag{26}$$

and doing the matrix-matrix multiplication the trace can be written in form of

$$\mathrm{Tr}[U_m(\mathcal{H})] \simeq \frac{1}{R}\sum_{r=1}^{R}\langle r|r\rangle_n \tag{27}$$

where

$$|r\rangle_n = U_n(\mathcal{H})|r\rangle \tag{28}$$

and $|r\rangle_n$ vector can be calculated recursively

$$|r\rangle_{n+1} = 2\mathcal{H}|r\rangle_n - |r\rangle_{n-1} \tag{29}$$

by matrix-vector multiplication. In the same manner, Γ_{mn} can be evaluated by

$$\Gamma_{mn}^{ab} = \frac{1}{R}\sum_{r=1}^{R}\langle r|\hbar v_a U_m(\mathcal{H})\hbar v_b U_n(\mathcal{H})|r\rangle. \tag{30}$$

Let's rewrite the expression as

$$\Gamma_{mn}^{ab} = \frac{1}{R}\sum_{r=1}^{R} {}_m\langle \bar{r}|\hbar v_b|r\rangle_n \tag{31}$$

where $|\bar{r}\rangle_n = U_n(\mathcal{H})|\bar{r}\rangle = U_n(\mathcal{H})\hbar v_a|r\rangle$. Keep in mind that $[U_n(\mathcal{H}), v_a] \neq 0$. To apply the velocity operator on the state, write the velocity in terms of the Hamiltonian of the system and $\mathbf{x}$ operator as

$$\hbar v_a = i[\mathcal{H}, x_a] \tag{32}$$

Since $|r\rangle$ can be considered random phase vector in real space representation, the velocity operator is constructed as

$$\begin{aligned}
\hbar(v_a)_{ij} &= i\sum[\mathcal{H}_{ik}x_{kj} - x_{ik}\mathcal{H}_{kj}] && (33)\\
&= i\sum[\mathcal{H}_{ik}x_j\delta_{kj} - x_i\delta_{ik}\mathcal{H}_{kj}] && (34)\\
&= i\sum\mathcal{H}_{ij}(x_j - x_i) && (35)
\end{aligned}$$

The diagonal symmetric element v_{ji} can be written as

$$\begin{aligned}
\hbar v_{ji} &= i\sum\mathcal{H}_{ji}(x_i - x_j) && (36)\\
&= -i\sum\mathcal{H}_{ji}(x_j - x_i) && (37)\\
&= -i\sum\mathcal{H}_{ij}^*(x_j - x_i) && (38)\\
&= \hbar v_{ij}^* && (39)
\end{aligned}$$

5 DOS in presence of applied magnetic field

5.1 Free 2D system

The Hamiltonian of 2D free particle system in presence of a perpendicular magnetic field is

$$\mathcal{H} = \frac{p_x^2}{2m} + \frac{1}{2m}(p_y - eA_y)^2 - \boldsymbol{\mu} \cdot \mathbf{B} \tag{40}$$

where vector potential can be chosen in Landau gauge as $A_y = B_0 x$. Since the Hamiltonian commute with p_y, it can be rewritten as

$$\mathcal{H} = \frac{p_x^2}{2m} + \frac{1}{2} m \left(\frac{eB}{m}\right)^2 (x - x_0)^2 \pm \Delta m_s \tag{41}$$

where $x_0 = \frac{\hbar k_y}{eB}$, and the Hamiltonian has the form of a simple harmonic oscillator with the frequency of $\omega_c^2 = \frac{eB}{m}$. The DOS is

$$\nu(E) = \frac{1}{L_x L_y} \sum_{n, m_s, k_y} \delta(E - E_{n, m_s, k_y}). \tag{42}$$

with eigenenergies $E_{n,s} = \hbar\omega_c(n + 1/2) \pm \Delta_s$ independent of k_y. The summation over k_y can be transformed to

$$\frac{1}{L_y} \sum_{k_y} = \int_0^? \frac{dk}{2\pi}. \tag{43}$$

To find the upper bound, we use the fact that $x - x_0$ must lie inside L_x. So

$$0 < x_0 < L_x \Rightarrow k_y < L_x / l^2 \tag{44}$$

where $l^2 = \frac{\hbar}{eB}$ is magnetic length. After evaluation of integral, the DOS will be

$$\nu(E) = \frac{eB}{\hbar} \sum_{n, m_s} \delta(E - E_{n, m_s}) \tag{45}$$

So by increasing the applied magnetic field, the ω_c and distance between the Landau's level will be increased (fig. (4)).

5.2 Graphene lattice around the Dirac points

The Hamiltonian of pristine graphene in tight-binding approximation is

$$\mathcal{H} - \epsilon_0 = \begin{pmatrix} 0 & -t\Gamma^* \\ -t\Gamma & 0 \end{pmatrix} \tag{46}$$

where $\Gamma = 1 + e^{i\mathbf{k}\cdot\mathbf{a}_1} + e^{i\mathbf{k}\cdot\mathbf{a}_2}$. The eigenenergies are

$$E = \pm t|\Gamma| \tag{47}$$

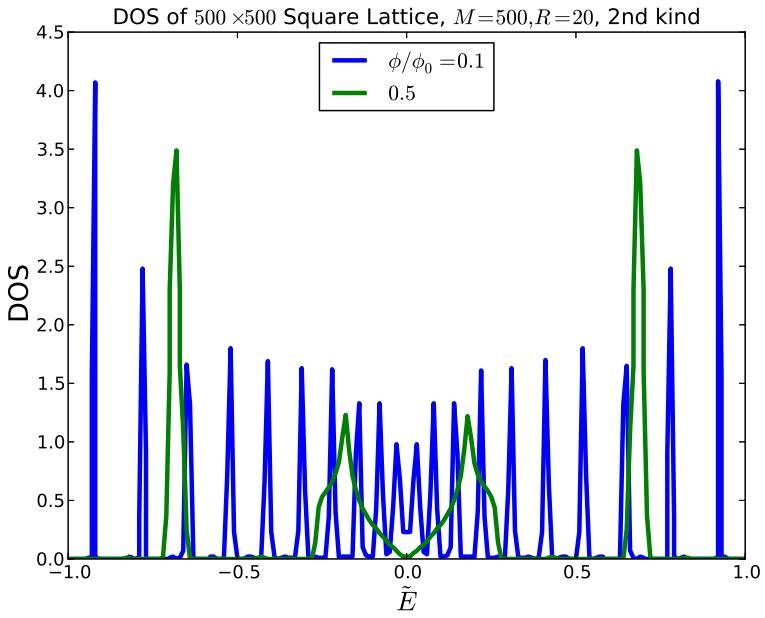

Figure 4: The DOS of a square lattice in presence of applied magnetic filed perpendicular to the lattice's space.

where Γ can be written as

$$\Gamma = 1 + 2\cos\left(\frac{ak_y}{2}\right) e^{i\sqrt{3}ak_x/2} \tag{48}$$

The zeros of Γ are $k_x = 0, k_y = \pm\frac{4\pi}{3a}$. To approximate the Hamiltonian around the Dirac's points, we have

$$\Gamma(\mathbf{k}+\mathbf{K}) \approx \boldsymbol{\nabla}_{\mathbf{k}}\Gamma|_{\mathbf{k}=\mathbf{K}} \cdot \mathbf{k} = -\frac{a\sqrt{3}}{2}(i\mathbf{k_x} \pm \mathbf{k_y}) \tag{49}$$

Factoring an i from Γ does not change the Hamiltonian

$$\mathcal{H}_D = \hbar v_F \begin{pmatrix} 0 & k_x \pm ik_y \\ k_x \mp ik_y & 0 \end{pmatrix} = \hbar v_F \mathbf{k} \cdot \boldsymbol{\sigma} \tag{50}$$

where $v_F = \frac{at\sqrt{3}}{2\hbar} \approx 10^6$. At corresponding K' the "helicity" is reverse $k_x \to k_x\,, k_y \to -k_y$. The behavior of carriers with energy in vicinity of Dirac point in the presence of applied magnetic field is governed by

$$\mathcal{H}_D = v_F \begin{pmatrix} 0 & p_x + i(p_y - eBx) \\ p_x - i(p_y - eBx) & 0. \end{pmatrix} \tag{51}$$

Since $[\mathcal{H}_D, k_y] = 0$, the wavefunction can be written as

$$\psi(x,y) = e^{ik_y y} \begin{pmatrix} \phi_1(x) \\ \phi_2(x) \end{pmatrix} \tag{52}$$

Applying the Hamiltonian to the eigenfunction we have

$$\begin{cases} [p_x + ieB(x_0 - x)]\phi_2(x) = \frac{\epsilon}{v_F}\phi_1(x) \\ [p_x - ieB(x_0 - x)]\phi_1(x) = \frac{\epsilon}{v_F}\phi_2(x) \end{cases} \tag{53}$$

By inserting the second equation into the first one we get

$$[p_x + ieB(x_0 - x)][p_x - ieB(x_0 - x)]\phi_1(x) = \left(\frac{\epsilon}{v_F}\right)^2 \phi_1(x) \tag{54}$$

which is similar to the simple harmonic equation. The commutation of

$$[p_x + ieB(x_0 - x), p_x - ieB(x_0 - x)] = ieB[p_x, x] + ieB[-x, p_x] = 2ieB(-i\hbar) = 2eB\hbar \tag{55}$$

suggest to write the Hamiltonian in terms of the ladder operators as

$$2\hbar eBa^\dagger a\phi_1(x) = \left(\frac{\epsilon}{v_F}\right)^2 \phi_1(x) \tag{56}$$

The eigenenergies will be

$$\epsilon = \hbar\omega_c\sqrt{n}, \tag{57}$$

where

$$\omega_c^2 = \frac{2eBv_F^2}{\hbar} \tag{58}$$

By following the same procedure that is adopted in the previous section, the DOS is

$$\nu(\epsilon) = \frac{eB}{h}\sum_n \delta(\epsilon - \epsilon_n) \tag{59}$$

The number of carriers in term of DOS is

$$n_e(\epsilon) = \int \mathrm{d}\epsilon\nu(\epsilon)n_F(\epsilon - \mu) = \frac{eB}{h}\int \mathrm{d}\epsilon\nu(\epsilon)\frac{1}{e^{\beta(\epsilon-\mu)} + 1} \tag{60}$$

At $T = 0$ the number of carriers

$$n_e = \frac{eB}{h}\sum_n \theta(\epsilon_n - \mu) \tag{61}$$

5.3 Quantum Hall effect

Starting from the Drude's model for classical carriers, we have

$$m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t} = e(\mathbf{E} + \mathbf{v} \times \mathbf{B}) - \frac{m\mathbf{v}}{\tau} \tag{62}$$

Considering the external magnetic field in z direction and the fact that transverse velocity is zero, we can write

$$\begin{cases} E_y = v_x B_0 \\ eE_x = \frac{mv_x}{\tau} \end{cases} \tag{63}$$

So by definition the longitudinal and transverse conductivity are

$$\begin{cases} \sigma_{xx} = \frac{I_x}{V_x} = \frac{e^2 \tau n_e}{m} \\ \sigma_{xy} = \frac{I_x}{V_y} = \frac{B_0}{e n_e} \end{cases} \tag{64}$$

So the transverse conductivity will be

$$\sigma_{xy} = \frac{e n_e}{B} = \left(\frac{e^2}{h}\right) \sum_{n,m} \theta(\epsilon_n - \mu) \tag{65}$$

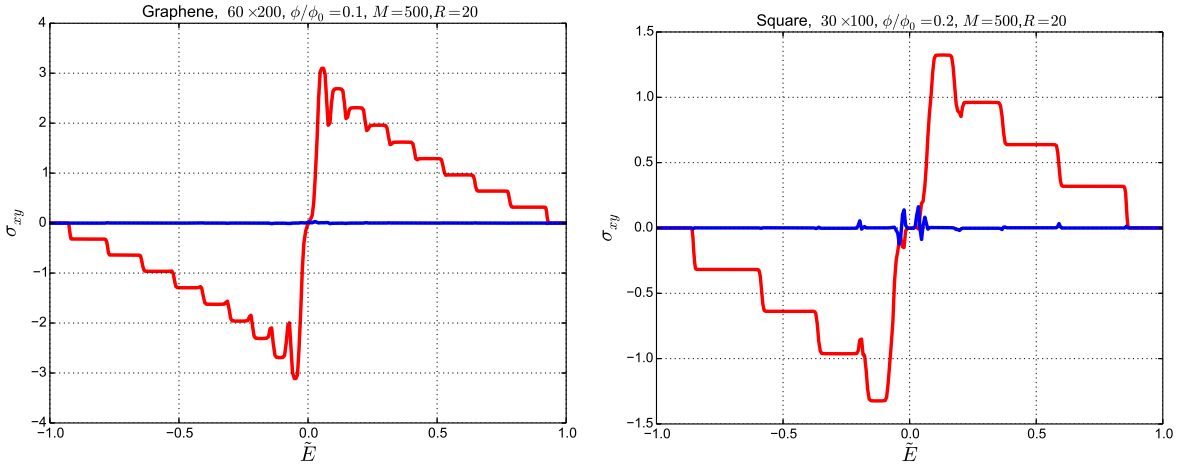

Figure 5: The number of plateaus and their locations are determined by the magnetic field strength and the type of lattice. Although a larger size lattice leads to sharper plateaus as we expect from the KMP technique.

6 The Local Density of State (LDOS)

To find the local DOS (LDOS), all diagonal elements of CBPs must be known. So the matrix-vector multiplication can not be used here . The matrix-matrix multiplication consume more memory resources and takes more time. In figure (6), some sites in the square lattice have lower energy which traps electron. As a result the LDOS is higher in the region with lower on-site potential. In addition, the LDOS is oscillating from the center which is due to the interference of wavefunctions. (Friedel's Oscillation)

7 Thechnical Consideration

7.1 Peierl's coefficient

An external magnetic field is imparted in the Hamiltonian as a shift in momentum

$$\mathbf{p} \rightarrow \mathbf{p} - \frac{e}{c}\mathbf{A}. \tag{66}$$

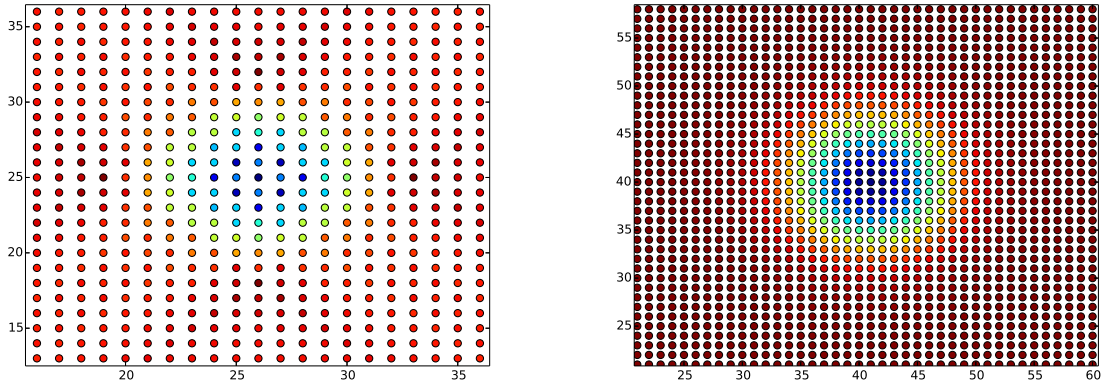

Figure 6: The LDOS of a square lattice with local lower on-site energy at central region at the Fermi energy.

Thus the translation operator in magnetic field reads

$$\tau(\mathbf{dx}) = e^{-i/\hbar(\mathbf{p}-\frac{e}{c}\mathbf{A})\cdot\mathbf{dx}} \tag{67}$$

The extra change of phase due to magnetic field is

$$e^{-i\frac{e}{\hbar c}\int_{\mathbf{r}_i}^{\mathbf{r}_j}\mathbf{A}\cdot\mathrm{d}\mathbf{r}} = e^{-i\frac{2\pi}{\Phi_0}\int_{\mathbf{r}_i}^{\mathbf{r}_j}\mathbf{A}\cdot\mathrm{d}\mathbf{r}} = e^{-i\frac{2\pi\Phi}{\Phi_0}} \tag{68}$$

which is Peierl's coefficient. Assuming an external constant magnetic field perpendicular to the surface of 2D system, the vector potential in the Landau's gauge will be $\mathbf{A} = (0, B_0 x, 0)$. To calculate the phase change through hopping along a straight line with coordinates $\mathbf{r}_i = (x_i, y_i)$, and $\mathbf{r}_j = (x_j, y_j)$ we have

$$\Phi = \int_{\mathbf{r}_i}^{\mathbf{r}_j}\mathbf{A}\cdot\mathrm{d}\mathbf{r} \tag{69}$$

$$= B_0\int_{y_i}^{y_j} x(y)\mathrm{d}y \tag{70}$$

The integral over line with slope

$$\tan\theta = \frac{y_j - y_i}{x_j - x_i} \tag{71}$$

give us

$$\Phi = \frac{B_0}{2}(y_j - y_i)(x_j + x_i) \tag{72}$$

7.2 Lattice and the Hamiltonian

The square lattice with $D = M \times N$ sites need a Hamiltonian matrix with $D \times D$ dimension. However only $N_z = 4NM = 4D$ elements are non-zero, considering periodic boundary condition in two dimensions. The number of non-zero elements of the matrix will vary in different calculation.

For example in the LDOS calculation, one needs to alter the on-side energies which will add the diagonal elements to non-zero elements. In all cases the Hamiltonian can be stored with three 1D arrays with N_z elements. Two integer arrays store the rows and columns of non-zero elements and one array stores the value.

7.3 Efficient Sparse Matrix-Matrix and Matrix-Vector multiplication

To perform fast sparse matrix-matrix and matrix-vector multiplication, the sparse matrix can be stored in three one dimensional arrays. Two integers arrays to store the column and row of the nonzero elements of the matrix and the third array which stores the values of the non-zero elements. The matrix-vector multiplication can be evaluated as

```
do ic = 1, size(indx)
      vec_reslt( indx(ic) ) = vec_reslt( indx(ic) ) + &
      values(ic) * vector( jndx(ic) )
end do
```

and in the same manner the matrix-matrix multiplication will be

```
do i = 1, dim_c(2)
   do in = 1, nnz
      c_res(indx(in),i) = c_res(indx(in),i) + &
          a_values(in) * b(jndx(in),i)
    end do
end do
```