Chiral *d*-wave Superconductivity in Doped Graphene

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Vetenskapsrådet

Swedish Foundation for Strategic Research

Wenner-Gren Stiftelserna

Carl Trygger Foundation

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Outline

- Introduction
- Superconductivity from electron repulsion in doped graphene
  - Mean-field theory
  - Renormalization group theory
- Properties of the chiral *d*-wave superconducting state in graphene
  - Edges
    - Chiral edge states, spontaneous currents
    - Majorana modes
  - Impurities
  - Proximity-effect enhancements

Recent review article (to appear in J. Phys.: Condens. Matter):
ABS and Honerkamp, arXiv:1406.0101

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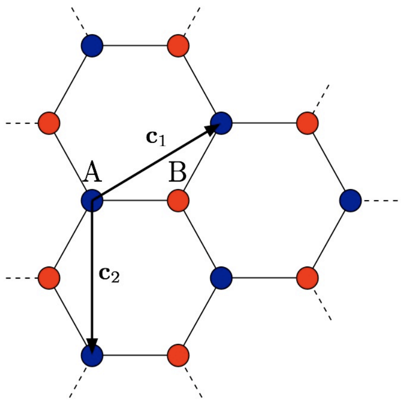
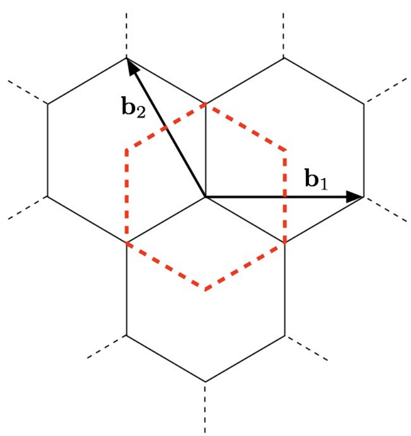
Free Electron Picture of Graphene

Honeycomb lattice:



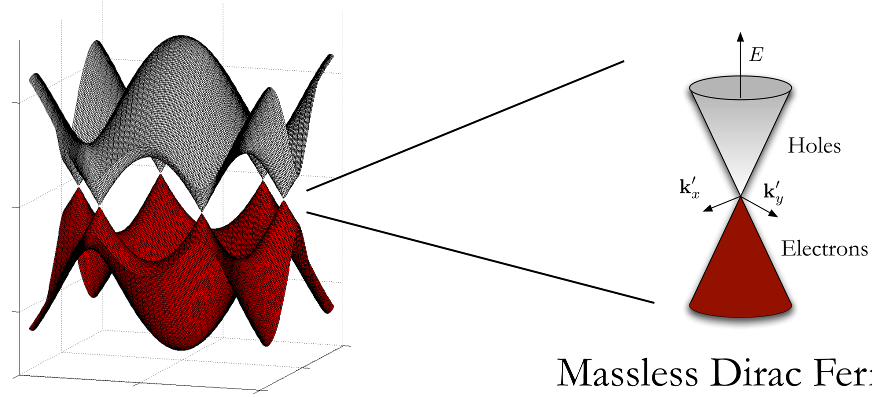
1st BZ:



sp^2 hybridization ⇒ $1p_z$ orbital per C atom left

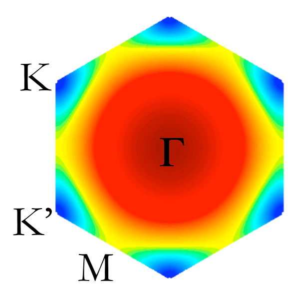
Tight-binding with nearest neighbor hopping only:

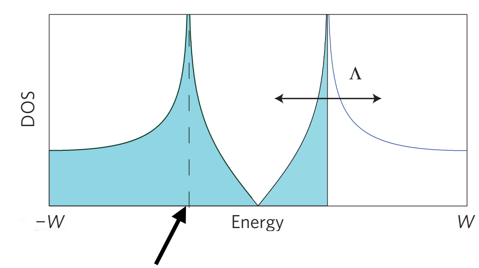
(Wallace, 1946)



Massless Dirac Fermions

($c \rightarrow v_F \sim c/300$)





Logarithmically diverging DOS

Superconductivity in Graphene?

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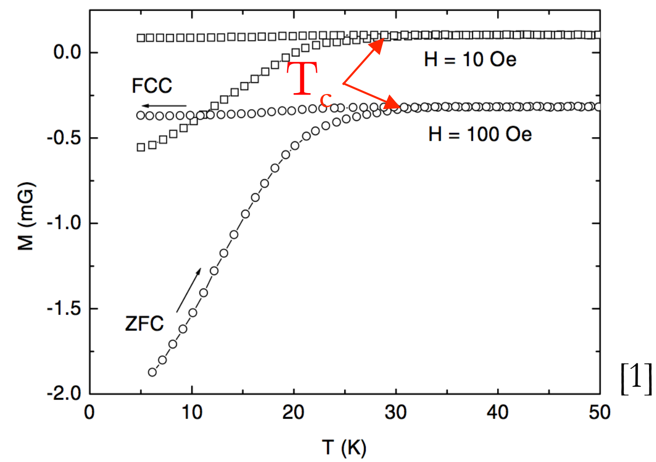
Intrinsic superconductivity in graphite-sulfur composites:



[1]

- T_c ~ 10-60 K
- SC located to the graphite planes
- 0.05% superconducting volume
- SC and FM co-exists

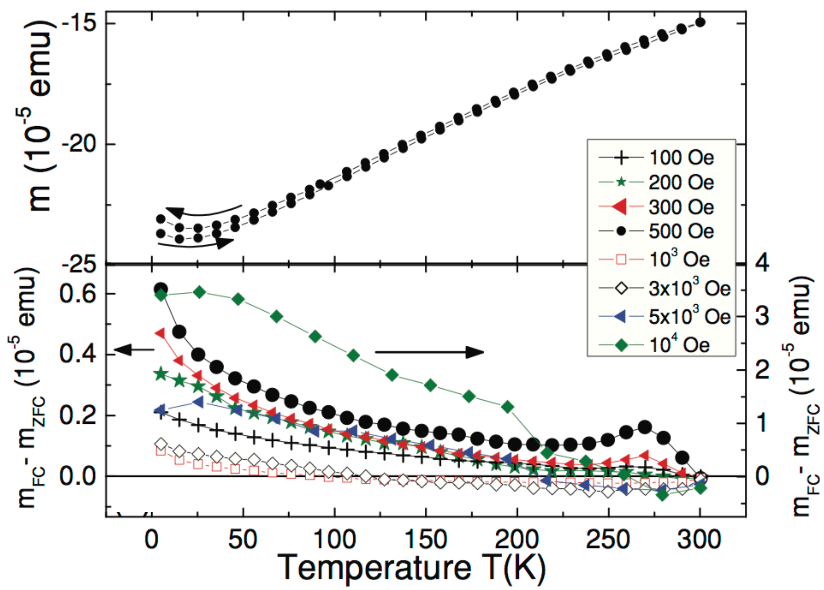
ADVANCED MATERIALS www.advmat.de

Materials Views www.MaterialsViews.com

Can Doping Graphite Trigger Room Temperature Superconductivity? Evidence for Granular High-Temperature Superconductivity in Water-Treated Graphite Powder

T. Scheike, W. Böhlmann, P. Esquinazi, J. Barzola-Quiquia, A. Ballestar, and A. Setzer*

[2]



[1]: da Silva et al., PRL 87, 147001 (2001), [2]: Scheike et al., Adv. Mater. 34, 5826 (2012)

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Electronic Correlations in Graphene

Electronic correlations should be important in graphite and graphene:

Nearest neighbor hopping t ~ 2.5 eV
On-site repulsion U ~ 6 - 10 eV [1]
} Intermediate coupling regime

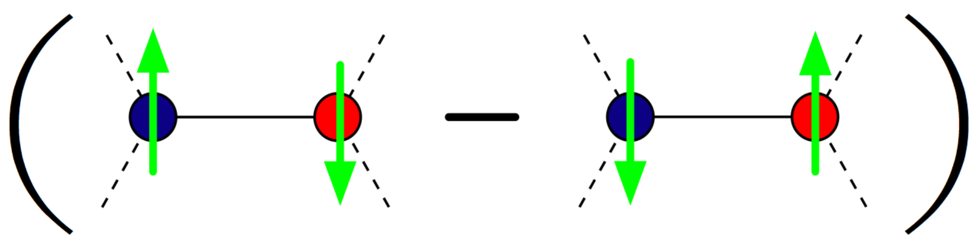
pπ-bonded planar organic molecules:

Nearest neighbor spin-singlet bonds (SB) encouraged compared to polar configurations
} Pauling's Resonance Valence Bond (RVB) idea

Give good estimates for:

Cohesive energy, C-C bond distance, singlet-triplet exciton energy differences etc.

SB =

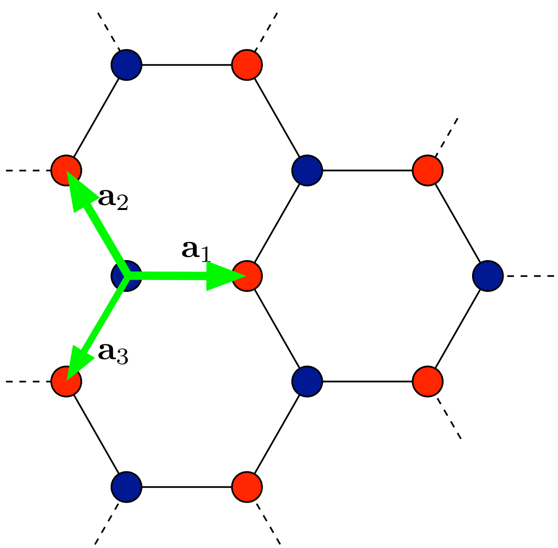


[1]: T. Wehling et al,. PRL 106, 236805 (2011)

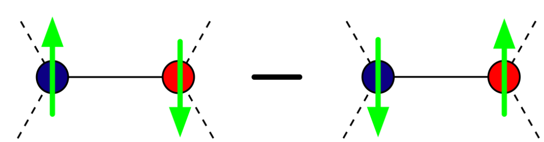
Modeling Correlation Effects

Effective model with SB pairing: [1]

$$H = -t \underbrace{\sum_{<i,j>,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + \mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma}}_{\text{Tight-binding band structure}} - 2J \underbrace{\sum_{<i,j>} h^\dagger_{ij} h_{ij}}_{\text{Favoring singlet bonds (SB)}}$$



$$h^\dagger_{ij} = \frac{1}{\sqrt{2}} (c^\dagger_{i\uparrow} c^\dagger_{j\downarrow} - c^\dagger_{i\downarrow} c^\dagger_{j\uparrow})$$

$h^\dagger_{ij} = \frac{1}{\sqrt{2}} \Big($  $\Big)$

$$\frac{J}{t} \sim 1$$

[1]: Baskaran, PRB 65, 212505 (2002)

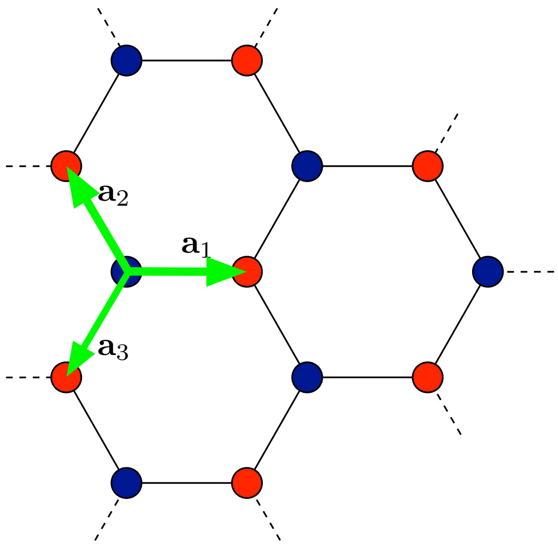
Mean-Field Approach

Effective model with SB pairing: [1]

$$H = -t \underbrace{\sum_{<i,j>,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + \mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma}} - 2J \underbrace{\sum_{<i,j>} h^\dagger_{ij} h_{ij}}$$

Tight-binding band structure

Favoring singlet bonds (SB)



Mean-field order parameters in the Cooper pairing channel:

$$\Delta_\alpha = \langle h^\dagger_{i,i+\mathbf{a}_\alpha} \rangle = \frac{1}{\sqrt{2}} \langle c^\dagger_{i\uparrow} c^\dagger_{i+\mathbf{a}_\alpha\downarrow} - c^\dagger_{i\downarrow} c^\dagger_{i+\mathbf{a}_\alpha\uparrow} \rangle$$

Expectation value of SB pair creation

[1]: Baskaran, PRB 65, 212505 (2002), ABS and Donaich, PRB 75, 134512 (2007)

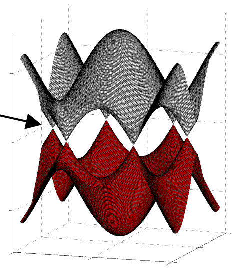
Mean-Field Superconductivity

BCS-type self-consistency equation:

Intraband pairing (regular BCS form)

$$\Delta^\dagger_\alpha = \frac{J}{N}\sum_{\mathbf{k}}\sum_{\gamma=1,2,3}\Bigg[\cos(\mathbf{k}\cdot\mathbf{a}_\alpha-\varphi_{\mathbf{k}})\cos(\mathbf{k}\cdot\mathbf{a}_\gamma-\varphi_{\mathbf{k}})\left(\frac{\tanh(\beta_c(t\epsilon_{\mathbf{k}}+\mu)/2)}{2(t\epsilon_{\mathbf{k}}+\mu)}+\frac{\tanh(\beta_c(t\epsilon_{\mathbf{k}}-\mu)/2)}{2(t\epsilon_{\mathbf{k}}-\mu)}\right)$$
$$+\sin(\mathbf{k}\cdot\mathbf{a}_\alpha-\varphi_{\mathbf{k}})\sin(\mathbf{k}\cdot\mathbf{a}_\gamma-\varphi_{\mathbf{k}})\left(\frac{\sinh(\beta_c\mu)}{2\mu\cosh(\beta_c(t\epsilon_{\mathbf{k}}+\mu)/2)\cosh(\beta_c(t\epsilon_{\mathbf{k}}-\mu)/2)}\right)\Bigg]\Delta^\dagger_\gamma$$

$$\epsilon_{\mathbf{k}} = |\sum_\alpha e^{i\mathbf{k}\cdot\mathbf{a}_\alpha}|$$
$$\varphi_{\mathbf{k}} = \arg(\sum_\alpha e^{i\mathbf{k}\cdot\mathbf{a}_\alpha})$$



Interband pairing, negligible contribution at low temperatures

3×3 eigenvalue problem for $\mathbf{\Delta}^\dagger = (\Delta^\dagger_1, \Delta^\dagger_2, \Delta^\dagger_3)^T$:

$$\frac{1}{J}\mathbf{\Delta}^\dagger = \begin{pmatrix} A & b & b \\ b & A & b \\ b & b & A \end{pmatrix}\mathbf{\Delta}^\dagger$$

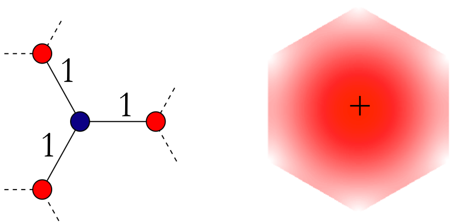
A = RHS for a = b
b = RHS for a ≠ b

ABS and Donaich, PRB 75, 134512 (2007)

Gap Symmetries

s-wave:

- $\Delta_\alpha = (1,1,1)$

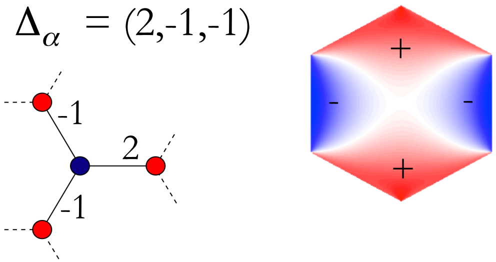


extended *s*-wave

- $\Delta \in A_{1g}$ of D_{6h}

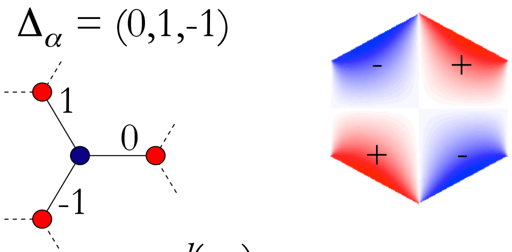
d-waves:

- $\Delta_\alpha = (2,-1,-1)$



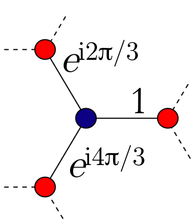
d(x^2-y^2)-wave

- $\Delta_\alpha = (0,1,-1)$



d(xy)-wave

- $\Delta \in E_{2g}$ of D_{6h}
  - Below T_c: $d(x^2-y^2)+id(xy)$

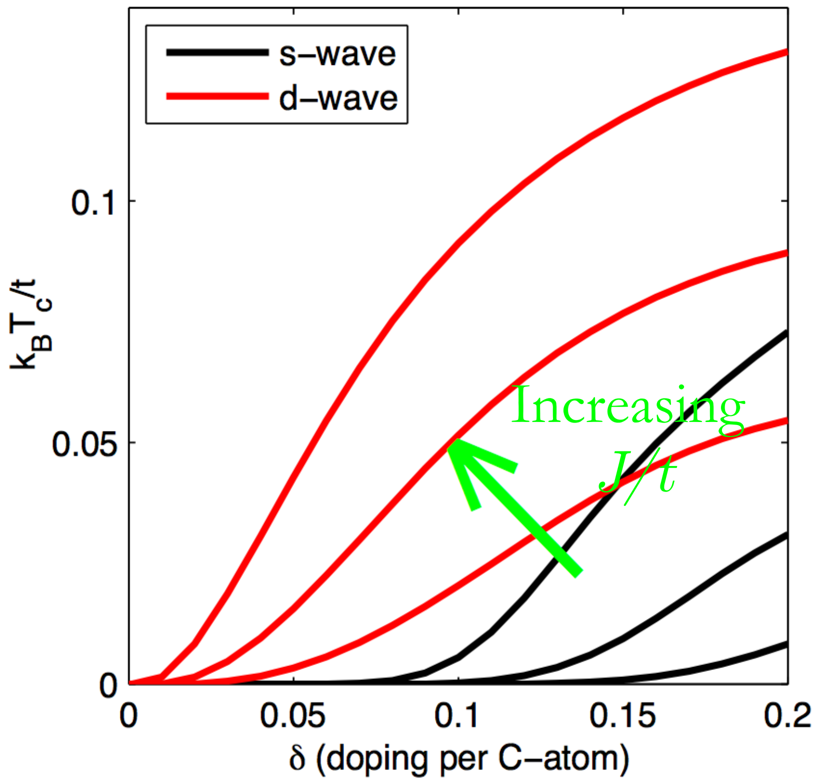


Chiral, time-reversal symmetry breaking state

ABS and Donaich, PRB 75, 134512 (2007)

Mean-Field Results

Transition temperature as a function of doping (δ) for coupling parameters $J/t = 0.8,\ 1.0,\ 1.2$:



Zero doping:

- QCP at $J/t = 1.91$
- *s*- and *d*-wave solutions degenerate

Finite doping:

- $T_c(d) >> T_c(s)$

ABS and Donaich, PRB 75, 134512 (2007)

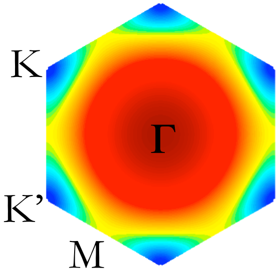
Realization of *d*-wave Superconductivity

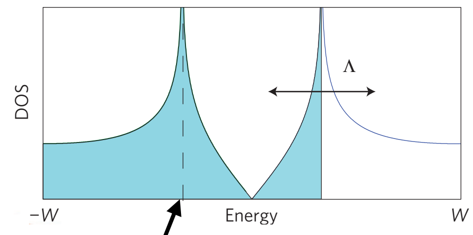
Need $\delta \sim 0.01$ for mean-field T_c(*d*-wave) ~ 10 K:

- Doping of a graphene sheet:
  - 3D graphite: $\delta \sim 10^{-4}$
  - Extended defects in graphene might induce self-doping [1]
  - Sulfur forms no chemical bonds but provides $\delta = 0.015$ holes/C-atom [2]

- Heavily doping of graphene:
  - Ad-atom deposition [3]
  - Electrolyte gating [4]

  } can approach van Hove singularity ($\delta = 0.25$, $\mu = t$)





Logarithmic diverging DOS

[1]: Peres et al., PRB 73, 125411 (2006), [2]: ABS and Doniach, PRB 75, 134512 (2007),
[3]: McChesney et al., PRL 104, 136803 (2010), [4]: Efetov et al., PRL 105, 256805 (2010)

Perturbative Renormalization Group

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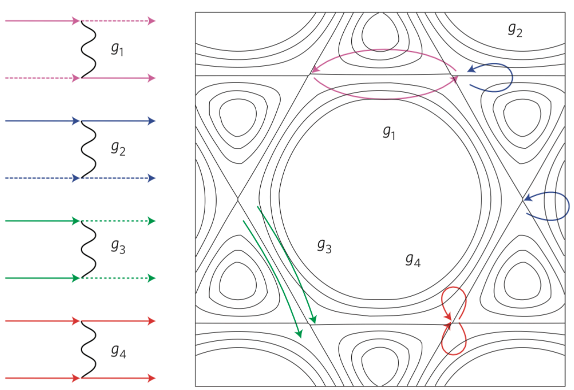
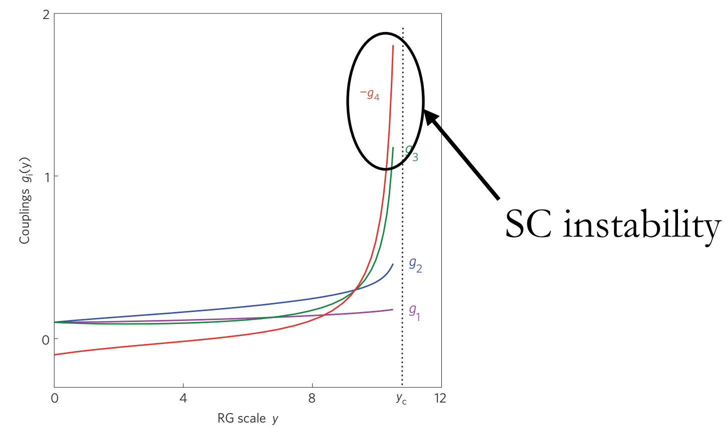
ARTICLES
PUBLISHED ONLINE: 22 JANUARY 2012 | DOI: 10.1038/NPHYS2208
nature physics

Chiral superconductivity from repulsive interactions in doped graphene

Rahul Nandkishore[1], L. S. Levitov[1] and A. V. Chubukov[2]*





Perturbative 3-patch RG:

- Low energy theory around M saddle points
- Short range interactions g_1, g_2, g_3, g_4
  - Marginal at tree level
  - Logarithmic corrections in perturbation theory

d-wave superconductivity = g_3-g_4 dominates over CDW, SDW

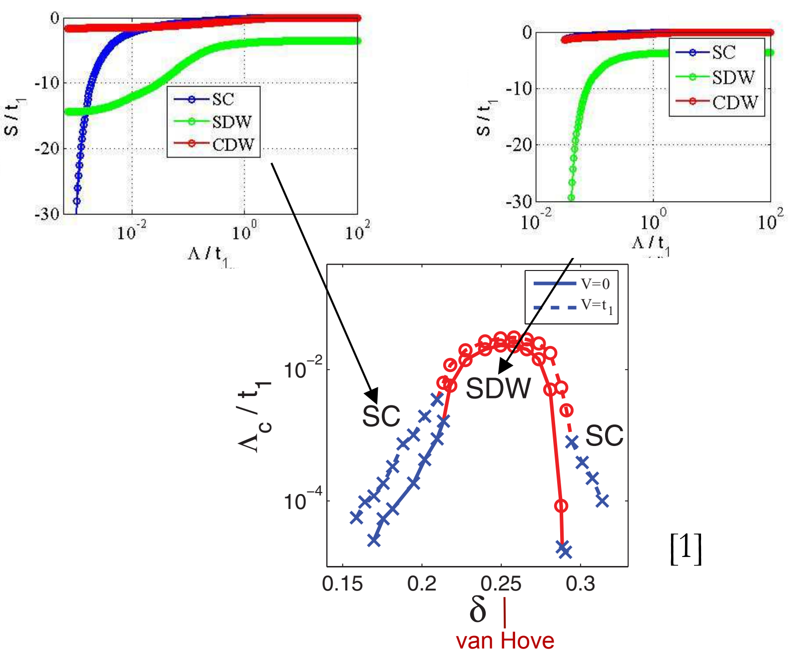
Functional Renormalization Group

Intermediate coupling regime ➔ functional RG

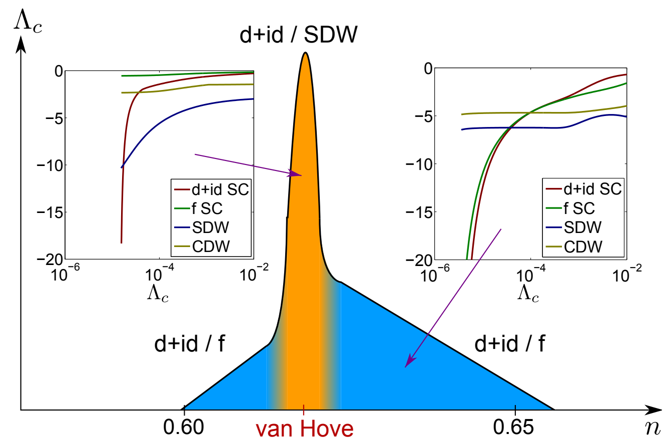
- Integrating out high-energy modes in the 4-point vertex function on the full Fermi surface

$$H = -\sum_{(ij)\sigma}(c_{i\sigma}^{\dagger} t_{ij} c_{j\sigma} + \text{H.c.}) - \mu N_e + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

$$+ \frac{1}{2} V \sum_{i\delta} n_i n_{i+\delta},$$



[1]



[2]

Chiral *d*-wave superconductivity close to van Hove singularity

- Pairing on NN, NNN, … bonds (depending on range of Coulomb interaction)

[1]: Wang et al., PRB 85, 035414 (2012), [2]: Kiesel et al., PRB 86, 020507 (2012)

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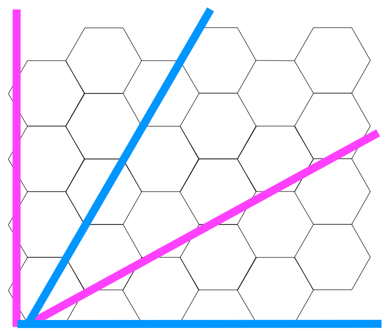
Edges and Impurities

The two *d*-wave solutions are degenerate on the honeycomb lattice

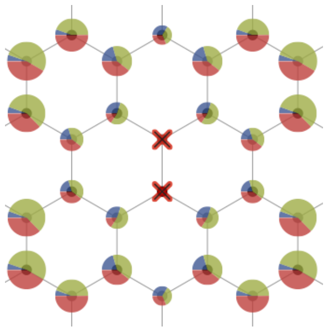
- Bulk: $d(x^2\text{-}y^2)+id(xy)$

What happens when translational symmetry is broken?

- Edges
  - Zigzag (ZZ)
  - Armchair (AC)



- Impurities
  - Singe-site vacancies
  - Bivacancies



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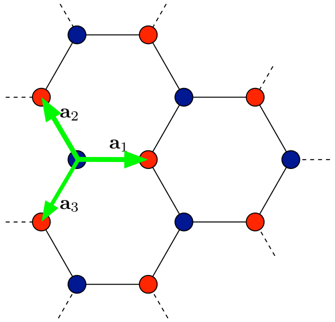
Bogoliubov-de Gennes Solution

Solve $$H = -t \sum_{<i,j>,\sigma} c^\dagger_{i\sigma} c_{j\sigma} + \mu \sum_{i,\sigma} c^\dagger_{i\sigma} c_{i\sigma} + \sum_{i,\alpha} \Delta_\alpha(i)(c^\dagger_{i\uparrow} c^\dagger_{i+\mathbf{a}_\alpha\downarrow} - c^\dagger_{i\downarrow} c^\dagger_{i+\mathbf{a}_\alpha\uparrow}) + \text{H.c.}$$

with site-dependent self-consistency criterion:

$$\Delta_\alpha(i) = -J\langle c_{i\downarrow} c_{i+\mathbf{a}_\alpha\uparrow} - c_{i\uparrow} c_{i+\mathbf{a}_\alpha\downarrow}\rangle$$

close to the van Hove singularity at $\mu = t$



ABS, PRL 109, 197001 (2012), Löthman and ABS, arXiv:1402.3195

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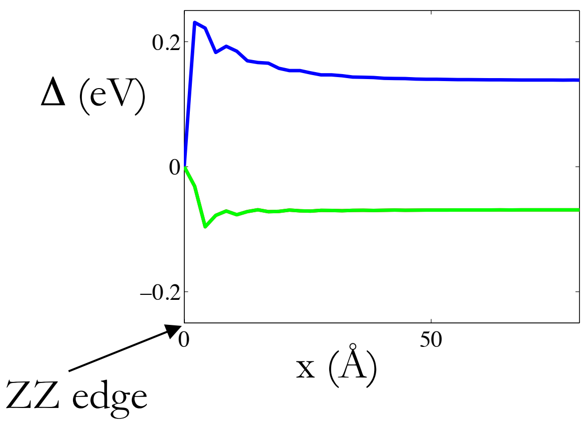
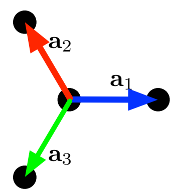
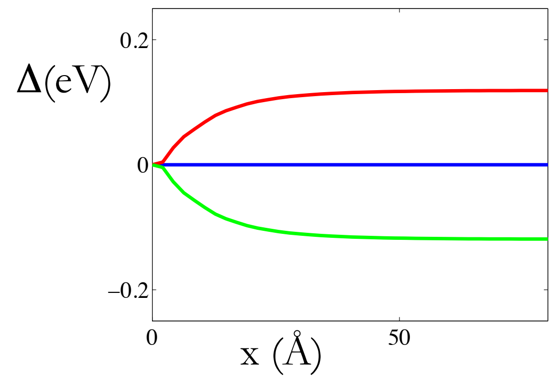
Superconductivity at the Edge

Real(Δ) $\approx$ $d(x^2-y^2)$ = (2,-1,-1)

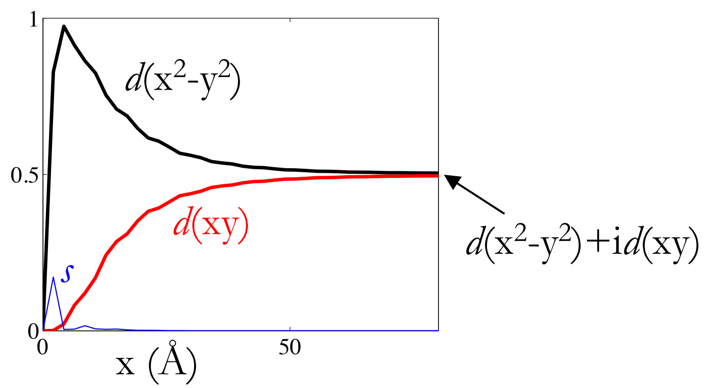




Imag(Δ) $\approx$ $d(xy)$ = (0,1,-1)



Character of Δ



ZZ and AC edges:

- Completely destroy $d(xy)$ part
- Enhance $d(x^2-y^2)$ part

➔ Pure $d(x^2-y^2)$-wave at the edge

➔ Graphene edges are not pair breaking

ABS, PRL 109, 197001 (2012)

$d(x^2-y^2)$-wave Edge State

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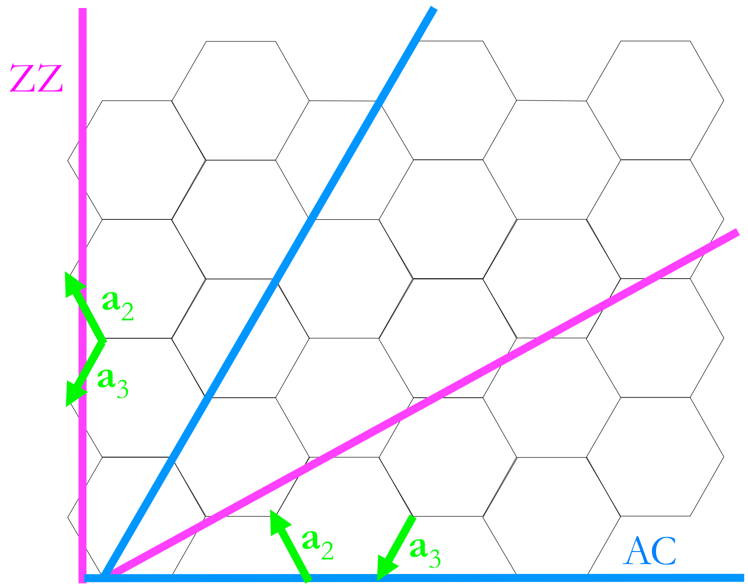
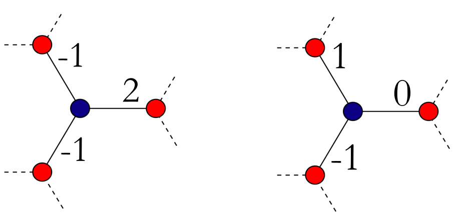
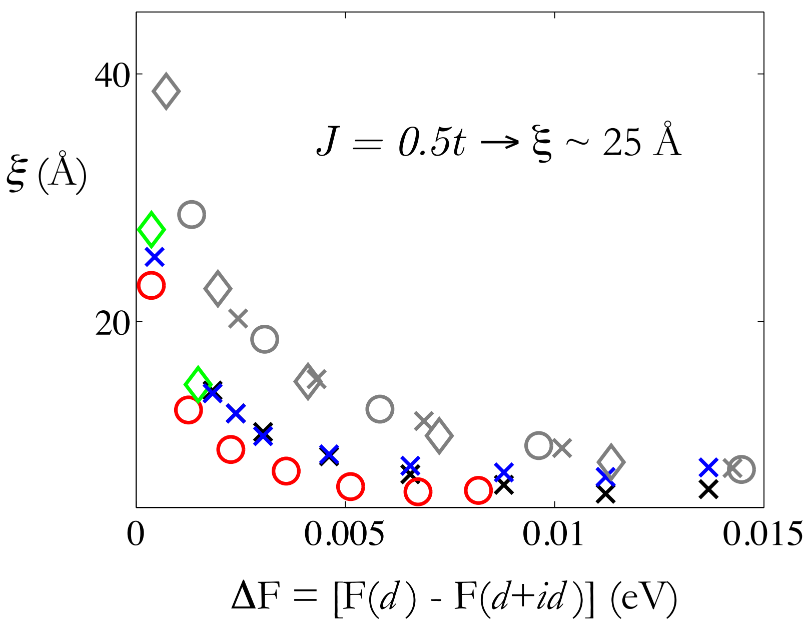


$\mathbf{a}_2 = \mathbf{a}_3$ for both AC and ZZ edges



➔ $d(x^2-y^2)$-wave preferred at any edge

Decay length



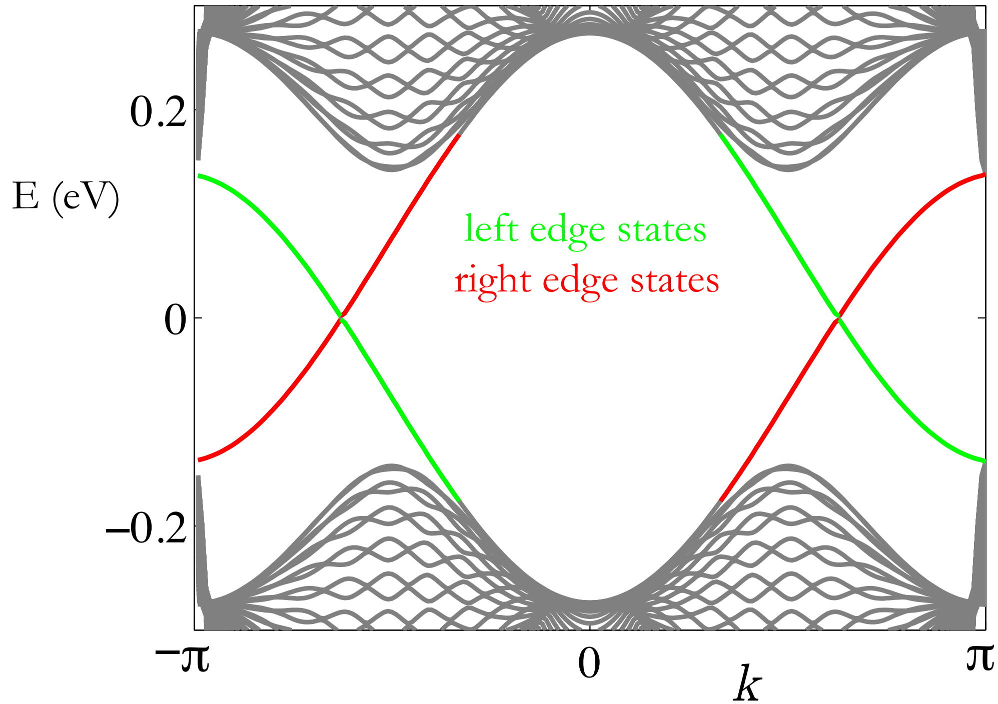
Long decay length for weak superconductivity

➔ Edge effects important even for macroscopic samples

ABS, PRL 109, 197001 (2012)

Chiral Edge States

Band structure for uniform $d(x^2\text{-}y^2)+id(xy)$ state



2 chiral (co-propagating) states per edge

➔ quantized thermal- and spin-Hall effects

ABS, PRL 109, 197001 (2012)

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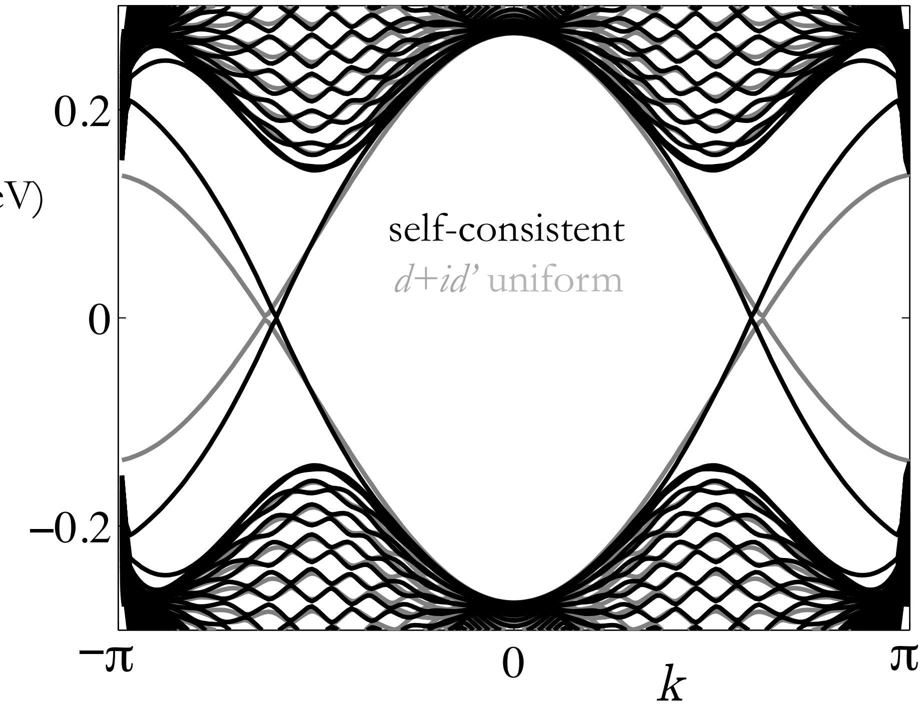
Chiral Edge States

Band structure self-consistent solution



ABS, PRL 109, 197001 (2012)

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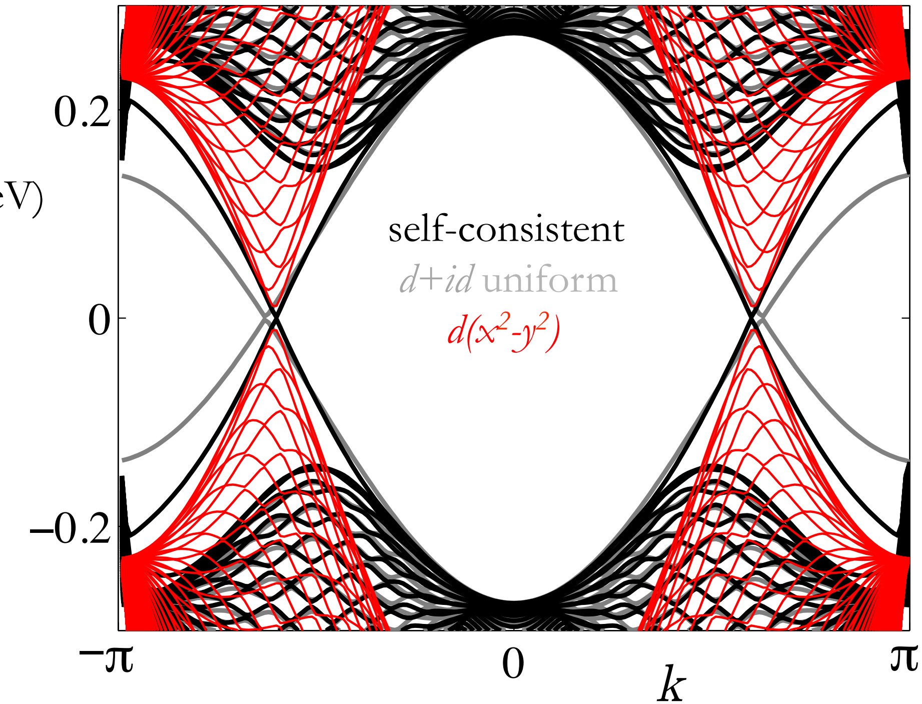
Chiral Edge States

Band structure self-consistent solution



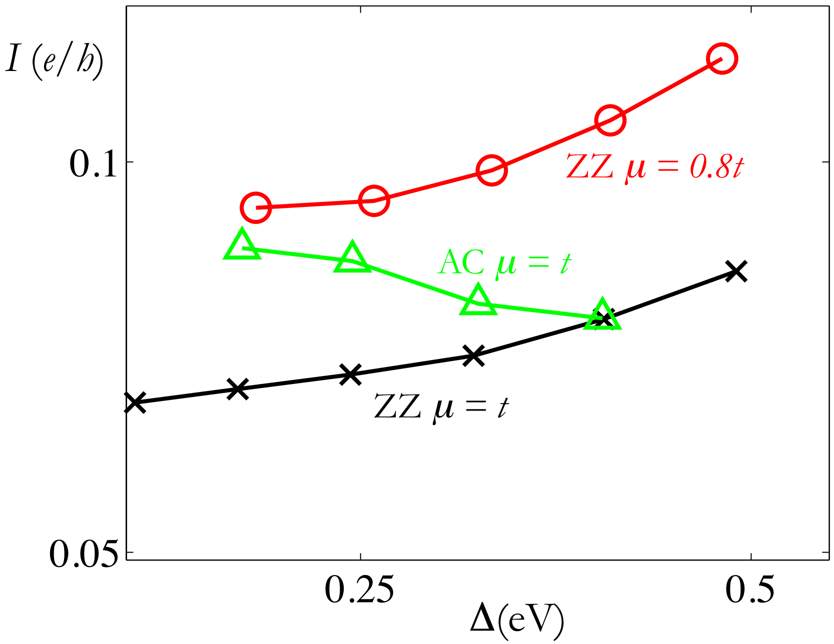
d(x^2-y^2) and *d+id'* solutions have similar edge band structures

- ➔ *d*(x^2-y^2) edge does not significantly modify the band structure
- ➔ Edge states well localized ~ 20 Å

ABS, PRL 109, 197001 (2012)

Spontaneous Edge Current

- Chiral edge states carry a spontaneous quasiparticle current
  - Broken time-reversal and parity symmetries
  - No quantized current



ABS, PRL 109, 197001 (2012)

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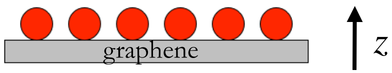
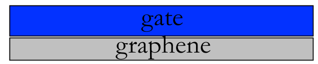
Rashba Spin-Orbit Coupling

Ad-atom deposition and electric gating break $z \rightarrow -z$ symmetry





➔ Allows Rashba spin-orbit coupling (SOC):

$$H_\lambda = i\lambda_R \sum_{\langle i,j\rangle,\sigma,\sigma'} \hat{z}\cdot(\mathbf{s}_{\sigma,\sigma'} \times \hat{\mathbf{a}}_{ij})c^\dagger_{i\sigma}c_{j\sigma'}$$

2D superconducting systems + Rashba SOC + Zeeman field

➔ Majorana modes at vortices and edges

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Majorana Modes

- Majorana modes
  - Real solution to a Dirac equation discovered by E. Majorana in 1937
  - $\gamma = \gamma^{\dagger}$
  - $c = \gamma_1 + i\gamma_2$ (1 electron ~ 2 Majorana)
  - Non-Abelian statistics ➔ fault-tolerant quantum computation

Majorana Edge States

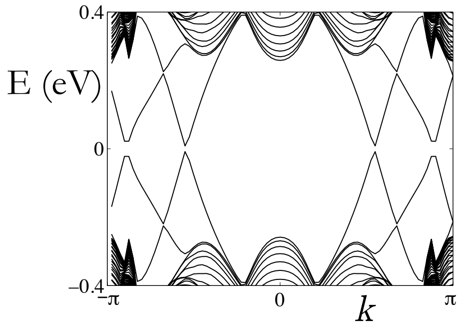
- Topological phase transition = bulk gap closing

Small Δ, λ_R, h $\rightarrow$ $h_c^2 = (\mu \pm t)^2 + (2\Delta)^2$

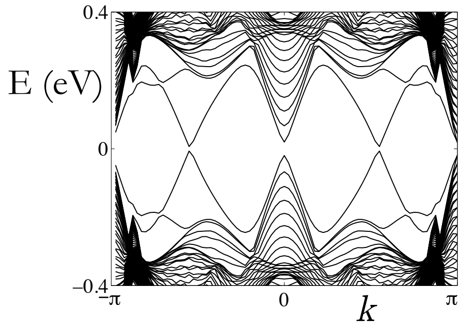
h_c — Zeeman field, h

Chiral *d*-wave superconductor
(2 chiral edge states)

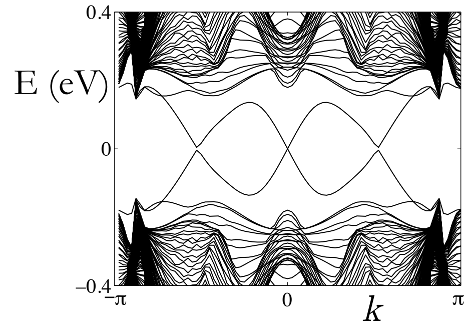
Majorana-supporting phase
(Majorana edge mode)



2 chiral edge states
(spin-split)



Bulk gap closing at
k = 0, π

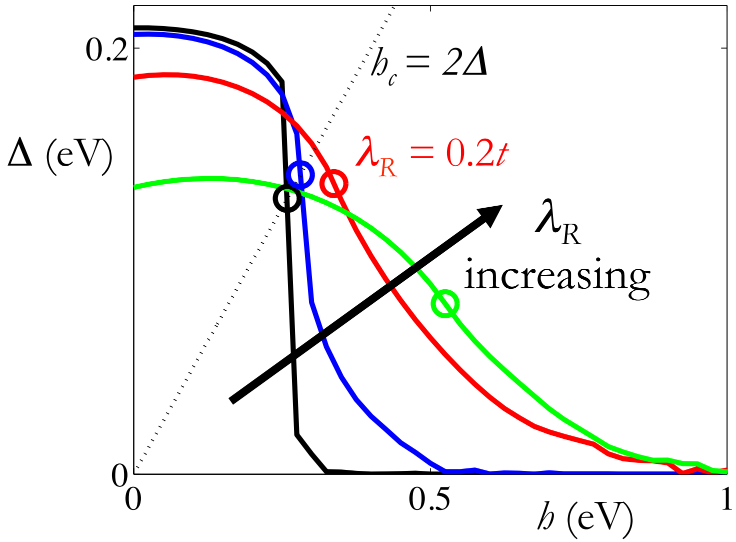


3 edge states (Majorana
+ 1 chiral state)

ABS, PRL 109, 197001 (2012)

Realizing the Majorana Phase

Superconducting state for finite Zeeman field, *h*:



- $\lambda_R \sim 0.2t$ for a superconducting state in Majorana-supported phase
  - Ad-atom induced SOC (?)
  - Electric field induced SOC (?)
- Zeeman field by proximity to ferromagnetic insulator

ABS, PRL 109, 197001 (2012)

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Outline

- Introduction

- Superconductivity from electron repulsion in doped graphene
  - Mean-field theory
  - Renormalization group theory

- Properties of the chiral *d*-wave superconducting state in graphene
  - Edges
    - Chiral edge states, spontaneous currents
    - Majorana modes
  - Impurities
  - Proximity-effect enhancements

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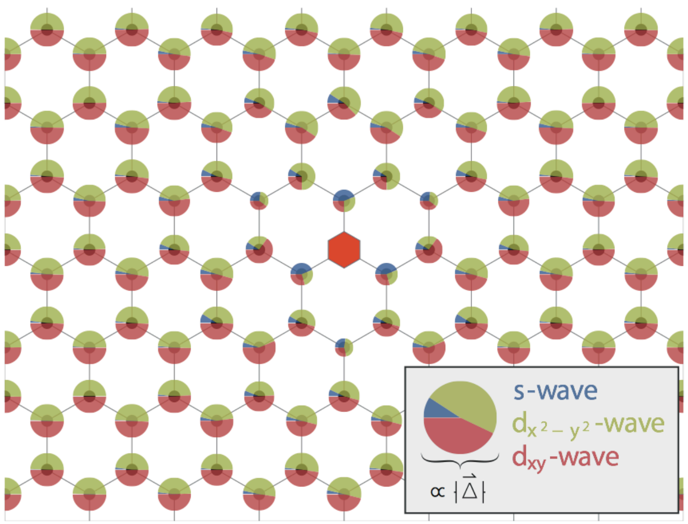
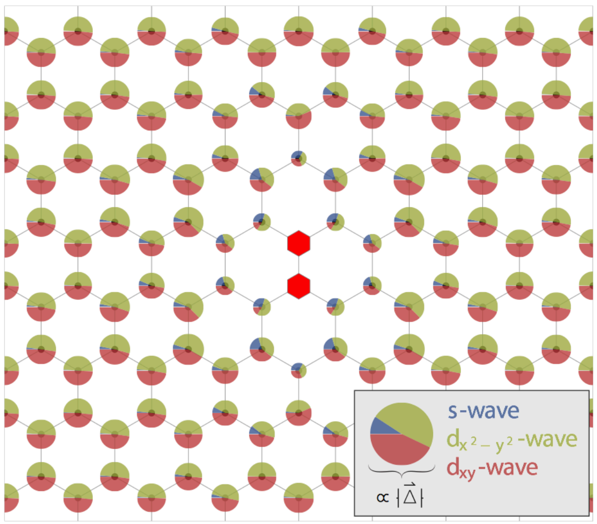
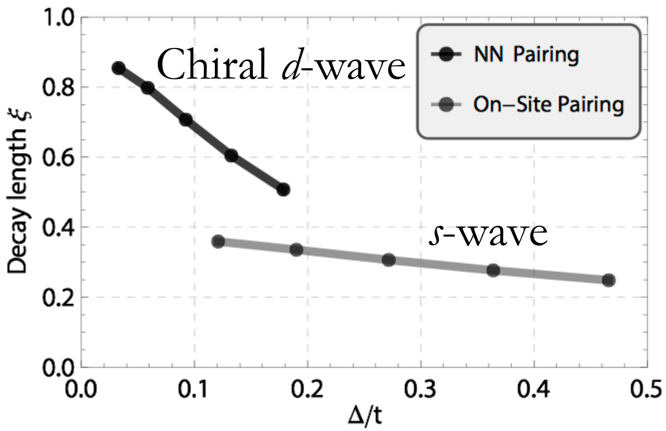
Vacancies

Single vacancy



Bivacancy





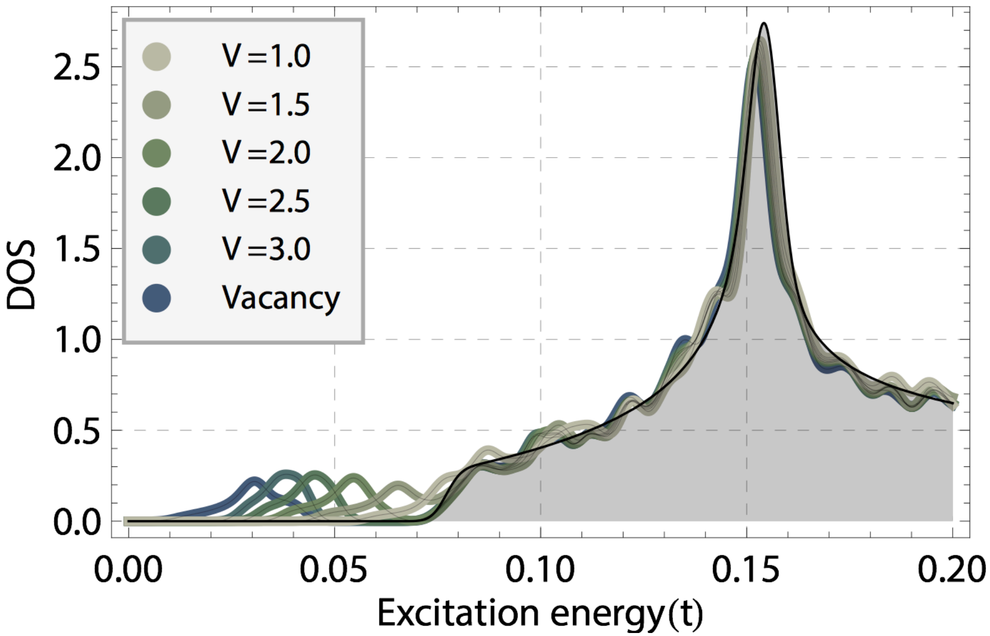
Chiral *d*-wave symmetry and amplitude restored quickly

➔ Chiral *d*-wave state resilient to defects

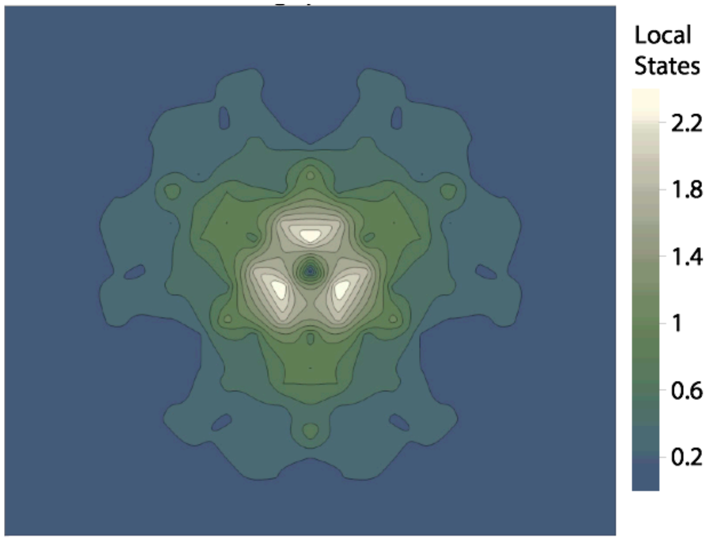
Löthman and ABS, arXiv:1402.3195

Impurity Mid-Gap States

DOS for chiral *d*-wave state with impurity



Spatial profile of mid-gap state



Löthman and ABS, arXiv:1402.3195

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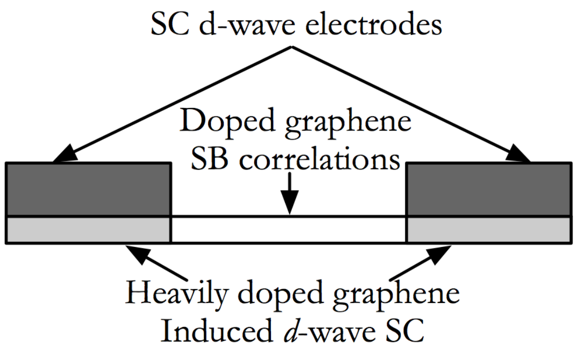
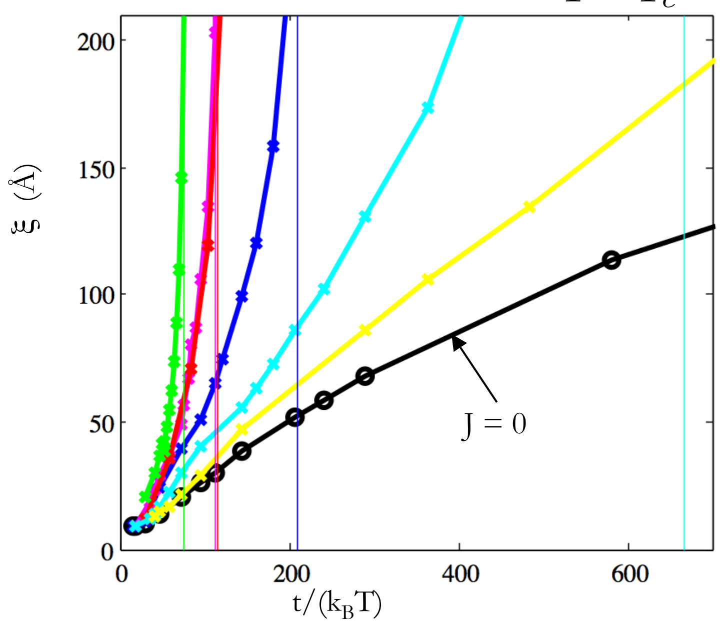
d-wave Josephson Junction

Proximity effect in a Josephson junction:

- Josephson junction with s-wave contacts does not enhance chiral *d*-wave correlations
- Josephson junction with *d*-wave contacts



Decay length in N: $\xi \sim \dfrac{1}{T - T_c}$



ABS and Doniach, PRB 81,014517 (2010)

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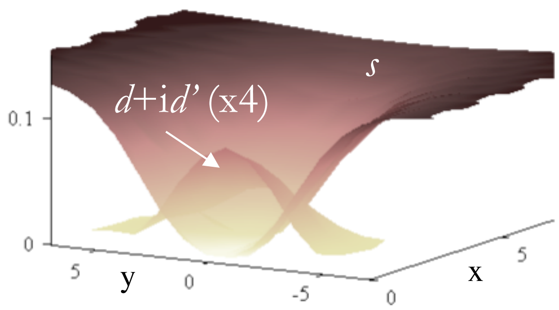
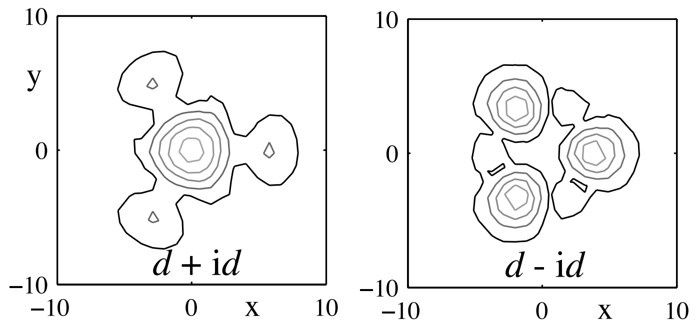
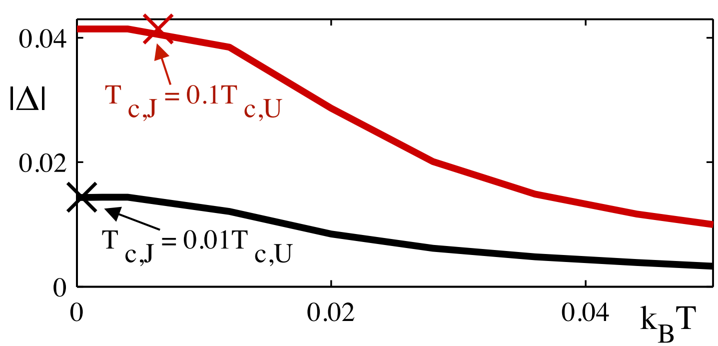
Double Quantized *s*-wave Vortex

- Doubly quantized vortex in an *s*-wave superconductor
  - n = 2 vortex winding angular momentum transferred to chiral *d*-wave state





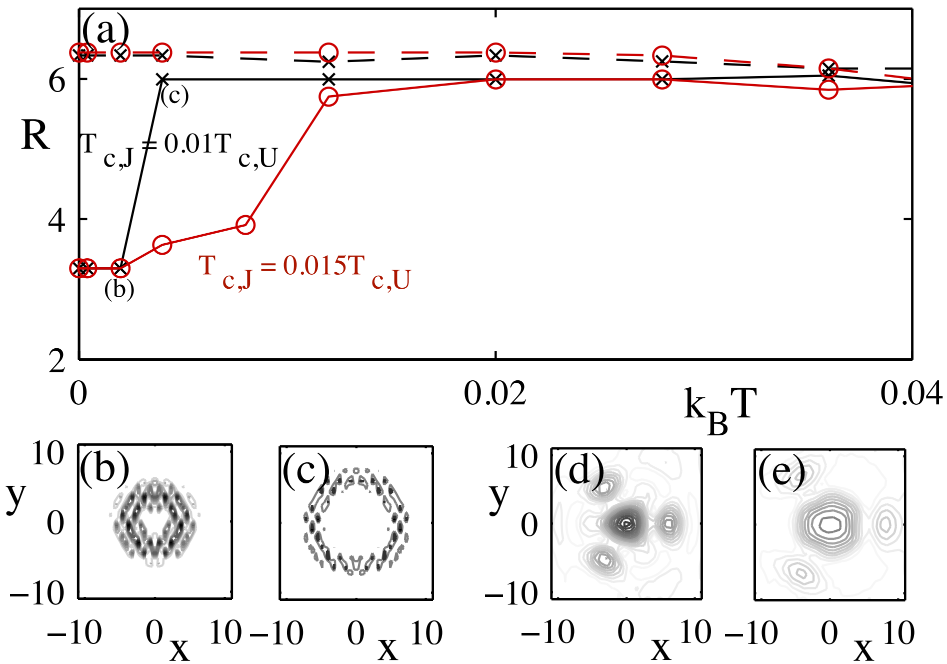
Temperature dependence: $\Delta(T) \sim \dfrac{\Delta(T=0)}{1+(T-T_c)^2/E_g^2}$



ABS, PRB 88, 104506 (2013)

Detecting the Chiral *d*-wave State

- Spatial profile for the lowest energy state in the vortex:
  - Without a chiral *d*-wave core: Vortex bound state $R_{core} \sim \xi_S$
  - With a chiral *d*-wave core: Chiral *d*-wave edge state $R_{edge} < R_{core}$



Spatial profile of the lowest energy state

Chiral *d*-wave order parameter

ABS, PRB 88, 104506 (2013)

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Summary

- Chiral $d(x^2\text{-}y^2)$+i$d(xy)$ superconductivity in heavily doped graphene
  - Mean-field result for an effective Hamiltonian
  - Perturbative RG and fRG results on extended Hubbard models
- Edges:
  - Pure $d(x^2\text{-}y^2)$-wave with long decay length
  - Two well-localized chiral edge states
  - Spontaneous, but not quantized, edge currents
  - Majorana fermions at the edge (Spin-orbit coupling & Zeeman field)
- Impurities
  - Chiral *d*-wave state resilient to impurities
- Enhancement of the chiral *d*-wave state by proximity effect
  - *d*-wave Josephson junctions
  - Doubly quantized vortices in *s*-wave superconductors

Recent review article (to appear in J. Phys.: Condens. Matter):
ABS and Honerkamp, arXiv:1406.0101