Ferromagnetism in Bernal stacked bilayer graphene

Khanh Pham, UC Berkeley
Faculty Advisor: Andrea Young, UCSB

Graphene

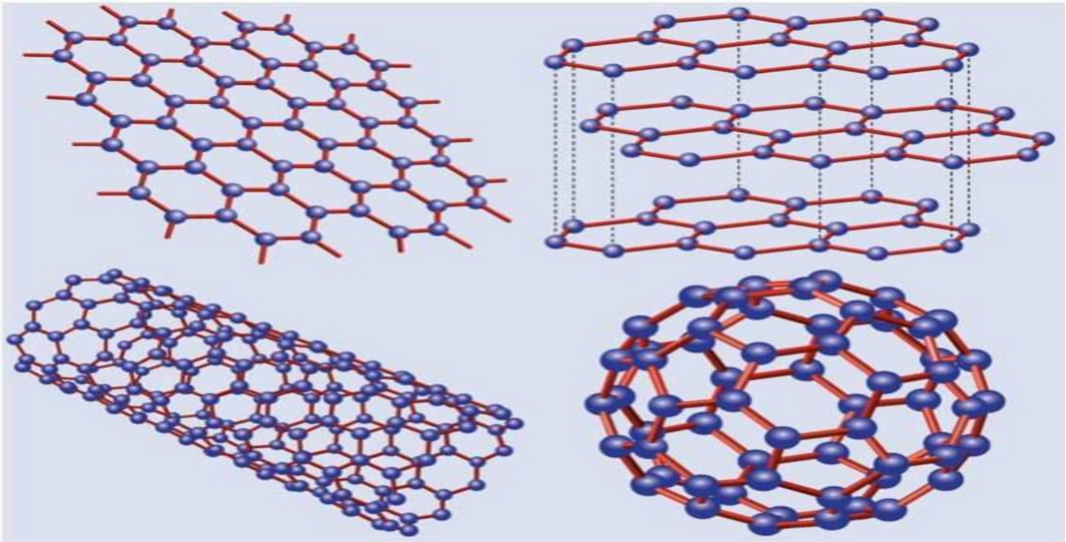
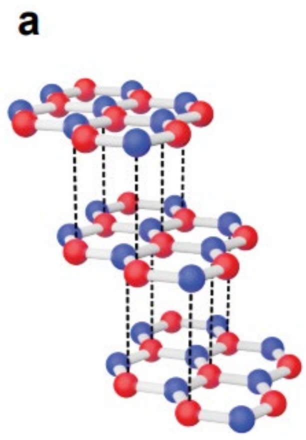


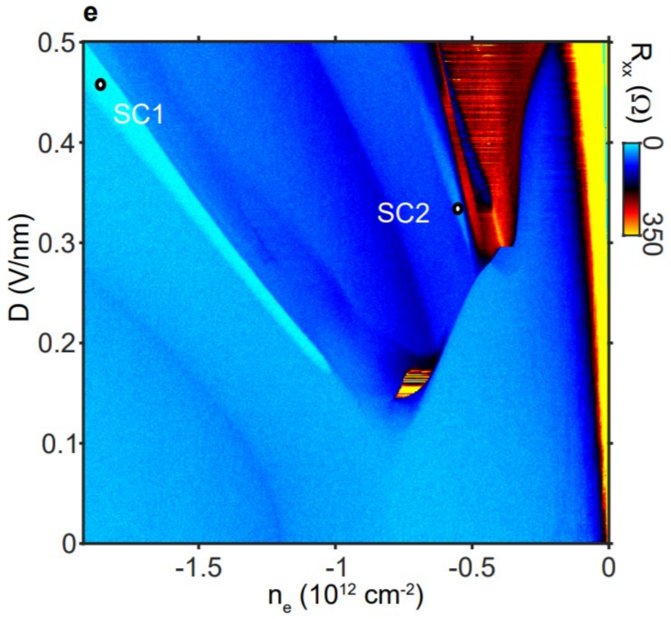
Image source: Figure 1 from A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim. The electronic properties of graphene. https://journals.aps.org/rmp/abstract/10. 1103/RevModPhys.81.109, 2009.

Recent work on ABC trilayer graphene



ABC trilayer graphene structure

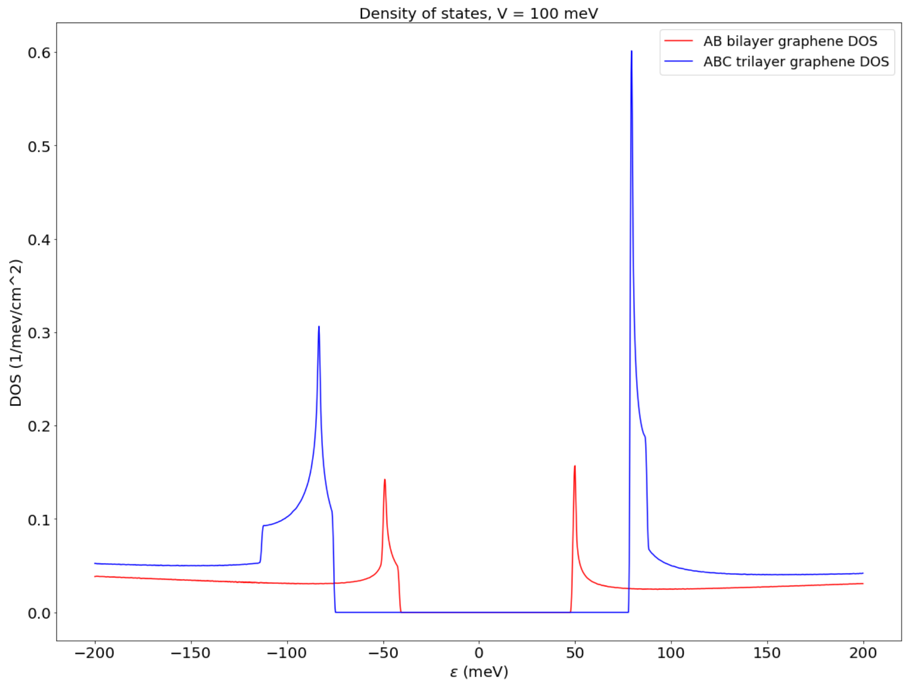
Figure 1a from Zhao, H. *et al*. Superconductivity in rhombohedral trilayer graphene. arXiv:2106.07640v1 [cond-mat.mes-hall] (2021)



Superconductivity

Figure 1e from Zhao, H. *et al*. Superconductivity in rhombohedral trilayer graphene. arXiv:2106.07640v1 [cond-mat.mes-hall] (2021)

Similarity of AB BLG and ABC TLG



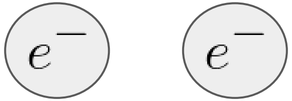
- Goal of the project: use theoretical models to explain experimental observations for ferromagnetism in bilayer graphene

What is ferromagnetism?

- A ferromagnetic material is one that reacts strongly to a magnetic field

$\uparrow\ \uparrow\ \uparrow\ \uparrow\ \uparrow\ \uparrow\ \uparrow\ \uparrow$	$\uparrow\ \downarrow\ \downarrow\ \uparrow\ \downarrow\ \uparrow\ \downarrow\ \uparrow$
ferromagnetic	paramagnetic

Origin of ferromagnetism

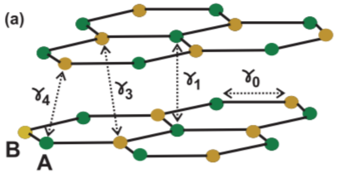


$$\frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle)$$

$$|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle, \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle)$$

Bilayer Graphene

- Structure of AB stacked bilayer graphene:



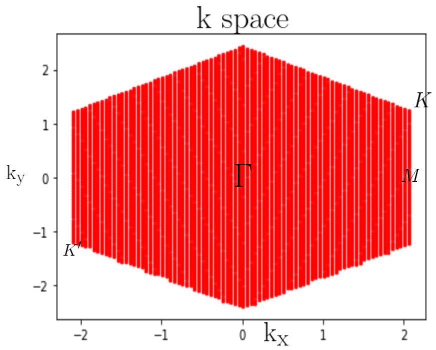
- Tight binding model: $\mathcal{H}_{t.b.} = -\gamma_0 \left(\sum_{\langle i,j \rangle, m} \hat{a}^{\dagger}_{m,i} \hat{b}_{m,j} + \hat{b}^{\dagger}_{m,j} \hat{a}_{m,i} \right) - \gamma_1 \left(\sum_{j} \hat{a}^{\dagger}_{1,j} \hat{a}_{2,j} + \hat{a}^{\dagger}_{2,j} \hat{a}_{1,j} \right) - \gamma_3 \left(\sum_{\langle i,j \rangle} \hat{b}^{\dagger}_{1,i} \hat{b}_{2,j} + \hat{b}^{\dagger}_{2,j} \hat{b}_{1,i} \right) - \gamma_4 \left(\sum_{\langle i,j \rangle} \hat{a}^{\dagger}_{1,i} \hat{b}_{2,j} + \hat{a}^{\dagger}_{2,i} \hat{b}_{1,j} + \hat{b}^{\dagger}_{1,j} \hat{a}_{2,i} + \hat{b}^{\dagger}_{2,j} \hat{a}_{1,i} \right)$

$$\mathcal{H}_{\mathrm{bi},\boldsymbol{k}} = \begin{bmatrix} -V/2 & -\gamma_0 f(\boldsymbol{k}) & \gamma_4 f(\boldsymbol{k}) & -\gamma_3 f(\boldsymbol{k})^* \\ -\gamma_0 f(\boldsymbol{k})^* & -V/2 + \Delta' & \gamma_1 & \gamma_4 f(\boldsymbol{k}) \\ \gamma_4 f(\boldsymbol{k})^* & \gamma_1 & V/2 + \Delta' & -\gamma_0 f(\boldsymbol{k}) \\ -\gamma_3 f(\boldsymbol{k}) & \gamma_4 f(\boldsymbol{k})^* & -\gamma_0 f(\boldsymbol{k})^* & V/2 \end{bmatrix}$$

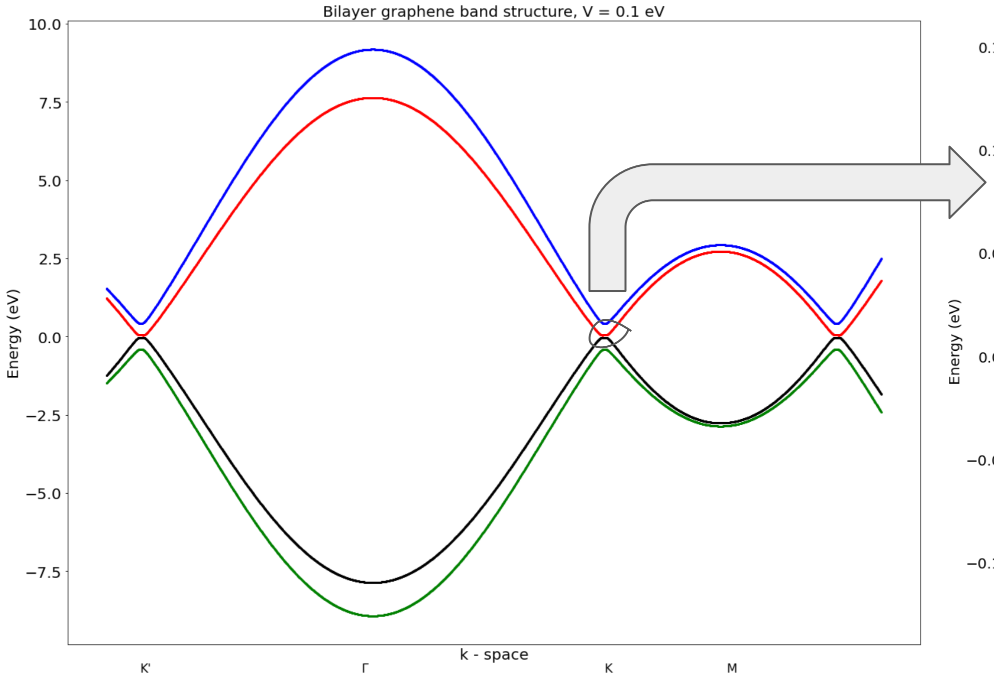
$$f(k) = e^{-ik_x a} \left[1 + 2e^{i3k_x a/2} \cos\left(\frac{\sqrt{3}}{2} k_y a \right) \right]$$

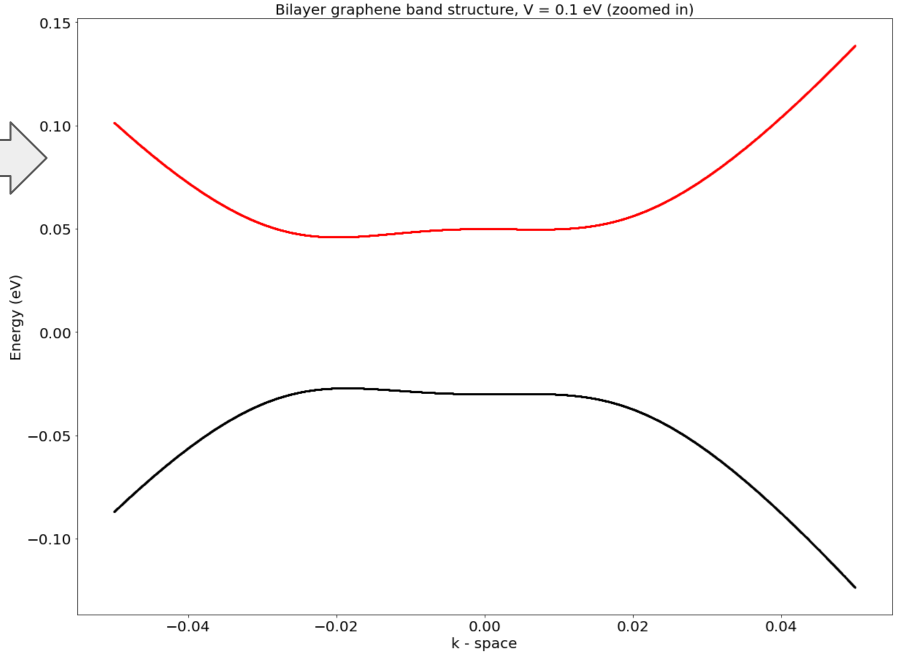
Image source: Figure 9 from A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim. The electronic properties of graphene. https://journals.aps.org/rmp/abstract/10. 1103/RevModPhys.81.109, 2009.

Band structure



- Band structure - allowed energy levels of the system

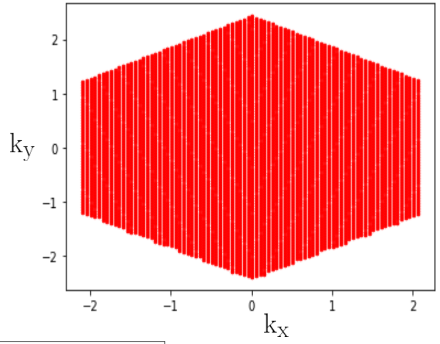




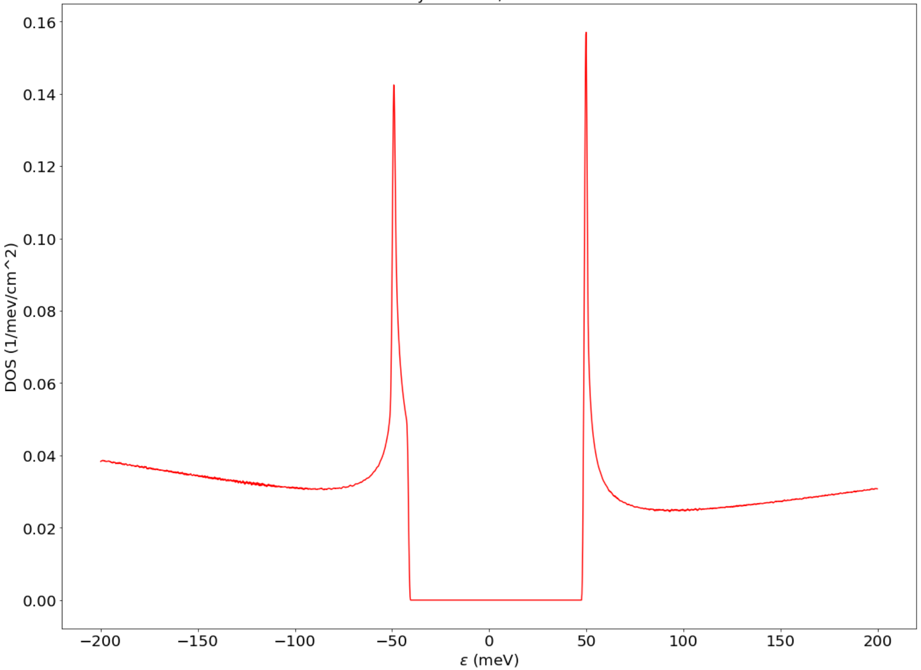
Density of states

$$\rho(\epsilon) = \frac{1}{A} \sum_{\vec{k}\in\mathrm{BZ}} \delta(\epsilon - \epsilon_{\vec{k}})$$

Brillouin zone



Density of states, V = 100 meV



Stoner model

Electron spin: $$|\uparrow,\uparrow\rangle, |\downarrow,\downarrow\rangle, \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle + |\downarrow,\uparrow\rangle), \frac{1}{\sqrt{2}}(|\uparrow,\downarrow\rangle - |\downarrow,\uparrow\rangle)$$

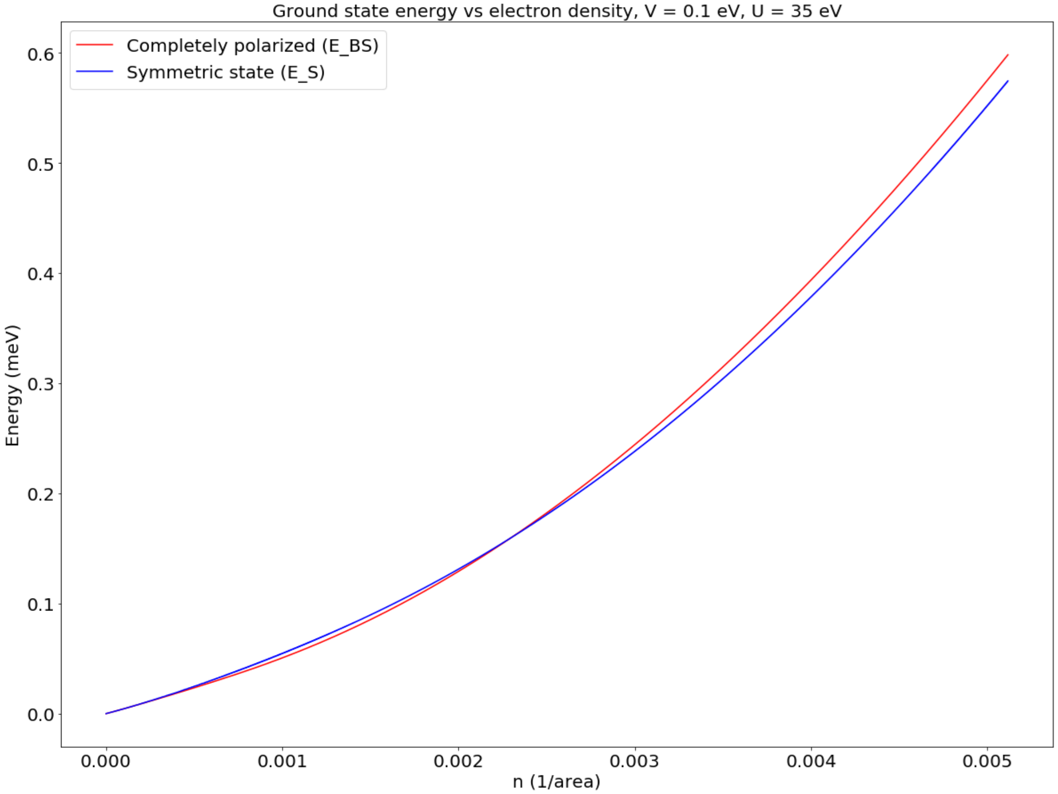
Kinetic energy: $$\langle E\rangle = \int_0^{n_\uparrow} \epsilon(n)\rho(n)\frac{d\epsilon}{dn}dn + \int_0^{n_\downarrow} \epsilon(n)\rho(n)\frac{d\epsilon}{dn}dn$$

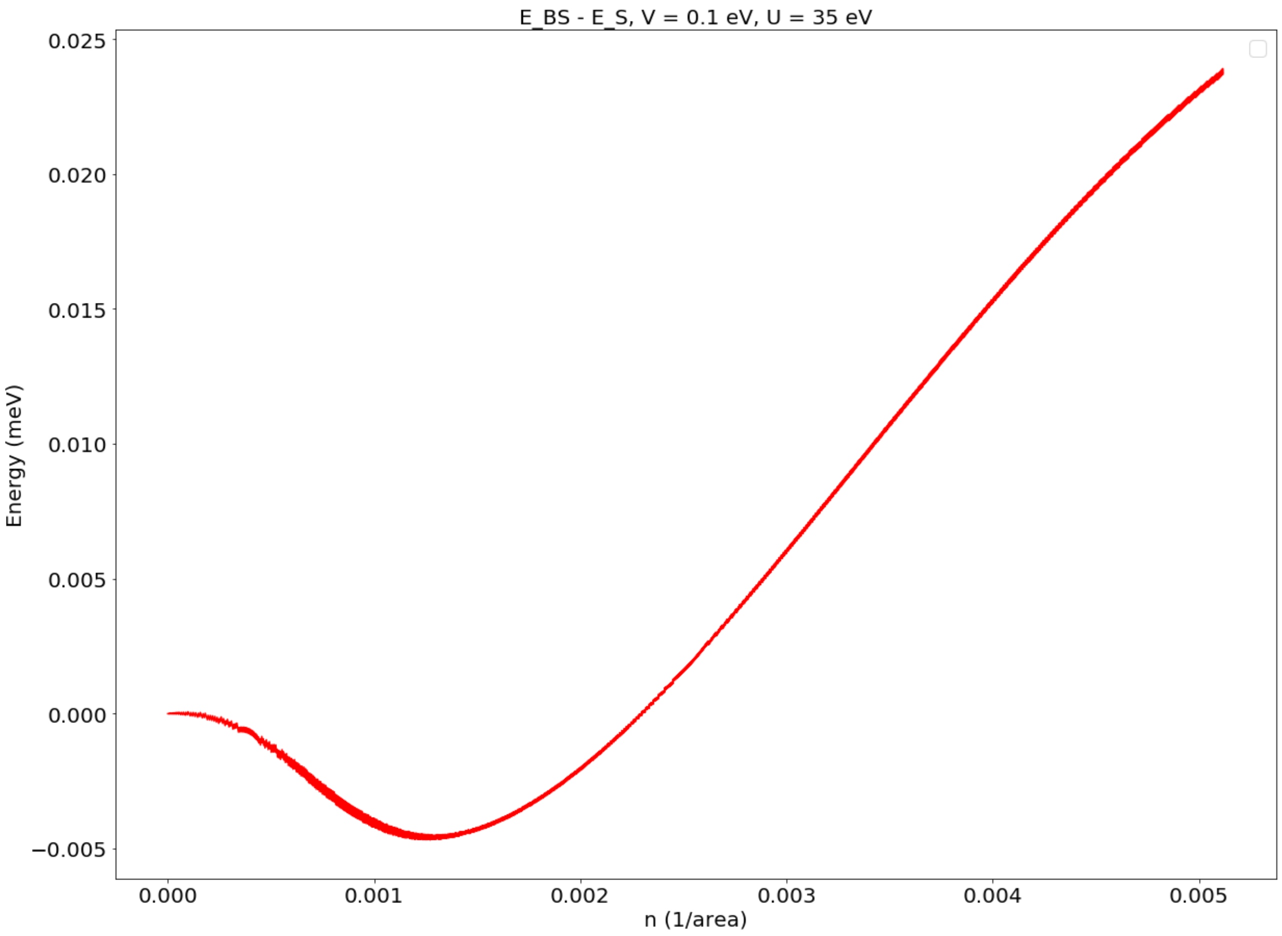
Coulomb interaction energy: $$V_{\text{int}} = \frac{UA_{\text{u.c.}}}{2}\sum_{\alpha\neq\beta} n_\alpha n_\beta$$

Grand potential per area: $$\frac{\Phi}{A} = \langle E\rangle + V_{\text{int}} - \mu\sum_\alpha n_\alpha$$

Phase transition

$$\frac{\Phi}{A} = \langle E \rangle + V_{\text{int}} - \mu \sum_{\alpha} n(\mu_\alpha)$$

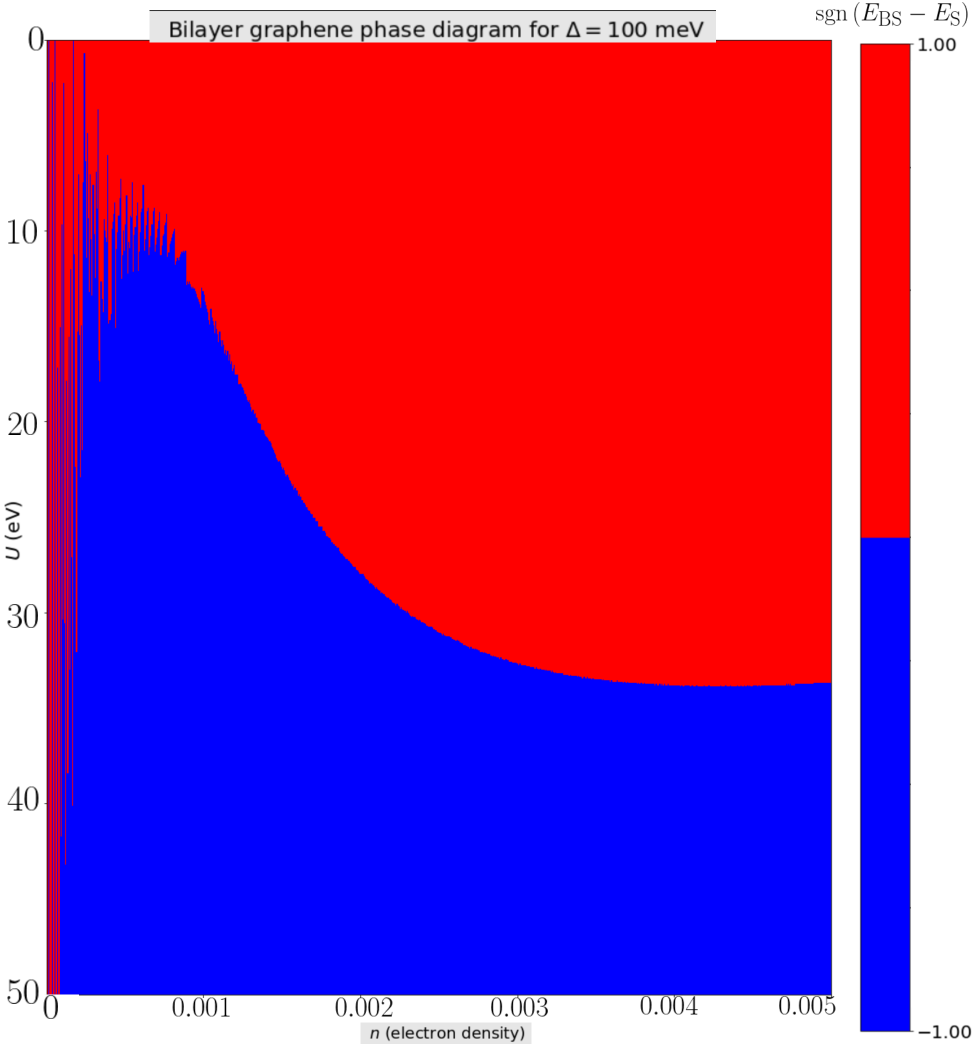



E_BS - E_S, V = 0.1 eV, U = 35 eV
Energy (meV)
n (1/area)
0.025
0.020
0.015
0.010
0.005
0.000
−0.005
0.000
0.001
0.002
0.003
0.004
0.005

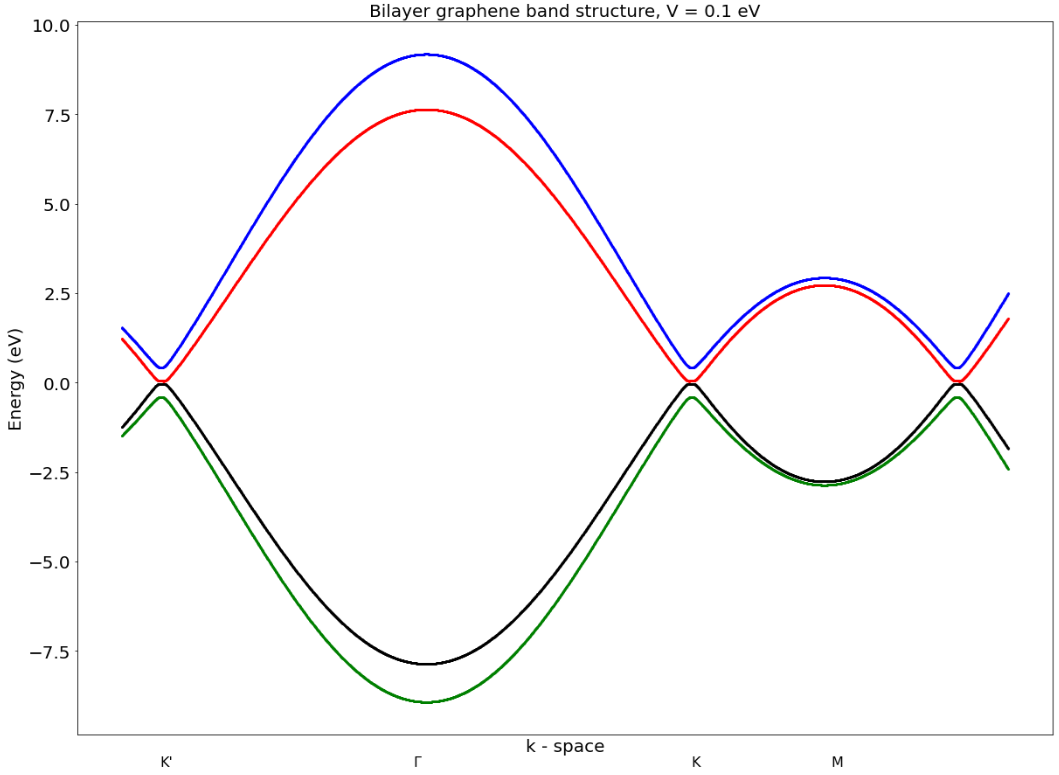
Phase Diagrams

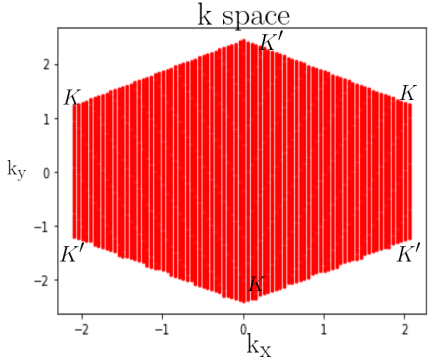
Stoner criterion for ferromagnetism:

$$U\rho(\epsilon) > 1$$



Electron valley





$$n_1 = \{\uparrow, K\}$$

$$n_2 = \{\uparrow, K'\}$$

$$n_3 = \{\downarrow, K\}$$

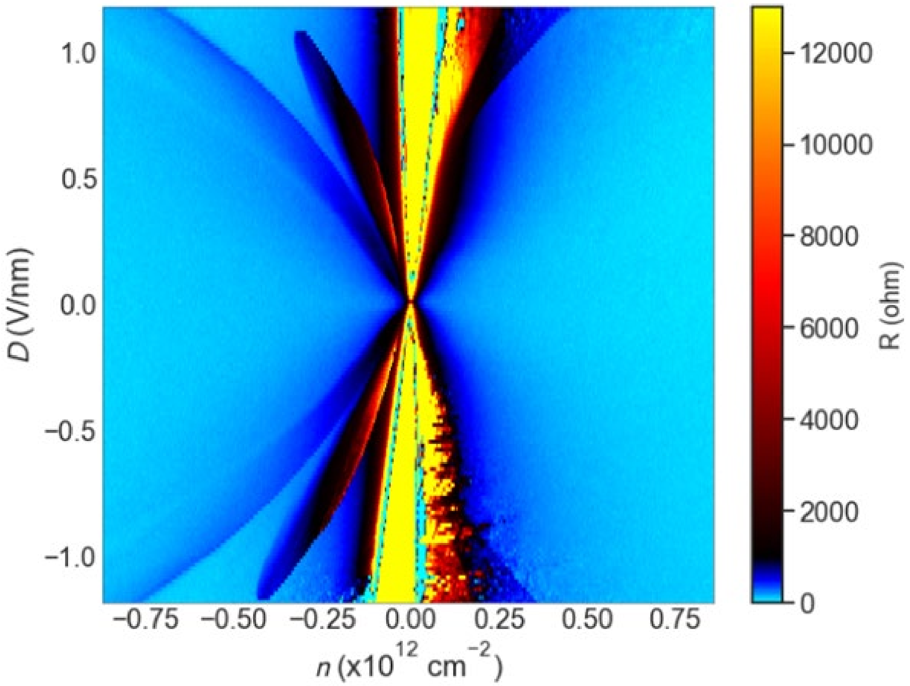
$$n_4 = \{\downarrow, K'\}$$

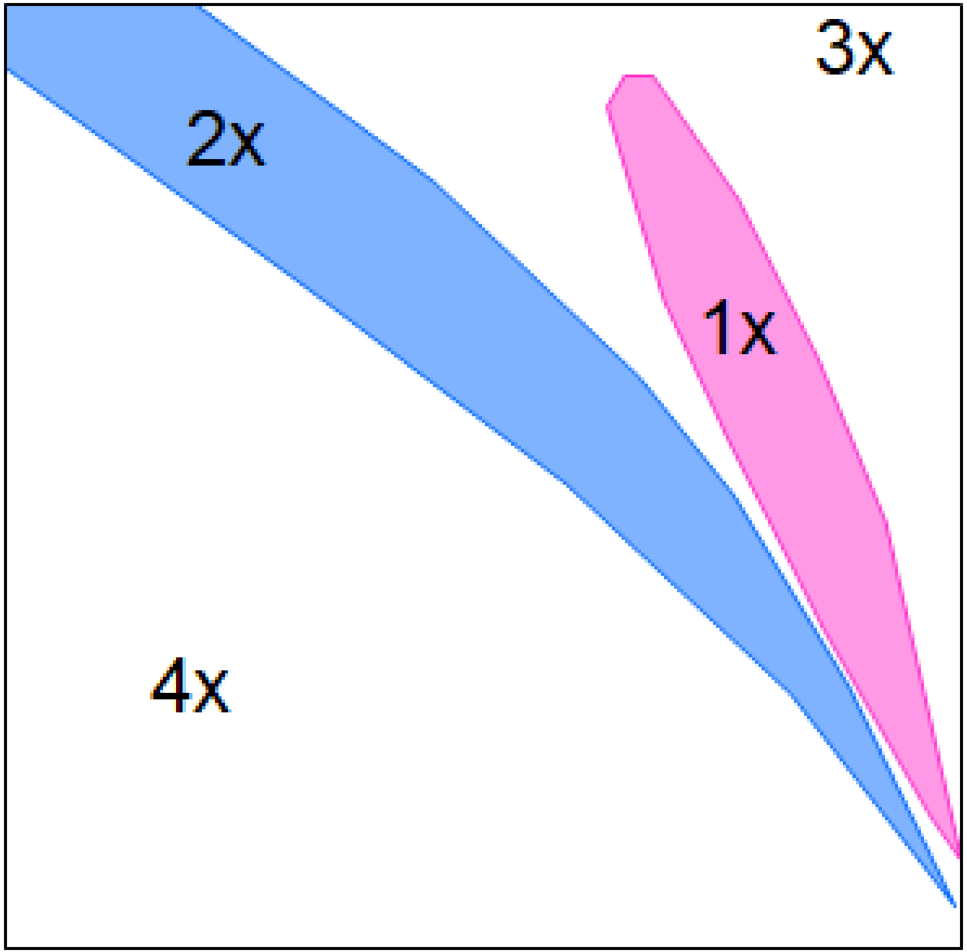
4 flavor Stoner model

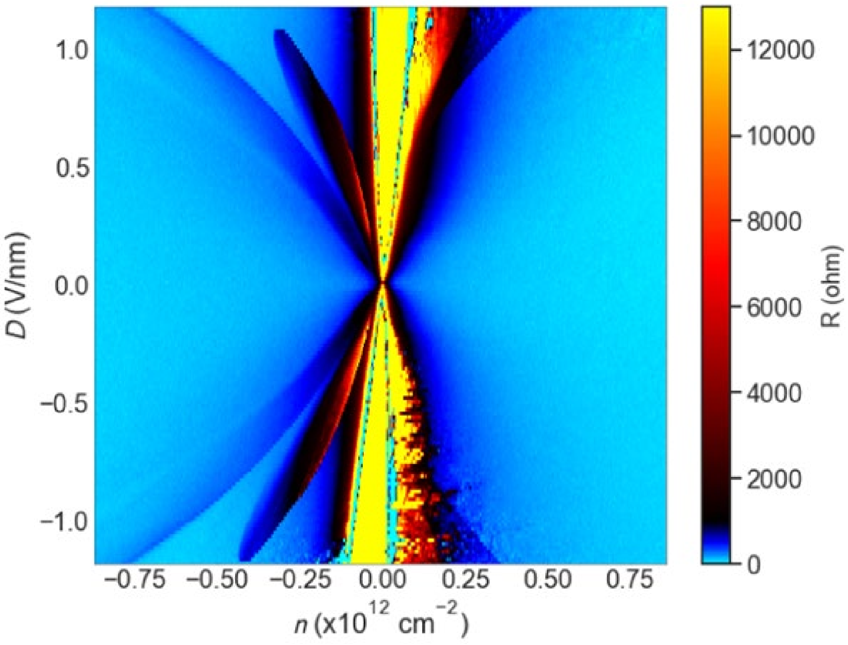
$$\frac{\Phi}{A} = \langle E \rangle + V_{\text{int}} - \mu \sum_{\alpha} n_{\alpha}$$

$$\langle E \rangle = \int_0^{n_1} \epsilon\rho(\epsilon)\frac{d\epsilon}{dn}dn + \int_0^{n_2} \epsilon\rho(\epsilon)\frac{d\epsilon}{dn}dn + \int_0^{n_3} \epsilon\rho(\epsilon)\frac{d\epsilon}{dn}dn + \int_0^{n_4} \epsilon\rho(\epsilon)\frac{d\epsilon}{dn}dn$$

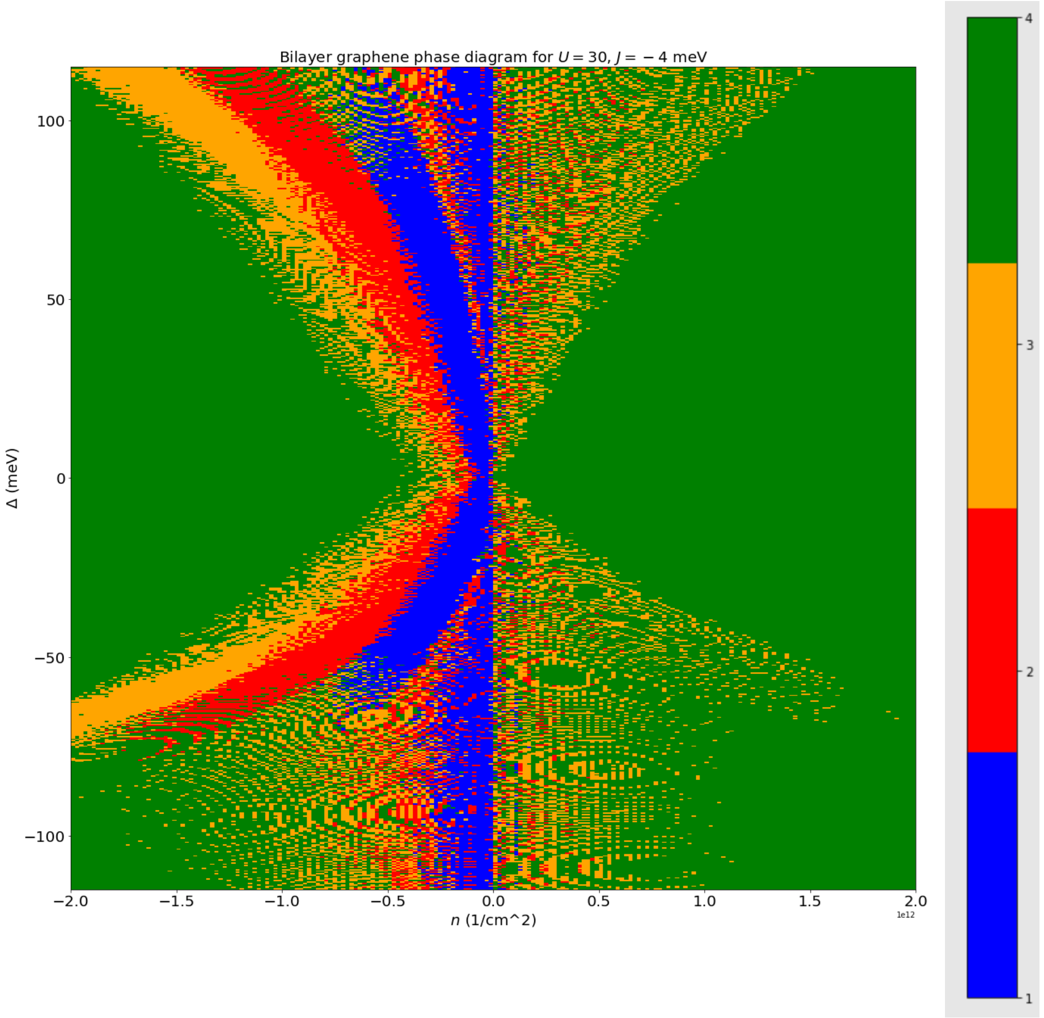
$$V_{\text{int}} = \frac{UA_{\text{u.c.}}}{2} \sum_{\alpha \neq \beta} n_{\alpha} n_{\beta} + JA_{\text{u.c.}}(n_1 - n_3)(n_2 - n_4)$$


1.0
0.5
0.0
−0.5
−1.0
D (V/nm)
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
n (x10^12 cm^−2)
12000
10000
8000
6000
4000
2000
0
R (ohm)

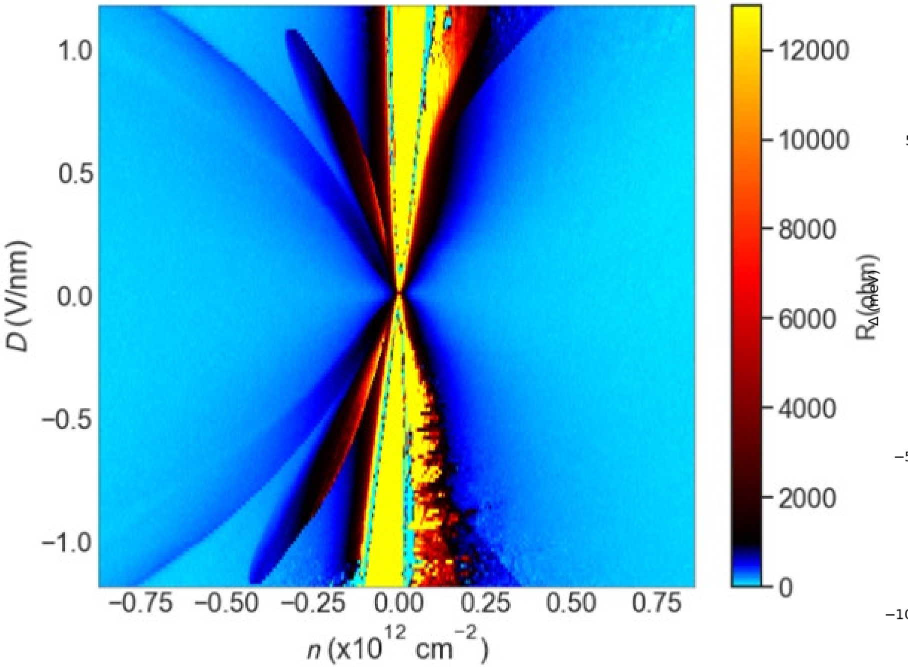

3x
2x
1x
4x



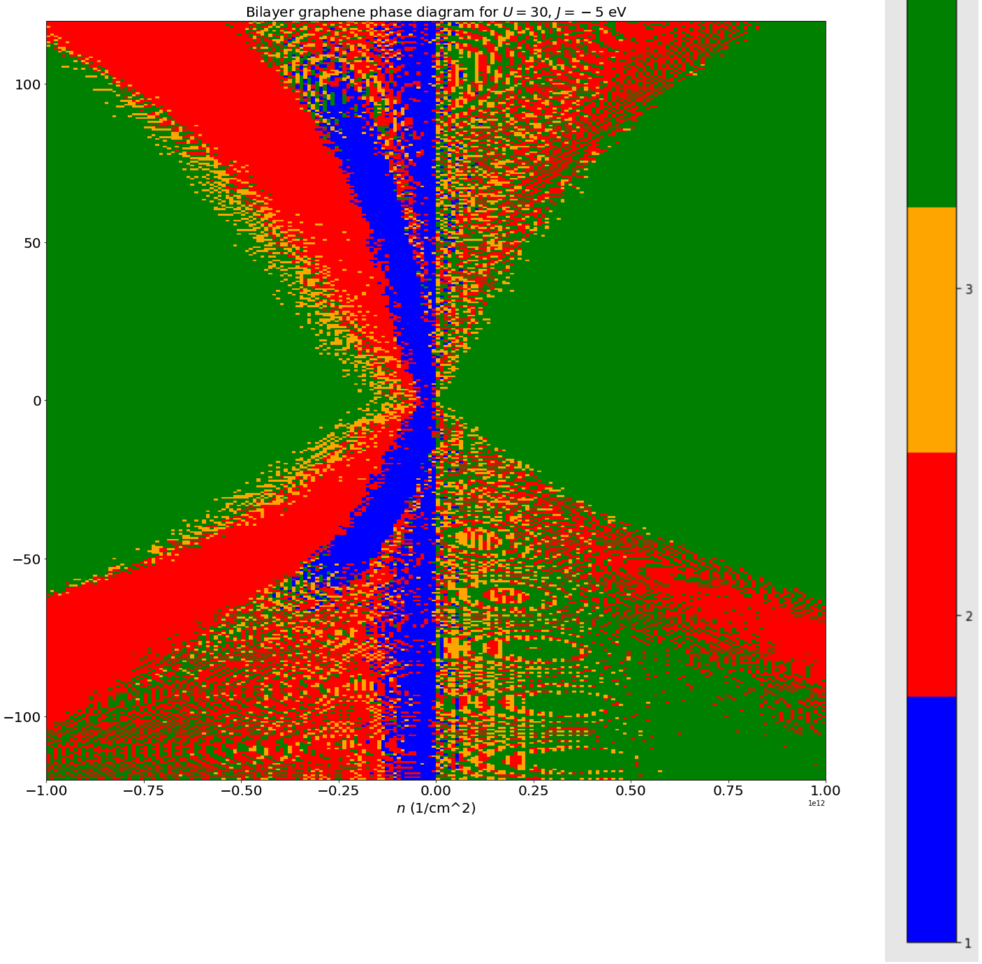
1.0
0.5
0.0
−0.5
−1.0
D (V/nm)
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
n (x10^12 cm^−2)
12000
10000
8000
6000
4000
2000
0
R (ohm)



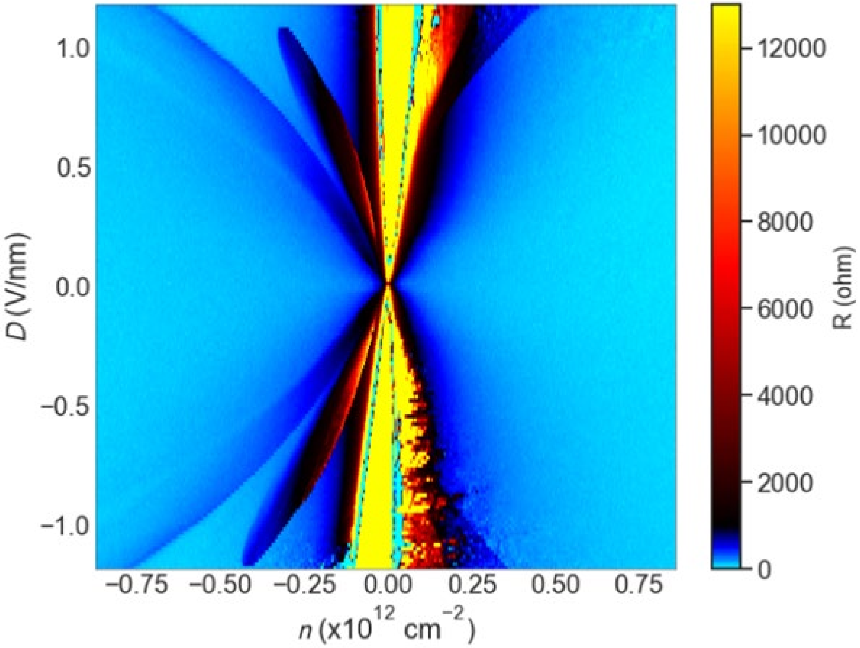
Bilayer graphene phase diagram for U = 30, J = −4 meV
100
50
0
−50
−100
Δ (meV)
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
1e12
n (1/cm^2)
4
3
2
1

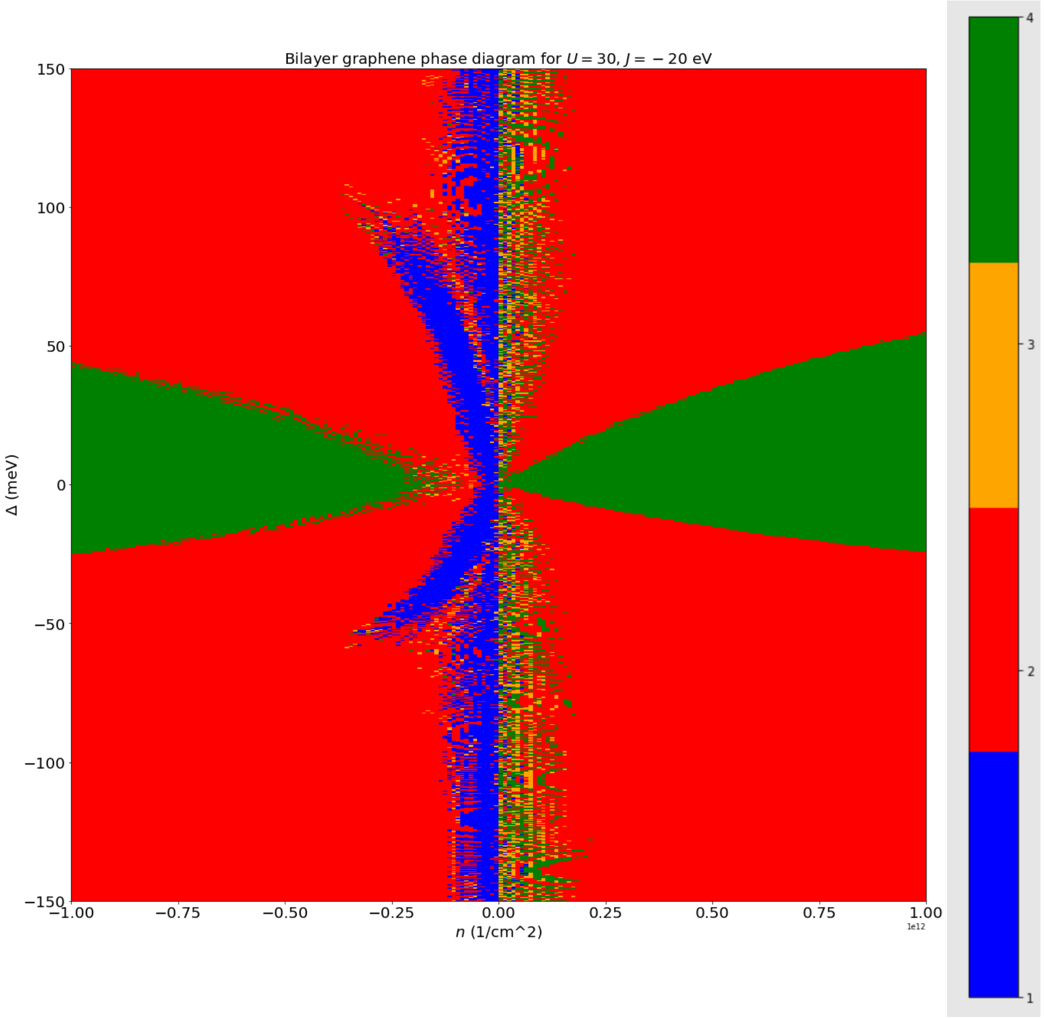


D (V/nm)
n (x10^12 cm^-2)
R_Δ (ohm)



Bilayer graphene phase diagram for U = 30, J = −5 eV
Δ (meV)
n (1/cm^2)
1e12


D (V/nm)
n (x10^12 cm^-2)
R (ohm)
12000
10000
8000
6000
4000
2000
0
1.0
0.5
0.0
−0.5
−1.0
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75


Bilayer graphene phase diagram for U = 30, J = −20 eV
Δ (meV)
n (1/cm^2)
1e12
150
100
50
0
−50
−100
−150
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
1
2
3
4

Next...

- Remove noise from phase transition (flipping constantly between phases with a region is not physical)

Acknowledgements

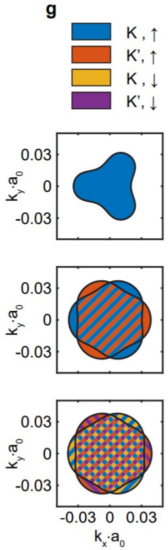
I would like to thank the following people:

- Andrea Young (Faculty advisor)
- Haoxin Zhou (Helpful grad student)
- Sathya Guruswamy (REU director)
- National Science Foundation and NSF REU grant PHY-1852574.

Resistance and phase transition

Conductivity: $\sigma = \dfrac{\nu e^2 \tau}{m^*}$

Fermi surface:



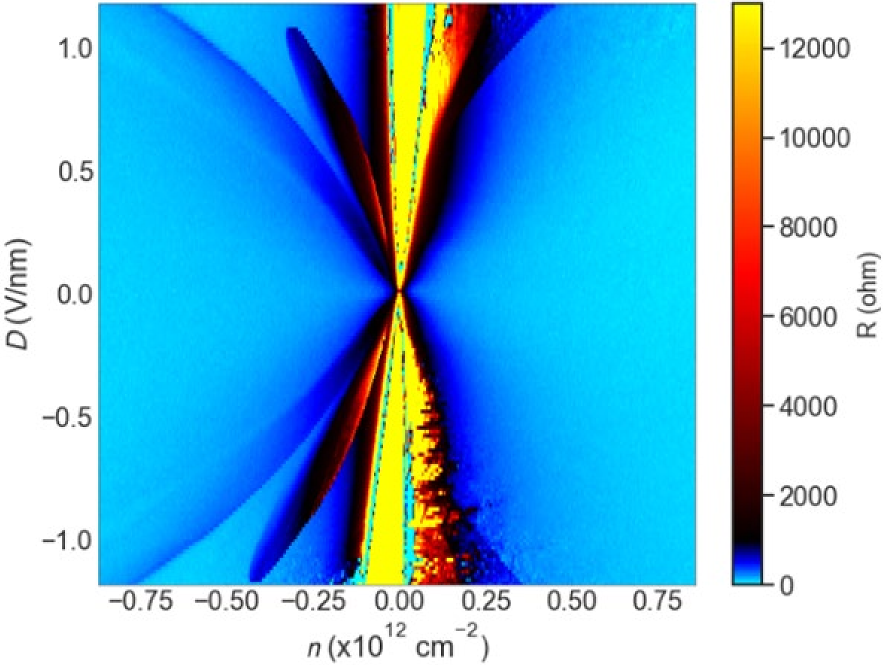
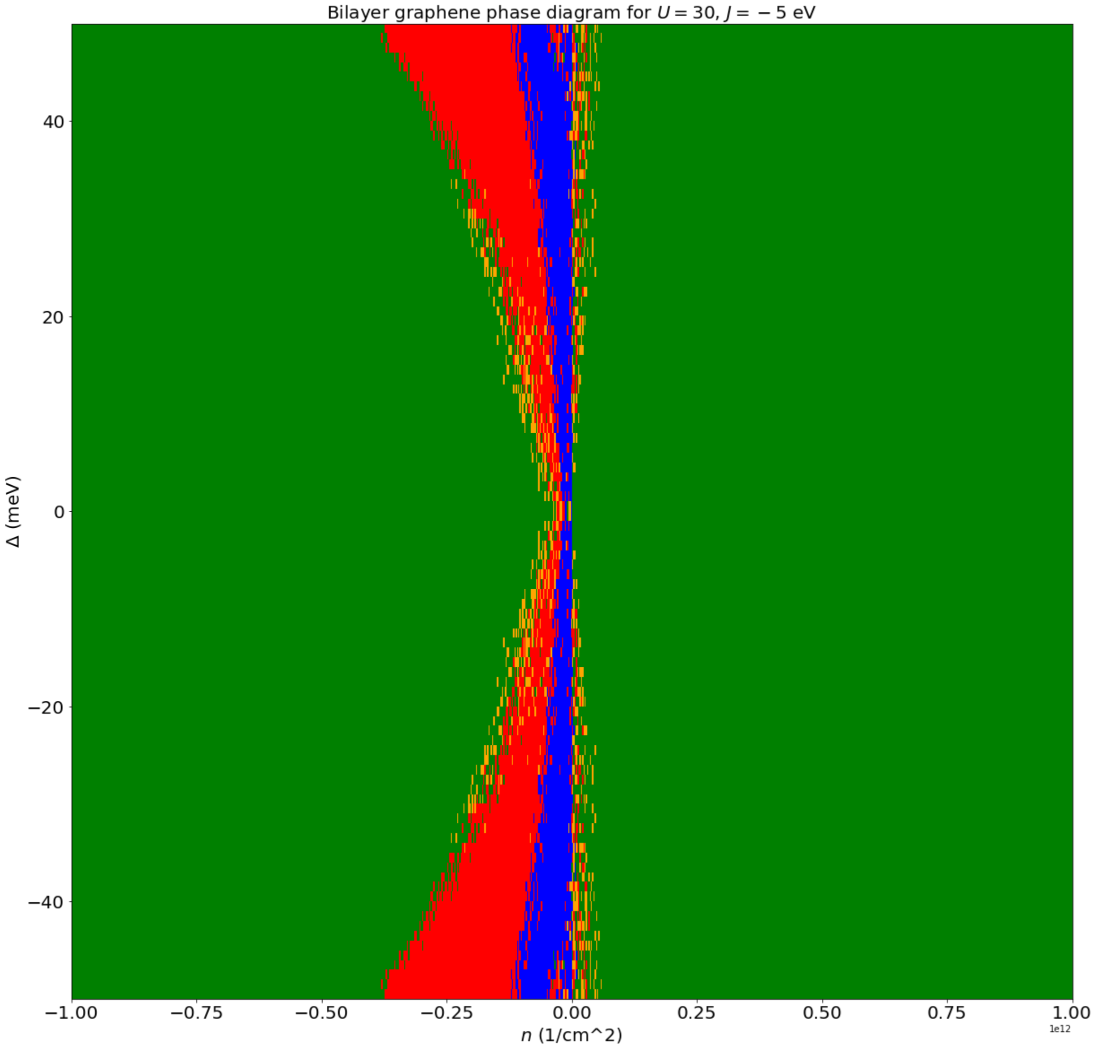
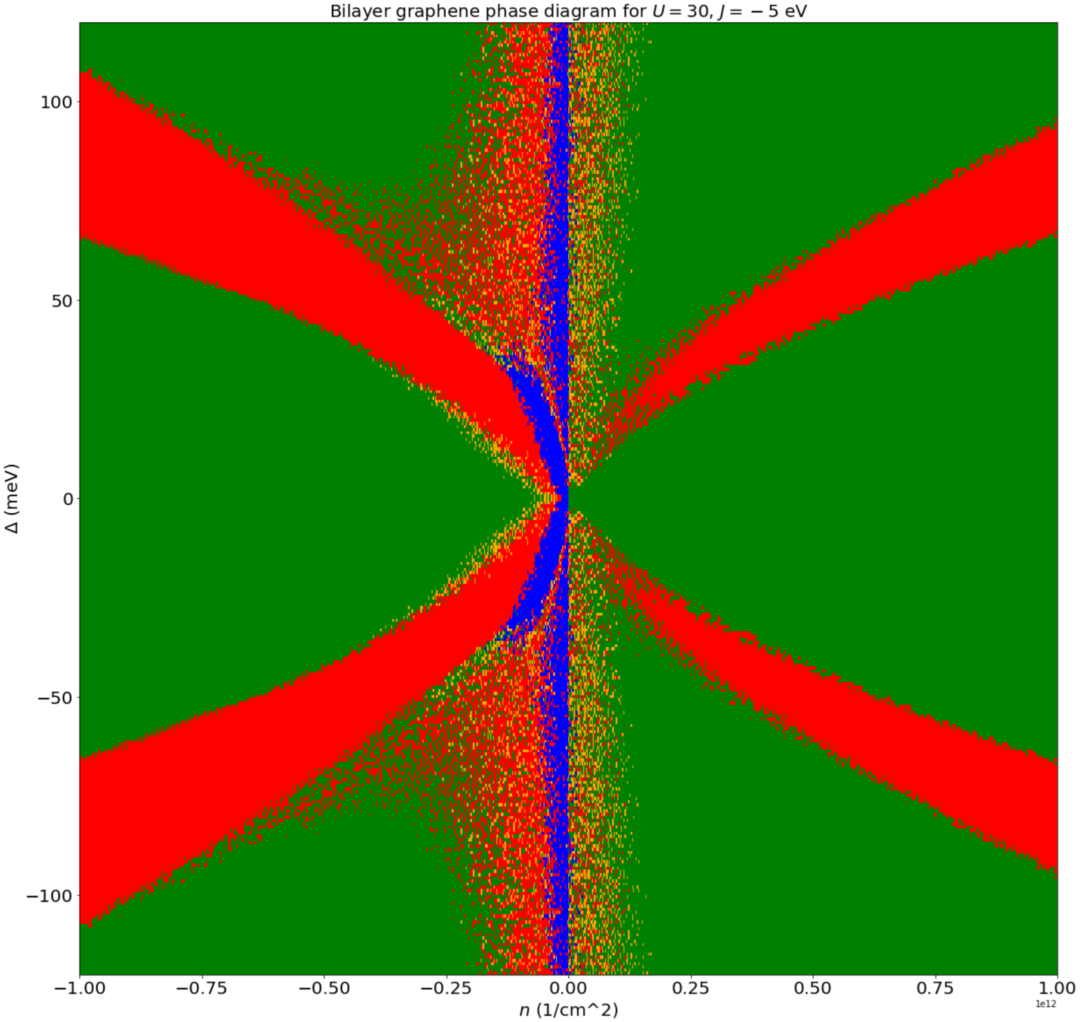


Image source: Figure 2g from Zhao, H. *et al*. Half and quarter metals in rhombohedral trilayer graphene. arXiv:2104.00653v3 [cond-mat.mes-hall] (2021)



Bilayer graphene phase diagram for $U = 30, J = -5$ eV
Δ (meV)
40
20
0
−20
−40
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
1e12
n (1/cm^2)



Bilayer graphene phase diagram for $U = 30$, $J = -5$ eV
100
50
0
−50
−100
Δ (meV)
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00
1e12
n (1/cm^2)