Ferromagnetism and on the Edges of Graphene Ribbons

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Outline

• Introduction, edge modes
• Including interactions
• Rigorous proof of ferromagnetism in 1D model
• Excitations: single particle and excitons
• More realistic models
• Edge-bulk interactions
• Conclusions
• Open Questions
Introduction

• Graphene is a single layer of carbon atoms
• Half-filled $\pi$-orbitals give simple honeycomb lattice tight-binding band structure
2 inequivalent Dirac points in Brillouin zone, where

$$E(\vec{k}) \approx \pm v_F \left| \vec{k} - \vec{K}_i \right| \quad (i=1,2)$$
Simple types of edges of ribbons:

- **Zigzag**
- **Armchair**
- **Bearded**
For non-interacting semi-infinite system with zigzag edge there are exact zero energy states localized near edge:

$$\phi(m,n) \propto \exp(ik_x m)[-2\cos(k_x/2)]^{-n}$$

n=0,1,2,... for |k|>2π/3.

N.B. k=±2π/3 are Dirac points
Proof: Wave-function only non-zero on A-sites

\[
\left( e^{ik/2} + e^{-ik/2} \right) \phi(n) + \phi(n + 1) = 0
\]
Including Interactions

• weak Hubbard interactions have little effect, with no boundaries even at half-filling, since 4-Fermi interactions are irrelevant in (2+1) dimensional Dirac theory ($\psi$ has d=1)
• Dirac liquid phase stable up to $U_c \sim 4t$
• But they have a large effect on flat edge bands which have effectively infinite interaction strength
• Mean field theory and numerical methods indicate ferromagnetic ordering on each edge
• Antiferromagnetic order between edges in ZZ case at half-filling
Actually, screening of long range Coulomb interaction is poor in graphene, especially with chemical potential at Dirac points. Should treat actual Coulomb interaction. This is marginal. Dimensionless coupling constant:

\[ \alpha_{\text{eff}} = \frac{e^2}{\hbar v_F \varepsilon} \approx 1 \]

since \( c/v_F \approx 100 \).
Projected 1D Hamiltonian

\[ H = \frac{U}{2} \sum_{k,k',q} \Gamma(k,k',q)[c_{k+q,\sigma}^c c_{k,\sigma} - \delta_{q,0}][c_{k'-q,\sigma'}^c c_{k,\sigma'} - \delta_{q,0}] \]

\[ \Gamma(k,k',q) \equiv \sum_{n=0}^{\infty} g_n(k)g_n(k')g_n(k+q)g_n(k'-q) \]

Schmidt & Loss (repeated spin indices summed)

Here \( g_n(k) \) is the wave-function of the edge state of momentum \( k \) at distance \( n \) from the edge:

\[ g_n(k) = \theta(\pi/3 - |k - \pi|)[2\cos(k/2)]^n \sqrt{1 - (2\cos(k/2))^2} \]

Due to restricted range of \( k \) this geometric series converges exponentially
• We can simply prove exact ground state of $H_{1D}$ is fully polarized ferromagnet
• This follows because we can write it as a sum of non-negative terms:

$$H = \frac{1}{2} \sum_{n,q} O_n^+(q)O_n(q), \quad [O_n^+(q) = O_{-n}(q)]$$

$$O_n(q) \equiv \sum_{k,\sigma} g_n(k)g_n(k+q)[c_{k+q,\sigma}^+c_{k,\sigma} - \delta_{q,0}]$$

• The fully polarized state is annihilated by all $O_n(q)$ operators
• Can prove this is unique ground state (up to spin rotation)
Uniqueness of ground state follows from observing that $O_n(q) \ket{\psi} \geq 0$ for all $n$ implies

$$
\left[ c_{k+q,\sigma}^+ c_{k,\sigma} + c_{-k,\sigma}^+ c_{-k-q,\sigma} - 2\delta_{q,0} \right] \ket{\Psi} \geq 0, \ \forall k
$$

We can then prove ferromagnetic states are only ones to satisfy these conditions for all $k,q$. 

• N.B.-unusual particle-hole symmetry: \( c_k \leftrightarrow c_k^+ \)
• Interaction energy and dispersion are both \( \text{O(U)} \)
• Energy to add (\( \downarrow \)) or remove (\( \uparrow \)) particle relative to fully polarized spin \( \uparrow \) state:

\[
E(k) = \frac{U}{2L} \sum_{k'} \Gamma(k,k',0)
\]
Since it is only a 2-body problem, it is feasible to study $\Delta M=-1$ exciton numerically despite complicated interactions ($L<602$)

Bottom of 2 particle continuum

Bound exciton

Near $q=2\pi/3$ we see free particle hole pair at band edges

![Graph showing E/U vs q for different $\eta$ values: $\eta=0$, $\eta=0.05$, $\eta=0.10$, and $\eta=0.109$.](image)
Graphene has 2\textsuperscript{nd} neighbour hopping: $t_2/t \sim 0.1$?

We might expect a potential acting near edge, $V_e$

For $U, t_2, V_e \ll t$, modification to edge Hamiltonian is:

$$\delta(H - \varepsilon_F N) = \frac{\Delta}{L} \sum_{k, \alpha} (2\cos k + 1) e^+_{k\alpha} e_{k\alpha}, \quad \Delta = t_2 - V_e$$

Here we assume $\varepsilon_F$ is held at energy of Dirac points, $\varepsilon_F = 3t_2$

This breaks particle-hole symmetry
For $\Delta>0$, energy to add a spin down electron is decreased near $k=\pi$ or for $\Delta>0$, energy to remove a spin up electron is decreased near $k=\pi$
• Increasing $\Delta$ causes the exciton to become unbound (except close to $q=0$)
• For $|\Delta| > \Delta_c \sim 0.109$ U the edge starts to become doped at $k$ near $\pi$ (while $\varepsilon_F$ is maintained at energy of Dirac points)
• Since exciton is unbound it is plausible that we get a non-interacting state with no spin down electrons for $\Delta < 0$ or filled band of spin up electrons, $\Delta > 0$
• We confirmed this by looking at $\Delta M = -2$ states near $\Delta = \Delta_c$ numerically ($L \leq 74$) – no bi-exiton bound states
• State with no spin down electrons (or no spin up holes) is non-interacting for our projected on-site Hubbard model since particle of same spin don’t interact with each other
• Gives simple magnetization curve

2\textsuperscript{nd} neighbor extended Hubbard interactions (must couple A to A sites) would turn this into a (one or two component) Luttinger liquid state
Effect of Edge-Bulk Interactions

• Decay of edge states into bulk states is forbidden by energy-momentum conservation
• But integrating out bulk electrons induces interactions between edge modes
We may calculate induced interactions for small $1/W$, $q$ and $\omega$ using Dirac propagators with correct boundary conditions (ignoring bulk interactions)
• Most important interactions involve spin operators of edge states $S_{U/L}(q,\omega)$ on upper and lower edges – like RKKY
• At energy scales $\ll v_F/W$, inter-edge interactions is simply

$$H_{\text{inter}} = J_{\text{inter}} \vec{S}_U \cdot \vec{S}_L, \quad J_{\text{inter}} = \pm 2 \frac{U^2}{tW^2}$$

• Ferromagnetic for zigzag-bearded ribbon or antiferromagnetic for zigzag-zigzag case
• Consistent with $S=(1/2)L$ or 0 for zigzag-bearded or zigzag-zigzag ribbon, respectively (Lieb’s Theorem)
Lieb’s Theorem:
Spin of ground state is $|N_A - N_B|/2$ for $U>0$ Hubbard model at half-filling with hopping between A and B sites only.

Ribbon with zigzag-bearded edges has $N_A - N_B = L$.

Ribbon with zigzag-zigzag edges has $N_A - N_B = 0$. 
• Intra-edge interaction induced by exchanging bulk electrons is long range and retarded but this effect is reduced for Dirac liquid compared to Fermi liquid
• Example: exciton dispersion gets a correction:

\[ E(q) \approx 0.36Uq^2 - \sqrt{3}(4 - \pi)(U^2 / t)q^2 \ln q^2 \]

• \(O(U^2)\) term increases energy of a spin flip, thus further stabilizing ferromagnetic state
• To investigate effects of edge-bulk interactions more systematically, I hope to develop a Renormalization Group method
• A type of boundary critical phenomenon in (2+1) dimensions:
  • Gapless (2+1) D Dirac fermions interacting with spin polarized semi-metallic edge states
  Like a Kondo or Anderson model in one higher dimension: Kondo: 0D impurity, interacting with 1D Dirac fermions
  Graphene: “impurity” is now 1D edge, interacting with 2D Dirac fermions
Conclusions

• Small U/t limit is a tractable starting point for studying graphene edge magnetism
• Rigorous result on 1D edge Hamiltonian indicate full polarization in simplest model
• $t_2$ and edge potential lead to edge doping but ground state may remain free for Hubbard model
• Edge-bulk interactions stabilize inter-edge magnetic ground state and introduce long range retarded interactions

Open Questions

- can higher orders in U/t be controlled? (Can we develop a renormalization group approach?)
- does ferromagnetism survive with:
  - long range Coulomb interactions
  - bulk doping away from Dirac points
  - chiral (rather than zigzag) edges
  [M. Schmidt, M, Golor, T. Lang, S. Wessel, PRB 87, 245431 (2013)]
  - disorder?
- will ferromagnetism be seen experimentally?
- will it be useful for spintronics?