Lattice Tight-Binding Bogoliubov-de Gennes Approach to Nonuniform Superconductivity:

Proximity-effect, Josephson junctions, and vortices

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Vetenskapsrådet

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Strategic Research

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Carl Trygger
Foundation

Outline

Self-consistent lattice tight-binding Bogoliubov-de Gennes method for nonhomogeneous superconductivity:

- SNS Josephson junctions in graphene
- Enhancing intrinsic pairing using an external superconductor
  - (Proposed) chiral *d*-wave state in doped graphene
- Majorana fermions in vortex cores

SNS Junctions in Graphene

Can we accurately model a SNS junction?

- Self-consistent lattice tight-binding Bogoliubov-de Gennes (TB-BdG) method
- Current-phase relation

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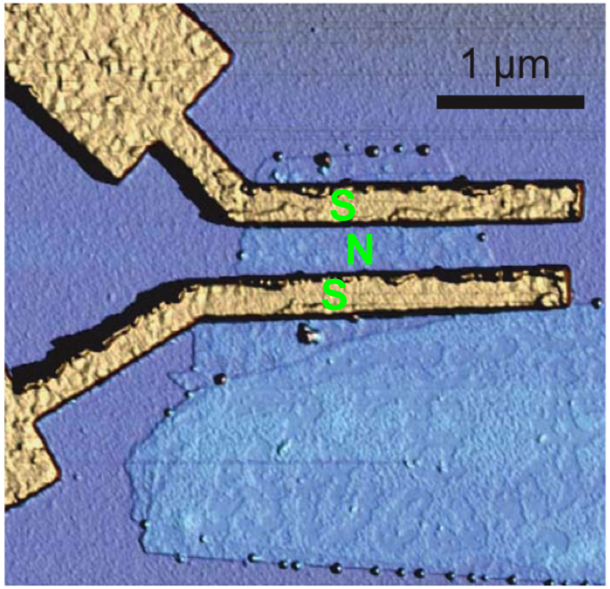
Proximity-Induced Superconductivity

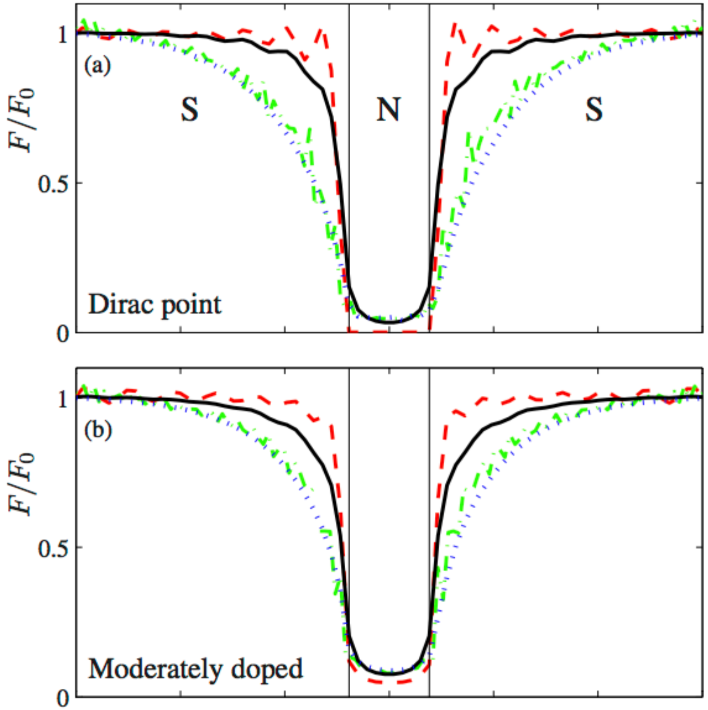
Inducing superconductivity in a non-superconducting material (N) by close contact to an external superconductor (S)

Graphene SNS (Josephson) junction:



[1]

Pair amplitude:

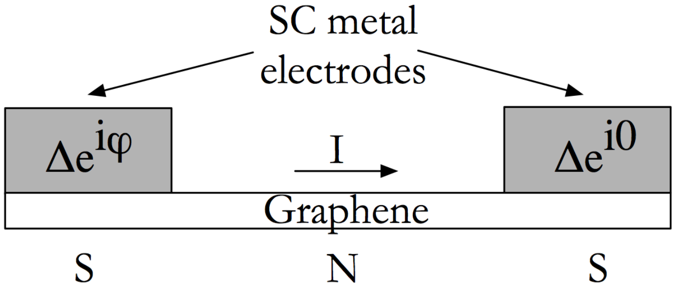


[2]

[1]: Heersche et al. Nature 446, 56 (2007), [2]: Linder, AMBS et al. PRB 80, 094522 (2009)

SNS Graphene (Josephson) Junctions

SNS graphene junction:



SC metal electrodes

$\Delta e^{i\varphi}$

I

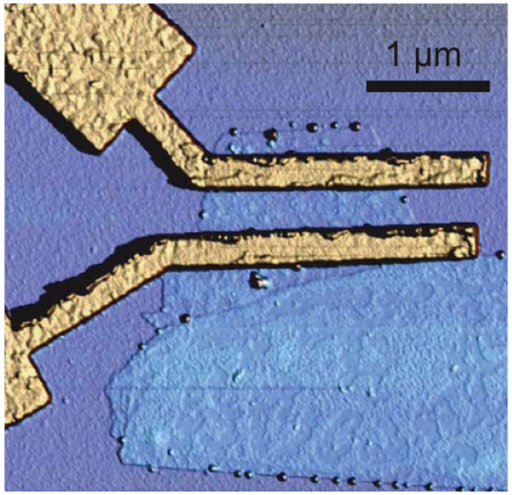
Δe^{i0}

Graphene

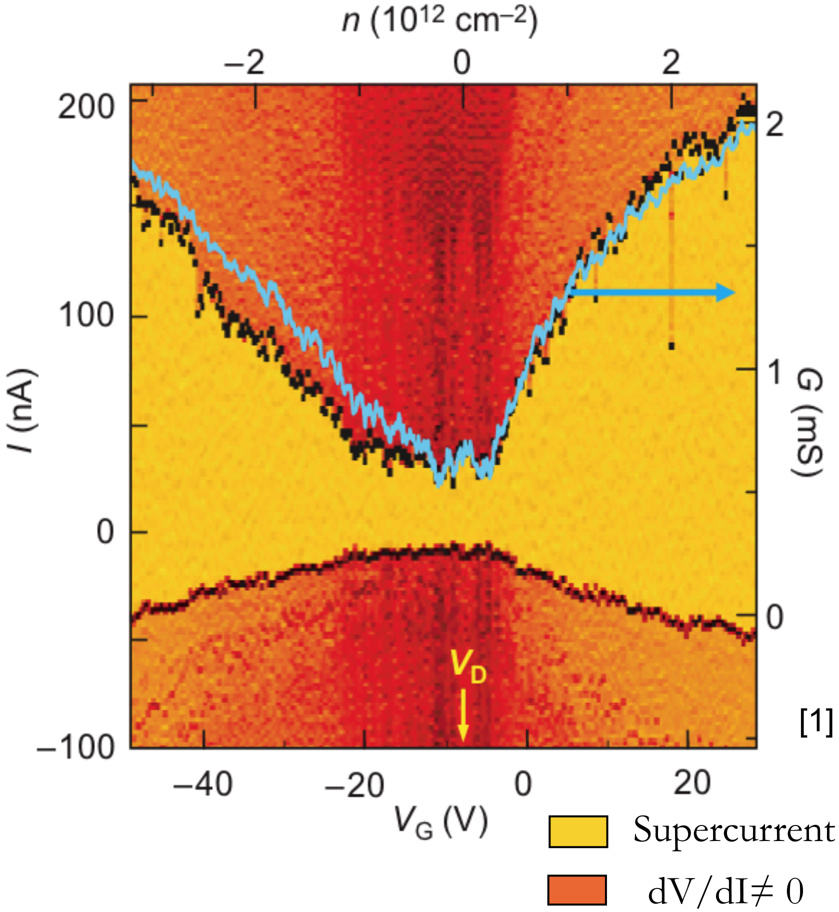
S

N

S



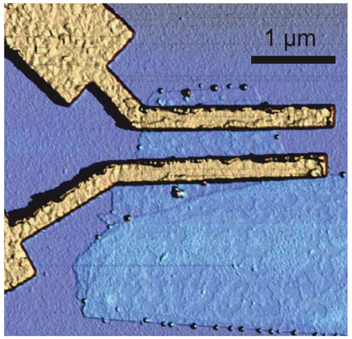
[1]

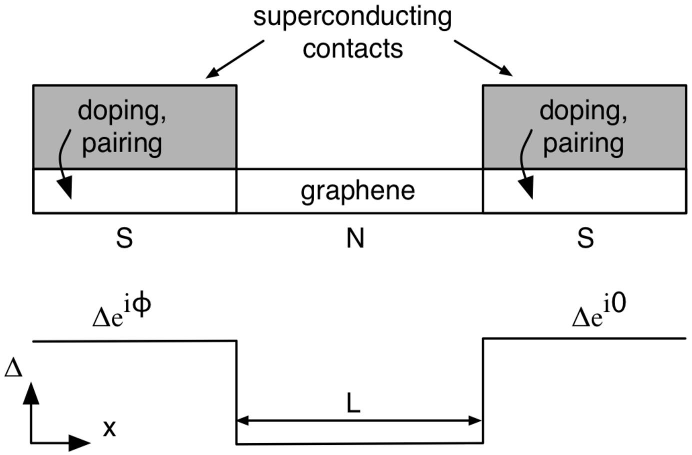


Uniform supercurrent even at the Dirac point

[1]: Heersche et al. Nature 446, 56 (2007)

Continuum Dirac-BdG Modeling





Neglects inverse proximity effect and current depairing

Assume Δ-profile (no self-consistency)

- Solve in S and N, match solutions at boundaries: Dirac-BdG formalism
- Current assumed to be carried by Andreev bound states

At Dirac point: $I(\phi) = \frac{e\Delta_0}{\hbar} \frac{2W}{\pi L} \cos(\phi/2) \operatorname{arctanh}[\sin(\phi/2)]$ [1]

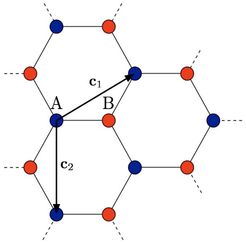
Traditional Josephson junction: $I = I_c \sin(\phi)$

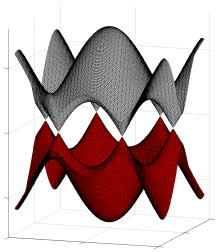
[1]: Titov et al., PRB 74 041401 (2006)

Tight-Binding BdG Formalism

Self-consistent TB-BdG on a lattice:

$$H_{\text{eff}} = -t\underbrace{\sum_{<i,j>,\sigma} c^{\dagger}_{i\sigma}c_{j\sigma} + \sum_{i,\sigma}\mu(i)c^{\dagger}_{i\sigma}c_{i\sigma}}_{\text{Tight-binding band structure}} - \underbrace{\sum_{i} U(i)c^{\dagger}_{i\uparrow}c_{i\uparrow}c^{\dagger}_{i\downarrow}c_{i\downarrow}}_{s\text{-wave pairing}}$$



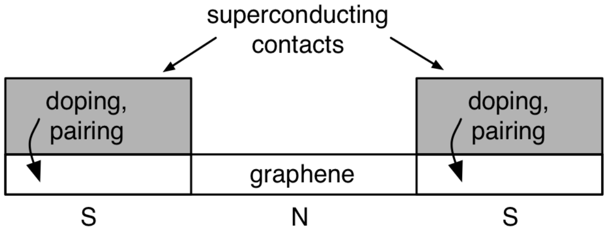


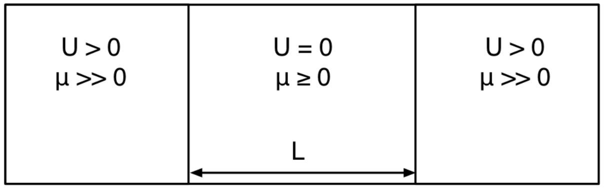
Mean-field theory

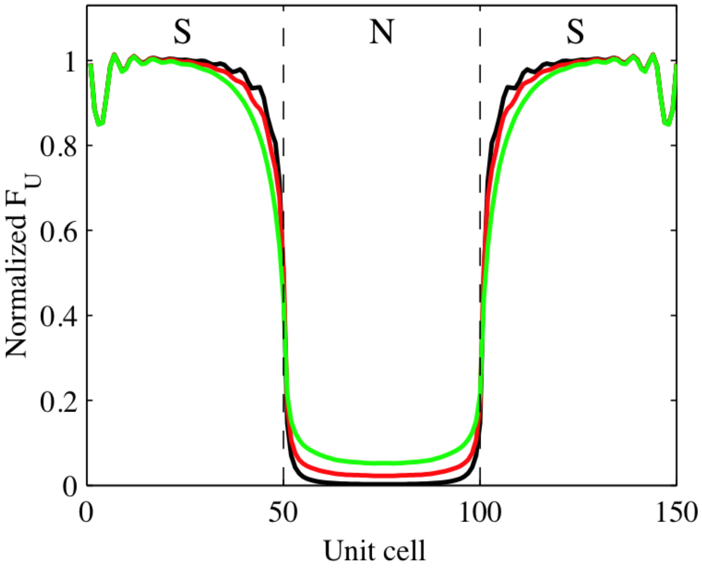
$$\Delta(i)c^{\dagger}_{i\uparrow}c^{\dagger}_{i\downarrow} + \text{H.c.}$$

$$\Delta(i) = -U(i)\langle c_{i\downarrow}c_{i\uparrow}\rangle$$

Pairing amplitude ($F_U = \langle c_{i\downarrow}c_{i\uparrow}\rangle$):



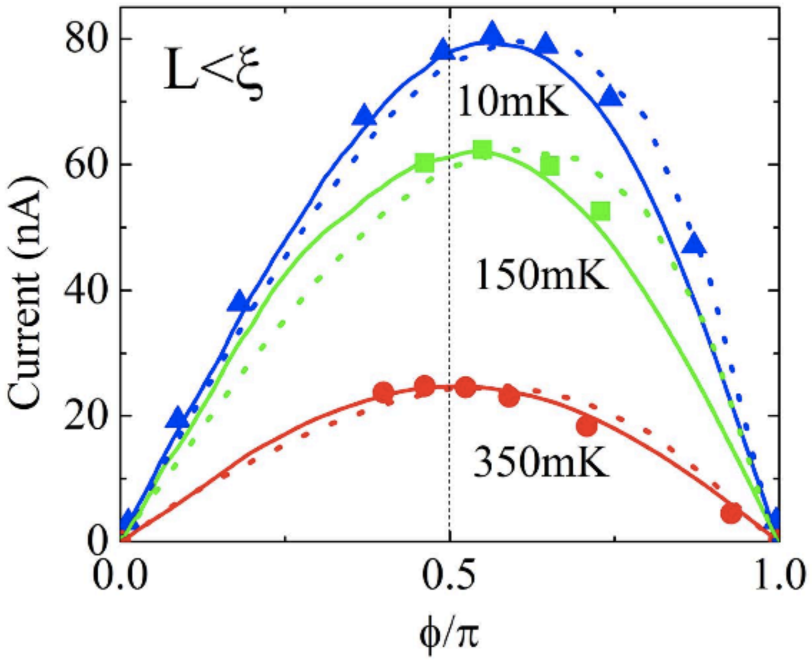




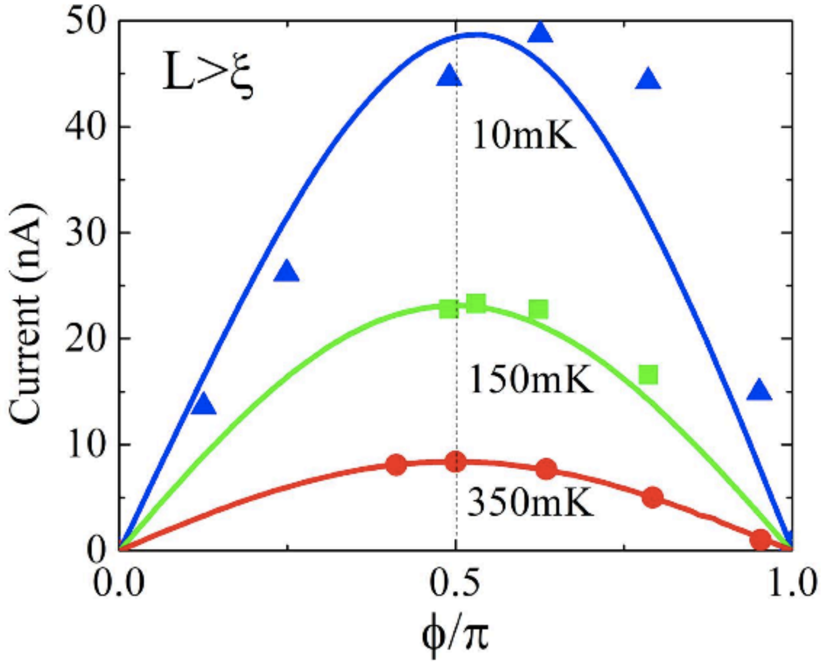
AMBS and Doniach, PRB 78, 024504 (2008)

Current-Phase Relation (CPR)

Short junctions



Long junctions



[1]

— Experiment (quasi-ballistic limit) [1]

---- DBdG results [2]

● Self-consistent results [3]

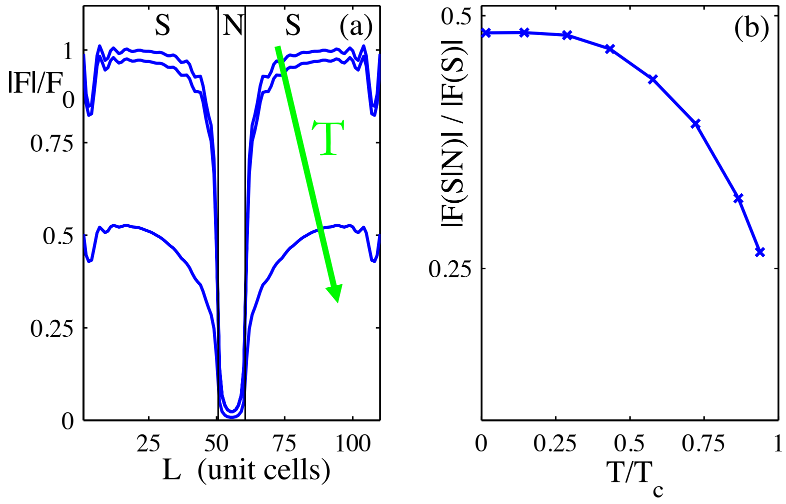
Self-consistent CPR less skewed than DBdG results

- Inverse proximity effect (IPE)
- Current depairing in short junctions

[1]: English et al., arXiv:1305.0327, [2]: Hagymasi et al., PRB 82, 134516 (2010),
[3]: AMBS and Linder, PRB 82, 184522 (2010)

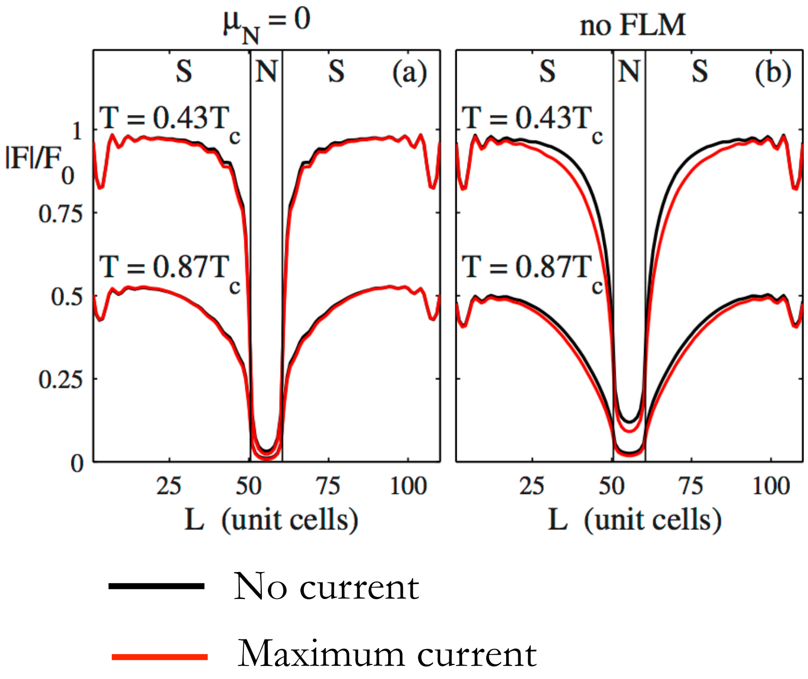
IPE and Current Depairing

Inverse proximity-effect (IPE):



Loss of superconductivity on the S side of the junction, worse with increasing T

Current depairing:



Current causes an overall loss of superconductivity

Need a self-consistent approach to capture IPE and current depairing

AMBS and Linder, PRB 82, 184522 (2010)

Intrinsic Pairing in Graphene

Interaction-driven chiral *d*-wave superconductivity in doped graphene

Can we enhance the intrinsic pairing using external superconductors?

- *d*-wave cuprate contacts
- Doubly quantized vortices in *s*-wave superconductors

Intrinsic Pairing in Graphene

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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:

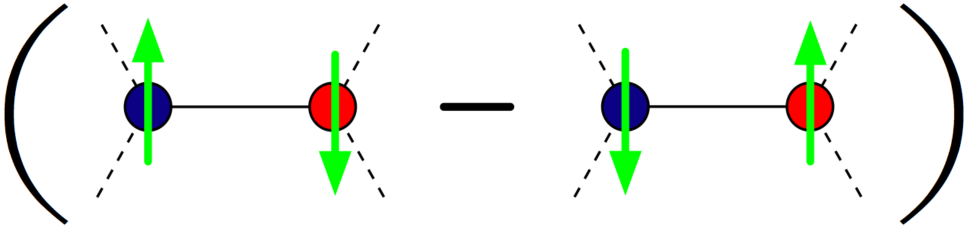
Nearest neighbor spin-singlet bonds (SB)
encouraged compared to polar configurations

} Pauling's Resonance Valence Bond (RVB) idea

Give good estimates for:

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

SB =



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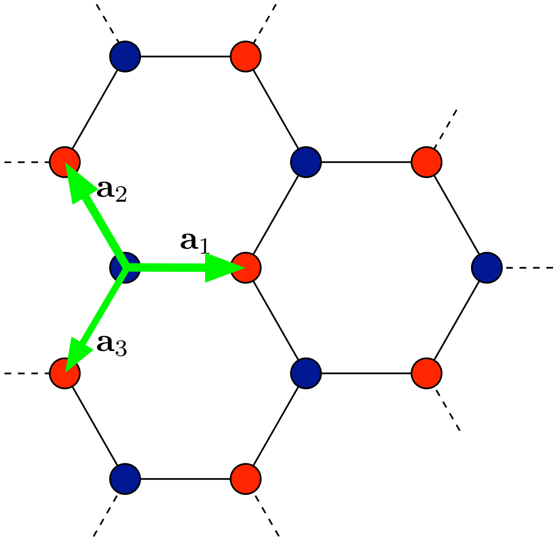
[1]: T. Wehling et al,. PRL 106, 236805 (2011)

Modeling Correlation Effects

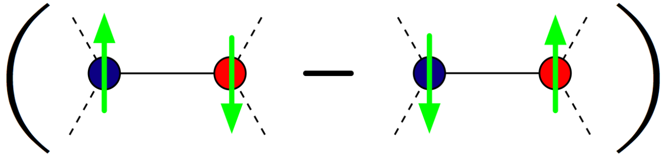
Effective model with SB pairing: [1]

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



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

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



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

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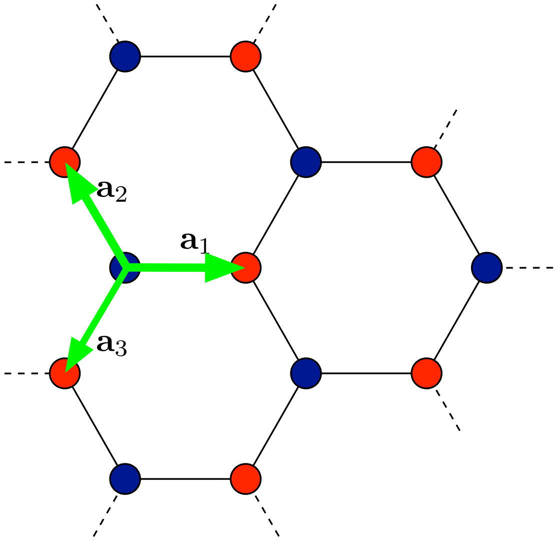
[1]: Baskaran, PRB 65, 212505 (2002)

Mean-Field Approach

Effective model with SB pairing: [1]

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



Mean-field order parameters in the Cooper pairing channel:

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

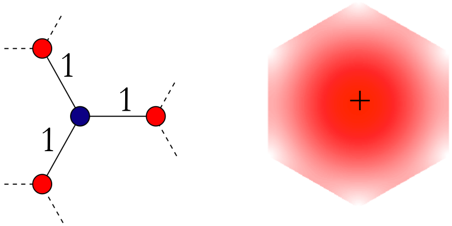
Expectation value of
SB pair creation

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

Gap Symmetries

s-wave:

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



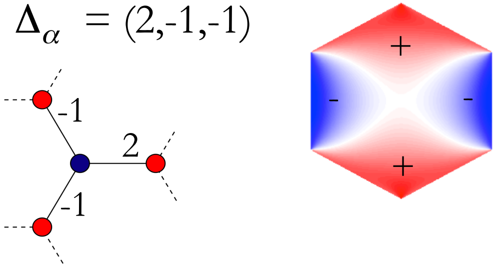
extended *s*-wave

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

ABS and Donaich, PRB 75, 134512 (2007)

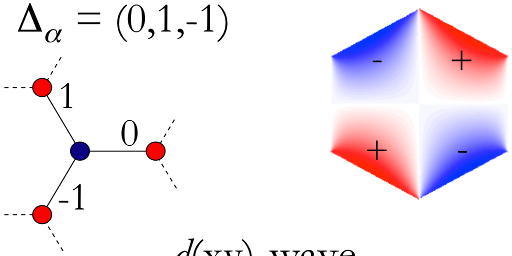
d-waves:

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



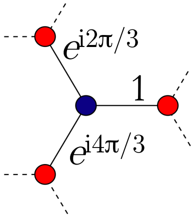
d(x^2-y^2)-wave

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



d(xy)-wave

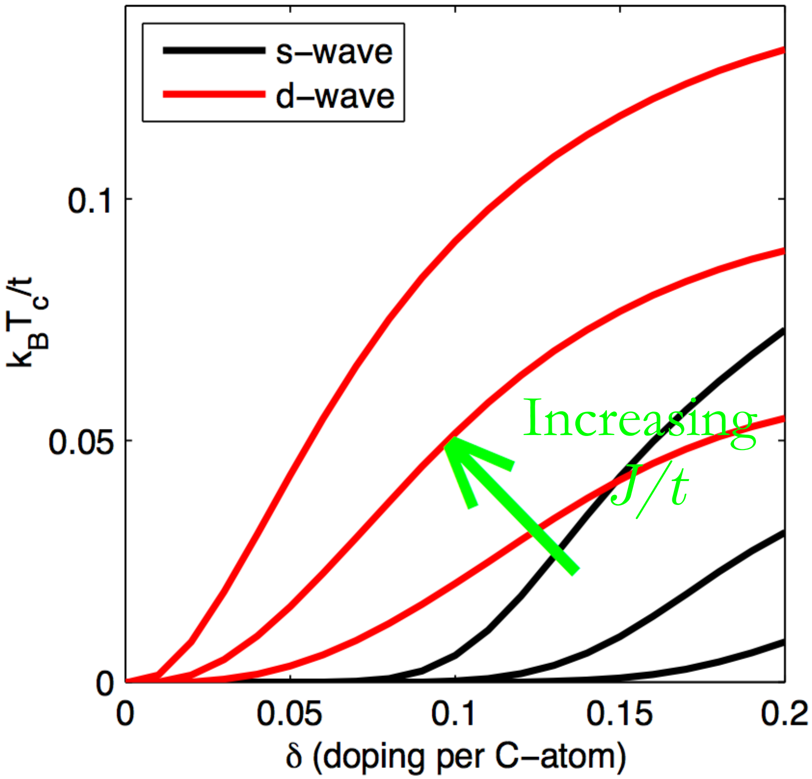
- $\Delta \in E_{2g}$ of D_{6h}
  - Below T_c: $d(x^2-y^2)+id(xy)$



Chiral, time-reversal symmetry breaking state

Mean-Field Results

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



Zero doping:

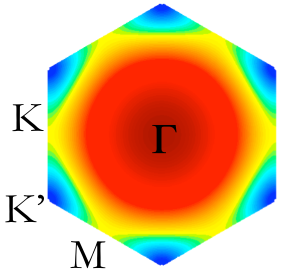
- QCP at $J/t = 1.91$
- *s*- and *d*-wave solutions degenerate

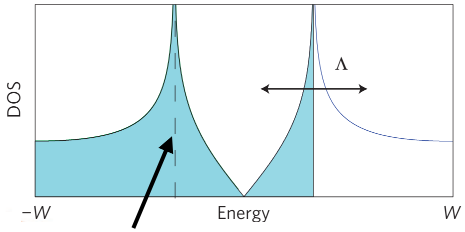
Finite doping:

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

Heavy doping can approach van Hove singularity ($\delta = 0.25$, $\mu = t$):

- Ad-atom deposition [1]
- Electrolyte gating [2]



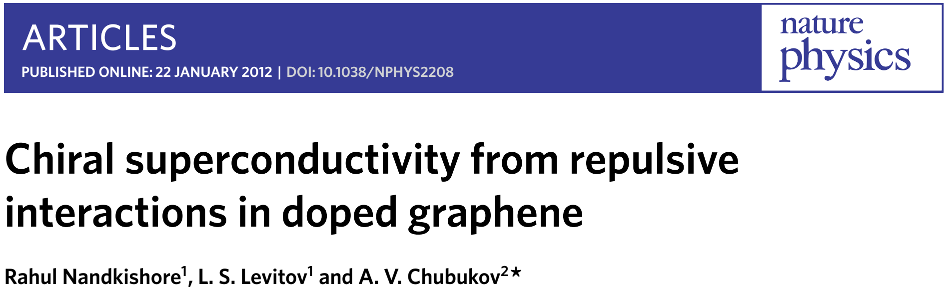


Logarithmic diverging DOS

ABS and Donaich, PRB 75, 134512 (2007), [1]: McChesney et al., PRL 104, 136803 (2010), [2]: Efetov et al., PRL 105, 256805 (2010)

RG Calculations at the van Hove point

Perturbative RG with contact interactions:



ARTICLES

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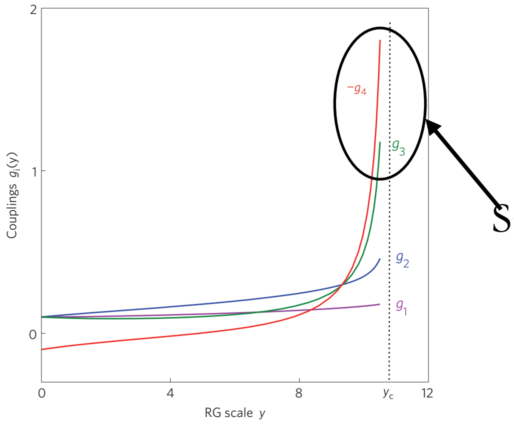
Chiral superconductivity from repulsive interactions in doped graphene

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

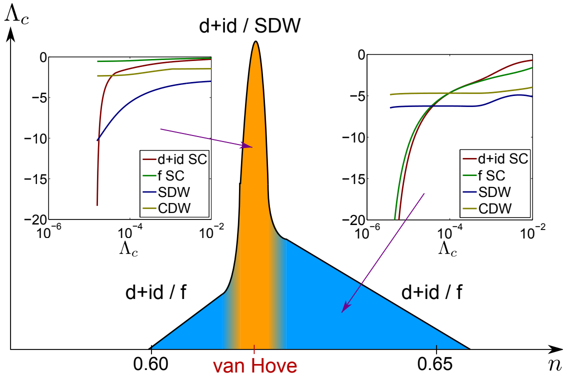


SC instability

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

Functional RG: [1,2]

$$H = -\sum_{(ij)\sigma}(c^\dagger_{i\sigma}t_{ij}c_{j\sigma} + \text{H.c.}) - \mu N_e + U\sum_i n_{i\uparrow}n_{i\downarrow}$$
$$+\frac{1}{2}V\sum_{i\delta} n_i n_{i+\delta},$$



Chiral *d*-wave superconductivity close to van Hove point in graphene

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

Intrinsic Pairing in Graphene

Interaction-driven chiral *d*-wave superconductivity in doped graphene

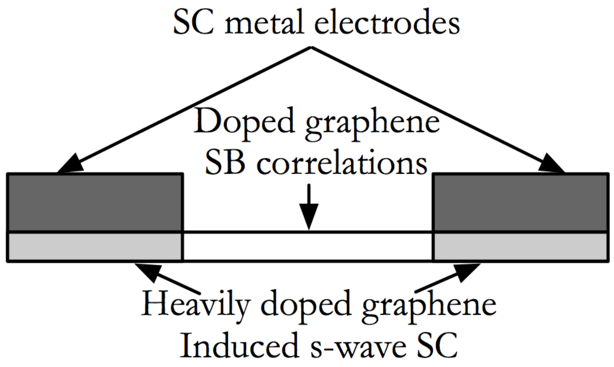
Can we enhance the intrinsic pairing using external superconductors?

- *d*-wave cuprate contacts
- Doubly quantized vortices in *s*-wave superconductors

Tight-Binding BdG Formalism

Effective Hamiltonian for conventional, *s*-wave contacts:

$$\begin{aligned} H_{\text{eff}} = & -t \sum_{<i,j>,\sigma} (f^{\dagger}_{i\sigma} g_{j\sigma} + g^{\dagger}_{i\sigma} f_{j\sigma}) + \sum_{i,\sigma} \mu(i)(f^{\dagger}_{i\sigma} f_{i\sigma} + g^{\dagger}_{i\sigma} g_{i\sigma}) \Big\} \ \text{Tight-binding band structure} \\ & -2 \sum_{<i,j>} J(i) h^{\dagger}_{ij} h_{ij} \Big\} \ \text{Intrinsic SB correlations} \\ & -\sum_{i} U(i)(n_{fi\uparrow} n_{fi\downarrow} + n_{gi\uparrow} n_{gi\downarrow}) \Big\} \ \text{Effective } s\text{-wave pairing} \end{aligned}$$



S	N	S
$U > 0$	$U = 0$	$U > 0$
$J = 0$	$J > 0$	$J = 0$
$\tilde{\mu} \gg 0$	$\tilde{\mu} > 0$	$\tilde{\mu} \gg 0$

Solve self-consistently for

on-site pair amplitude: $\Delta_U(i) = \dfrac{\langle f_{i\downarrow} f_{i\uparrow} + g_{i\downarrow} g_{i\uparrow} \rangle}{2}$

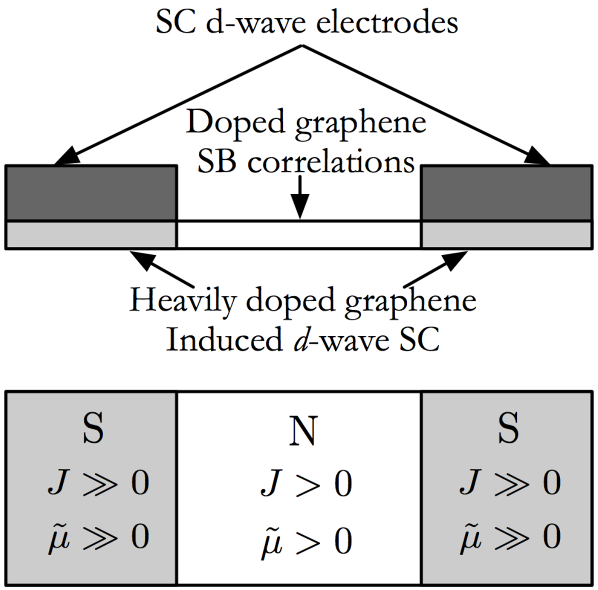
SB pair amplitude: $\Delta_{Ja}(i) = \langle h_{i,i+a} \rangle$

Can the SB correlations be enhanced by *external* superconducting contacts?

d-wave Josephson Junction

Proximity effect in a Josephson junction:

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

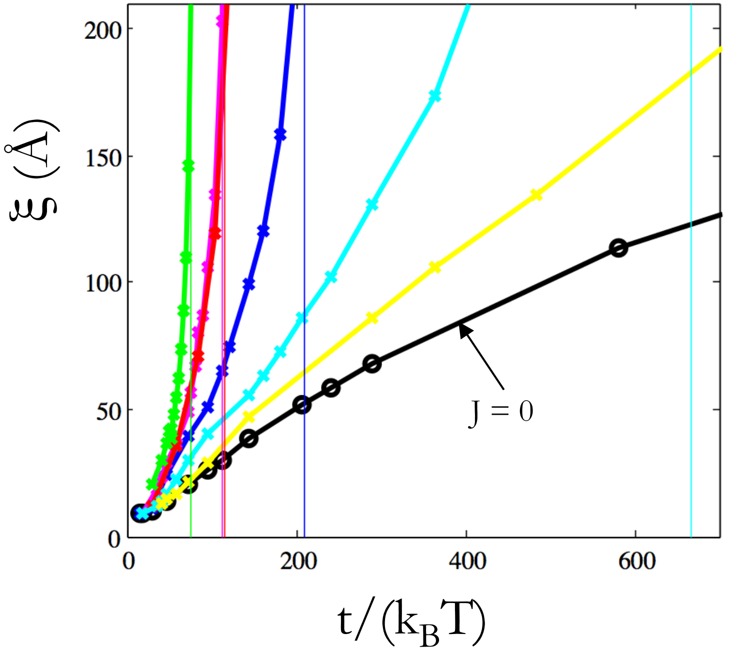

SC d-wave electrodes

Doped graphene
SB correlations

Heavily doped graphene
Induced *d*-wave SC

S	N	S
$J \gg 0$	$J > 0$	$J \gg 0$
$\tilde{\mu} \gg 0$	$\tilde{\mu} > 0$	$\tilde{\mu} \gg 0$

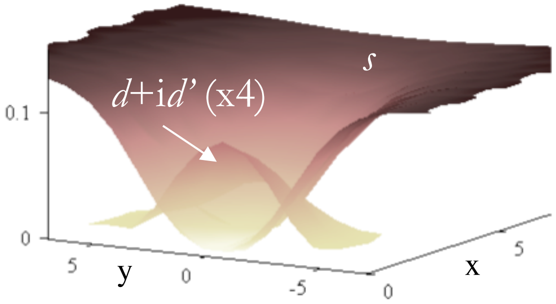
Decay length in N: $\xi \sim \dfrac{1}{T - T_c}$

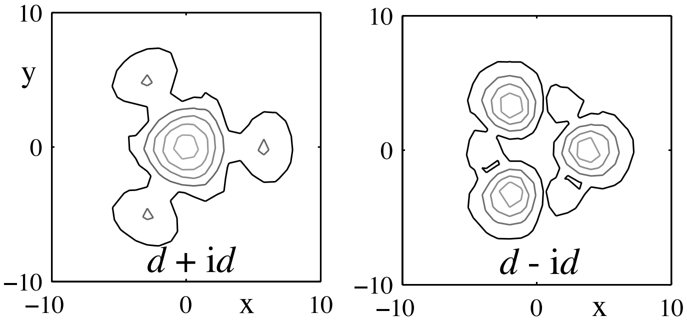


ABS and Doniach, PRB 79, 064502 (2009), PRB 81,014517 (2010)

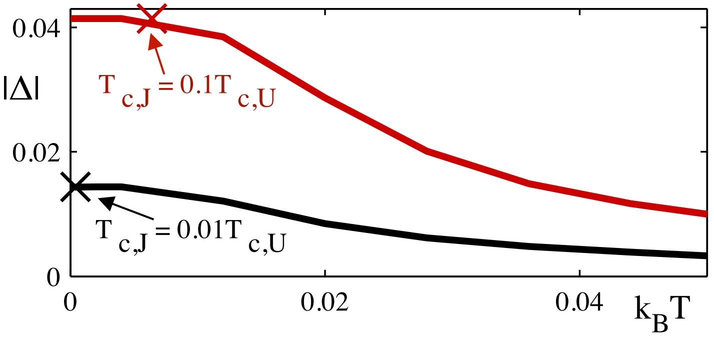
Double Quantized *s*-wave Vortex

- Doubly quantized vortex in an *s*-wave superconductor
  - Force a 4π rotation on the sample edges of the *s*-wave order parameter
  - 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)

Majorana Fermion in Vortex Cores

Self-consistent lattice TB-BdG method solution for a vortex in a spin-orbit coupled semiconductor – superconductor hybrid structure

- Accurate value of the superconducting order parameter
- Additional phase transition in the vortex core region

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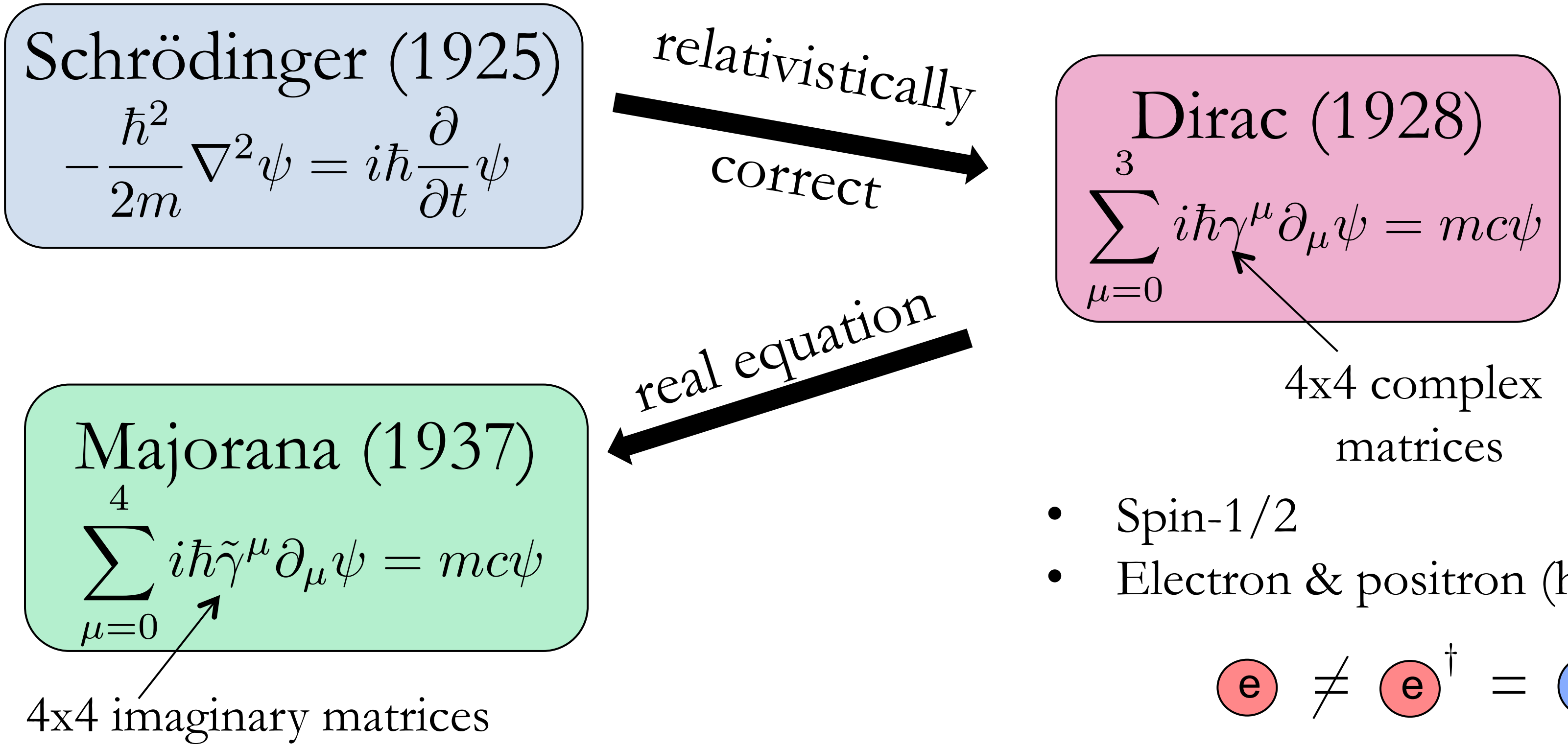
Schrödinger, Dirac, and Majorana



Schrödinger (1925)

$$-\frac{\hbar^2}{2m}\nabla^2\psi = i\hbar\frac{\partial}{\partial t}\psi$$

relativistically

correct

Dirac (1928)

$$\sum_{\mu=0}^{3} i\hbar\gamma^\mu\partial_\mu\psi = mc\psi$$

4x4 complex
matrices

real equation

Majorana (1937)

$$\sum_{\mu=0}^{4} i\hbar\tilde{\gamma}^\mu\partial_\mu\psi = mc\psi$$

4x4 imaginary matrices

- Spin-1/2
- Electron & positron (hole)

$$e \neq e^\dagger = h$$

- Particle = Antiparticle: $M = M^\dagger$
- Electron "=" 2 Majorana fermions: $e = M_1 + i\, M_2$

Majorana Fermion

Where do we find Majorana fermions?

- Fundamental particle (neutrino?)

- Quasiparticle excitations in condensed matter systems
  - Particle = antiparticle → Zero-energy states in superconductors
  - No degeneracy → Effectively spinless *p*+i*p*’-wave superconductor

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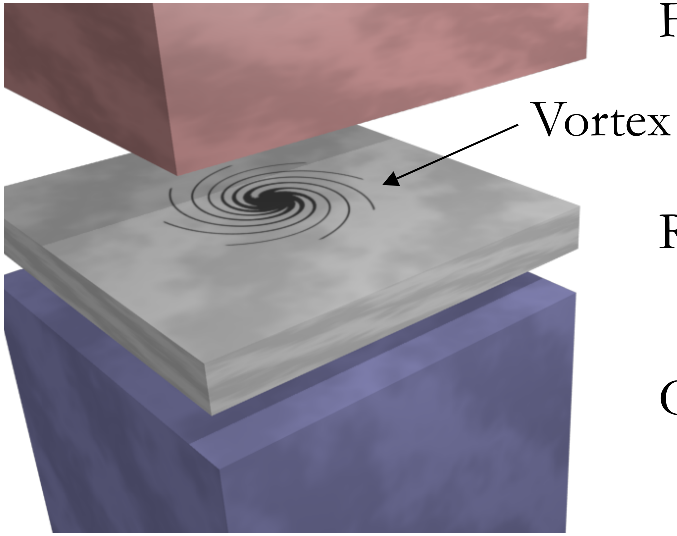
Spin-Orbit Coupled Semiconductors – Superconductor Hybrid Structures



Ferromagnetic insulator

Rashba spin-orbit coupled 2D semiconductor

Conventional *s*-wave superconductor

$$
\begin{aligned}
\mathcal{H} &= \mathcal{H}_{\text{kin}} + \mathcal{H}_{V_z} + \mathcal{H}_{\text{SO}} + \mathcal{H}_{\text{sc}}, \\
\mathcal{H}_{\text{kin}} &= -t \sum_{\langle \mathbf{i},\mathbf{j}\rangle,\sigma} c_{\mathbf{i}\sigma}^{\dagger} c_{\mathbf{j}\sigma} - \mu \sum_{\mathbf{i},\sigma} c_{\mathbf{i}\sigma}^{\dagger} c_{\mathbf{i}\sigma}, \\
\mathcal{H}_{V_z} &= -V_z \sum_{\mathbf{i},\sigma,\sigma'} (\sigma_z)_{\sigma\sigma'} c_{\mathbf{i}\sigma}^{\dagger} c_{\mathbf{i}\sigma'}, \\
\mathcal{H}_{\text{SO}} &= -\frac{\alpha}{2} \sum_{\mathbf{i}} [(c_{\mathbf{i}-\hat{x}\downarrow}^{\dagger} c_{\mathbf{i}\uparrow} - c_{\mathbf{i}+\hat{x}\downarrow}^{\dagger} c_{\mathbf{i}\uparrow}) \\
&\quad + i(c_{\mathbf{i}-\hat{y}\downarrow}^{\dagger} c_{\mathbf{i}\uparrow} - c_{\mathbf{i}+\hat{\mathbf{y}}\downarrow}^{\dagger} c_{\mathbf{i}\uparrow}) + \text{H.c.}], \\
\mathcal{H}_{\text{sc}} &= \sum_{\mathbf{i}} \Delta_{\mathbf{i}} (c_{\mathbf{i}\uparrow}^{\dagger} c_{\mathbf{i}\downarrow}^{\dagger} + \text{H.c.}).
\end{aligned}
$$

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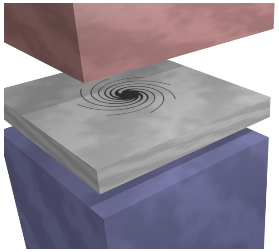
Rashba SO + *s*-wave SC + Zeeman field:

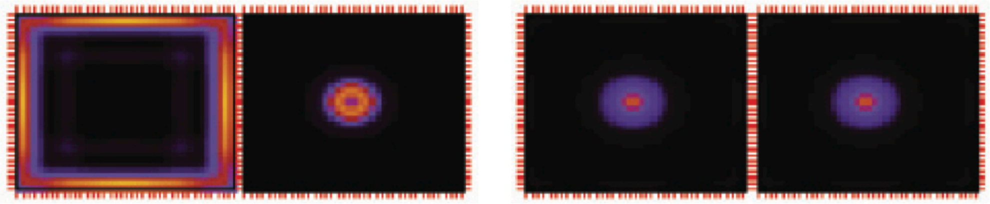
→ Effective spinless *p*+i*p*'-wave superconductivity

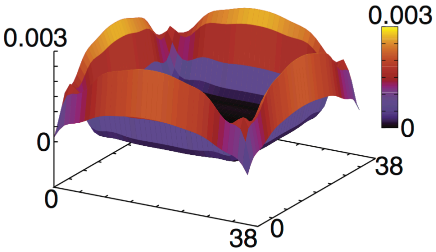
→ Majorana fermions at edges and vortices

Majorana Fermion in a Vortex Core

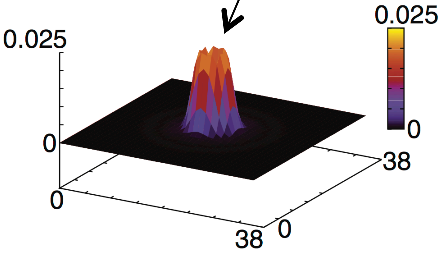


Probability density of the lowest energy eigenstates:





Majorana on the sample edge



Majorana in the vortex core

2 Majorana = 1 electron

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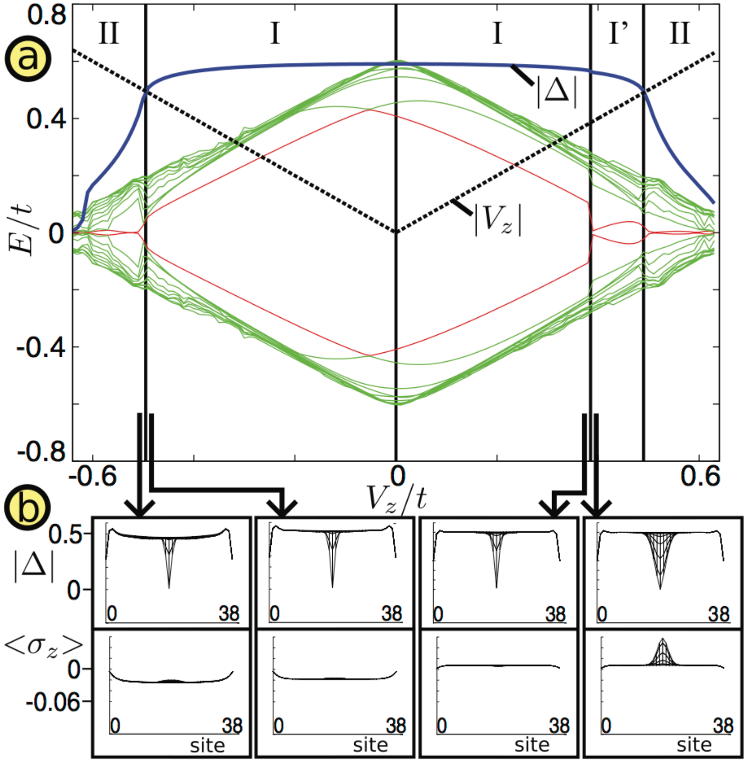
Self-Consistent Solution of Vortex Core

I: Toplogically trivial region, $\Delta > V_z$
II: Non-trivial region (Majorana), $\Delta < V_z$



Self-consistent solution gives:

- Accurate value of Δ
- Additional region I':
  - Local phase transition in the vortex core
  - Two low-energy solutions (Majorana) inside vortex core → 1 electron state

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Summary

Self-consistent lattice tight-binding Bogoliubov-de Gennes solution:

- Microscopically accurate superconducting state for inhomogeneous systems
  - SNS graphene Josephson junctions
    - Proximity effect (leakage of pairing into N)
    - Inverse proximity effect (loss of pairing in S)
    - Current depairing (loss of pairing in S due to supercurrent)
  - Vortex in a spin-orbit coupled semiconductor-superconductor hybrid structure
    - Local phase transition in vortex core before the formation of the Majorana fermion
- Easy to incorporate additional pair correlations
  - Intrinsic chiral *d+id'*-wave-wave pairing in graphene proximity-enhanced by external superconductors