RKKY Interactions on Dirac Surfaces

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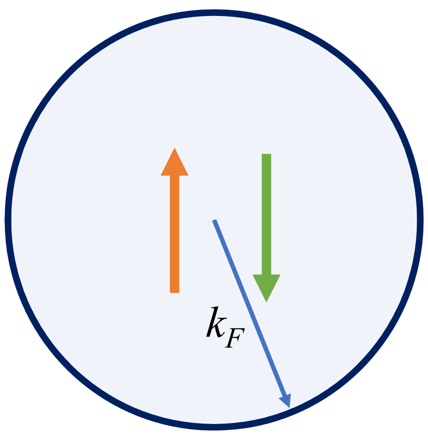
Outline

1. Introduction: Spin exchange via conduction electrons (the RKKY phenomenon)
2. The Paradigm for Dirac electrons: RKKY interactions in graphene
3. RKKY in graphene in (pseudo-)magnetic fields
4. RKKY on topological crystalline insulator surfaces
5. Spin stiffness, domain walls, and gap-breaching states
6. Summary

Ruderman-Kittel-Kasuya-Yosida (RKKY) Interactions in Metals

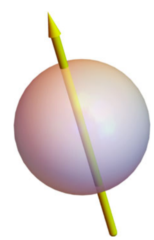
- Indirect exchange mechanism between local magnetic moments (impurities, nuclear moments)

Ingredients: Start with Fermi gas of spinful electrons…



$\vec{s}(\boldsymbol{r})$

..add magnetic impurities...
(dilute; assumed classical)



$\overrightarrow{S_1}$

…and couple them via *sd* Hamiltonian.

$$H_{sd}(\vec{S}_1) = J\vec{S}_1 \cdot \hat{\vec{s}}\,\delta(\vec{r}-\vec{r}_1)$$

Spin susceptibility

- $\overrightarrow{S_1}$ enters as a local magnetic field at $\vec{r}_1$, inducing spin response in the Fermi gas

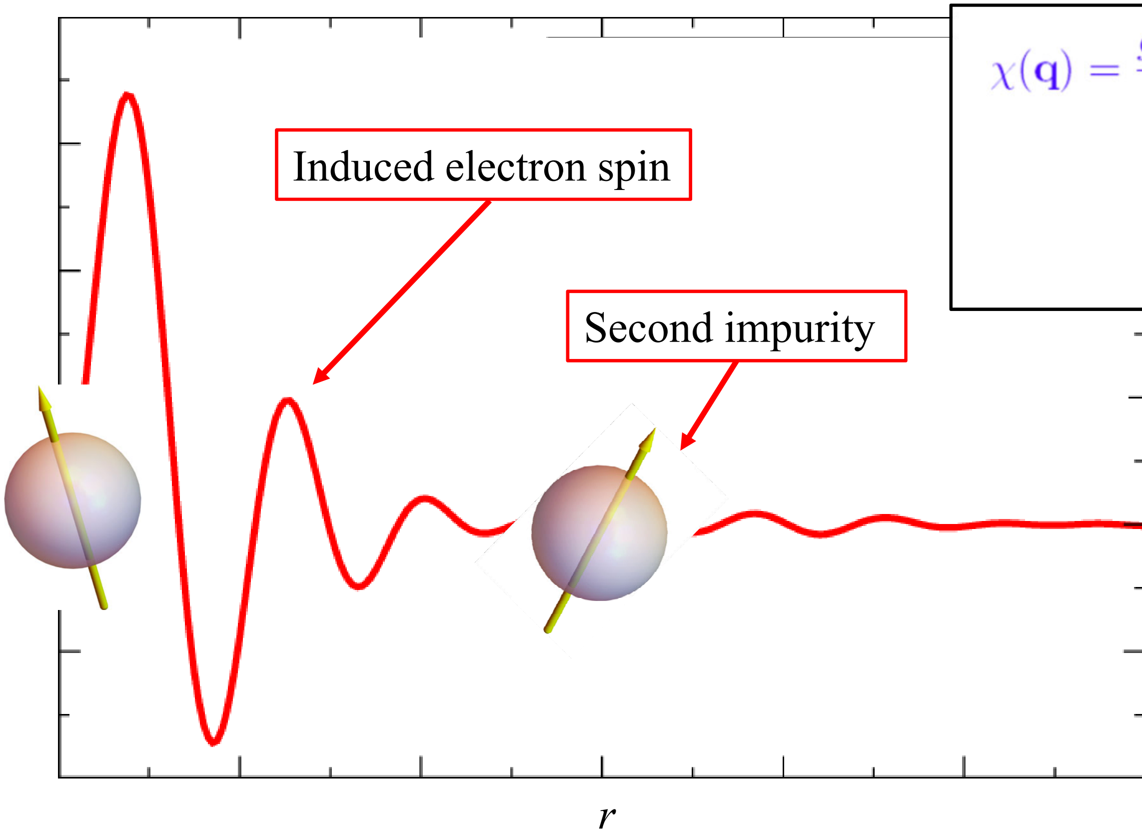
$$\mathcal{H}_{sd} = g\mu_B \sum_i \mathbf{H}_{\text{eff}} \cdot \mathbf{s}_i \qquad \mathbf{H}_{\text{eff}} = -\frac{J}{g\mu_B}\mathbf{S}_1\delta(\mathbf{r}) \qquad \mathbf{M}(\mathbf{r}) = \int d^3r'\,\chi(\mathbf{r}-\mathbf{r}')\mathbf{H}_{\text{eff}}(\mathbf{r}') = -\frac{J}{g\mu_B}\chi(\mathbf{r})S_\alpha$$

Effective spin-spin interaction

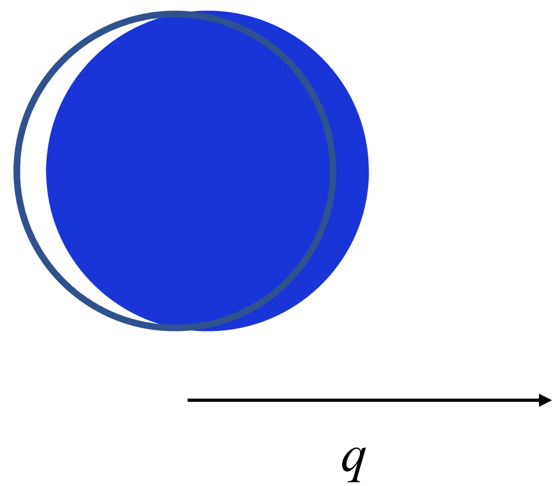
Why are there oscillations?

$$\chi(\mathbf{q}) = \frac{g^2\mu_B^2}{\mathcal{V}} \sum_{\mathbf{k}} \frac{f_{\mathbf{k}} - f_{\mathbf{k+q}}}{\epsilon_{\mathbf{k+q}} - \epsilon_{\mathbf{k}}} = \frac{3g^2\mu_B^2(N/\mathcal{V})}{8\epsilon_F} F\left(\frac{q}{2k_F}\right)$$

$$F(x) = \frac{1}{2} + \frac{1-x^2}{4x} \ln\left|\frac{1+x}{1-x}\right| .$$



$$\mathcal{H}_{\mathrm{RKKY}} = -\frac{J^2}{g^2\mu_B^2}\chi(\mathbf{r})\,\mathbf{S}_\alpha \cdot \mathbf{S}_\beta$$



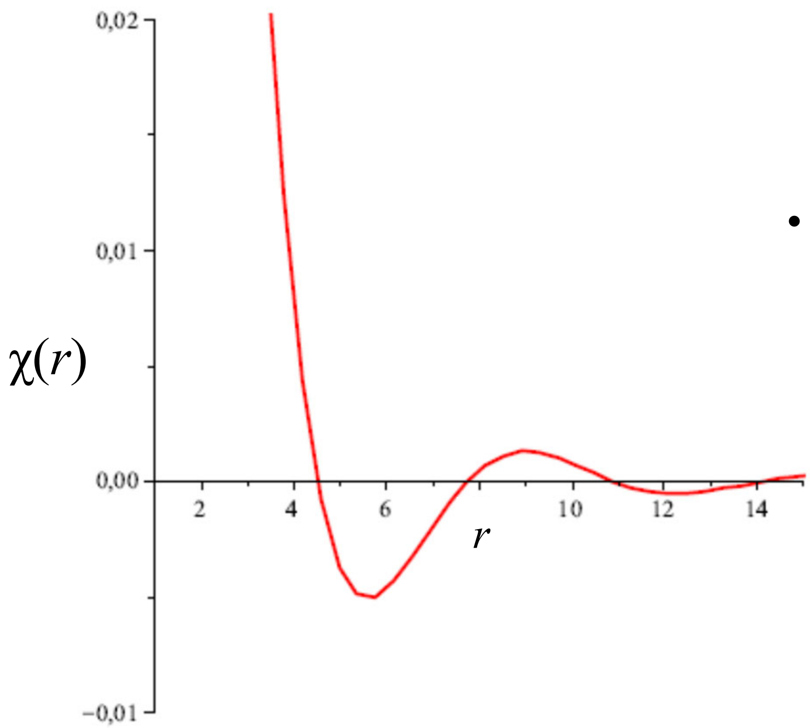
“Kohn anamoly” at $q = 2k_F$

Another (completely equivalent) approach: second order perturbation theory

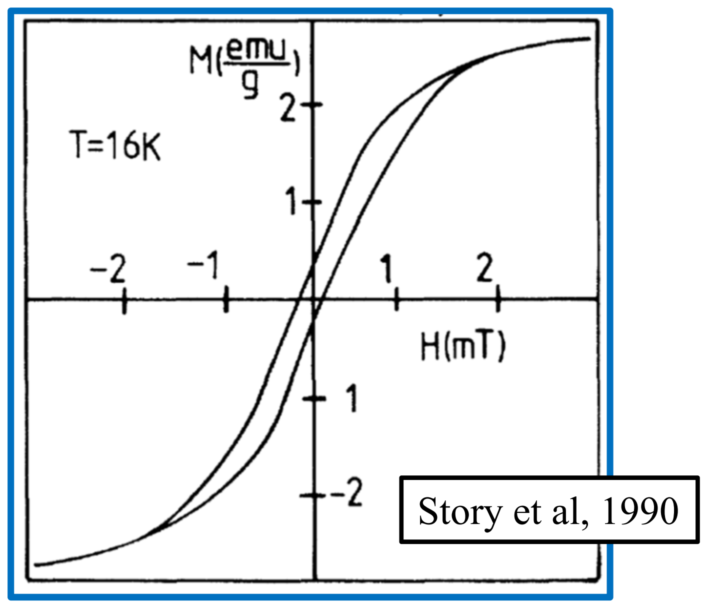
$$\Delta E^{spin\ coupling} = \sum_{\alpha\ occ} \sum_{\beta\ unocc} \frac{\left\langle \alpha \middle| H_{sd}\left(\vec{S}_1\right) \middle| \beta \right\rangle \left\langle \beta \middle| H_{sd}\left(\vec{S}_2\right) \middle| \alpha \right\rangle + c.c.}{E_\alpha^{(0)} - E_\beta^{(0)}}$$

- RKKY interaction is the (spin-dependent part of) the change in energy of the electron gas due to its coupling to the spin impurities

$$\mathcal{H}_{\mathrm{RKKY}} = -\frac{J^2}{g^2\mu_B^2}\,\chi(\mathbf{r})\,\mathbf{S}_\alpha \cdot \mathbf{S}_\beta$$

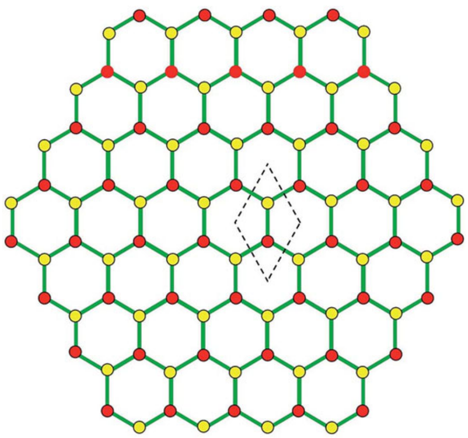


- Effective coupling oscillates; positive at short distance → ferromagnetism when impurities are sufficiently close; spin glass when dilute
- Magnetic moments usually dopants as well ⟹ electron and dopant density tied together (semiconductors)
- Basic mechanism for many dilute magnetic semiconductors (spintronic systems)

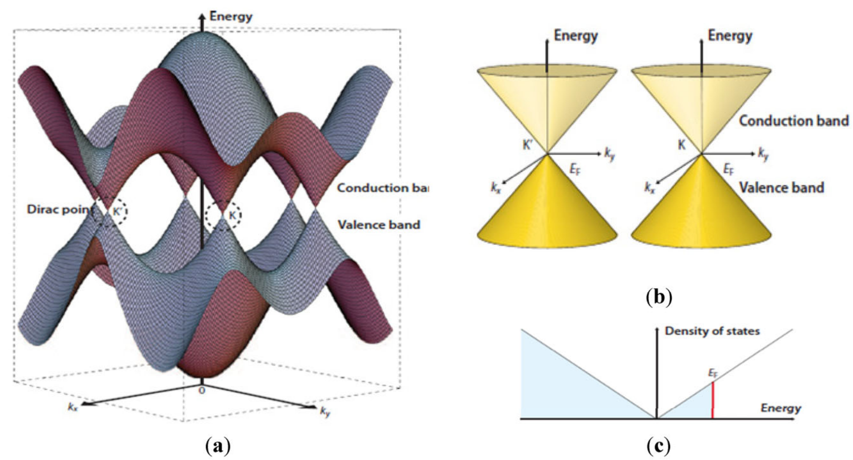


RKKY Interactions in Graphene: A Paradigm for Dirac Surfaces

What is different about graphene?



1. Two sublattices: Electron wavefunctions are *spinors*
2. "Light-cone" spectrum + Dirac points



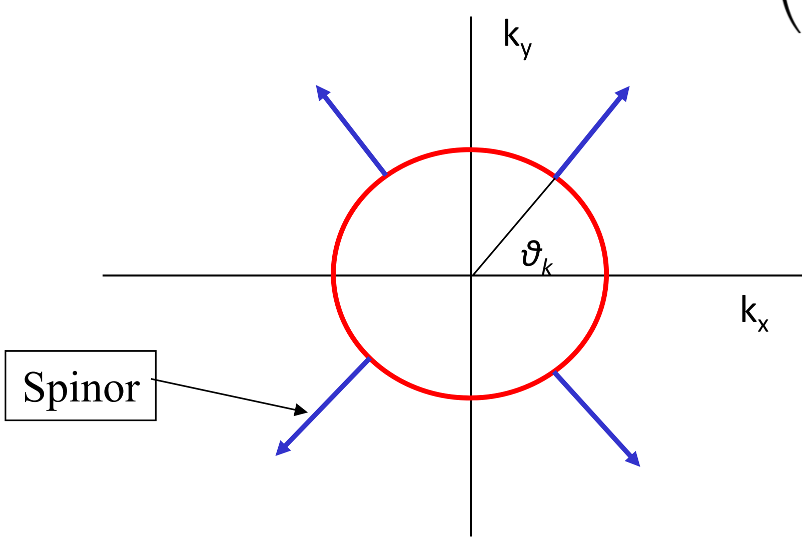
- Fermi energy is adjustable with a gate
- Fermi surface can shrink to a point but cannot vanish

3. Electron wavefunctions are *helical*

Near: **k=K** **k=K'**

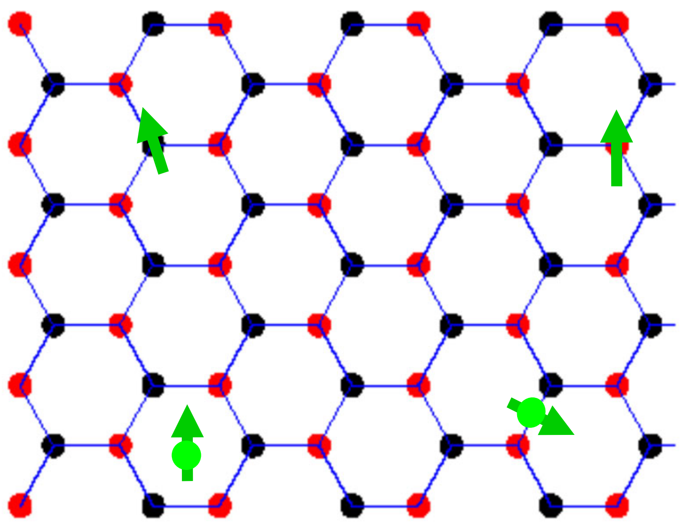
$$H_0 = -a_0 \frac{\sqrt{3}}{2} t \begin{pmatrix} 0 & k_x - ik_y \\ k_x + ik_y & 0 \end{pmatrix} \qquad H_0 = -a_0 \frac{\sqrt{3}}{2} t \begin{pmatrix} 0 & -k_x - ik_y \\ -k_x + ik_y & 0 \end{pmatrix}$$

$$\psi_{(\tau=+,\mathbf{k})}(i) = e^{i\mathbf{K}\cdot\mathbf{R}_i} e^{i\mathbf{k}\cdot\mathbf{R}_i} \begin{pmatrix} e^{-i\frac{\theta_{\mathbf{k}}}{2}} \\ \pm e^{i\frac{\theta_{\mathbf{k}}}{2}} \end{pmatrix} \qquad \psi_{(\tau=-,\mathbf{k})}(i) = e^{i\mathbf{K}'\cdot\mathbf{R}_i} e^{i\mathbf{k}\cdot\mathbf{R}_i} \begin{pmatrix} e^{i\frac{\theta_{\mathbf{k}}}{2}} \\ \mp e^{-i\frac{\theta_{\mathbf{k}}}{2}} \end{pmatrix}$$



- Orthogonality of spinors at **k** and –**k** tends to suppress backscattering: graphene is an excellent conductor

4. Different possible locations for spin impurities:
sd exchange coupling to multiple sites possible



$$\chi^0_{\mu,\nu}(q) = -g_v \frac{1}{N} \sum_{s,s',\mathbf{k}} \frac{f(\epsilon_{\mathbf{k},s}) - f(\epsilon_{\mathbf{k+q},s'})}{\epsilon_{\mathbf{k},s} - \epsilon_{\mathbf{k+q},s'}} F^{\mu,\nu}_{s,s'}(\mathbf{k},\mathbf{q})$$

Valley degeneracy (2)

Sublattice

Electron, hole band

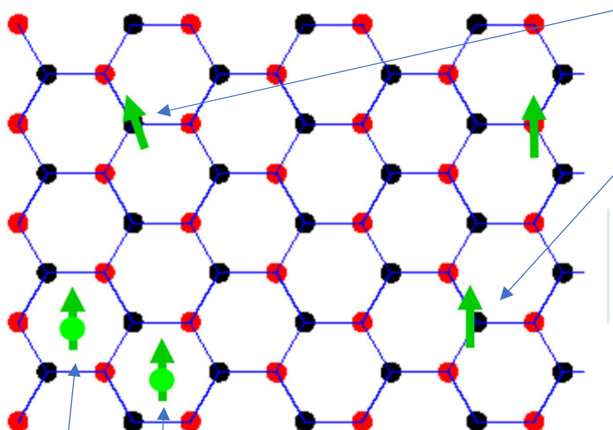
$$F^{AA}_{ss'}(\vec{k},\vec{k}+\vec{q}) = F^{BB}_{ss'}(\vec{k},\vec{k}+\vec{q}) = \frac{1}{4}(0,s')\begin{pmatrix}0\\ s\end{pmatrix}(0,s')\begin{pmatrix}0\\ s\end{pmatrix} = \frac{1}{4}$$

$$F^{AB}_{ss'}(\vec{k},\vec{k}+\vec{q}) = (e^{i\theta_{\vec{k}}},0)\begin{pmatrix}e^{-i\theta_{\vec{k}+\vec{q}}}\\ 0\end{pmatrix}(0,s)\begin{pmatrix}0\\ s'\end{pmatrix} = \frac{1}{4}ss'e^{i\theta}$$

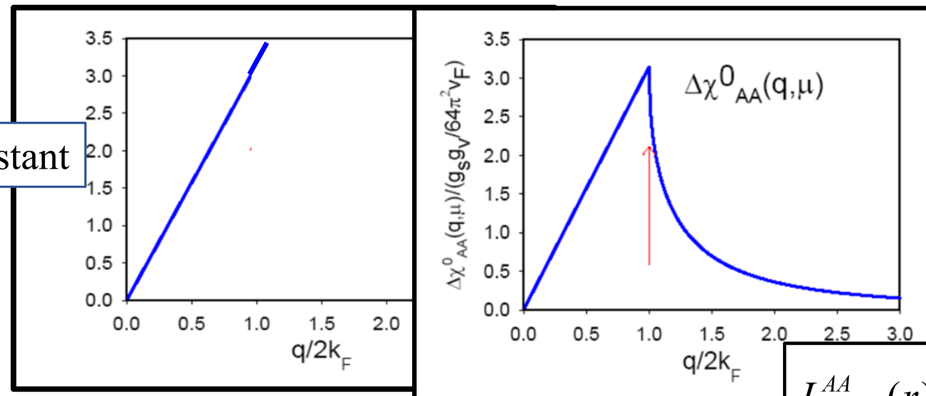
$\Longrightarrow$ RKKY coupling depends on details of impurity locations in the lattice

So AA response is *different* than AB response

$$\chi^0_{AA}(q,\mu) = \chi^0_{AA}(q,\mu=0) + \Delta\chi^0_{AA}(q,\mu)$$

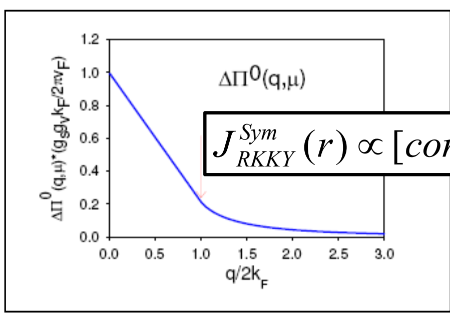


-χ_0- constant

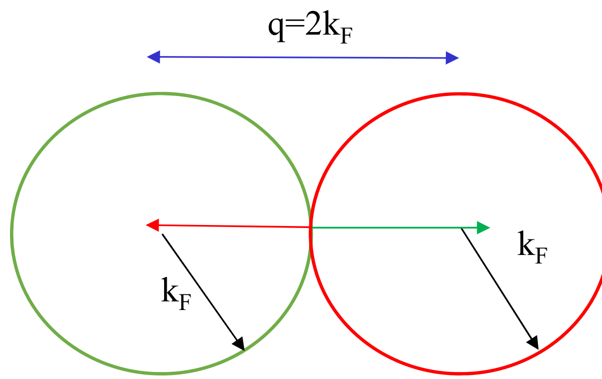


$$J^{AA}_{RKKY}(r) \propto \frac{\sin(2k_F r)}{r^2}$$

$$\Pi^0 = \chi^0_{AA} + \chi^0_{AB} = \Pi^0(q,\mu=0) + \Delta\Pi^0(q,\mu=0)$$



$$J^{Sym}_{RKKY}(r) \propto [const + \cos(2k_F r)]/r^3$$



Absence of backscattering lifts discontinuity!

$$\chi^0_{AB}(q,\mu) = -\chi^0_{AA}(q,\mu) + \text{Smooth function of q}$$

$$J^{\mu\nu}_{RKKY}(\vec{r}) \propto \int d^2\vec{q}\, e^{i\vec{q}\vec{r}} \chi^0_{\nu\mu}(q,\mu)$$

Discontinuity introduces long-range power-law tail
in effective coupling constant.

$$J^{AA}_{RKKY}(r) \propto \frac{\sin(2k_F r)}{r^2}$$

$$J^{AB}_{RKKY}(r) \propto -\frac{\sin(2k_F r)}{r^2}$$

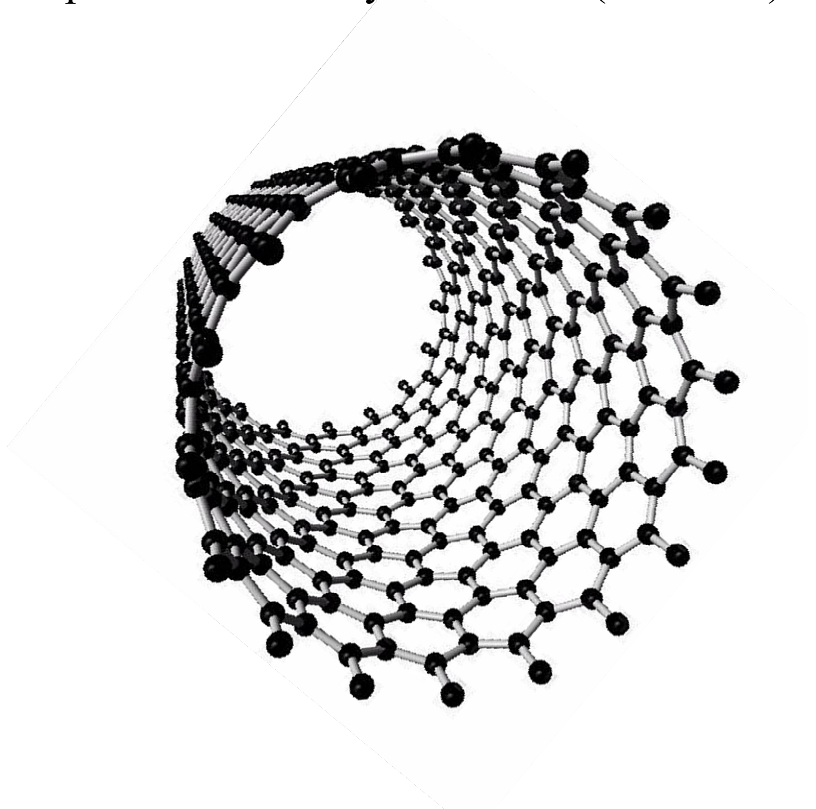
Strong local antiferromagnetic correlations from **single particle physics.**

- Undoped case ($k_F \to 0$)

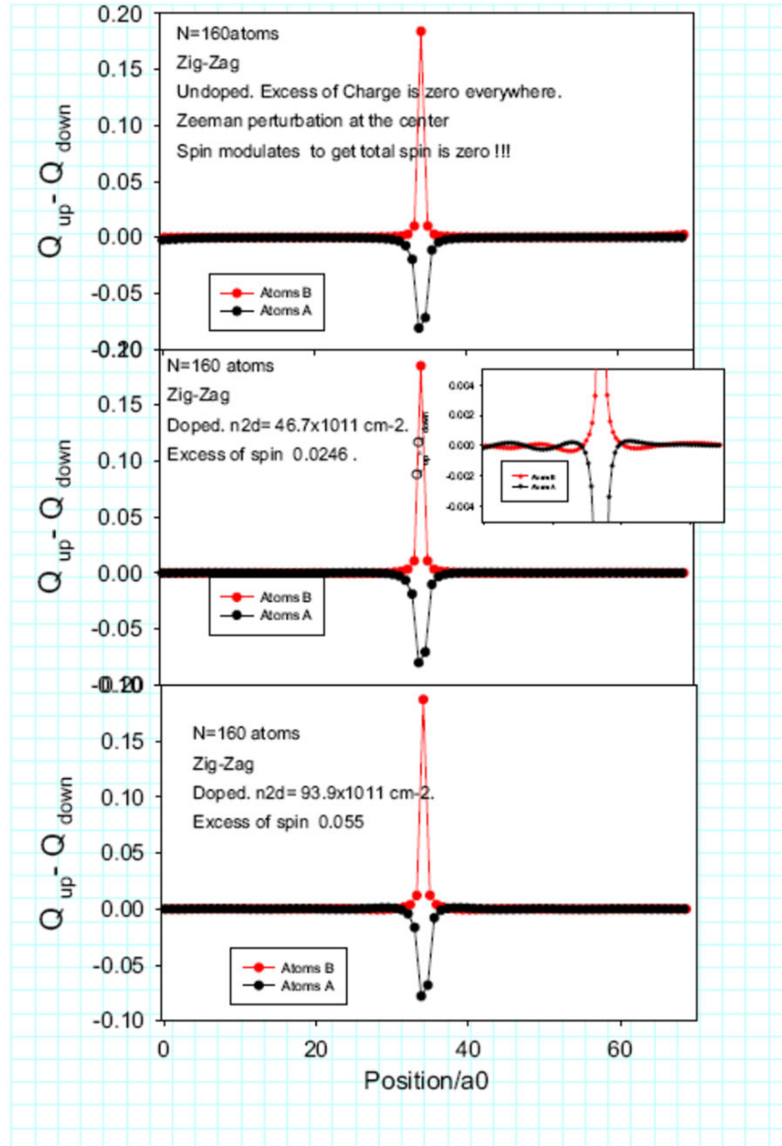
$$J^{AA}_{RKKY}(r) \propto \frac{1}{r^3} \qquad J^{AB}_{RKKY}(r) \propto -\frac{1}{r^3}$$

(Equal and opposite in this case.)

Numerical check: graphene sheet with periodic boundary conditions (nanotube)



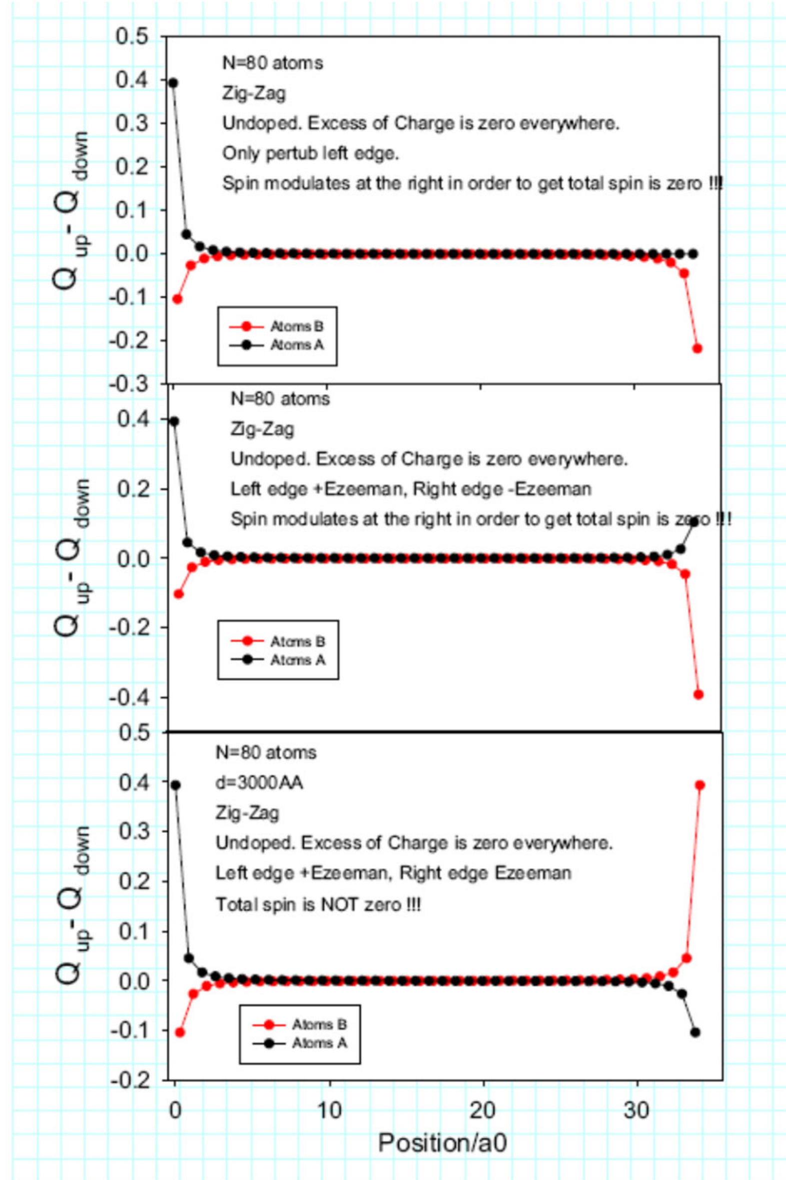
Introduce local perturbations and obtain charge and spin density profile.



- Local Zeeman field induces **no** net spin for undoped ribbon
- Spin induced in ribbon proportional to doping

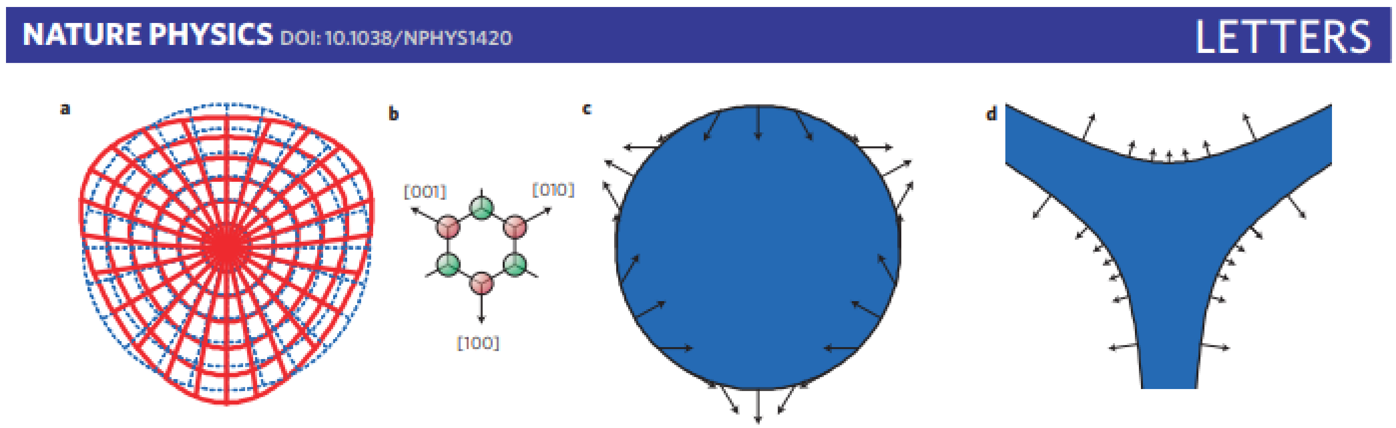
• Interesting effect for undoped zigzag ribbons:

Zeeman field applied at only one edge induces a spin response at the other!



Can we induce **ferromagnetism** in graphene? Need to break symmetry between sublattices.

One way: use strain!



F. Guinea et al, Nature Physics (2009)

- Strain creates a pseudo-magnetic field: ~40T @ ~ 10% strain
- Opposite orientations for opposite valley
- Effective field creates **Landau levels**

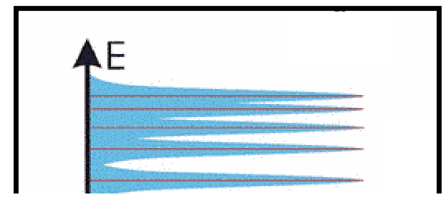
Quantum States in a (Real) Magnetic Field

$$\Psi(+,n) = e^{ik_x x}\begin{pmatrix} \pm\phi_{n-1}(y-k_x\ell^2) \\ \phi_n(y-k_x\ell^2) \end{pmatrix} \qquad \Psi(-,n) = e^{ik_x x}\begin{pmatrix} \pm\phi_{n}(y-k_x\ell^2) \\ \phi_{n-1}(y-k_x\ell^2) \end{pmatrix}$$

$$\Psi(+,0) = e^{ik_x x}\begin{pmatrix} 0 \\ \phi_0 \end{pmatrix} \qquad \Psi(-,0) = e^{ik_x x}\begin{pmatrix} \phi_0 \\ 0 \end{pmatrix}$$

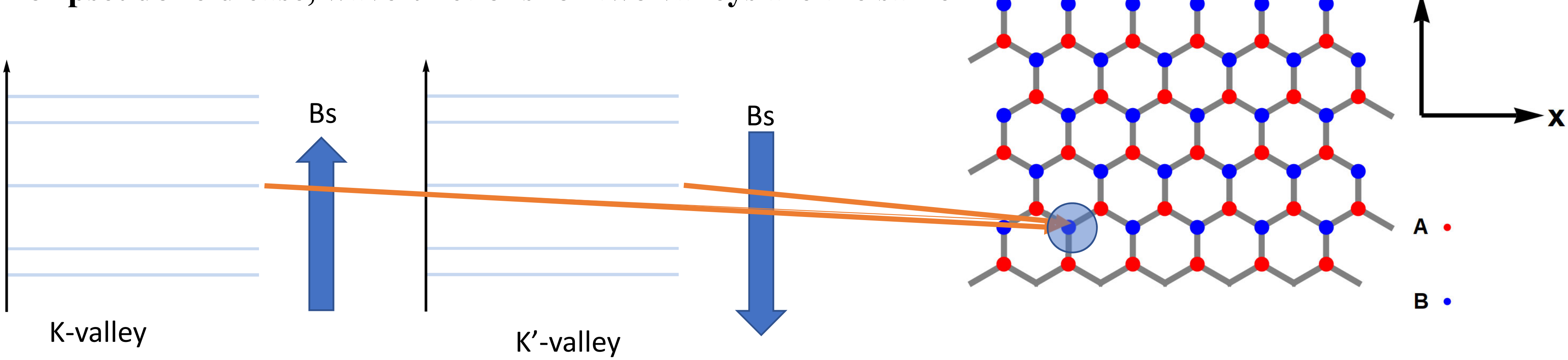
<u>Energies:</u>

$$\varepsilon(\tau,n) = \pm\sqrt{3\,|n|}\;\frac{a}{\ell}t$$



- With valley and spin indices, each Landau level hosts 4×(# flux quanta) states
- Valley degeneracy restores symmetry between sublattices

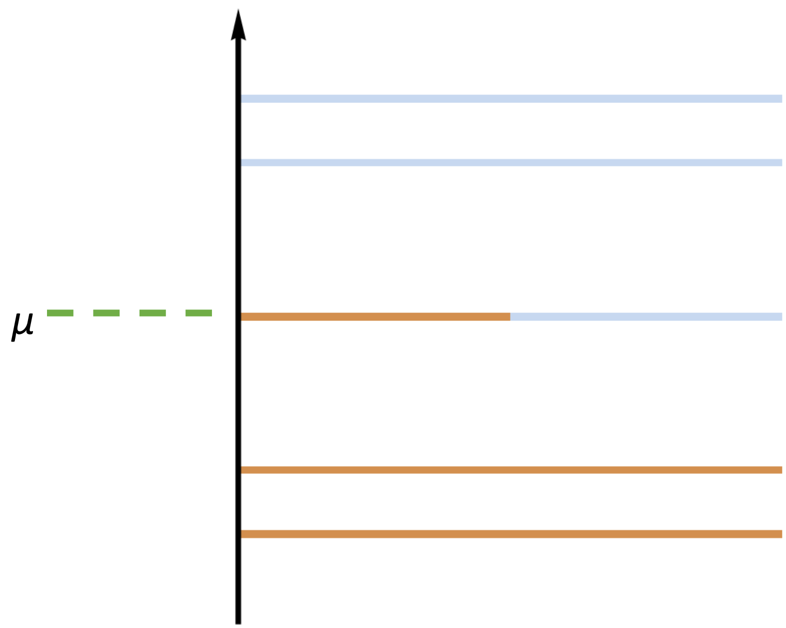
For pseudofield case, wavefunctions for two valleys are the same



Problem: Breakdown of second order perturbations theory

Recall $$\Delta E^{spin\ coupling} = \sum_{\alpha\ occ} \sum_{\beta\ unocc} \frac{\langle \alpha | H_{sd}(\vec{S}_1) | \beta \rangle \langle \beta | H_{sd}(\vec{S}_2) | \alpha \rangle + c.c.}{E_\alpha^{(0)} - E_\beta^{(0)}}$$

Landau level degeneracy $\Longrightarrow$ divergences (2^{nd} order perturbation theory)



Strategy: Compute energy of many-body electron state for two impurities with fixed spin orientations

- Find energies of states in n=0 Landau level e*xactly*
- Compute effect of impurities on filled $n \neq 0$ levels in 2^{nd} order perturbation theory

… a problem when n=0 level partially occupied

Hilbert Space of states in LLL: M angular momentum states

$n=0$ wave functions:

$$z = \frac{x-iy}{l_B} \quad \phi_{n=0,m}(z) \propto z^m e^{-\frac{|z|^2}{4}} \quad m = 0, 1, 2, .., M-1$$ (on one sublattice)

Impurities @ z_1, z_2. States of the form

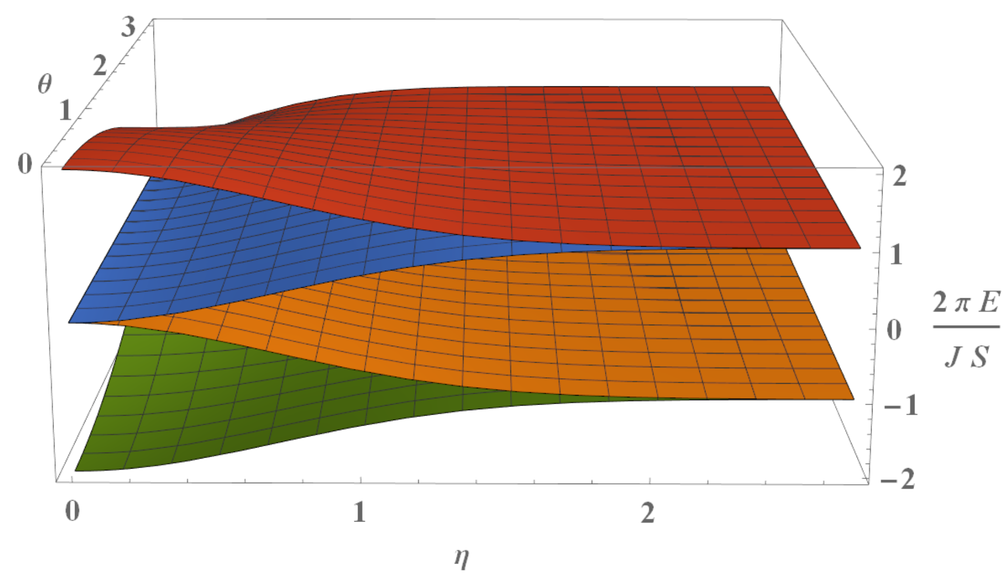
$$\phi \sim z^{\tilde{m}}(z-z_1)(z-z_2)e^{-\frac{|z|^2}{4}}$$

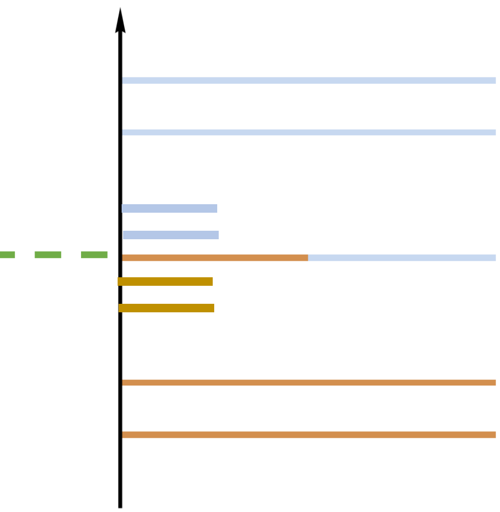
are *unaffected* by the impurities. There are M-2 of these.

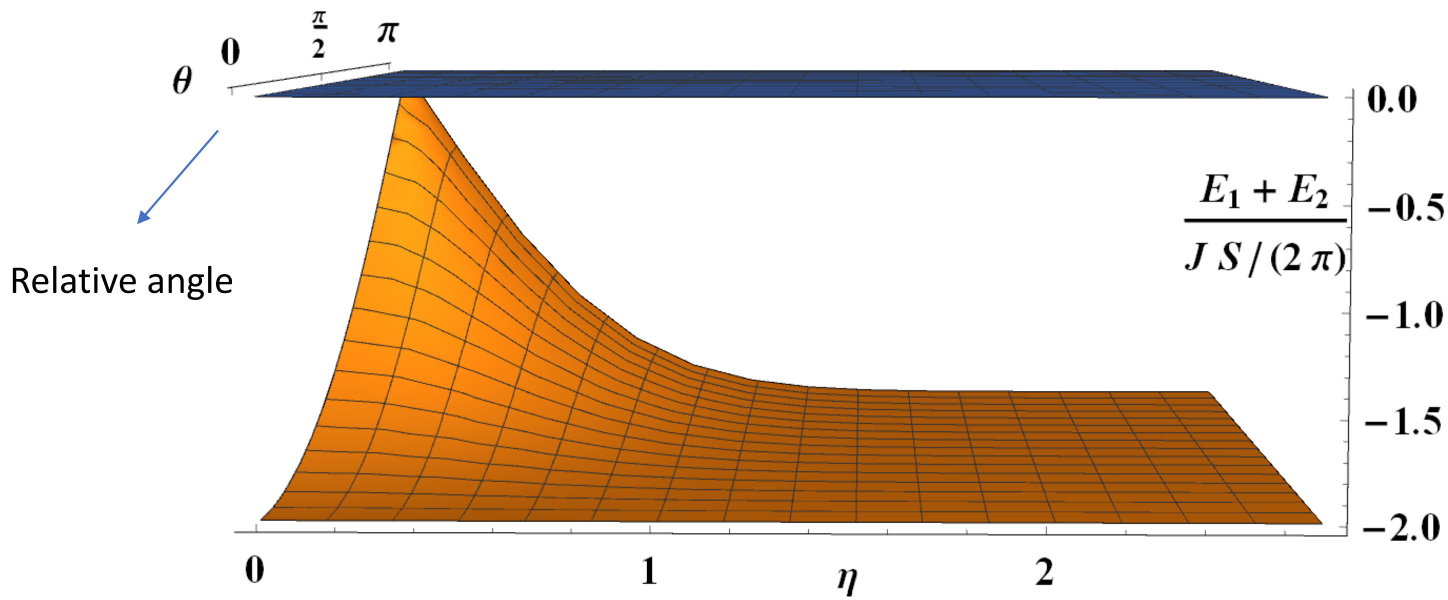
⇒ Only 2 states "touch" the impurities

Including spin, only 4 states affected by impurities

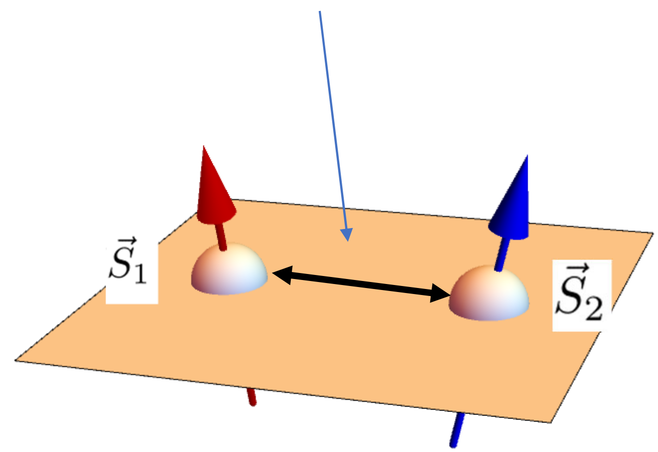
⟹ Must solve a 4×4 matrix equation







- Linear in J
- Strong ferromagnetic RKKY coupling up to distance ℓ, falls off as a Gaussian
- Non-analytic in $\vec{S}_1 \cdot \vec{S}_2$
- Acts on spins on only one of the two sublattices



Remaining Landau levels handled by perturbation theory:

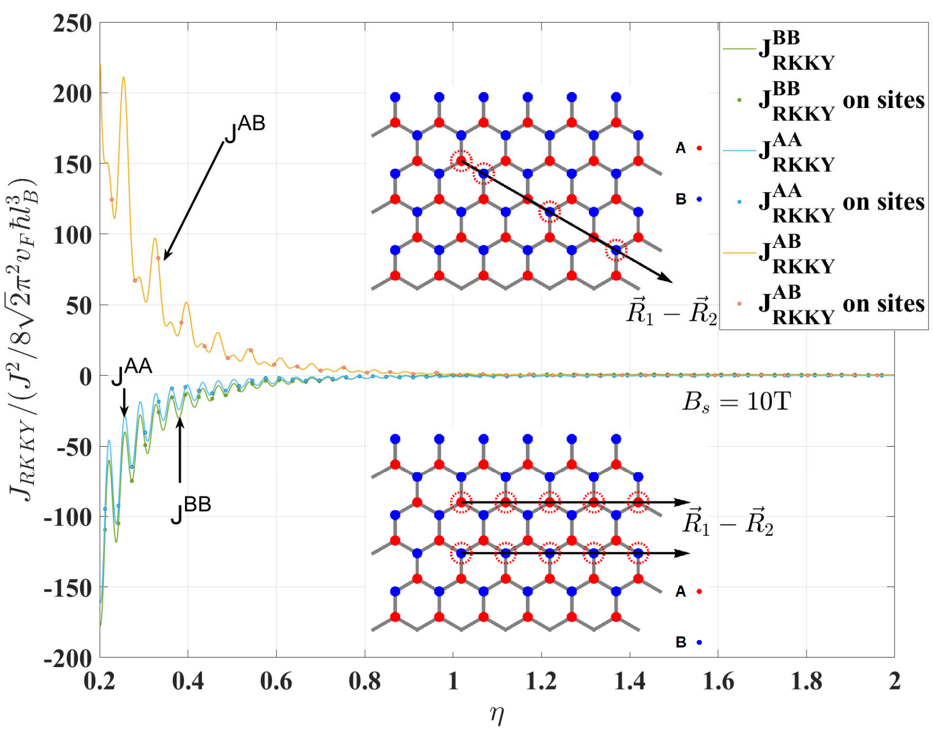
Gives another contribution to RKKY

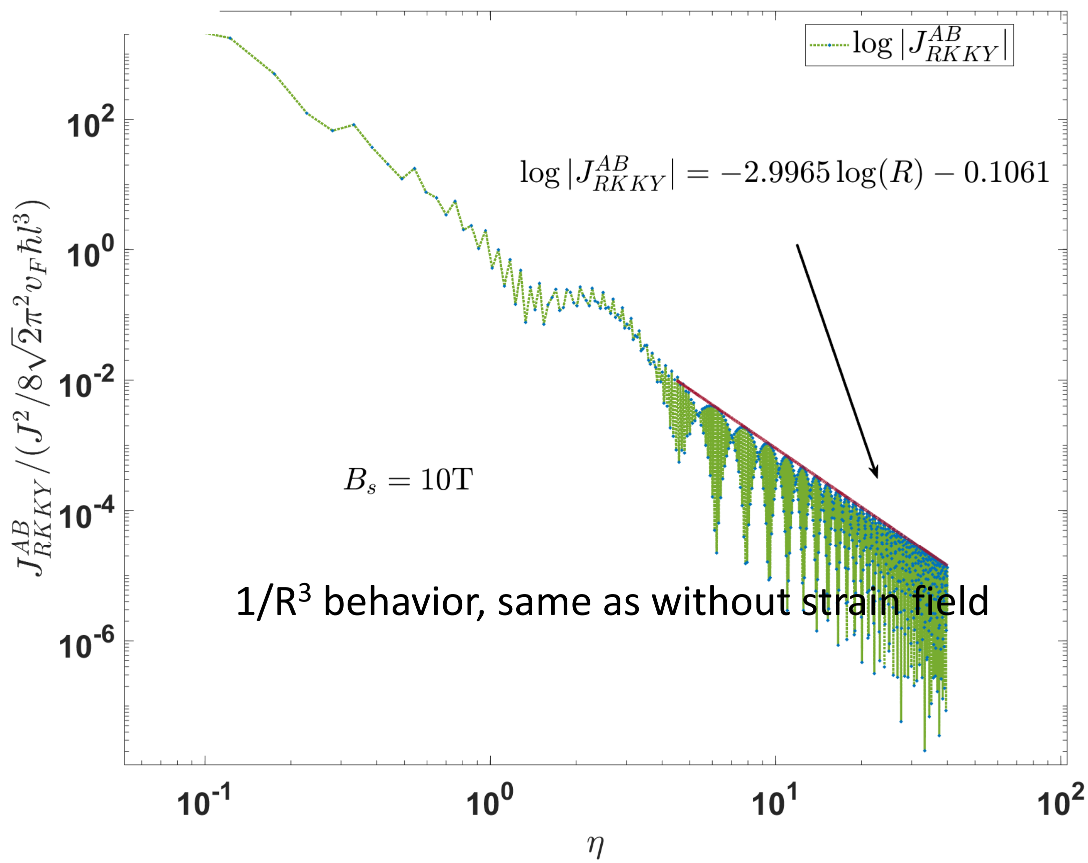
$$E^{(2)}_{\mathrm{RKKY}} = J_{\mathrm{RKKY}} \vec{S}_1 \cdot \vec{S}_2$$

Numerical Sum up to cut off

$$\Delta E^{(2)} = \sum_{\substack{n<0,\\ n'\neq n}} \sum_{k,k'} \sum_{s,s'} \sum_{\tau,\tau'} \frac{|V_{n'k's'\tau',nks\tau}|^2}{E^{(0)}_n - E^{(0)}_{n'}}$$

Landau level cut off gives oscillations





Mean-field theory for RKKY interactions in strained graphene

Pairwise RKKY interaction =

LLL nonperturbative part + 2nd order perturbative part

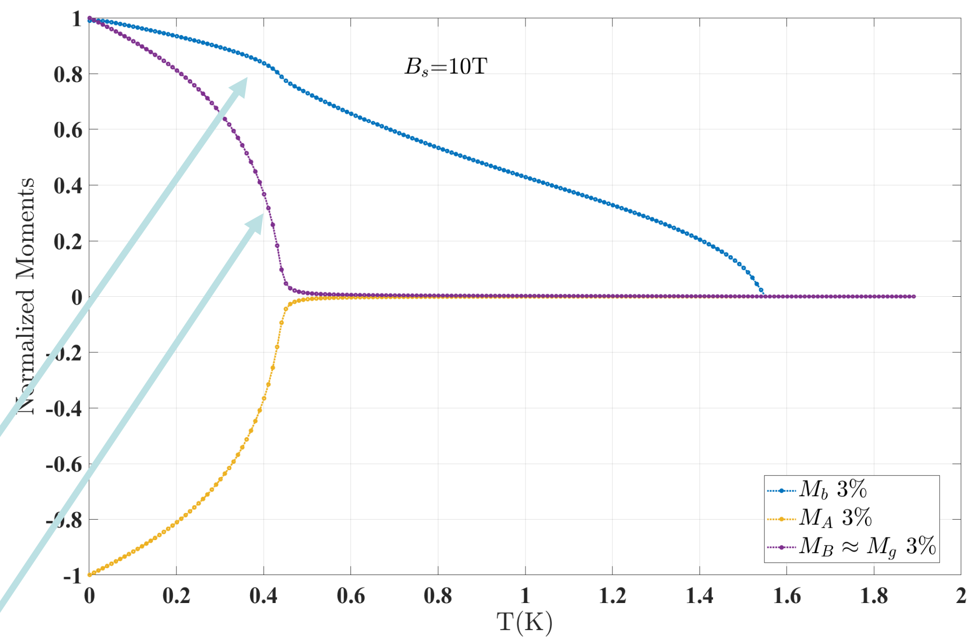
Problem: For typical sample, impurity density > 1%,

if B< 1000T, # states in LLL < # impurities

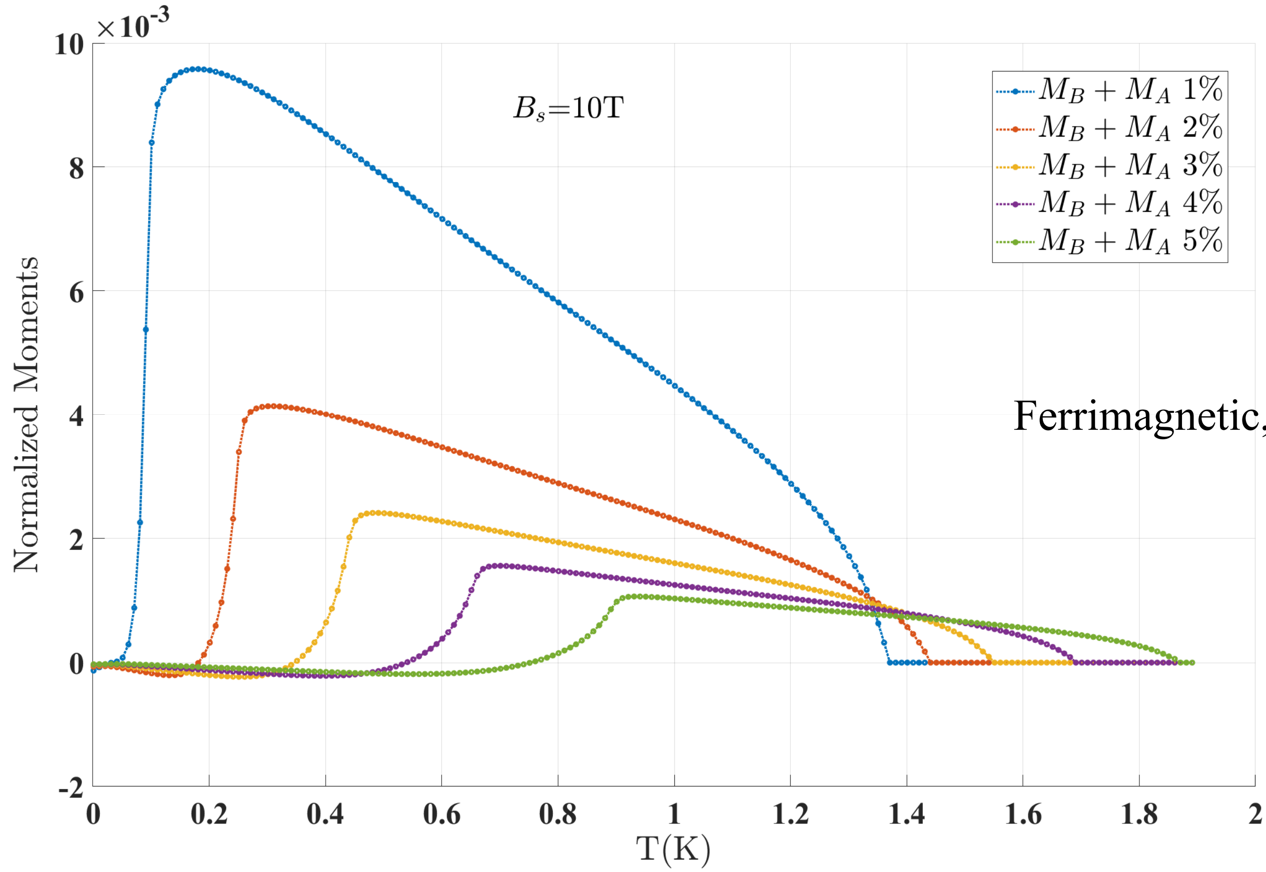
Tiny portion of impurities have electrons in LLL bound to them.

f_b fraction of B site impurities binding LLL electrons

$1 - f_b$ fraction of B site impurities interacting only by the perturbative part (not utilizing LLL)



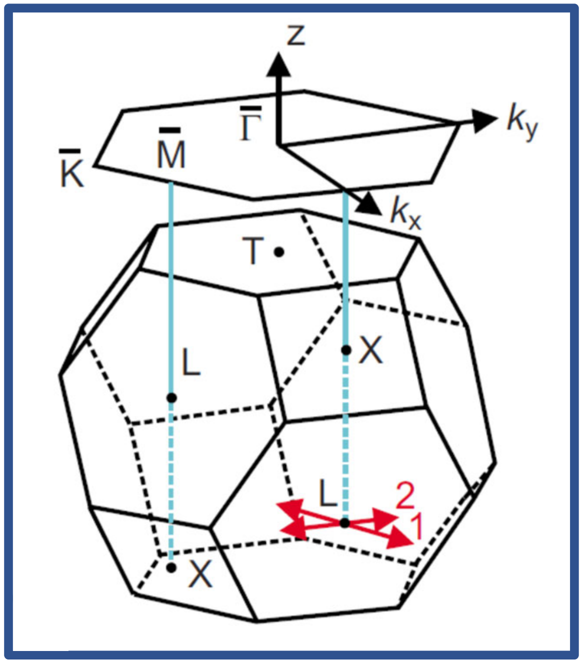
Net Moment



Ferrimagnetic, but small net moment.

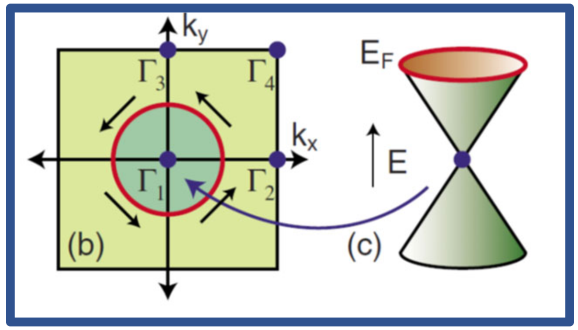
Dirac Surfaces on Topological Insulators

I. <u>Surface states protected by time-reversal symmetry</u>



From Hassan and Kane, RMP (2010)

- Paradigm: $Bi_{1-x}Sb_x$
- Projection of time-reversal invariant points onto surface guaranteed to be doubly degenerate ("Kramer's doublet")
- Away from these points states repel ⇒ surface Dirac cone



- Gapless nature of surface states protected by *time-reversal symmetry*

- Difference from graphene: Dirac spinors directly contain spin content
- Coupling of magnetic impurities to Dirac electrons works differently than graphene

Mean-field approach: Treat impurity spins as a continuous effective field (anticipates spin ordering)

Recall for conventional electron gas: $H = H_0 + H_{sd}$ with $\mathcal{H}_{sd} = g\mu_B \sum_i \mathbf{H}_{\text{eff}} \cdot \mathbf{s}_i$ $\quad \mathbf{H}_{\text{eff}} = -\frac{J}{g\mu_B}\mathbf{S}_1 \delta(\mathbf{r})$

Single impurity

- Ignore spatial localization of impurities

Graphene: $H = v_F \vec{k} \cdot \vec{\sigma} + \left[\frac{1}{2}(\vec{H}_{eff}^A + \vec{H}_{eff}^B) \cdot \vec{s}\right] + \left[\frac{1}{2}(\vec{H}_{eff}^A - \vec{H}_{eff}^B) \cdot \vec{s}\right] \sigma_z$

Sublattice

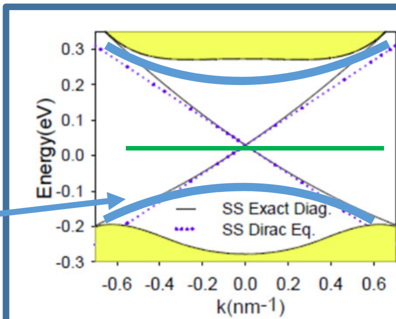
Electron spin

Antiferromagnetic alignment: $\vec{H}_{eff}^A = -\vec{H}_{eff}^B$

Topological insulator: $H = v_F \left(\vec{k} + \vec{H}_{eff}^{\parallel}\right) \cdot \vec{\sigma} + H_{eff}^z \sigma_z$

- Connection between H_{eff} and impurity magnetization $\vec{S}(\vec{r})$ can be complicated
- Magnetization shifts Dirac point *and* opens gap

Antiferromagnetic order
$\Rightarrow$ net lowering of energy

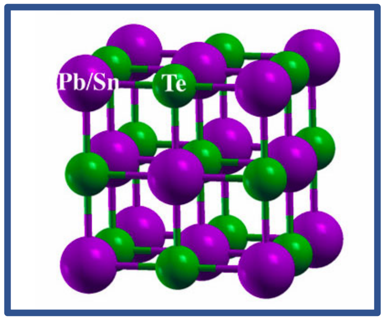


E_F

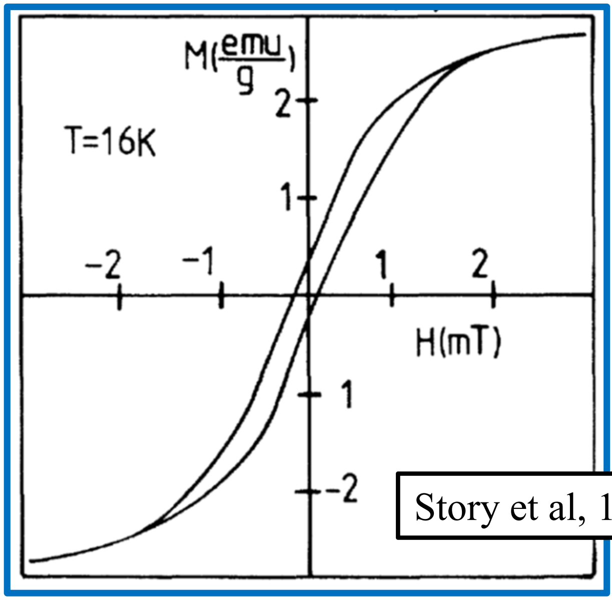
Topological crystalline insulators (TCI)

(Liang Fu, 2012)

- Paradigm: $Sn_{1-x}Pb_xTe$: Rocksalt structure
- System is topological for range of x
- Surface states protected by *mirror* symmetry



- (Sn,Pb)Te doped with sufficient magnetic impurity (Mn,Eu) concentration long-known to be ferromagnetic
- Impurities substitute for (Sn,Pb) → Uniform impurity environment
- Magnetic impurities are also hole dopants: impurities interact with holes via *s*-*d* Hamiltonian, leading to RKKY interaction:

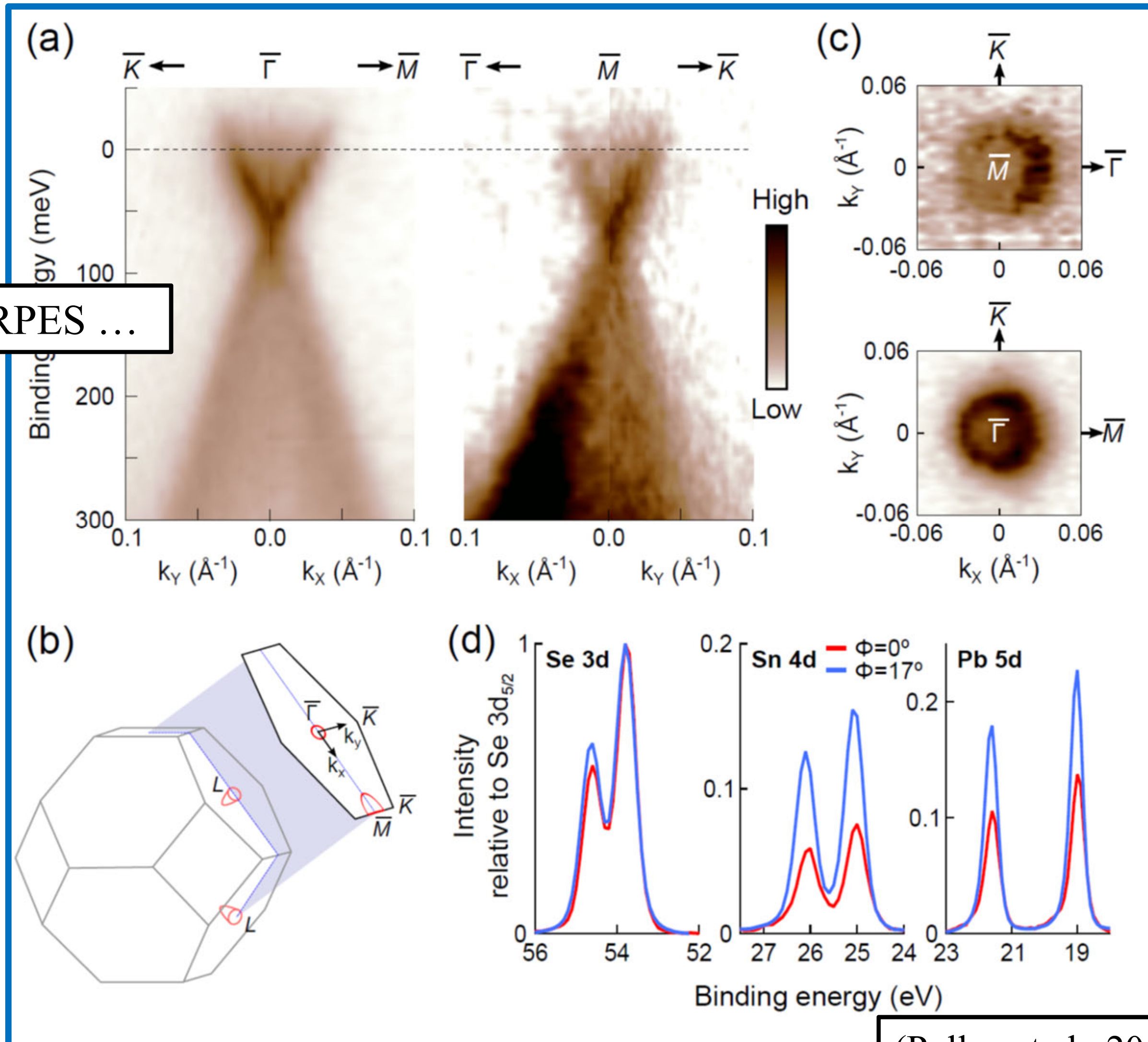


Story et al, 1990

In topological regime…

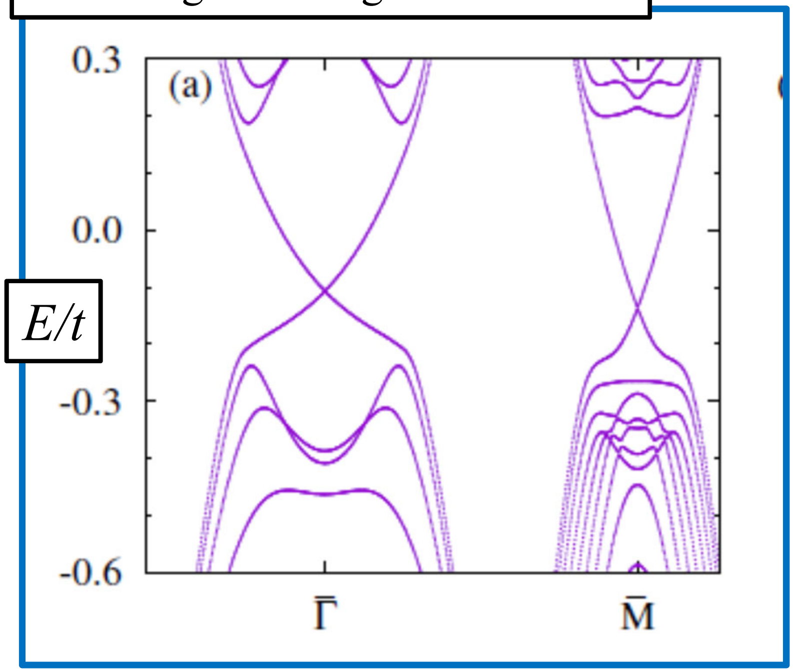
For (111) surface: Dirac points present at $\bar{\Gamma}$ and $\bar{M}$ (3 of these) points

Surface states confirmed in ARPES …



(Polley et al., 2014)

… and tight binding calculations.



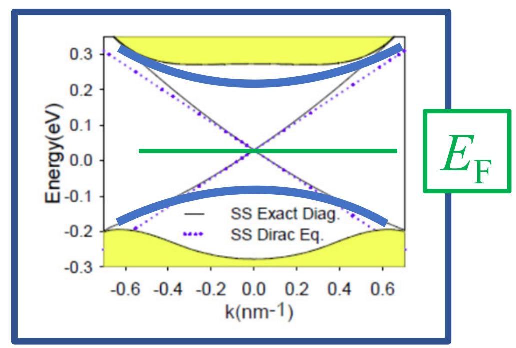
Suppose the system is compensation doped to remove mobile holes from bulk:
$\Longrightarrow$ No magnetic order in bulk. **But there can be magnetic order on the surface.**

$$H_{\bar{\Gamma}} \to B\left[(q_1 - a_1)\tilde{\sigma}_2 + (q_2 - a_2)\tilde{\sigma}_1\right] + b_3\tilde{\sigma}_3 + E_{\bar{\Gamma}}$$

$$H_{\bar{M}} \to \frac{AB}{\sqrt{A^2+\eta^2 B^2}}\left[\left(\eta^2-1\right)(q_2 - a_2)\tilde{\sigma}_1 + (q_1 - a_1)\tilde{\sigma}_2\right] + b_3\tilde{\sigma}_3 + E_{\bar{M}}$$

- $\vec{H}_{eff}^{\parallel} \sim (a_1, a_2)$ proportional to components of $\vec{S}(\vec{r})$ perpendicular to $\Gamma - L$ direction
- b_3 proportional to component of $\vec{S}(\vec{r})$ along $\Gamma - L$ direction
- $\eta = 2\sqrt{2}/3$ anisotropy factor for $\bar{M}$ surface Dirac points

- Gaps of size $2b_3$ open at Dirac points: Mirror symmetry broken by $\vec{S}$!

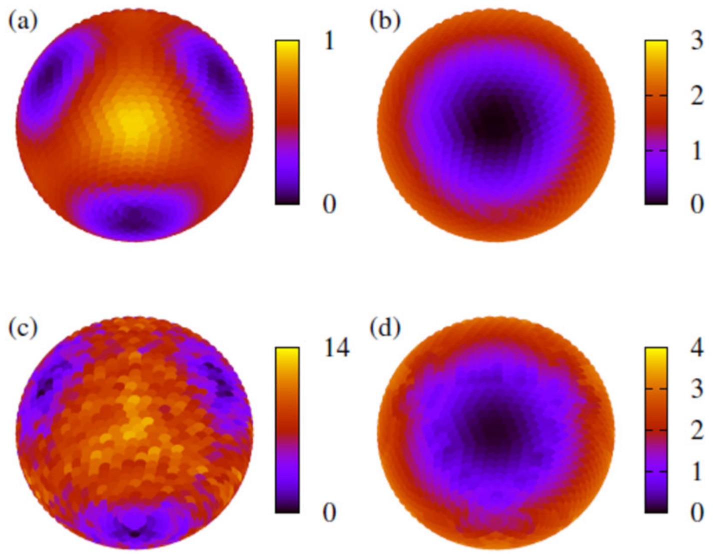


Slab geometry:total (free) energy computed for different $\vec{S}$ orientations

All $\vec{S}$ same within a layer.

Fixed N

Fixed μ



$E_F \sim E_{\bar{M}}$

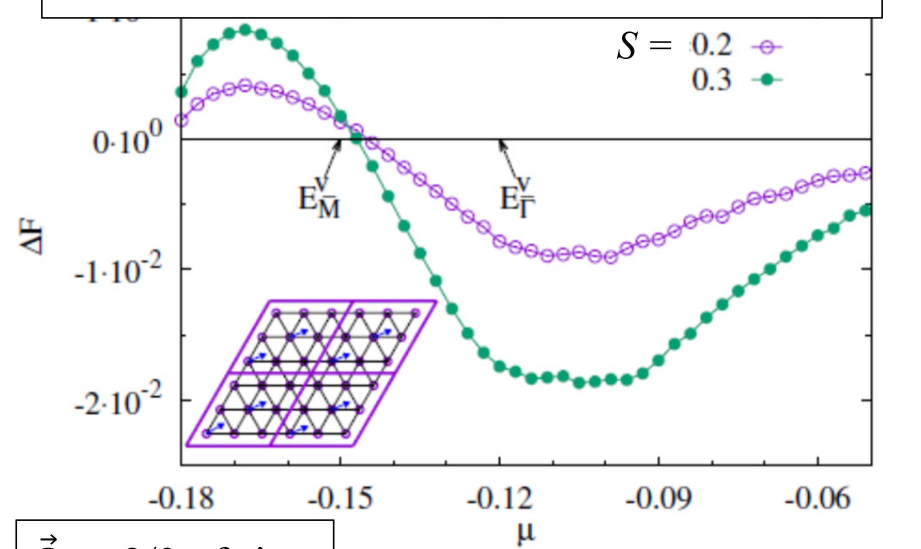
$E_F \sim E_{\bar{\Gamma}}$

6-state (KT transition)

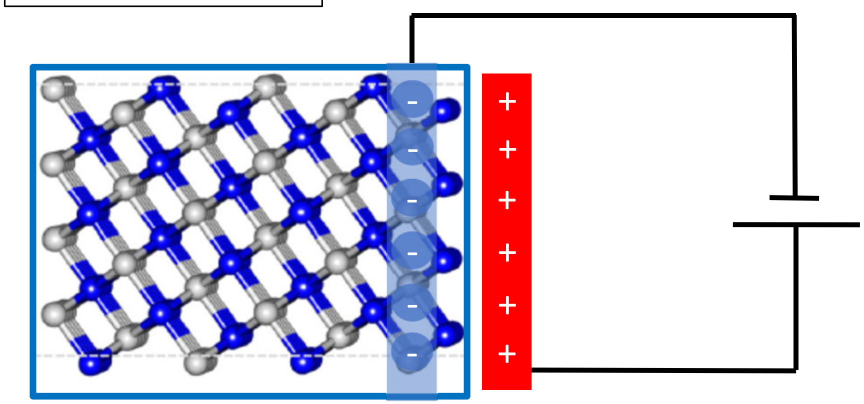
Ising

So direction of magnetization can be manipulated using an electric gate!

Free difference between $\bar{\Gamma}$ and $\bar{M}$ orientations



$\vec{S}$ on 2/9 of sites



Is uniform magnetization best?

- Spin-orbit coupled system: $$H = v_F\left\{\left(-i\frac{\partial}{\partial x} - b_y\right)\sigma_1 + \left(-i\frac{\partial}{\partial y} - b_x\right)\sigma_2 + b_z\sigma_3\right\}$$

- Consider uniform and oscillating part: $$\mathbf{b} = b_z\hat{z} + \delta\mathbf{b}\cos\mathbf{Q}\cdot\mathbf{r}.$$

- Change in energy due to this oscillation:
For chemical potential in gap, always positive

$$\Delta E(\mathbf{Q}) - \Delta E(0) = (\delta b_x \delta b_y)\begin{pmatrix} g^{xx}_{xx}Q_x^2 + g^{xx}_{yy}Q_y^2 & g^{xy}_{xy}Q_xQ_y \\ g^{xy}_{xy}Q_yQ_x & g^{yy}_{xx}Q_x^2 + g^{yy}_{yy}Q_y^2 \end{pmatrix} \times \begin{pmatrix}\delta b_x \\ \delta b_y\end{pmatrix}$$

But there is something strange: Stiffness coefficients *diverge* as $b_z \to 0$

$$g^{zz}_{xx} = g^{zz}_{yy} = 2b_z^2\int\frac{d^2q}{(2\pi)^2}\frac{q^2}{\varepsilon_0(q)^7} = \frac{8}{15\pi b_z}$$

$$g^{xx}_{xx} = g^{yy}_{yy} = \frac{4}{5\pi b_z},\quad g^{yy}_{xx} = g^{xx}_{yy} = g^{xy}_{xy} = \frac{16}{5\pi b_z}$$

Recall for undoped graphene:

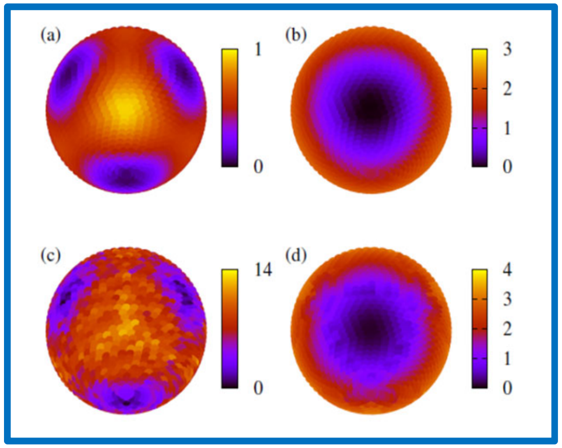
$$J^{\mu\nu}_{RKKY}(r) \propto \pm\frac{1}{r^3}$$

For smooth spin density, yields a Coulomb-like stiffness: ~ $$\int d^2r_1\int d^2r_2\frac{\partial S(r_1)\partial S(r_2)}{|r_1 - r_2|} \Leftrightarrow \int d^2q|S(q)|^2q$$

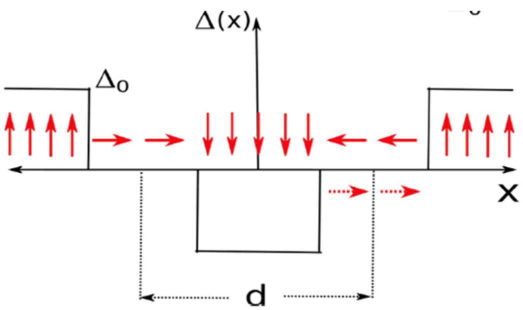
… up to distance set by b_z (non-perturbative effect)

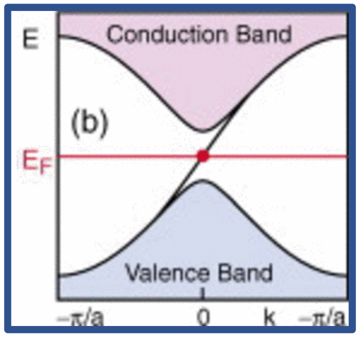
Implications for Domain-walls: TCI

➢ Spin-orbit coupled systems: broken SU(2) symmetry (e.g., SnTe 111 surface)



➢ Domain wall on the surface: expect a logarithmic interaction up to a cut-off determined by magnetization (large for small impurity density)



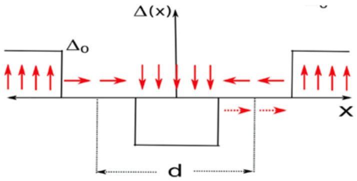


- Jackiw-Rebbi mid-gap states
- Number of channels depends on how many b_z's change sign
- Should be detectable in surface conductivity

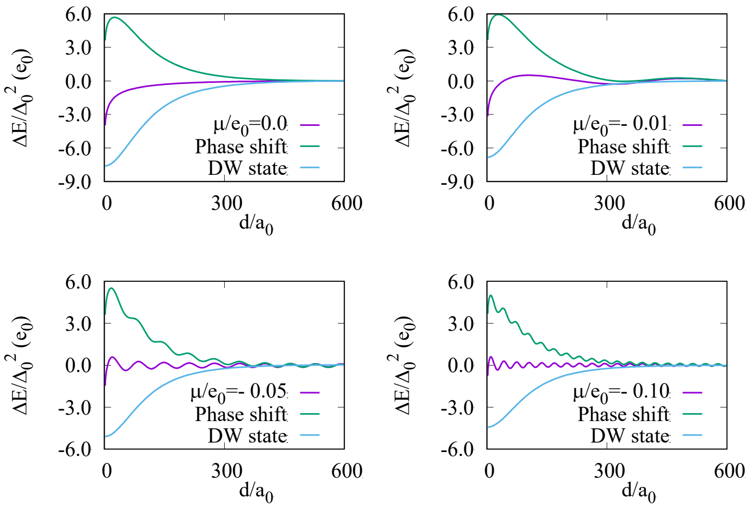
Domain wall energetics: Transfer matrix method

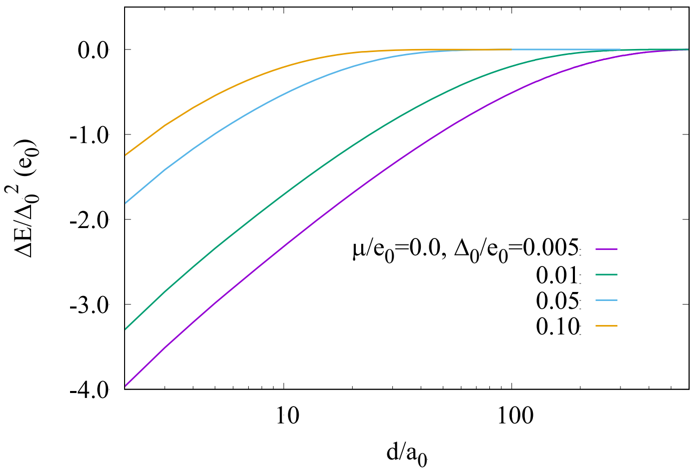
- Single Dirac point with SOC
- Two contributions: in-gap bound states and scattering states

Transfer Matrix
$$\begin{pmatrix} T_{AA} & T_{AB} \\ T_{BA} & T_{BB} \end{pmatrix}$$



Boundary condition
$$\frac{T_{AA}e^{ik_xL} - T_{AB}}{T_{BB}e^{-ik_xL} - T_{BA}} = 1$$

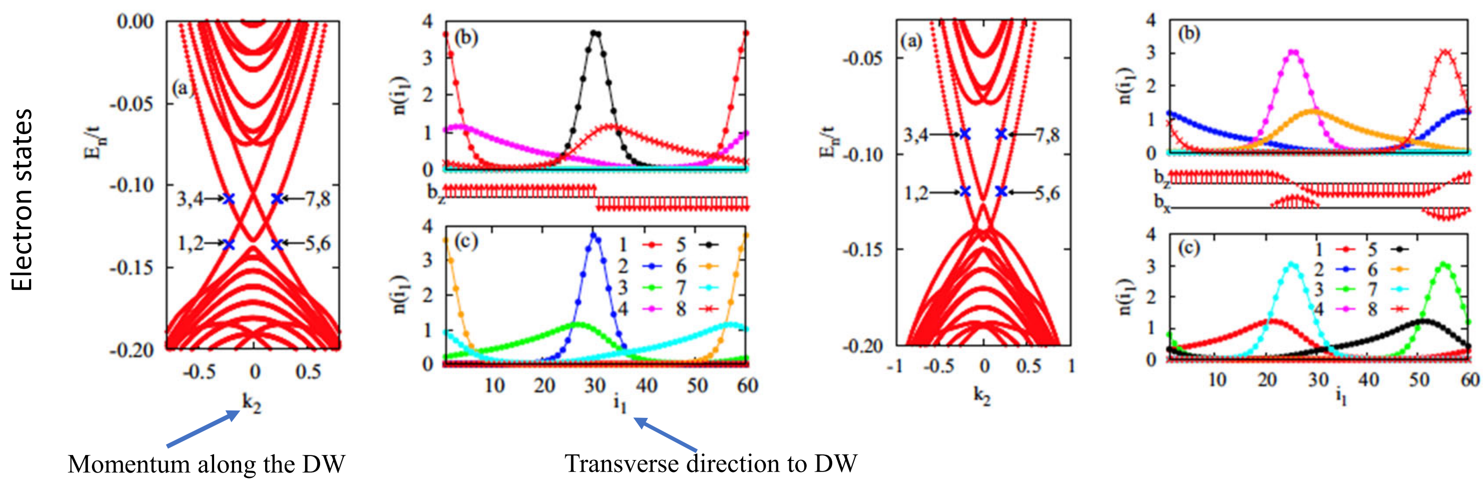




- Similar results are obtained for tight-binding graphene model with antiferromagnetic domain walls

Domain walls on TCI (111) surfaces

- Tight binding slab with (111) surface
- Magnetic impurities arranged in DW configuration on surface



- One in-gap state for every DW and every Dirac point for which mass changes sign
- Individual DW do have net chirality
- Consistent with Chern number calculations

Many thanks to ….

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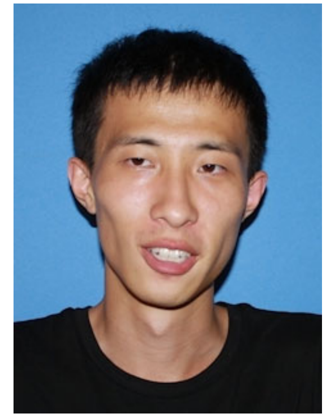
Sankar Das Sarma - Maryland



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Summary

- Dirac electrons offer a new paradigm for RKKY interactions with interesting differences from conventional electron systems
- Graphene: Strong antiferromagnetic correlations across sublattices
- Topological insulators: Spin-orbit coupling breaks SU(2) symmetry
  * Multiple groundstate directions
  * Gate controllable
  * Different thermal disordering transitions possible

- Spin stiffness from Dirac electrons: Emergent long-range form
  * Effect on DW energetics: subtle interplay of bound state energies and phase shifts
  * Multiple in-gap current-carrying states

References: L. Brey, HAF and S. Das Sarma, PRL **99**, 116802 (2007).
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THANK YOU!