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Innovations in Strongly Correlated Electronic Systems: School and Workshop

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Collective instabilites in doped graphene

Andrey CHUBUKOV

University of Wisconsin-Madison
Department of Physics
Madison
U.S.A.

Collective instabilities in doped graphene

Andrey Chubukov

University of Wisconsin

Trieste, August 16, 2012

Collaborators

Rahul Nandkishore, MIT/Princeton

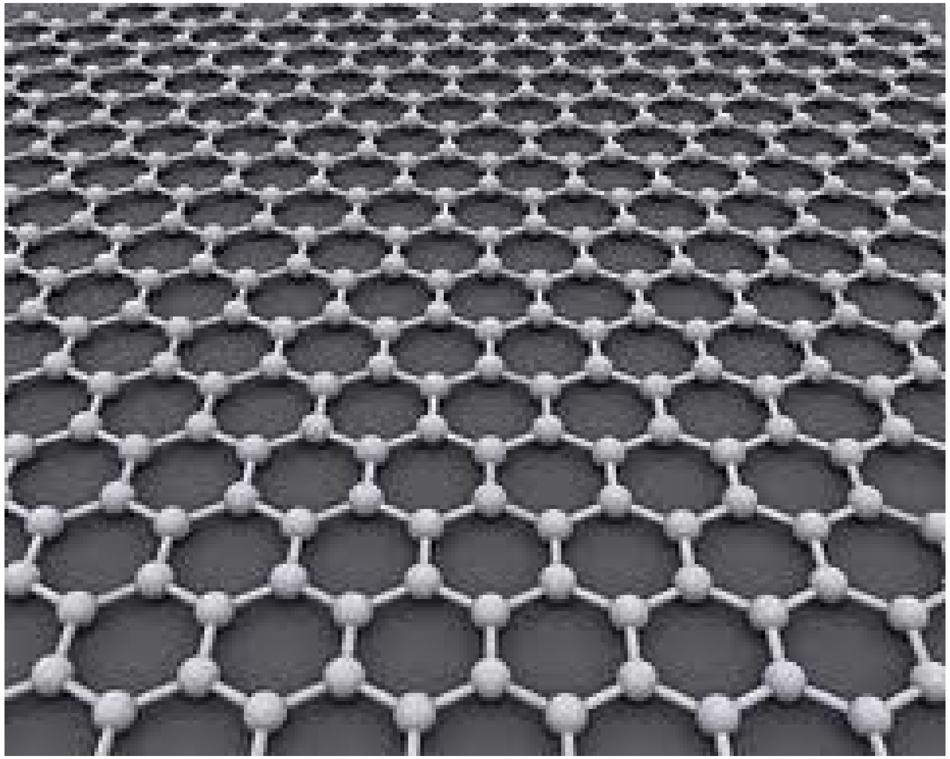
Leonid Levitov, MIT

Rafael Fernandes,
Columbia/LANL/
Minnesota

Gia-Wei Chern,
Madison/LANL

This will be the story about
superconductivity and SDW
in single-layer graphene
doped to van-Hove point

Graphene -- an atomic-scale honeycomb lattice made of carbon atoms.

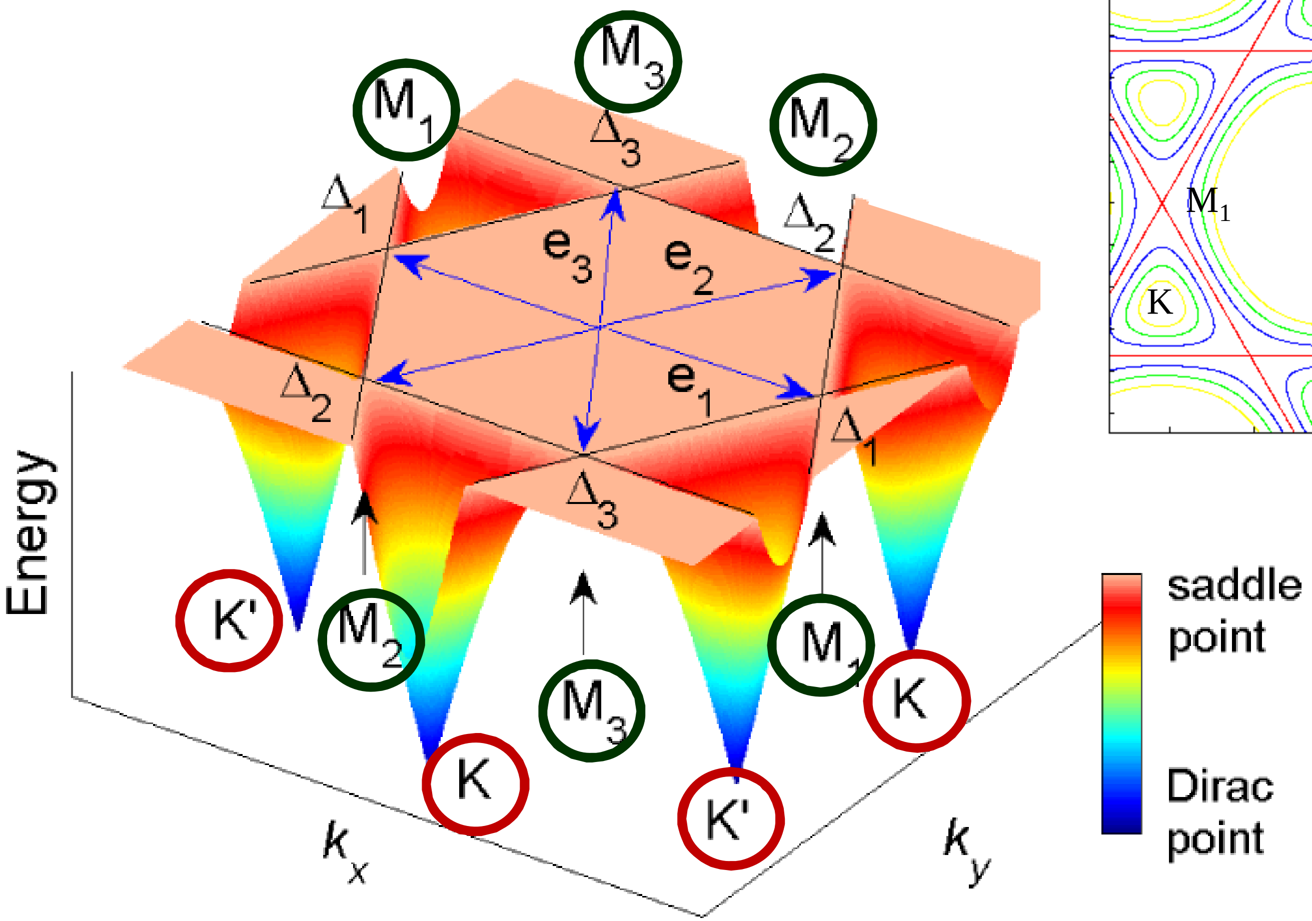


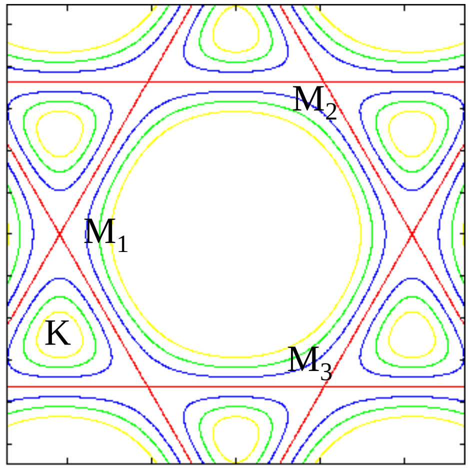
Nobel Prize 2010
Andre Geim, Konstantin Novoselov

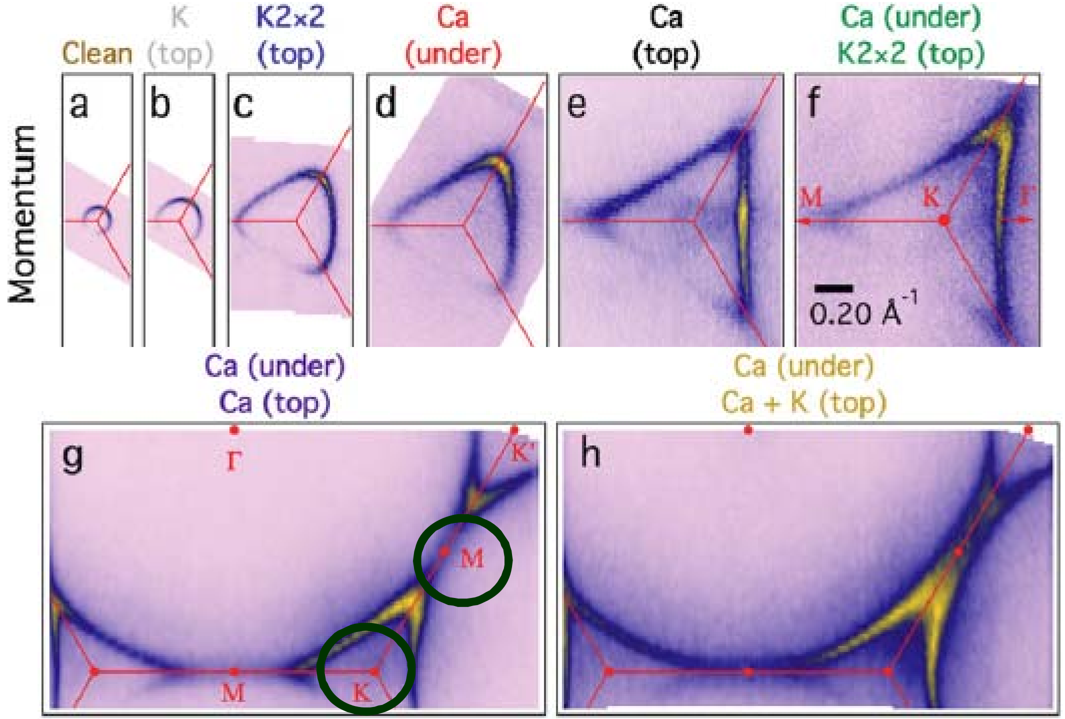
$$\varepsilon(\mathrm{k}) = t_1\sqrt{1 + 4\cos\frac{k_y\sqrt{3}}{2}\cos\frac{3k_x}{2} + 4\cos^2\frac{k_y\sqrt{3}}{2}} - \mu$$

$\mu = 0$, Dirac points

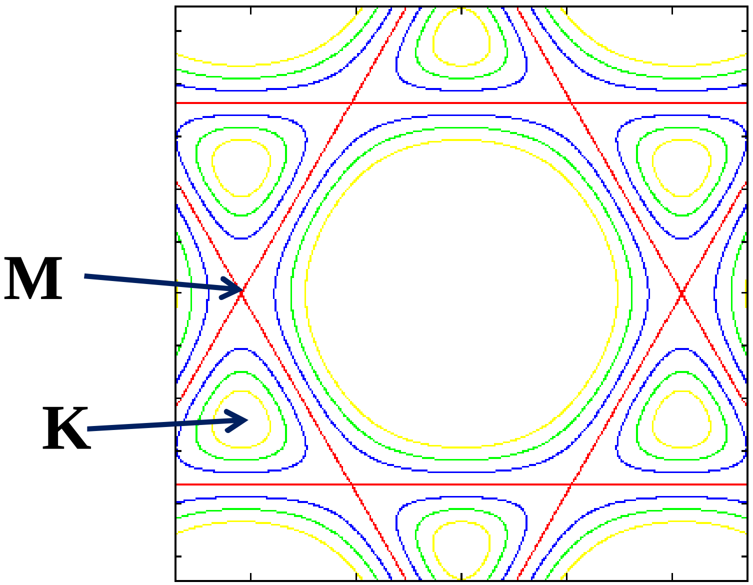
$\mu = t_1$, van Hove points







E. Rotenberg et al
PRL 104, 136803 (2010)



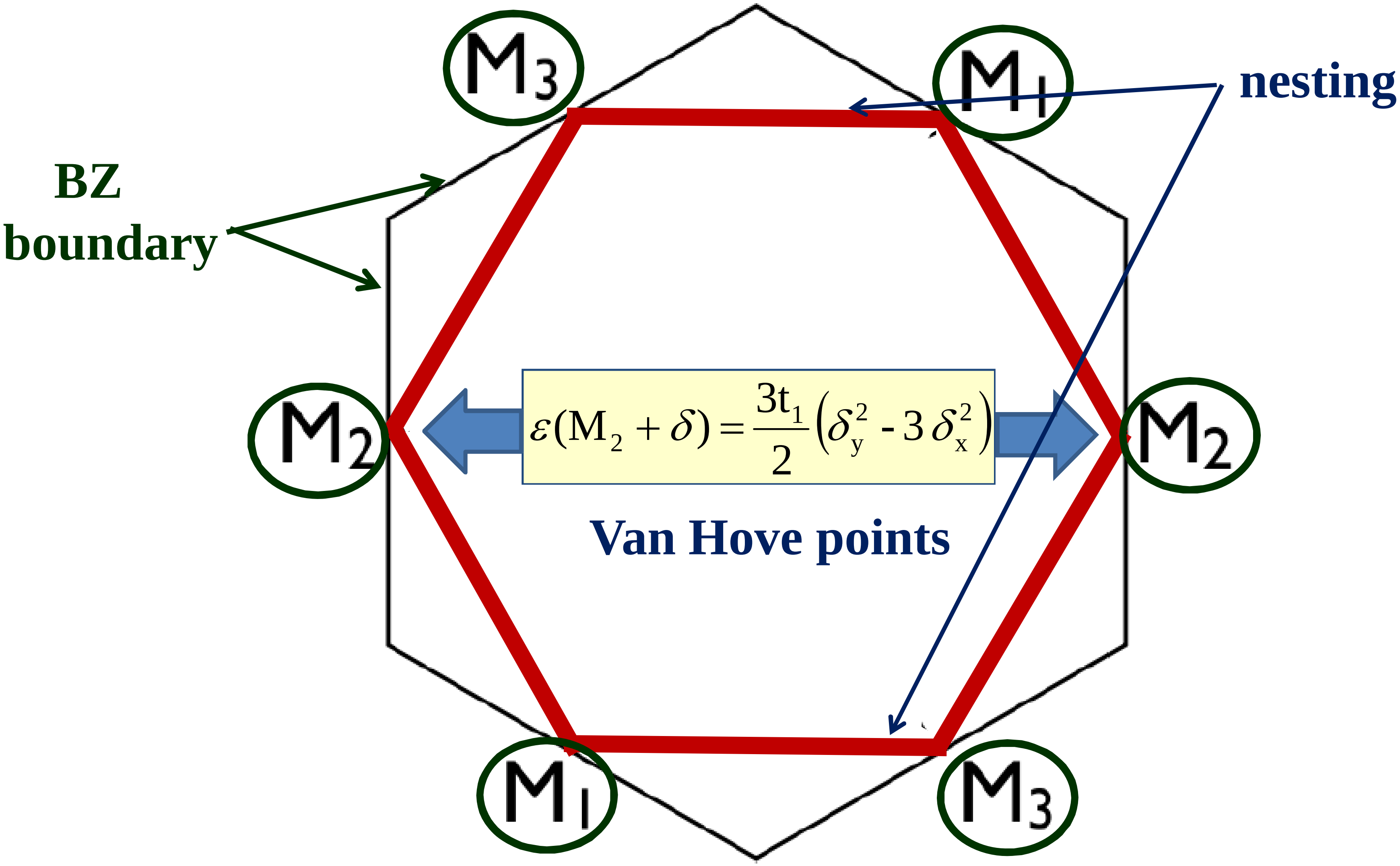
Ca can create additional subbands and cause a phonon SC, like in CaC_6

Mazin & Balatsky

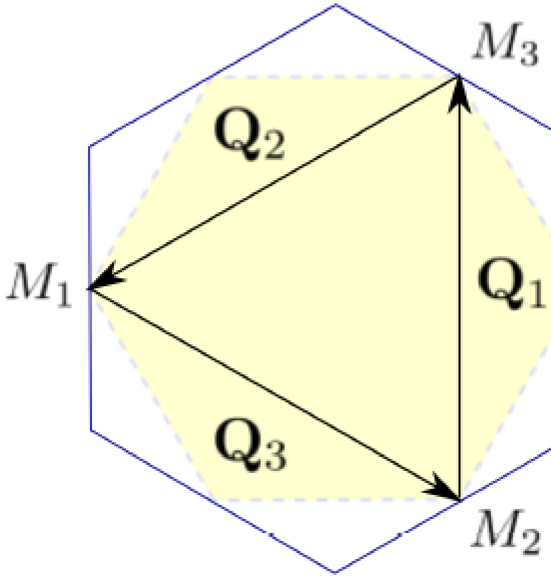
But let's assume that the only effect of doping is the change of electronic structure

At van Hove doping

$$\varepsilon(\mathrm{k}) = t_1\sqrt{1+4\cos\frac{k_y\sqrt{3}}{2}\cos\frac{3k_x}{2}+4\cos^2\frac{k_y\sqrt{3}}{2}} - t_1$$



$$\varepsilon(M_2+\delta) = \frac{3t_1}{2}\left(\delta_y^2 - 3\,\delta_x^2\right)$$



Because of van-Hove points

- superconducting susceptibility gets an extra boost:

$$\Pi_{pp}(0) \propto \log^2 \frac{\Lambda}{T}$$

Because of nesting and van-Hove points

- more exotic susceptibilities are also log-singular

$$\Pi_{pp}(Q_i) \propto \log \frac{\Lambda}{T},$$

$$\Pi_{ph}(0) \propto \log \frac{\Lambda}{T}$$

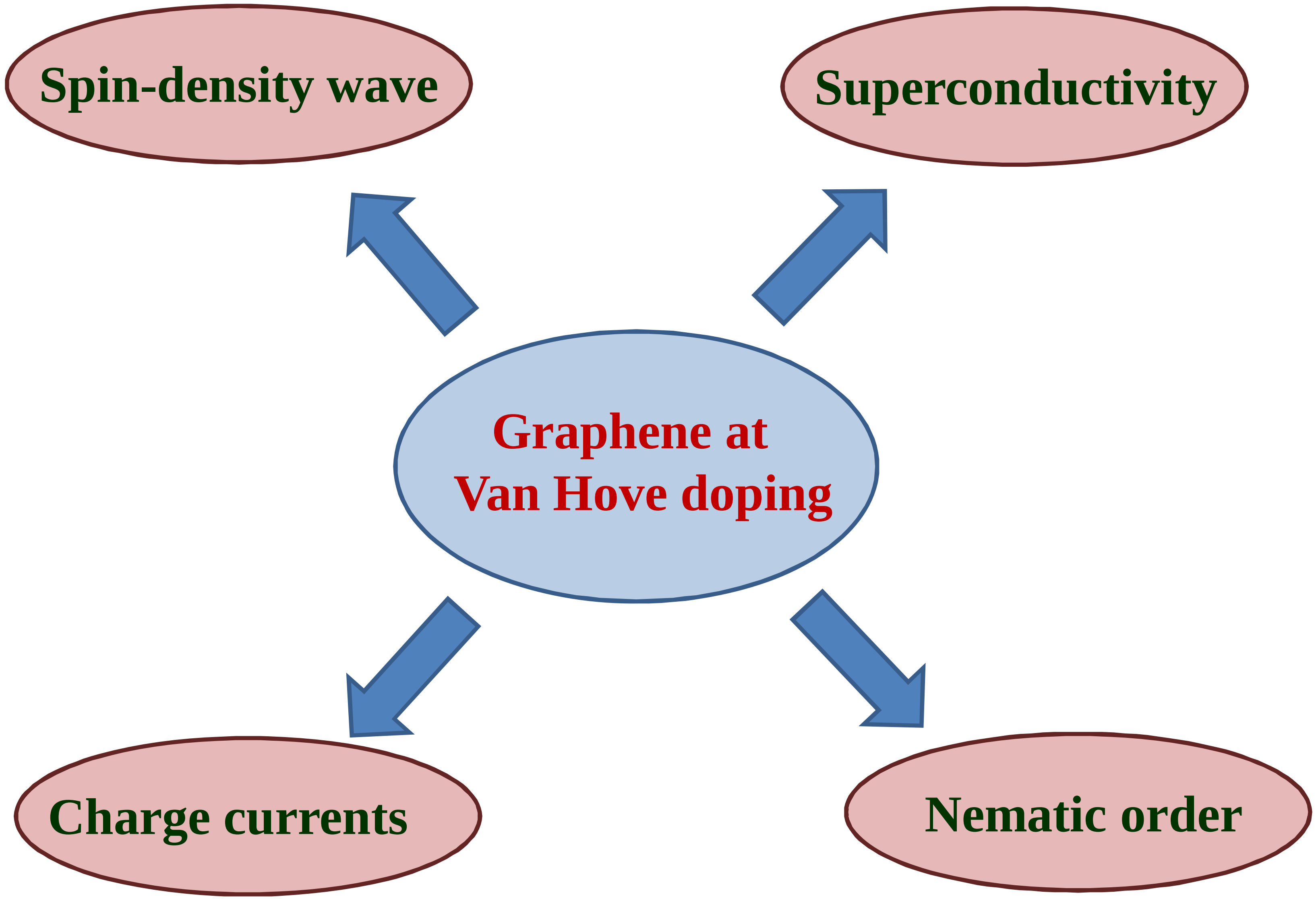
- density-wave susceptibilities also get extra boosts:

$$\Pi_{ph}(Q_i) \propto \log^2 \frac{\Lambda}{T}$$ perfect nesting

$$\Pi_{ph}(Q_i) \propto \log \frac{\Lambda}{T} \log \frac{\Lambda}{\max(T, t_3)}$$ imperfect nesting

t_3: 3rd neighbor hopping

Self-consistent approach will give a solution for each order



Suppose we consider weak el-el interaction.
What is the leading instability?

This is a typical parquet RG problem: there are logarithms in particle-hole and particle-particle channels.

Bare level:
pairing interaction is generally repulsive in all channels,
interactions in SDW and current CDW channels are attractive
density-wave order (SDW) is the instability at the RPA level

But, interactions flow to new values at low energies, and which one will eventually win remains to be seen

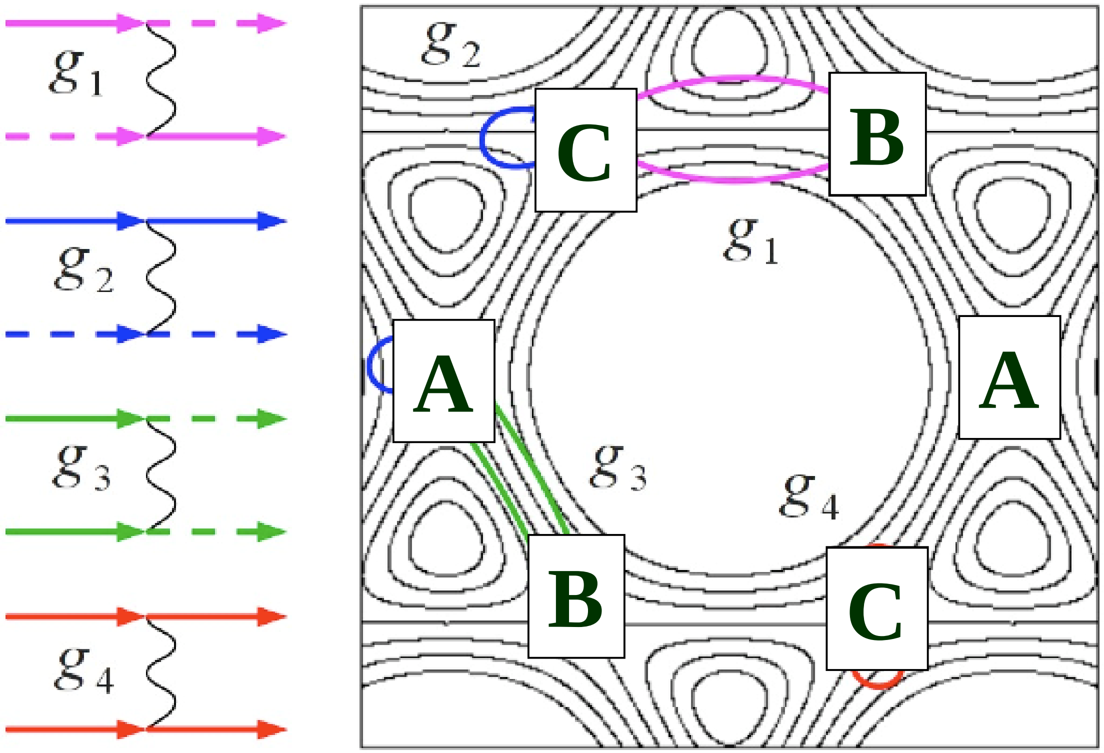
A similar story in bi-layer graphene: Lemonic, Aleiner, Fal'ko
Cvetkovic, Throckmorton, Vafek

How one should do this:

Introduce all possible interactions between low-energy fermions

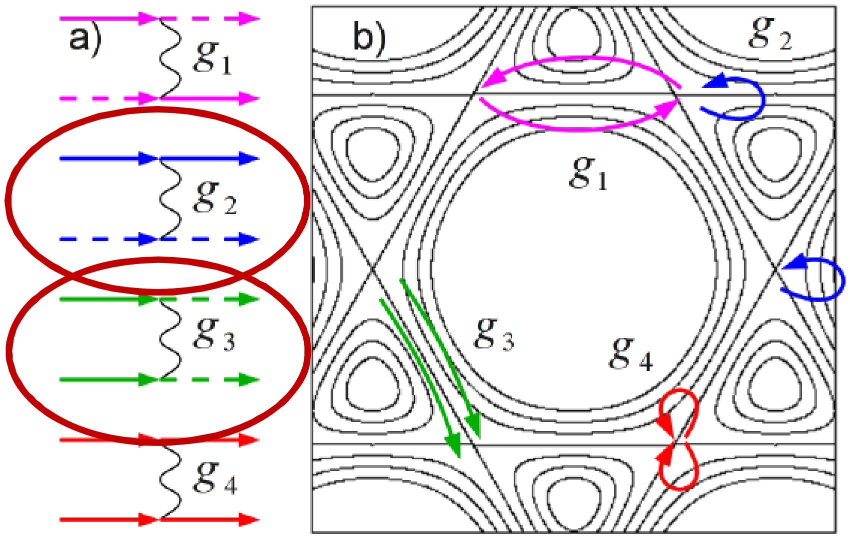
$$H_{two-particle} = \sum_{\alpha,\beta=1}^{3} \frac{g_1}{2} \psi^+_\alpha \psi^+_\beta \psi_\alpha \psi_\beta + \frac{g_2}{2} \psi^+_\alpha \psi^+_\beta \psi_\beta \psi_\alpha + \frac{g_3}{2} \psi^+_\alpha \psi^+_\alpha \psi_\beta \psi_\beta$$

$$+ \sum_{\alpha=1}^{3} \frac{g_4}{2} \psi^+_\alpha \psi^+_\alpha \psi_\alpha \psi_\alpha$$



3 patches

RG equations (perfect nesting)



Particle-hole and particle- particle channels

Only particle-hole channel

$$\dot{g}_2 = g_2^2 + g_3^2$$

$$\dot{g} = dg/d\,(\log\,(\Lambda/E))^2$$

$$\dot{g}_3 = g_3\left(4g_2 - 2g_1 - 2g_4 - g_3^2\right)$$

$$\dot{g}_1 = 2\,g_1\left(g_2 - g_1\right)$$

$$\dot{g}_4 = -2\,g_3^2 - g_4^2$$

RG equations (non-perfect nesting)

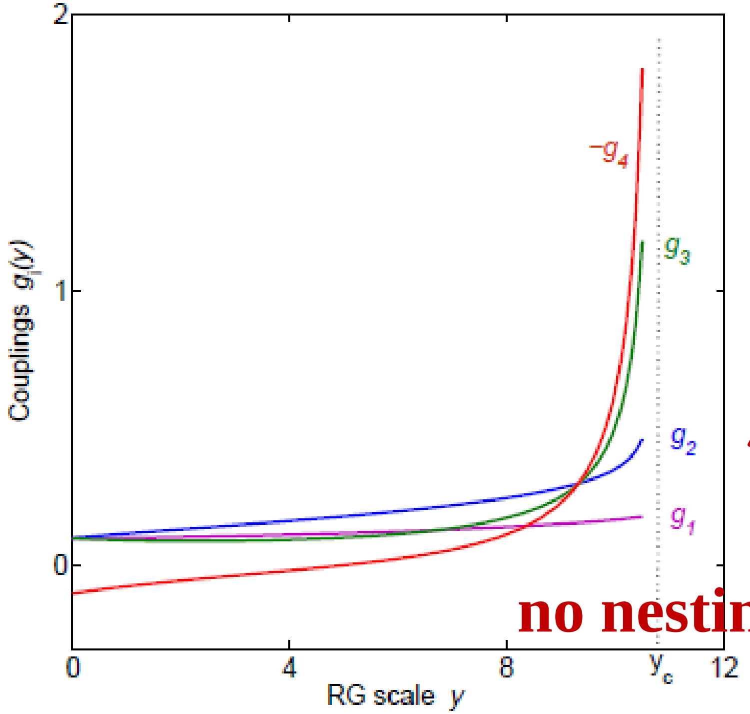
$$\frac{dg_1}{dy} = 2d_1 g_1(g_2 - g_1), \qquad \frac{dg_2}{dy} = d_1(g_2^2 + g_3^2),$$

$$\frac{dg_3}{dy} = -(n-2)g_3^2 - 2g_3 g_4 + 2d_1 g_3(2g_2 - g_1), \qquad \frac{dg_4}{dy} = -(n-1)g_3^2 - g_4^2.$$

$d_1(y) = d\Pi_{\text{pl}}$

measures non-p

$\Pi_{\text{ph}}(Q_i) \propto \log \frac{\Lambda}{E}$ l



n=3 is the # of patches

d_1 as a parameter

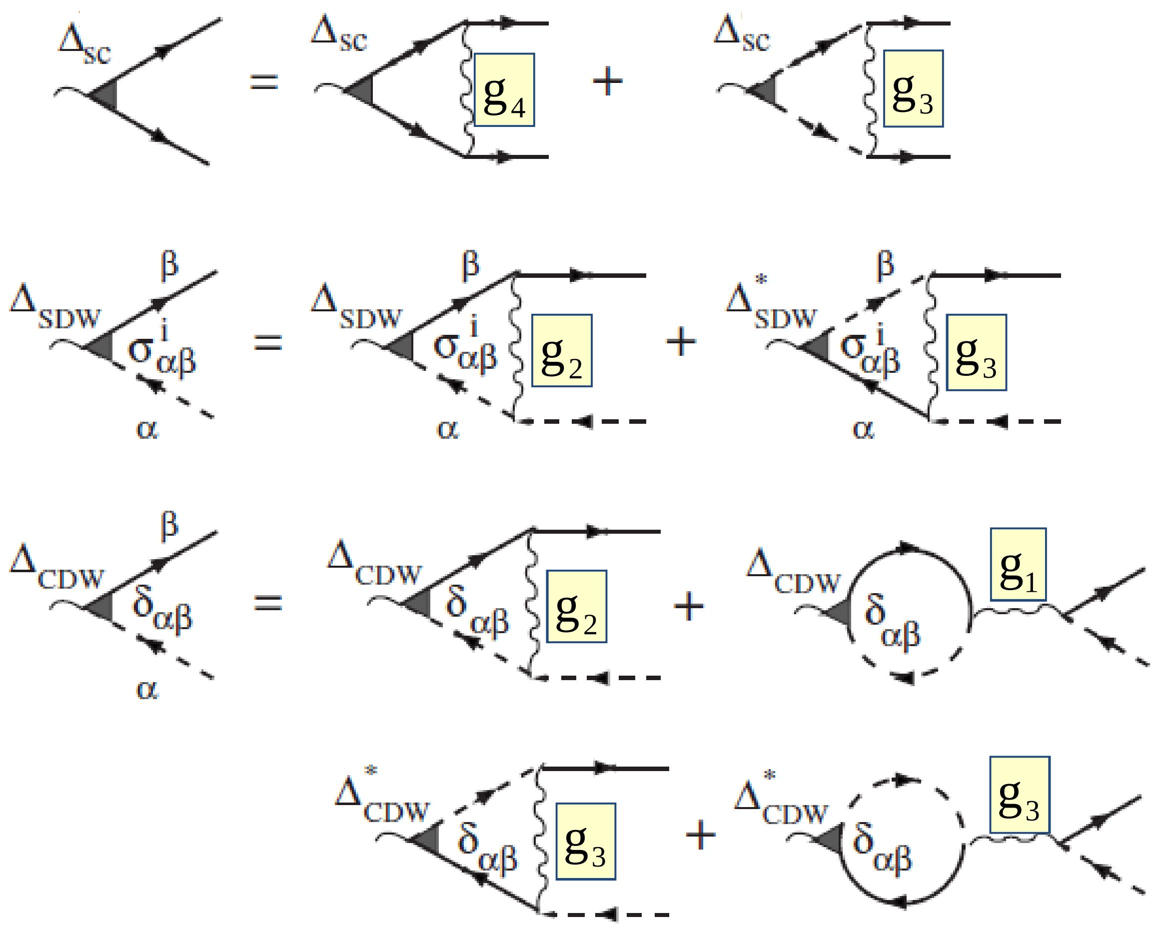
< d_1 <1

no nesting **perfect nesting**

all couplings diverge at a particular scale

similar eqs for square lattice (n=2): Le Hur & Rice, Dzyaloshinskii, Yakovenko, Schulz ….

SDW, CDW, and SC vertices



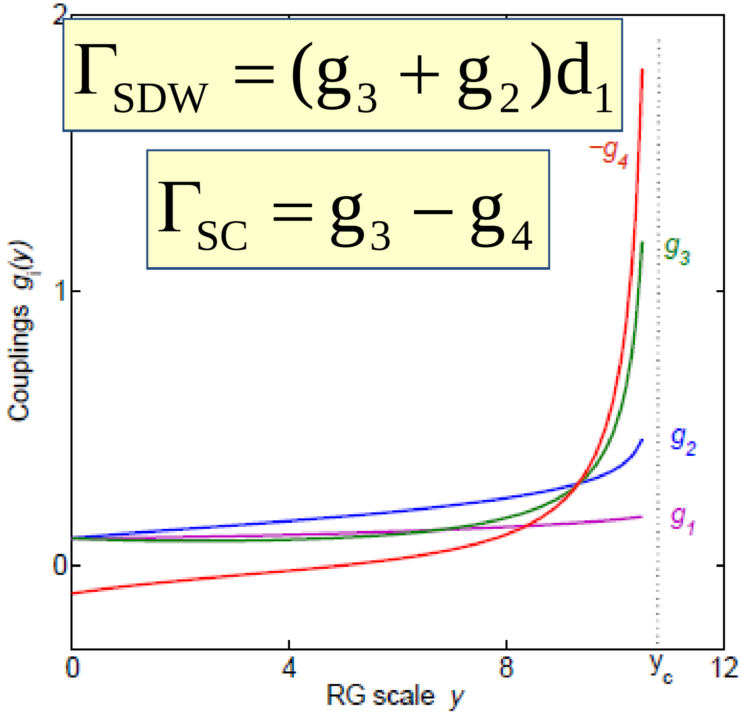
$$\Delta_j = \Delta^0_j \left(1 + \Gamma_j \log^2 \frac{\Lambda}{E}\right)$$

$$\Gamma_{SDW} = (g_3 + g_2)d_1$$

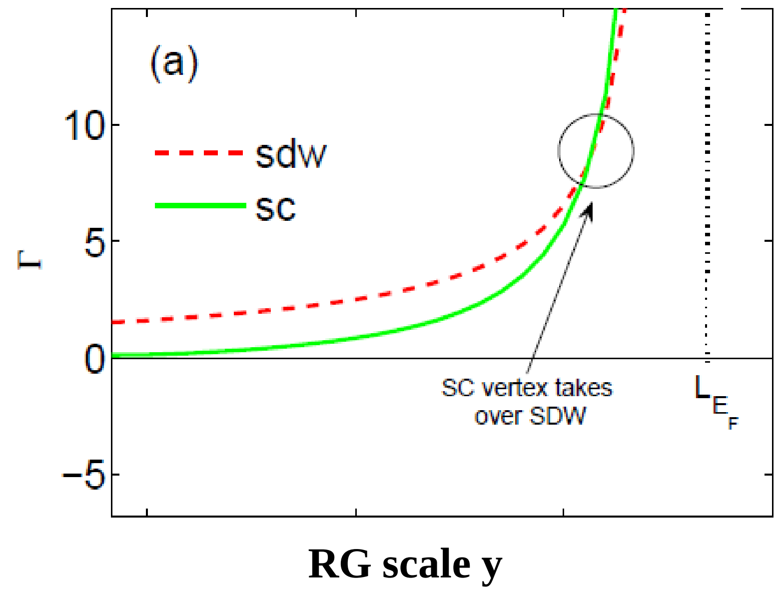
$$\Gamma^a_{SC} = (g_3 - g_4), \Gamma^b_{SC} = (-2\, g_3 - g_4)$$

$$\Gamma_{SDW} = (g_3 + g_2)d_1$$

$$\Gamma_{SC} = g_3 - g_4$$



Need $\Gamma > 0$ for instability

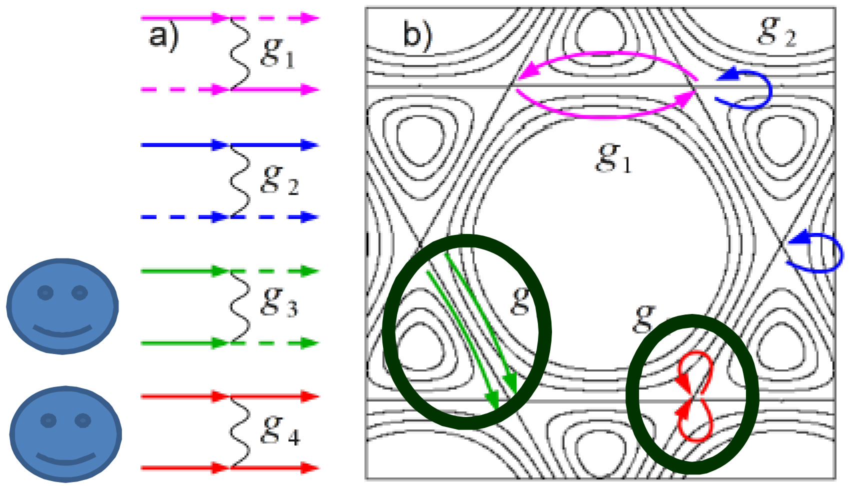


• The two leading instabilities are SDW and spin-singlet SC

• The SDW vertex is the largest one at intermediate energies

• The superconducting vertex eventually takes over and becomes the leading instability at low energies, both at perfect and imperfect nesting

Superconductivity



$$\Gamma^{a}_{SC} = (g_3 - g_4),\ \Gamma^{b}_{SC} = (-2\,g_3 - g_4)$$

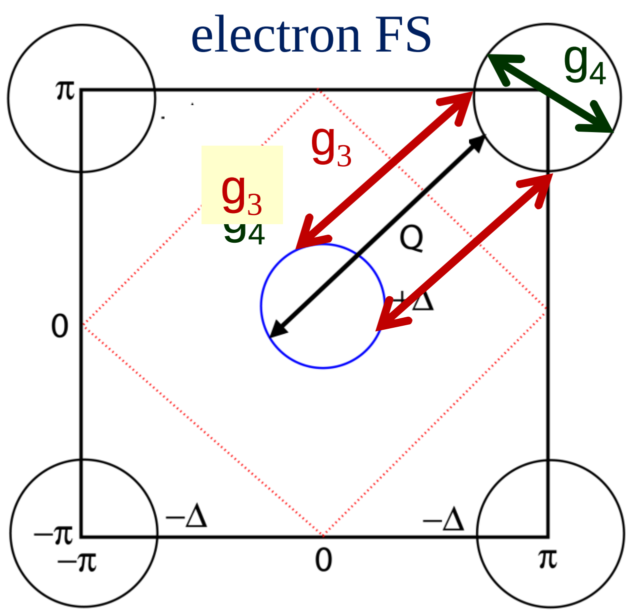
g_4 is against any pairing

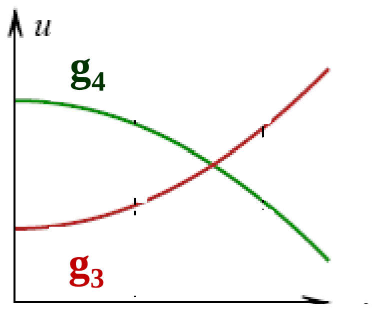
g_3 is not against ANY pairing:

$\Gamma^{a}_{sc} > 0$ if $g_3 > g_4$

Re flow:

Pnictides: 2 “hot spots”





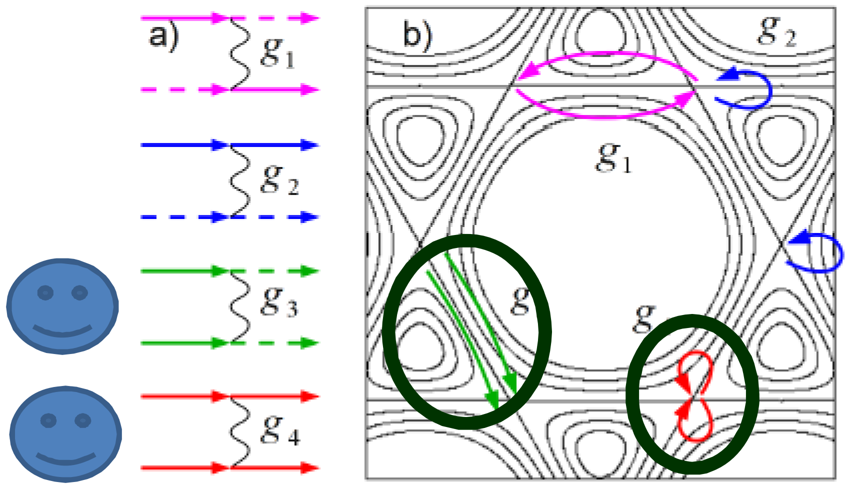
$\Gamma_1 = -g_4 - 2\,g_3$

$\Gamma_{2,3} = -g_4 + g_3$

$\Gamma > 0$ for pairing

$\Gamma_{s+-} > 0$

sign-changing s-wave



$$\Gamma^a_{SC} = (g_3 - g_4),\ \Gamma^b_{SC} = (\text{-}2\,g_3 - g_4)$$

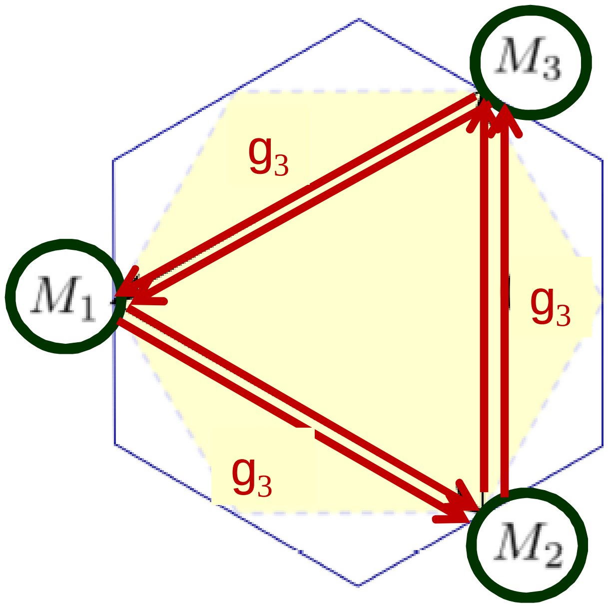
g_4 is against any pairing

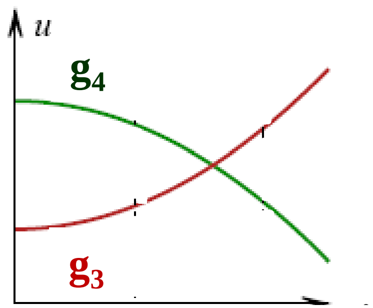
g_3 is not against ANY pairing:

$\Gamma^a{}_{sc} > 0$ if $g_3 > g_4$

Re flow:

Our case: 3 “hot spots”





$$\Gamma_1 = \text{-}g_4 \text{-} 2\,g_3$$
$$\Gamma_{2,3} = \text{-}g_4 + g_3$$
$\Gamma > 0$ for pairing

$$\Gamma_{2,3} = g_3 \text{-} g_4 > 0$$

doubly degenerate solution for SC

$$\frac{\partial}{\partial y}\begin{bmatrix}\tilde{\Delta}_1\\ \tilde{\Delta}_2\\ \tilde{\Delta}_3\end{bmatrix} = -2\begin{bmatrix} g_4 & g_3 & g_3\\ g_3 & g_4 & g_3\\ g_3 & g_3 & g_4\end{bmatrix}\begin{bmatrix}\tilde{\Delta}_1\\ \tilde{\Delta}_2\\ \tilde{\Delta}_3\end{bmatrix}$$

Eigenfunctions

$$\tilde{\Delta}_a = \frac{\tilde{\Delta}}{\sqrt{2}}(0,1,-1), \quad \tilde{\Delta}_b = \sqrt{\frac{2}{3}}\tilde{\Delta}\left(1,-\frac{1}{2},-\frac{1}{2}\right)$$

$$\tilde{\Delta}_c = \frac{\tilde{\Delta}}{\sqrt{3}}(1,1,1).$$

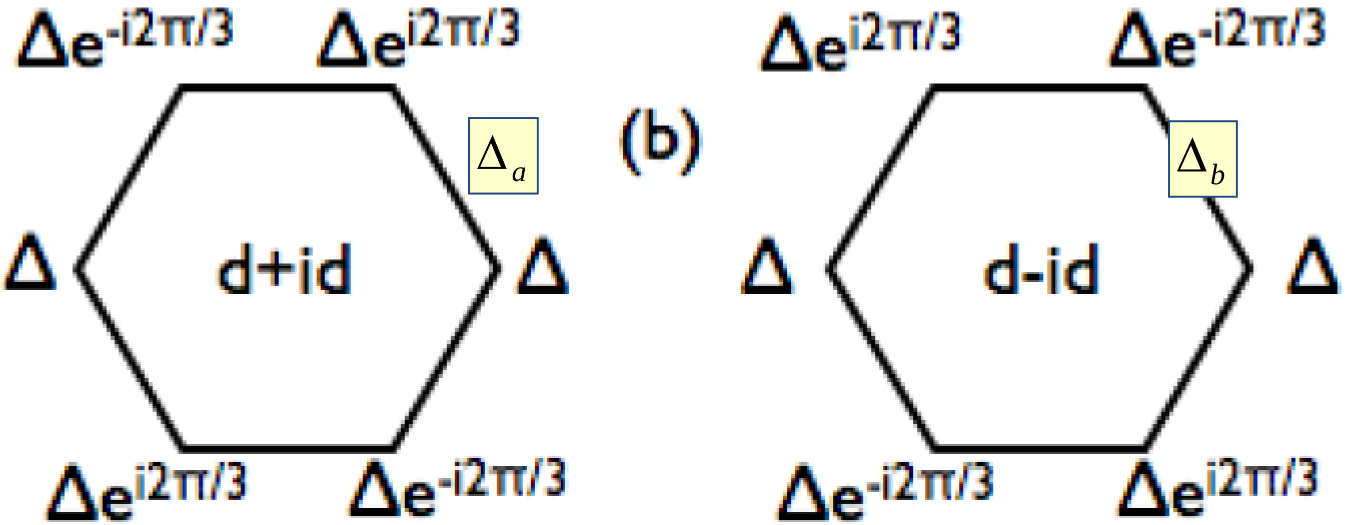
Eigenvalues

$$\Gamma_1 = -g_4 - 2g_3$$

$$\Gamma_{2,3} = -g_4 + g_3$$

s-wave (repulsion)

$\Gamma_{2,3} > 0$
doubly degenerate
solution for SC



The two d-wave solutions are degenerate by symmetry

Gonzales

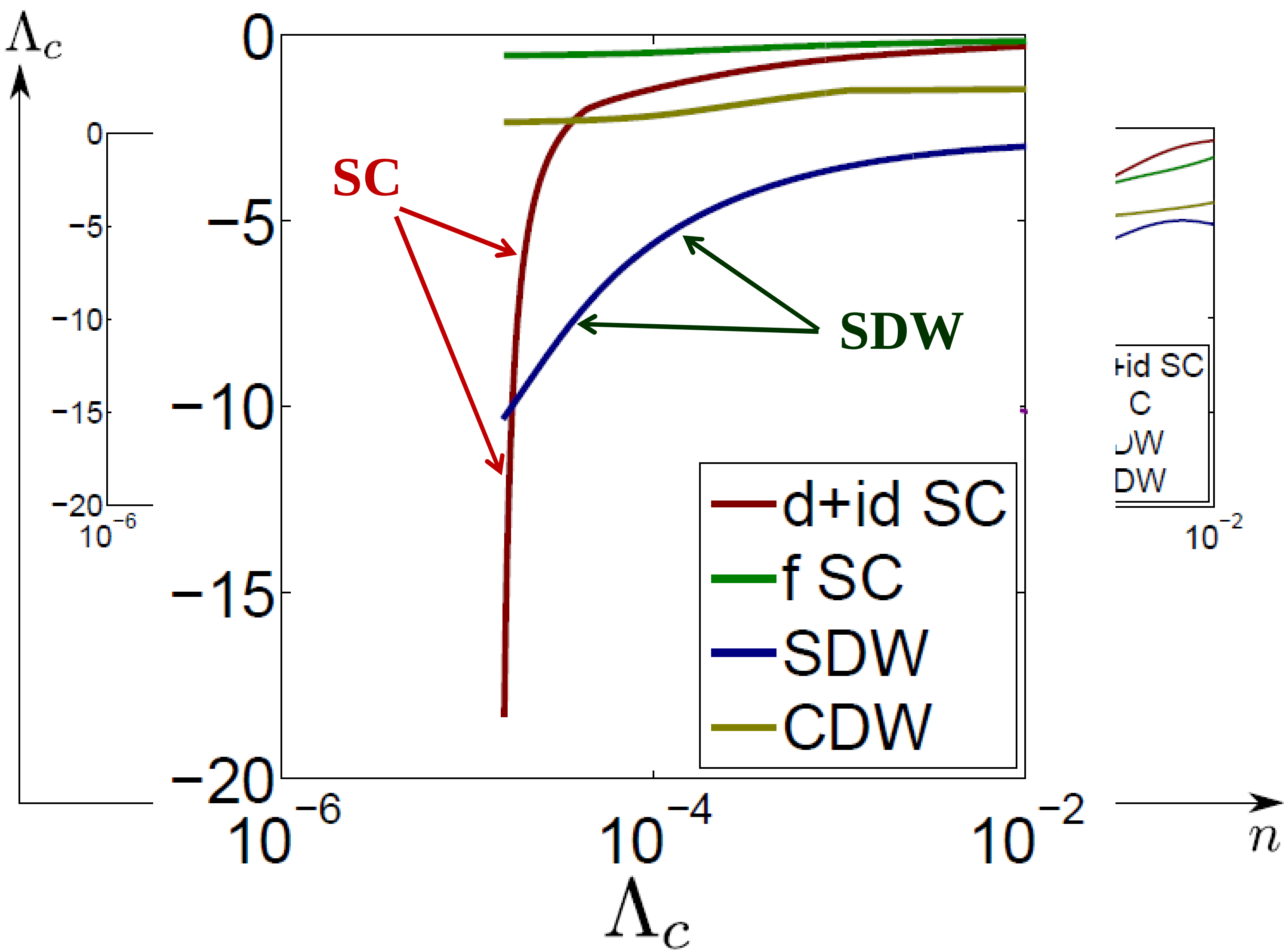
Landau-Ginzburg expansion

$$F = \alpha(T - T_c)(|\Delta_a|^2 - |\Delta_b|^2) + K_1\left(|\Delta_a|^2 + |\Delta_b|^2\right)^2 + K_2|\Delta_a^2 + \Delta_b^2|^2 + O(\Delta^6)$$

d+id state wins

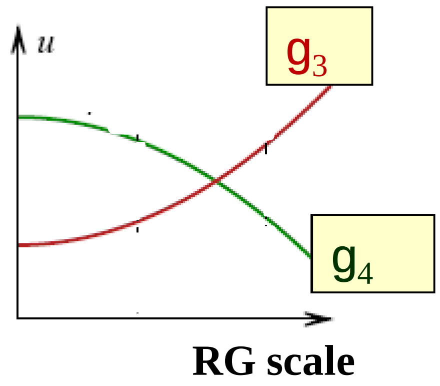
Functional RG – the same result

Thomale et al



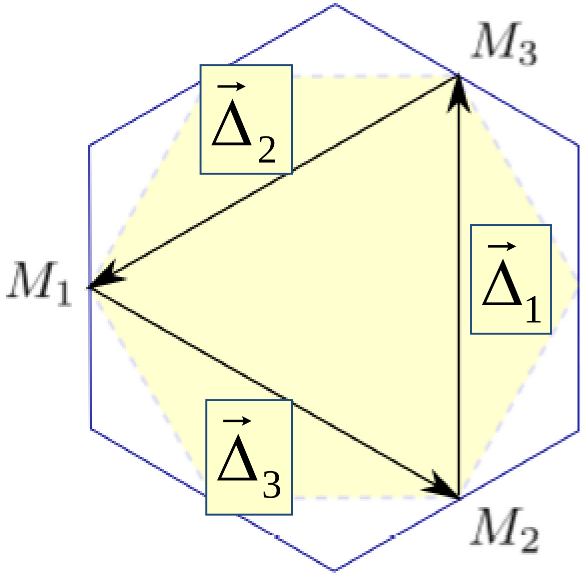
Spin density wave

Away from van Hove filling, RG stops at some scale



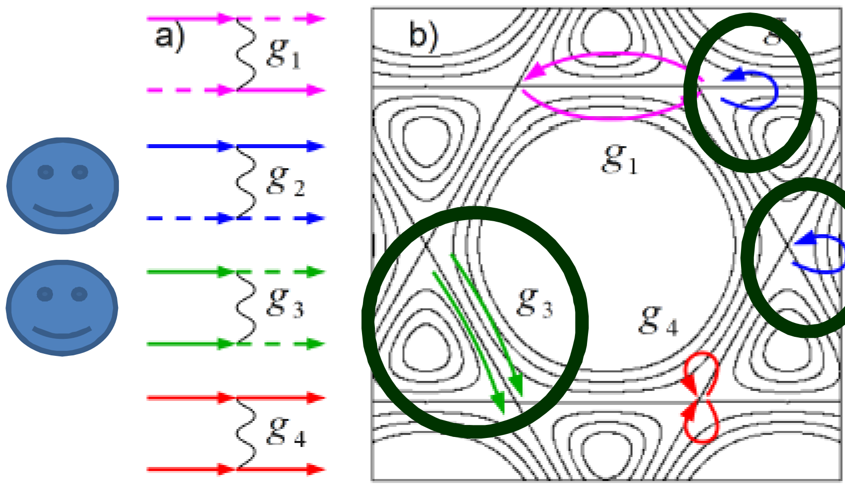
Need $g_3 > g_4$ for SC

d-wave SC may or may not develop, but SDW channel is attractive anyway and is always dominant at intermediate scales



$$\Pi_{ph}(Q_i) \propto \log \frac{\Lambda}{T} \log \frac{\Lambda}{\max(T, t_3)}$$

$$\vec{\Delta}_i = \sum_k < c^{+}_{k+Q_i,\alpha} \, \vec{\sigma}_{\alpha\beta} c_{k\beta} >$$

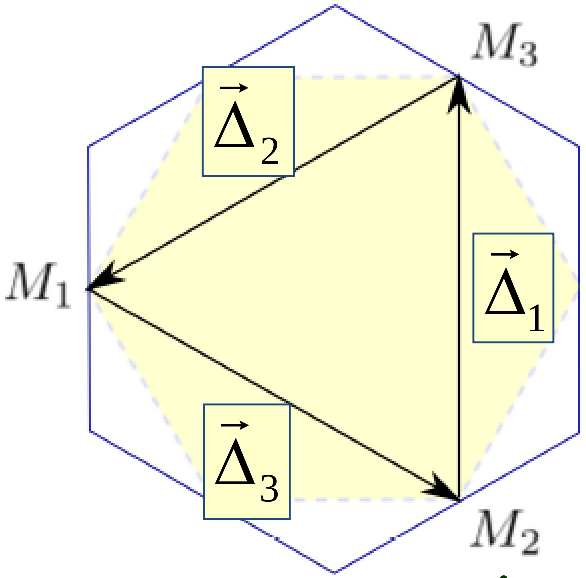


$$\lambda_{SDW} = g_2 + g_3 > 0$$

The issue is what kind of SDW order emerges

$$\mathcal{L} \propto \alpha(T - T_N) \sum \Delta_i^2$$

leaves infinite number of possible SDW states



Previous works on this and similar models:

non-coplanar, chiral SDW state with a nonzero $\mathbf{\Delta_1} \cdot \mathbf{\Delta_2} \times \mathbf{\Delta_3}$

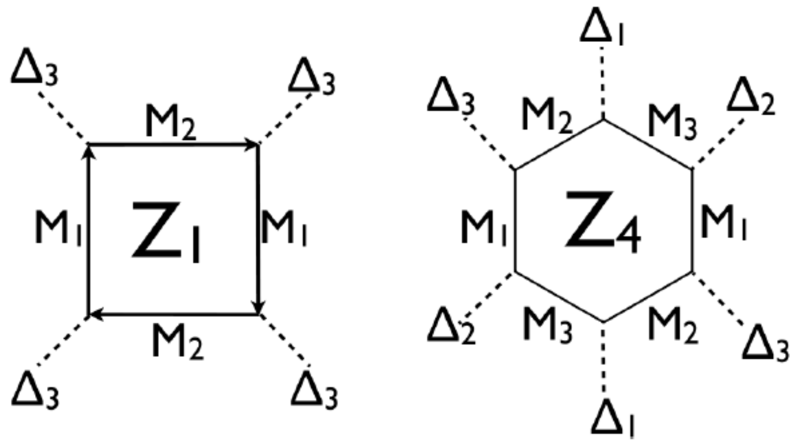
Li, Morais Smith et al, Batista & Martin…

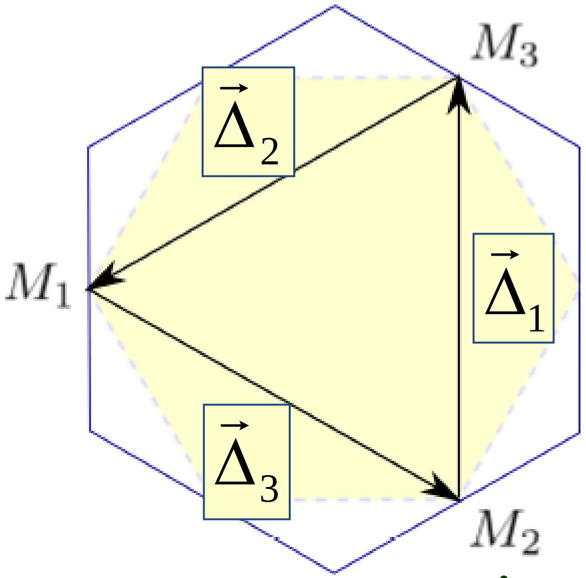
We found different SDW order:

we integrated out electrons and obtained Landau functional

$$\mathcal{L} \propto \alpha(T - T_N) \sum_i \mathbf{\Delta}_i^2 + Z_1(\mathbf{\Delta}_1^2 + \mathbf{\Delta}_2^2 + \mathbf{\Delta}_3^2)^2 + 2(Z_2 - Z_1 - Z_3)(\mathbf{\Delta}_1^2\mathbf{\Delta}_2^2 + \mathbf{\Delta}_2^2\mathbf{\Delta}_3^2 + \mathbf{\Delta}_3^2\mathbf{\Delta}_1^2)$$

$$+ \; 4Z_3\left((\mathbf{\Delta}_1 \cdot \mathbf{\Delta}_2)^2 + (\mathbf{\Delta}_2 \cdot \mathbf{\Delta}_3)^2 + (\mathbf{\Delta}_3 \cdot \mathbf{\Delta}_1)^2\right) - 4Z_4\left(\mathbf{\Delta_1} \cdot \mathbf{\Delta_2} \times \mathbf{\Delta_3}\right)^2 + \cdots$$





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we integrated out electrons and obtained Landau functional

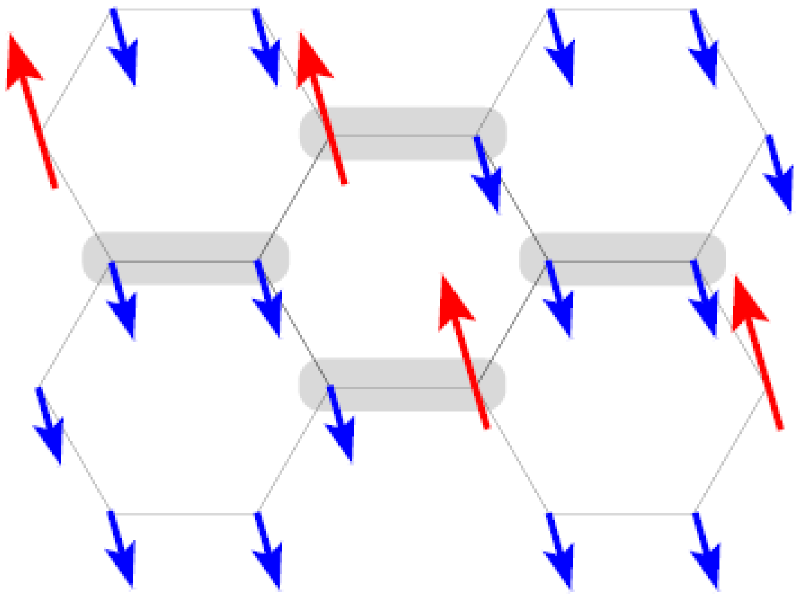
$$\mathcal{L} \propto \alpha(T-T_N)\sum_i \boldsymbol{\Delta}_i^2 + Z_1(\boldsymbol{\Delta}_1^2+\boldsymbol{\Delta}_2^2+\boldsymbol{\Delta}_3^2)^2 + 2(Z_2-Z_1-Z_3)\underline{(\boldsymbol{\Delta}_1^2\boldsymbol{\Delta}_2^2+\boldsymbol{\Delta}_2^2\boldsymbol{\Delta}_3^2+\boldsymbol{\Delta}_3^2\boldsymbol{\Delta}_1^2)}$$
$$+\ 4Z_3\underline{\left((\boldsymbol{\Delta}_1\cdot\boldsymbol{\Delta}_2)^2+(\boldsymbol{\Delta}_2\cdot\boldsymbol{\Delta}_3)^2+(\boldsymbol{\Delta}_3\cdot\boldsymbol{\Delta}_1)^2\right)} - 4Z_4\underline{\left(\boldsymbol{\Delta}_1\cdot\boldsymbol{\Delta}_2\times\boldsymbol{\Delta}_3\right)^2} + \cdots$$

(blue underline) **either only one of Δ_i appears, or all 3 appear with equal amplitudes**

(green underline) **either the state is chiral or co-planar**

Our result: the SDW state is co-planar (non-chiral), uni-axial, and with equal magnitudes of all Δ_i

$$\vec{\Delta}_1 = \vec{\Delta}_2 = \vec{\Delta}_3 = \Delta \sigma_z$$



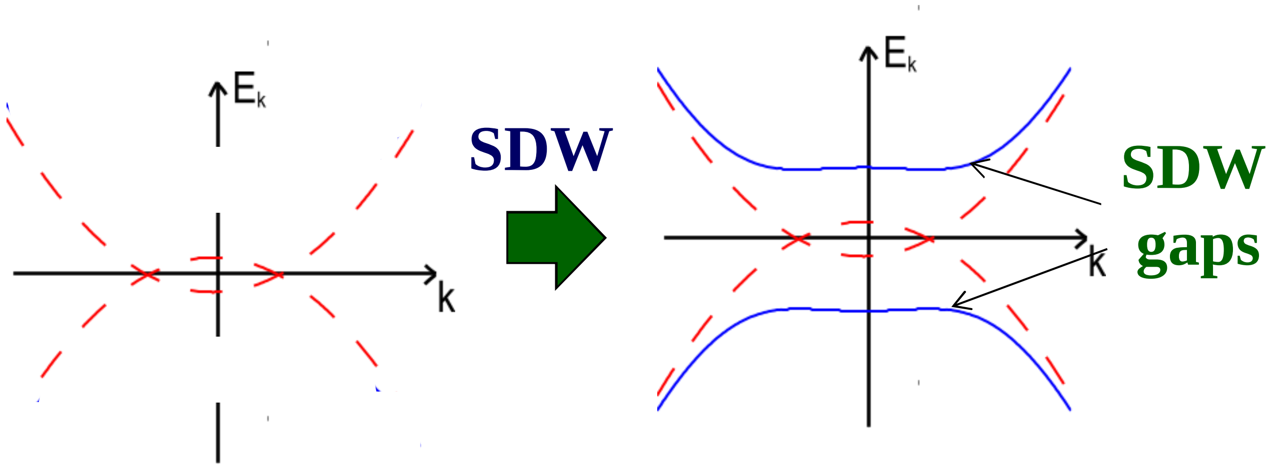
8-site unit cell with moments +3Δ and –Δ and zero magnetization

One cannot get this order in localized spin models

Is this state a metal or an insulator?

$$\vec{\Delta}_1 = \vec{\Delta}_2 = \vec{\Delta}_3 = \Delta\,\sigma_z$$

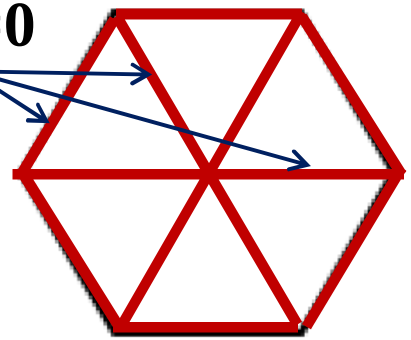
If there was a single SDW order parameter

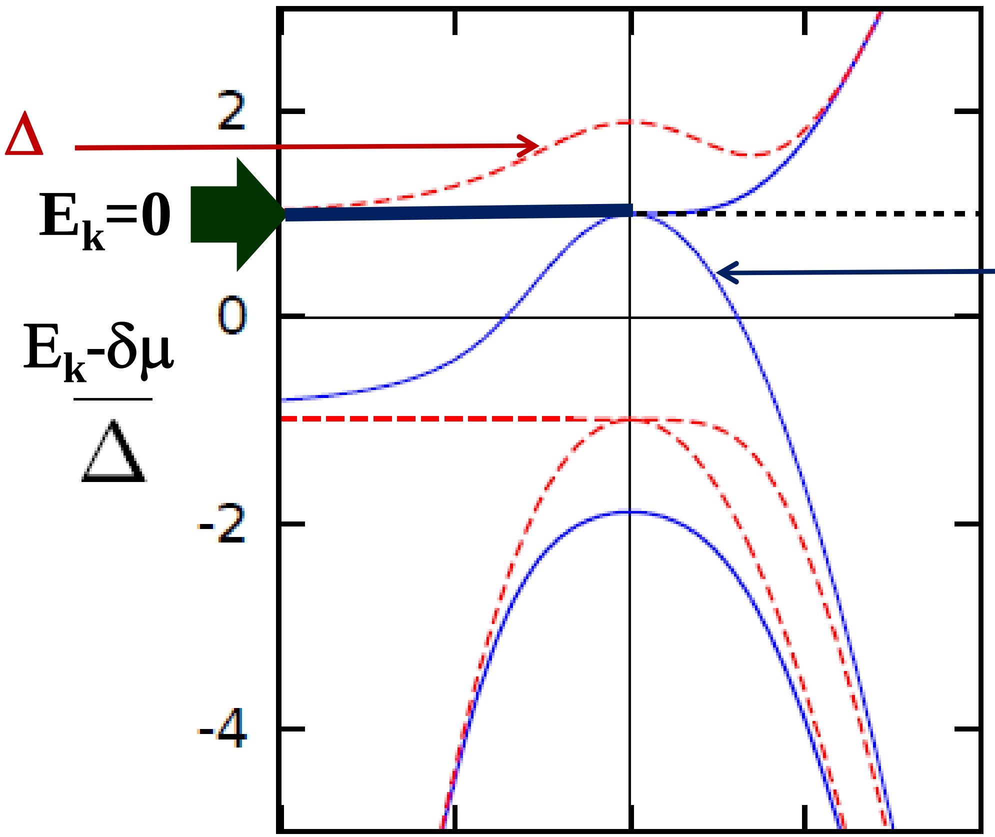


All states would be gapped (insulator)

Is this state a metal or an insulator?

$$\delta\mu = -\Delta$$





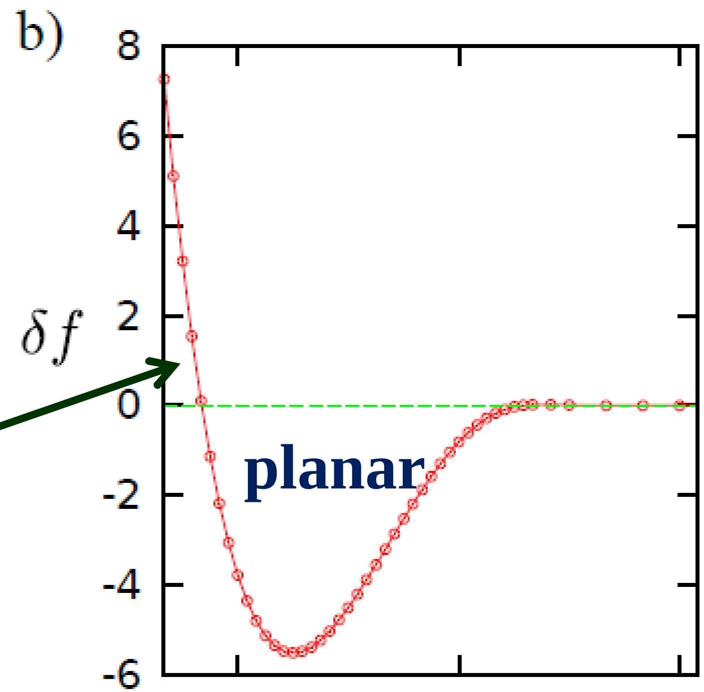
δμ is the change of the chemical potential

The SDW state is half-metal: for spin-up excitations (red) all states are gapped, for spin-down excitations (blue), the full FS survives

Charge currents are necessary spin currents

This story has one extra chapter:

Planar SDW exists only in a finite range of temperatures

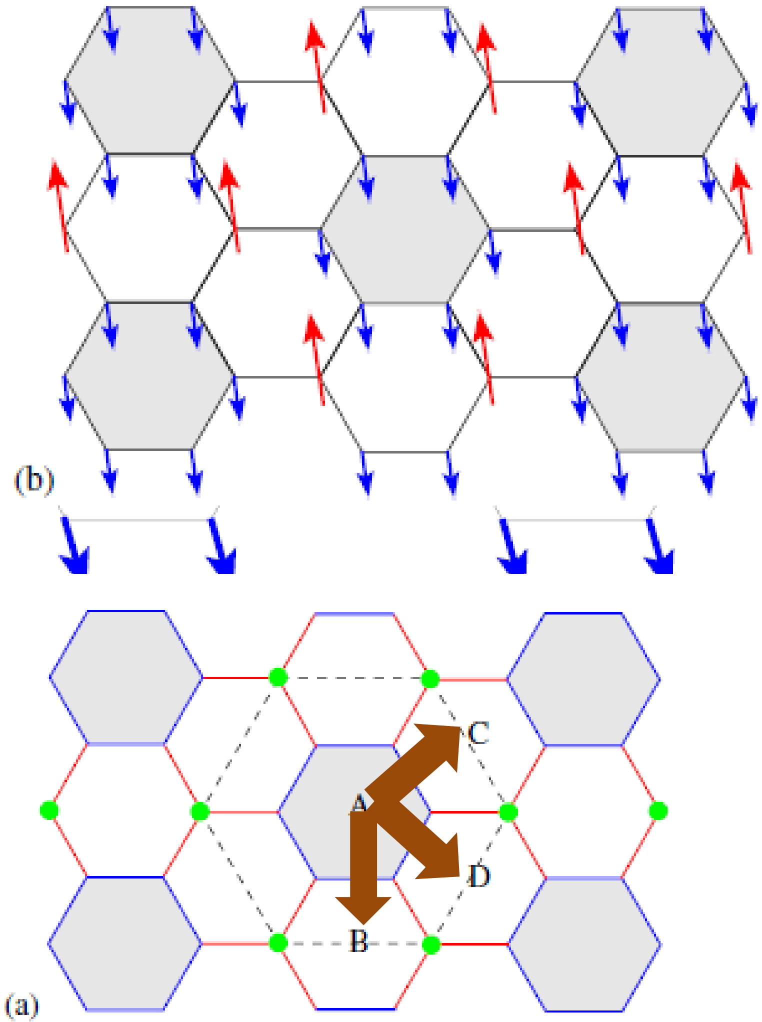


temperature

non-planar chiral SDW

Explanation:
Batista & Chern

Pre-emptive nematic order:



$O(3) \times Z_4$

(Δ, Δ, Δ)

$(\Delta, -\Delta, -\Delta), \quad (-\Delta, \Delta, -\Delta),$

$(-\Delta, -\Delta, \Delta)$

Z_4 order breaks translational symmetry, but leaves rotational lattice symmetry intact

Can the system break Z_4 before it breaks O(3)?

Yes!

$$\frac{S[r,\phi]}{NV} = -\frac{(r-r_0)^2}{2u} + \frac{3\phi^2}{2g} + \frac{3r}{8\pi}$$
$$+\frac{1}{8\pi}\left[(r-2\phi)\log\frac{\Lambda^2}{r-2\phi} + 2(r+\phi)\log\frac{\Lambda^2}{r+\phi}\right]$$

$, \phi_3),$ where $\phi_i = g\left(\mathbf{\Delta}_j \cdot \mathbf{\Delta}_k\right) \quad \psi \propto \mathbf{\Delta}_1^2 + \mathbf{\Delta}_2^2 + \mathbf{\Delta}_3^2$

$$S[\psi, \boldsymbol{\phi}] = \int_x \left(\frac{|\boldsymbol{\phi}|^2}{2g} - \frac{\psi^2}{2u}\right) + \frac{3}{2}\int_q \log\left(\det \hat{\mathcal{X}}\right)$$

$$\hat{\mathcal{X}} = \begin{pmatrix} \tilde{\chi}_q^{-1} & -\phi_3 & -\phi_2 \\ -\phi_3 & \tilde{\chi}_q^{-1} & -\phi_1 \\ -\phi_2 & -\phi_1 & \tilde{\chi}_q^{-1} \end{pmatrix} \qquad \tilde{\chi}_q^{-1} = r_0 + \psi + q^2 \equiv r + q^2$$

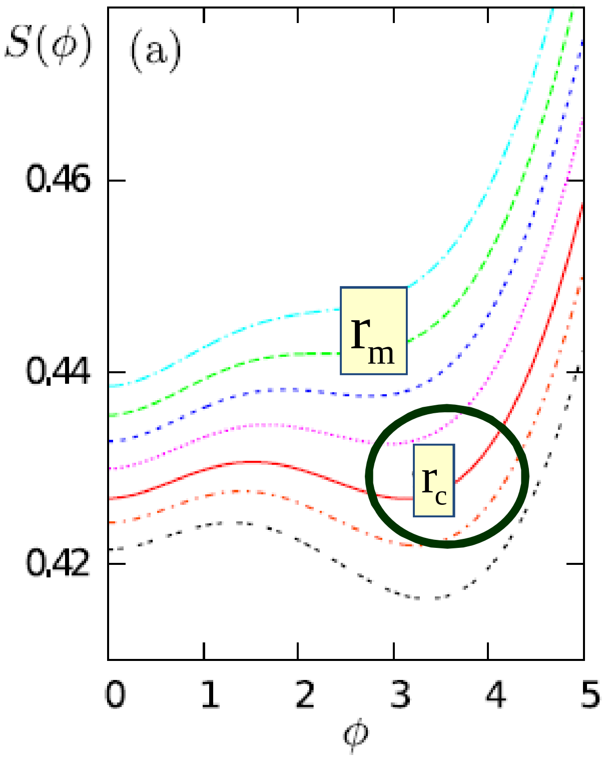
Can the system break Z_4 before it breaks O(3)?

Yes!

$$\frac{S[r,\phi]}{NV} = -\frac{(r-r_0)^2}{2u} + \frac{3\phi^2}{2g} + \frac{3r}{8\pi} + \frac{1}{8\pi}\left[(r-2\phi)\log\frac{\Lambda^2}{r-2\phi} + 2(r+\phi)\log\frac{\Lambda^2}{r+\phi}\right]$$

SDW order sets at r = 0

If $<\phi> \neq 0$ at r > 0 $\Rightarrow$ pre-emptive nematic order



1st order transition into a nematic state which breaks Z4 translational symmetry, but preserves O(3) spin rotational symmetry and also preserves lattice rotational symmetry

SDW — **Nematic** → **T**

O(3) broken
Z_4 broken

O(3) unbroken
Z_4 (translational) broken

Details:

Beyond mean-field: the transition is in the universality class of 4 state Potts model.

Potts model in 2D: the transition exists, is 2nd order, with $\beta = 1/12$ for $\phi \sim (T_c - T)^{\beta}$, almost 1st order

How to detect the nematic order?

Static spin susceptibility $\chi(Q)$ jumps at the nematic transition

$$\chi(\bar{r}_0) = \frac{1}{r}\left[1 + \left(\frac{\phi}{r}\right)^2 + \cdots\right]$$

Conclusions

Doped graphene is a wonderful playground to study truly unconventional superconductivity and SDW order

d+id superconductivity

semi-metallic SDW with spin-dependent excitations

pre-emptive nematic order

What's next: **f-wave (l=3) superconductivity ?**

co-existence of SDW and SC ?

THANK YOU