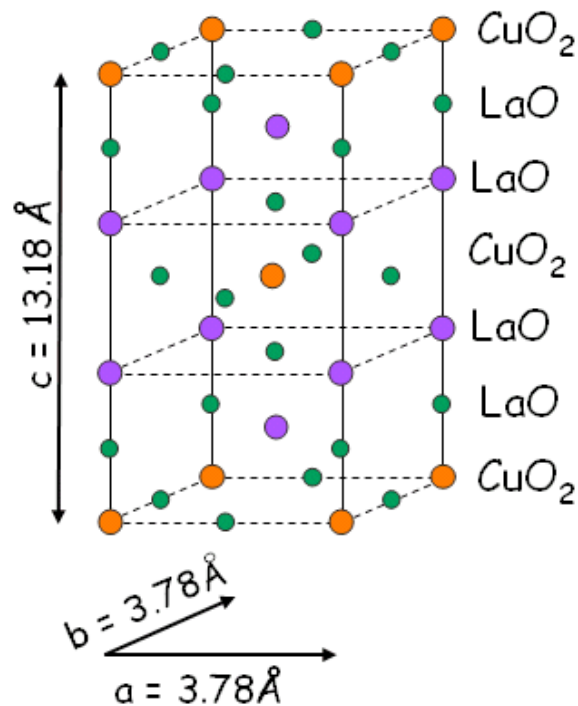
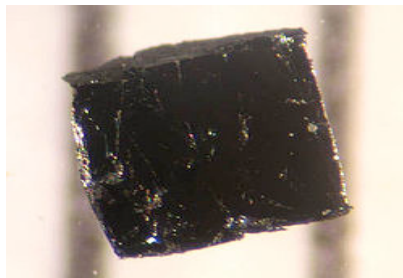


# High-Tc Superconductivity and the Hubbard model

Why is the 2D Hubbard model difficult to solve?  
Can we increase Tc?

Karyn Le Hur  
Yale

collaborators



T. Maurice Rice


C.-H. Chung (Yale)

I. Paul (Grenoble)

# Content

- BCS superconductors
- Introduction to High-Tc superconductors
- Link to John Hubbard and cold atoms

Unsolved problems in physics:  
*What is the responsible mechanism  
that causes certain materials to  
exhibit superconductivity at temperatures  
above 50 kelvin?*



Karyn Le Hur and T. Maurice Rice, arXiv:0812.1581 (98 pages)

Annals of Physics, Special Issue (2009)

Bilayer: K. Le Hur, C.-H. Chung, I. Paul and T. M. Rice, in progress

# Brief history of Superconductivity

1911: Kamerlingh Omnes

Hg becomes superconducting at 4K

1913: He won the Nobel price in physics



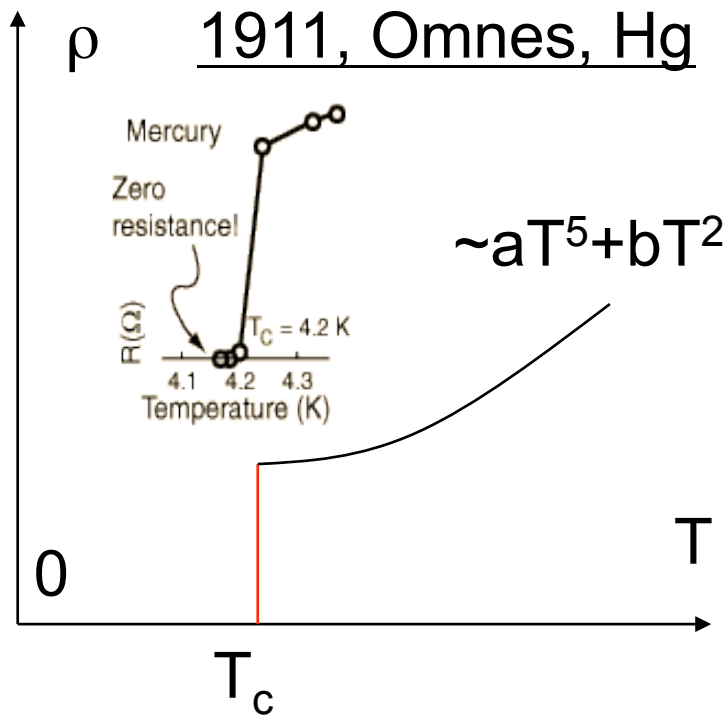
1933: Meissner effect

1941: niobium-nitride,  $T_c=16K$



Ginzburg-Landau (1950)

2 types of superconductors: Abrikosov (1957)



(below  $H_c$ : type I Scs  
below  $H_{c1}$ : type II Scs)

$$\vec{B} = \mu_0(\vec{H} + \vec{M}) = \vec{0}$$

$$\vec{M} = \chi \vec{H} \rightarrow \chi = -1$$

Perfect  
diamagnetism

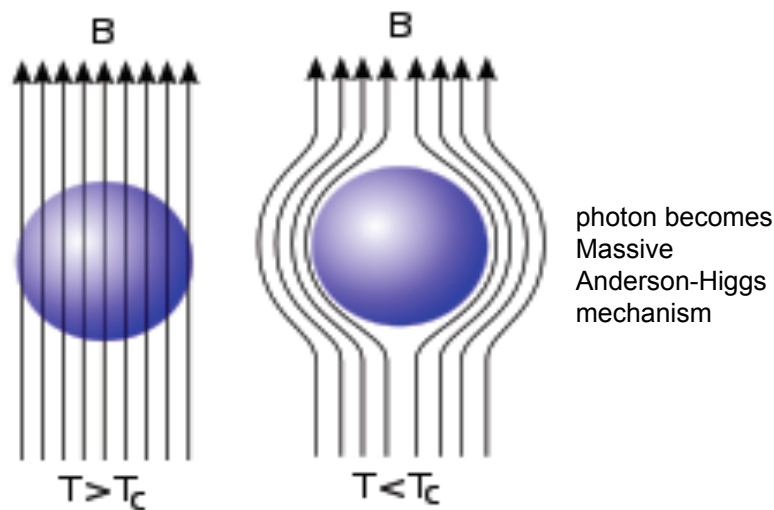
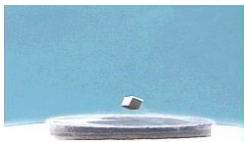
London & London (1935)  
(transport without dissipation)

$$\vec{j}_s(\vec{r}) = -\frac{n_s e^2}{m} \vec{A}(\vec{r})$$

$$\vec{\nabla} \times \vec{B} = \mu_0 \vec{j}_s$$

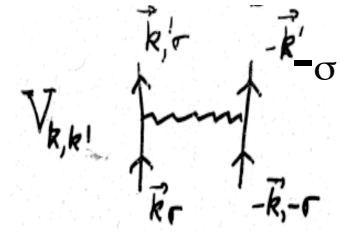
$$\vec{\nabla}^2 \vec{B} = \frac{1}{\lambda_L^2} \vec{B}$$

$$\lambda_L^2 = \frac{m}{\mu_0 n_s e^2} \quad (\text{SI})$$



Meissner-Ochsenfeld (1933)

# Lattice Vibrations...



Simple model of screening: compute the full  $\epsilon...$  (1950)

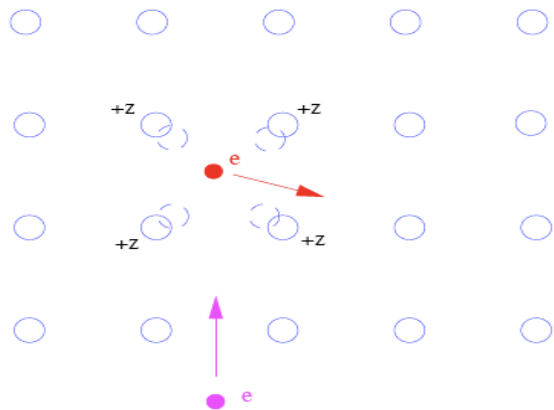
$$V_{\vec{k},\vec{k}'} = \frac{4\pi e^2}{(\vec{k} - \vec{k}')^2 + k_c^2} \left( 1 + \frac{\hbar^2 \omega^2 (\vec{k} - \vec{k}')}{(\epsilon_{\vec{k}} - \epsilon_{\vec{k}'})^2 - \hbar^2 \omega^2 (\vec{k} - \vec{k}')} \right)$$

Thomas Fermi wave-vector

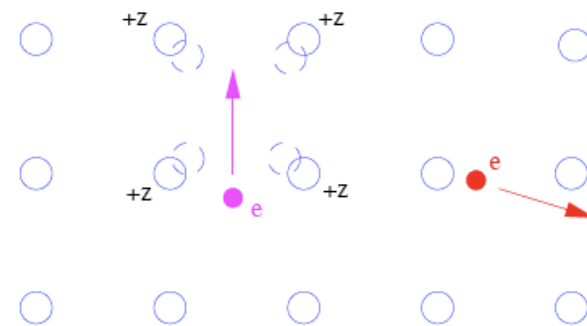
Ion contribution

Possible attractive interaction

$$\omega = (\epsilon_{\vec{k}} - \epsilon_{\vec{k}'})/\hbar < \omega(\vec{k} - \vec{k}') < \omega_D$$



$$\omega(\vec{k}) = \frac{\Omega_p^2}{1 + \frac{k_c^2}{k^2}}$$



Fröhlich (1950), Bardeen-Pines (1955),...

# Basic steps of BCS theory

Tinkham or De Gennes book,...

$$E_D = \hbar\omega_D$$
$$H - \mu N = \sum_{\vec{k}\sigma} \xi_{\vec{k}} n_{\vec{k}\sigma} - \sum_{\vec{k}\vec{p}} V c_{\vec{k}\uparrow}^\dagger c_{-\vec{k}\downarrow}^\dagger c_{-\vec{p}\downarrow} c_{\vec{p}\uparrow}$$

$$|\psi_G\rangle = \prod_{\vec{k}} \left( u_{\vec{k}} + v_{\vec{k}} c_{\vec{k}\uparrow}^\dagger c_{-\vec{k}\downarrow}^\dagger \right) |\phi_0\rangle$$

Determination of BCS coefficients through variational approach

$$\Delta = V \sum_{\vec{k}} \langle \Psi_G | c_{-\vec{k}\downarrow} c_{\vec{k}\uparrow} | \Psi_G \rangle = V \sum_{\vec{k}} u_{\vec{k}} v_{\vec{k}} = V \sum_{\vec{k}} \frac{\Delta}{2\sqrt{\xi_{\vec{k}}^2 + \Delta^2}}$$

Quasiparticle energy

$$E_{\vec{k}} = (\xi_{\vec{k}}^2 + \Delta^2)^{1/2}$$

$$\Delta \sim 2\omega_D \exp(-1/N_o V)$$

Zero temperature evaluation of the gap

# BCS Theory, 1957



Bogoliubov, 1958

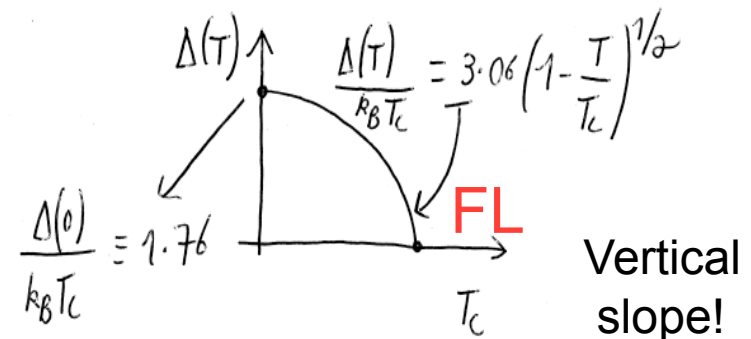
BCS theory assumes some attraction between electrons

Coupling of electrons to the vibrating crystal lattice (**phonons**)

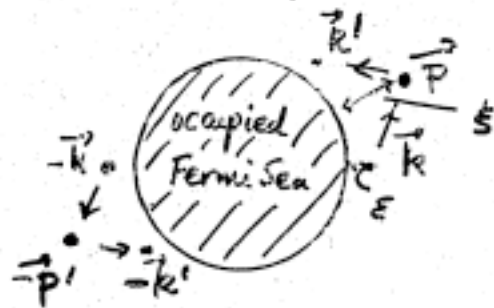
Fermi liquid to SC at:  $k_B T_c = 1.1 E_D \exp -1/N(0)V \quad 2e^\gamma/\pi \approx 1.13$

$$\frac{1}{V} = \frac{1}{2} \sum_{\vec{k}} \frac{\tanh(\beta E_{\vec{k}}/2)}{E_{\vec{k}}}$$

Gap at T=0 grows with  $T_c$   
Debye energy not high: 100K



## Landau Theory



Matrix Element connecting initial and final states

$$\Gamma(\epsilon) = V + \frac{V^2}{\Omega} \sum_{\xi < D} \frac{2}{P} \frac{1}{2(\epsilon - \xi)} + \dots$$

D: Energy Cutoff.

## Scaling Hypothesis

$$\Gamma\left(\frac{\epsilon}{D}, V\right) = \Gamma\left(\frac{\epsilon}{D'}, V'\right)$$

works with

$$V \mapsto V' = \frac{V}{1 + \frac{mk_F \cdot V \cdot \ln\left(\frac{D}{D'}\right)}{2\pi^2}}$$

• attractive Interactions  
E1-Phonon  $D \sim D_D$  scale to  $-\infty$

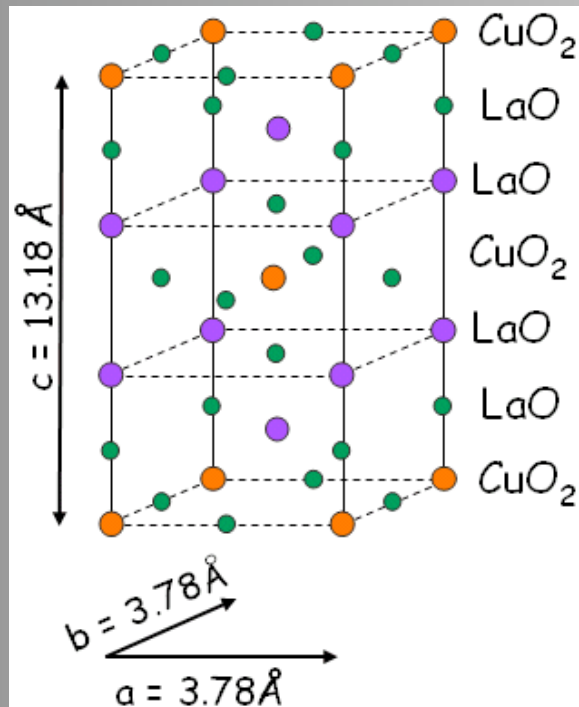
→ BCS Theory based on Cooper Instability of an s-wave pair

L. Cooper (1956)  
Hides RG formulation

Anderson-Higgs 1963, 1964



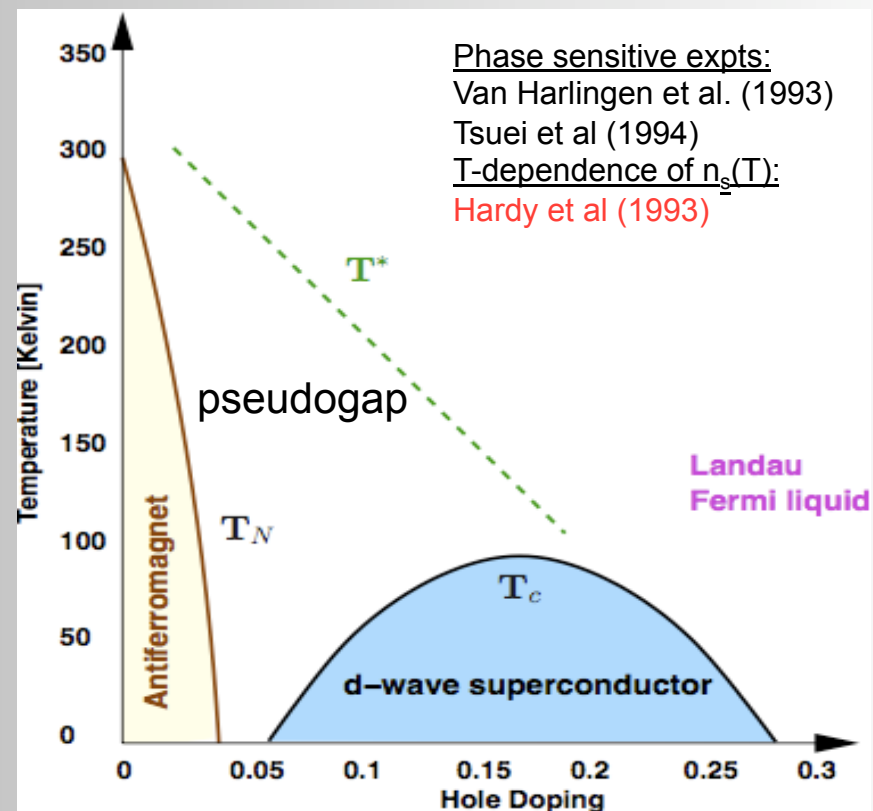
# High Temperature Superconductors



1986



- Coupled  $\text{CuO}_2$  layers
- Doping with holes leads to SC
- Nonmonotonic  $T_c$  versus doping
- Maximum  $T_c \sim 150 \text{ K}$
- Electronic SC without phonons?
- Normal phase is not a Fermi liquid at low doping: gap does not follow  $T_c$ !



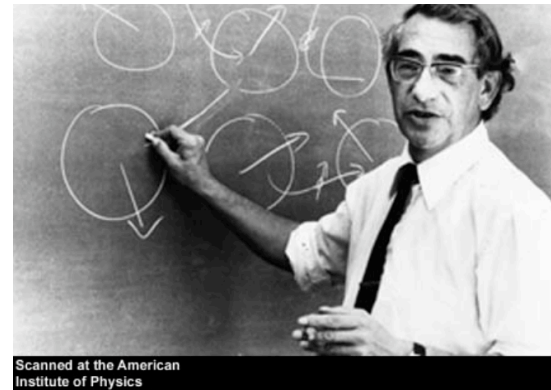
# Hubbard model or t-J model

$$H = \sum_{\langle i;j \rangle, s} -t c_{is}^\dagger c_{js} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Large on-site interaction  $U$ : t-J model

$$H = \sum_{\langle i;j \rangle, s} -t c_{is}^\dagger c_{js} + \mathbf{J} \sum_{\langle i;j \rangle} \vec{S}_i \cdot \vec{S}_j$$

$$J = \frac{4t^2}{U}$$
$$\vec{S}_i = c_{is}^\dagger \sigma_{ss'} c_{is'}$$

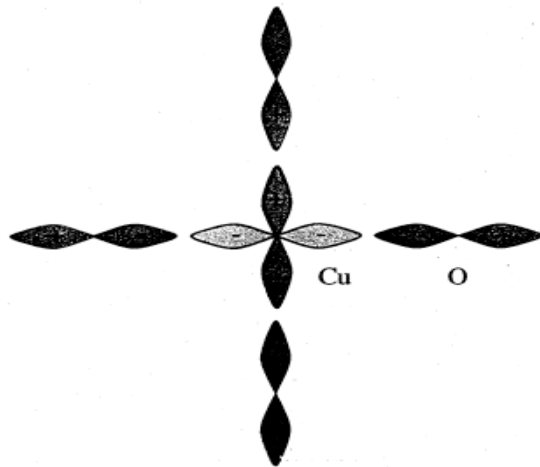


**BIOGRAPHY OF  
JOHN HUBBARD**  
(1931 - 1980)

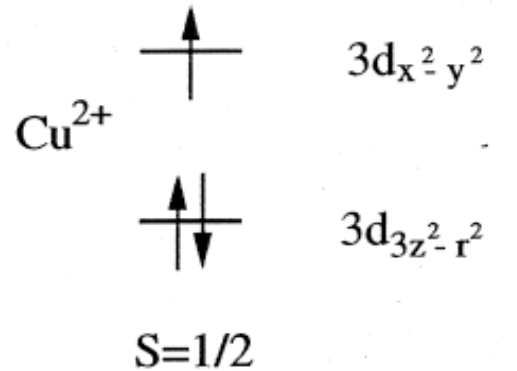
born Oct. 27, 1931,  
London, England.  
died Nov. 27, 1980, San  
Jose, CA., U.S.

# Planar cuprates

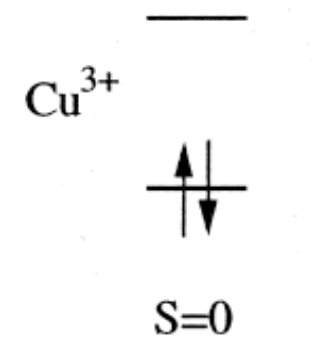
Octahedral crystal field:  $e_g$   
Square planar distortion



## Oxidation States:



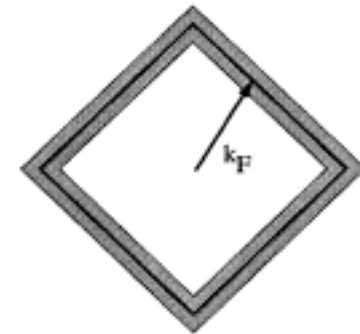
(9 d-electrons & 5 orbitals)



charge +1e1

Zhang-Rice singlets

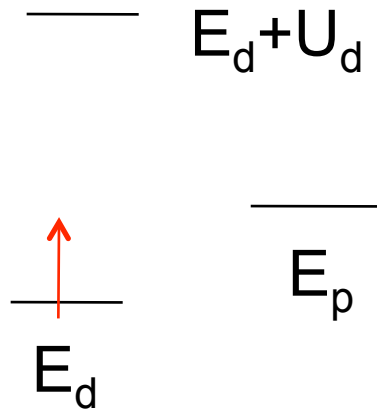
- Stoichiometric Oxides:  
all  $\text{Cu}^{2+} \rightarrow$  AF Mott Insulators.
- Hole doped Oxides:  
 $\sim 15\% \text{Cu}^{3+} \rightarrow$  High- $T_c$  Superconductors.



t-J model or Hubbard model at large U

Zhang-Rice (1988)

# Hole picture



$$H_{eff} = J \sum_{\langle i;j \rangle} \left( \vec{S}_i \vec{S}_j - 1/4 \right)$$

$$U_d = 10.5 \text{ eV}$$

$$E_p - E_d \sim 3.6 \text{ eV}$$

$$t_{pd} \sim 1.3 \text{ eV}$$

Schlüter et al

## Hubbard parameters:

$$t \sim 0.4 \text{ eV} \quad \text{P. Fleury, Z. Fisk et al}$$

$$J \sim 0.145 \text{ eV} \quad (0.13 - 0.15 \text{ eV})$$

(Debye T for Cu  $\sim 315 \text{ K}$ )

$$U \sim E_p - E_d \quad (2 - 4 \text{ eV})$$

$$J = \frac{4t_{pd}^4}{(E_p - E_d)^2} \left( \frac{1}{U_d} + \frac{1}{E_p - E_d} \right)$$

$$t = \frac{t_{pd}^2}{E_p - E_d}$$

# t-J model

$$H = -t \sum_{\langle i,j \rangle} d_{is}^\dagger d_{js} - \mu \sum_{i,s} d_{is}^\dagger d_{is} + J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

Trial wavefunction and physical properties must reflect that the (effective) on-site interaction is large (Anderson, 1987)

Superconductivity can be described through **P|BCS>**, where

$$P = \prod_i (1 - n_{i\uparrow} n_{i\downarrow}) \quad |BCS\rangle = \prod_{\vec{k}} (u_{\vec{k}} + v_{\vec{k}} d_{\vec{k}}^\dagger d_{-\vec{k}}^\dagger) |Vac\rangle$$

Gutzwiller approximation (1963): statistical weighting factors

$$H = -t g_t \sum_{\langle i,j \rangle} d_{is}^\dagger d_{js} - \mu \sum_{i,s} d_{is}^\dagger d_{is} + J g_s \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j$$

$\langle d_{is}^\dagger d_{js} \rangle = g_t \langle d_{is}^\dagger d_{js} \rangle_0$
$\langle \vec{S}_i \cdot \vec{S}_j \rangle = g_s \langle \vec{S}_i \cdot \vec{S}_j \rangle_0$

$g_t = 2\delta/(1+\delta)$  and  $g_s = 4/(1+\delta)^2$       Rice et al. 1988

review: Anderson, Rice, Lee et al (2004)

$$H_{mf} = - \sum_{\langle i;j \rangle} (tg_t + \chi_{ij}) d_{is}^\dagger d_{js} - \sum_{is} \mu d_{is}^\dagger d_{is} + \sum_{\langle i;j \rangle} \Delta_{ij} (d_{i\uparrow}^\dagger d_{j\downarrow}^\dagger - d_{i\downarrow}^\dagger d_{j\uparrow}^\dagger) + h.c.$$

2 order parameters:  $\chi_{ij} = (3g_s J/4) \langle d_{is}^\dagger d_{js} \rangle$  and  $\Delta_{ij}$

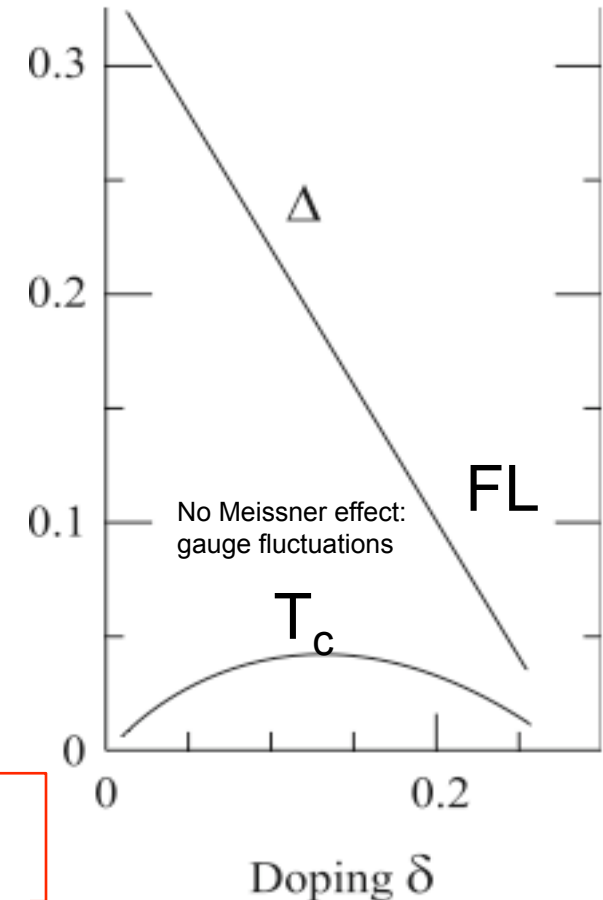
$$\Delta_{\vec{k}} = \frac{3}{4} g_s J \sum_{\vec{k}'} \gamma_{\vec{k}-\vec{k}'} \frac{\Delta_{\vec{k}'}}{2E_{\vec{k}'}}$$

$$\chi_{\vec{k}} = \frac{3}{4} g_s J \sum_{\vec{k}'} \gamma_{\vec{k}-\vec{k}'} \frac{-\xi_{\vec{k}'}}{2E_{\vec{k}'}}$$

$(\Delta(\cos k_x - \cos k_y))$  and  $\gamma_{\vec{k}} = 2(\cos k_x + \cos k_y)$

$\xi_{\vec{k}} = g_t \epsilon_{\vec{k}} - \mu - \chi_{\vec{k}}$  and  $\epsilon_{\vec{k}} = -t\gamma_{\vec{k}}$

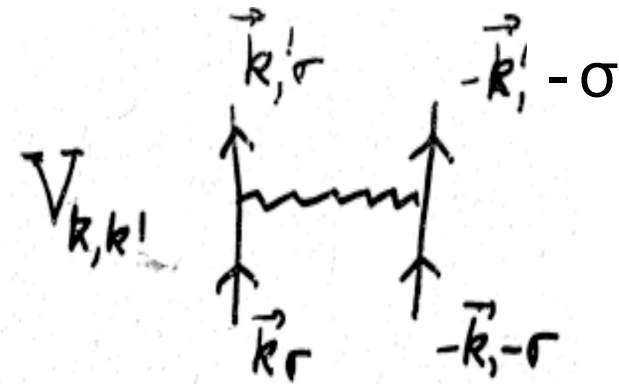
$$(T_c)^2 = \langle BCS | P(d_{i\uparrow}^\dagger d_{j\downarrow}^\dagger d_{i+l\uparrow} d_{j+l\downarrow}) P | BCS \rangle = g_t^2 \Delta^2$$



# D-wave superconductivity...

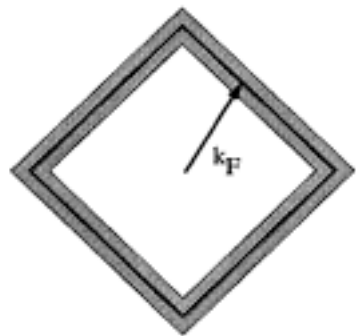
$$\Delta(\vec{p}) = - \sum_{\vec{p}'} V_S(\vec{p} - \vec{p}') \frac{\Delta(\vec{p}')}{2E_{\vec{p}'}}$$

$$V_S(\vec{Q}) = -\frac{6}{4}g_s J(\cos Q_x + \cos Q_y)$$



Spin fluctuations make the singlet channel interaction more positive (repulsive) at  $(\pi, \pi)$ :  $V_S(\pi, \pi) > 0$

$$\Delta(\pi, 0) < 0$$



$$\Delta(0, \pi) > 0$$

Very general argument!

example of Kohn-Luttinger attraction

- Superconducting  $T_c = g_t \cdot \Delta$

$T_c$  must go to zero at zero doping: insulator

$T_c$  must go to zero at large doping: Fermi liquid

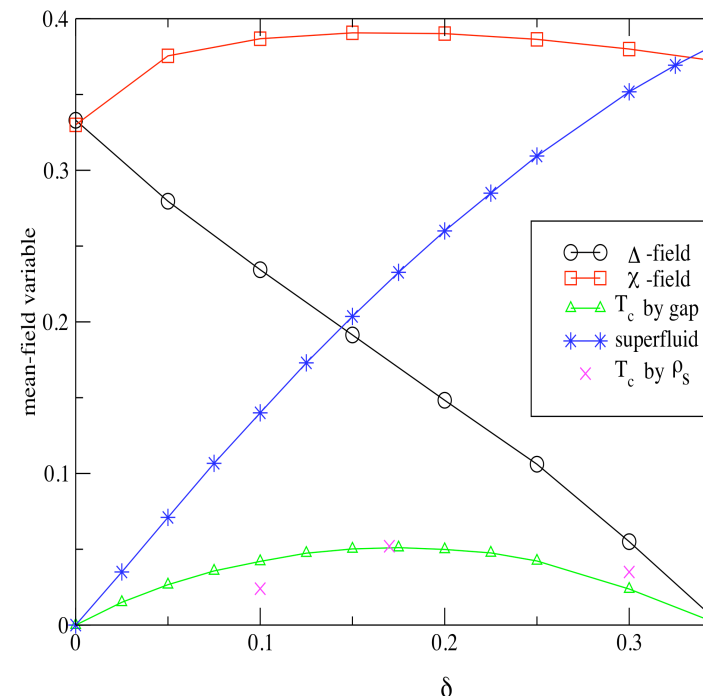
Maximum  $T_c$  at optimal doping  $T_c \sim g_t J/2 \sim 169K$

- d-wave quasiparticles: reduction of superfluid density  $n_s(T_c)=0$

$$n_s(T) = n_s(0) - AT, \quad A \propto v_F/v_\Delta$$

$T_c$  follows  $n_s(T=0) \sim g_t$  and  $\Delta$

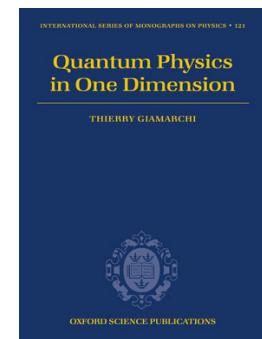
Lee and Wen (1997); Millis, Girvin, et al (1998)



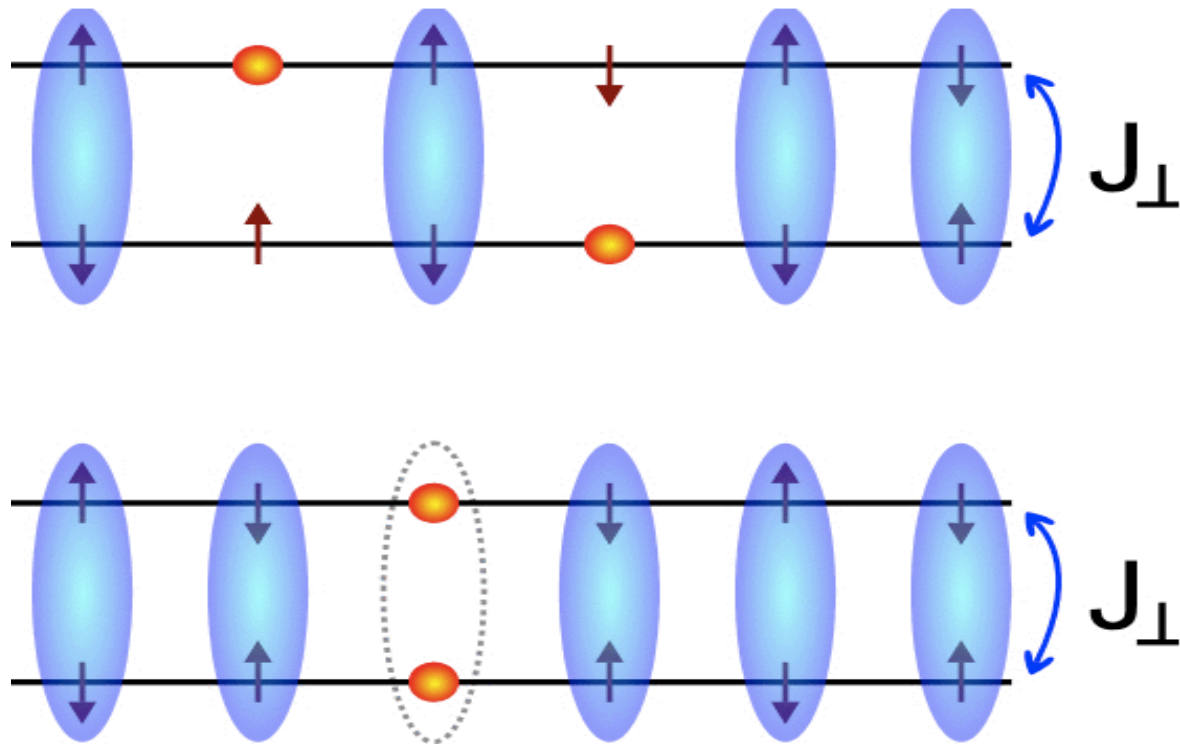


# D-wave Superconductivity

- Weak-coupling argument: RPA approach
- Numerical methods: DMFT and extensions
- Gauge theories
- Renormalization Group methods
- Quasi-1D limit



# Rigorous Limit: Ladder



Strong Interaction Limit

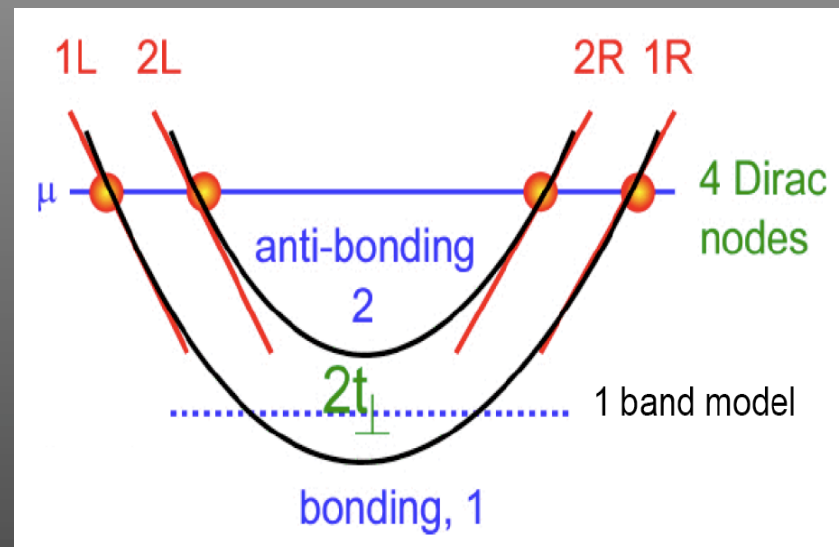
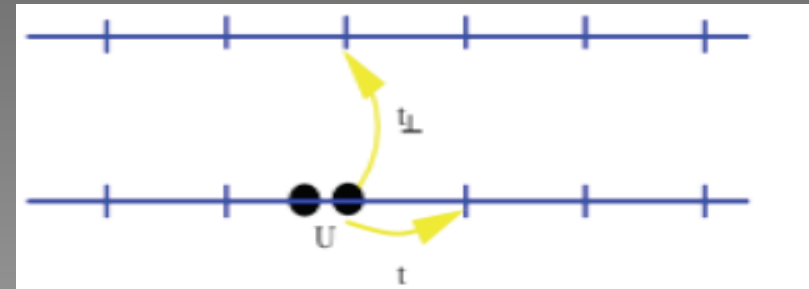
# Weak coupling regime

First, diagonalize the spectrum

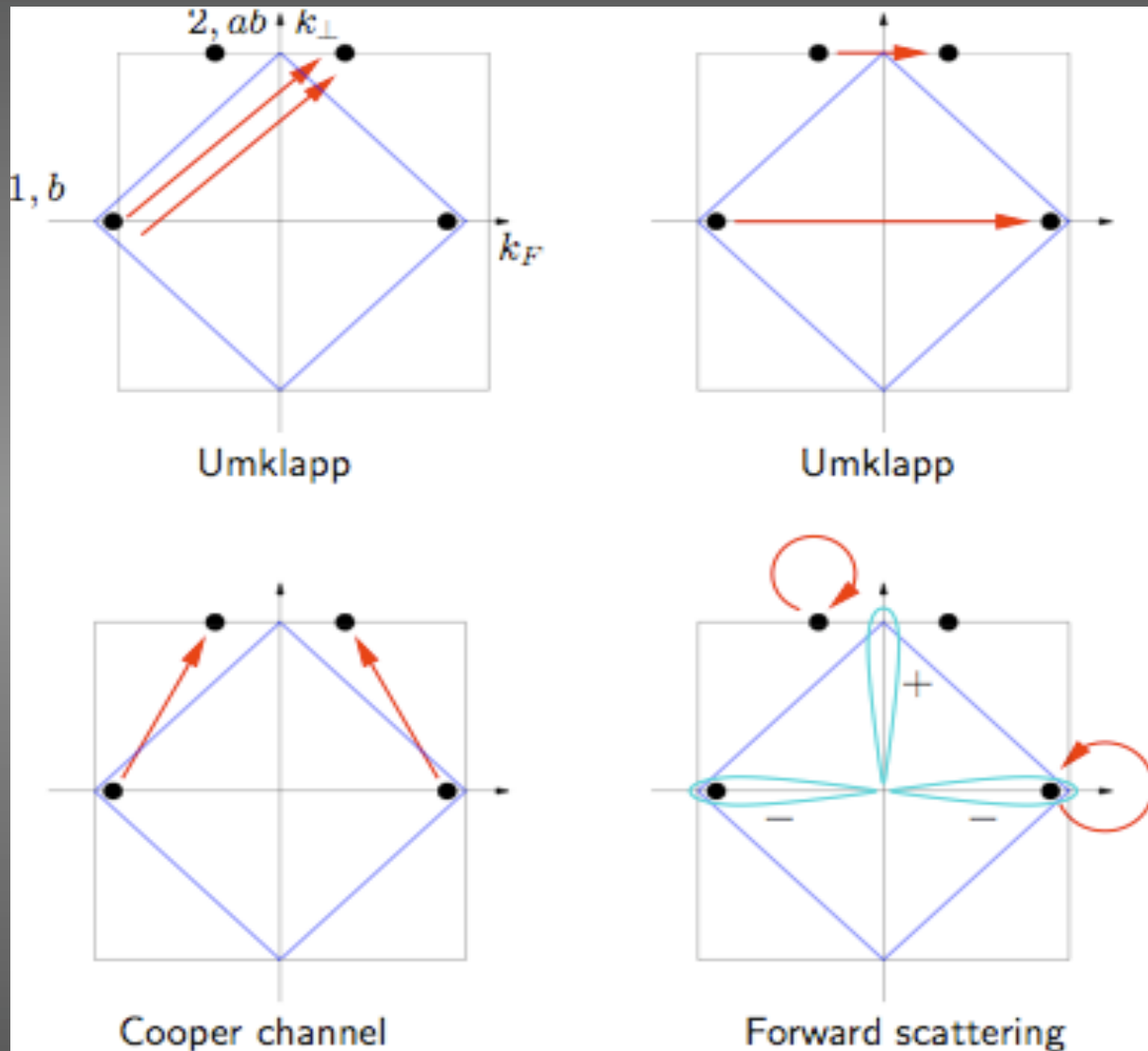
$$\epsilon_j(k) = \mp t_{\perp} - 2t \cos(k)$$

Half-filling:  $\nu_1 = \nu_2$   
and  $k_{F1} + k_{F2} = \pi$

Large Doping:  $\nu_2 \ll \nu_1$



# 2D Interpretation of couplings



Competing channels: RG approach

# Example: RG for spinless fermions

Urs Ledermann & K. Le Hur, PRB 61, 2497 (2000)

Away from Half-filling

$$\begin{aligned}
 H_{Int} = & \int dk_1 dk_2 dk_3 dk_4 \delta(k_1 + k_3 - k_2 - k_4) \\
 & \times [c_1 \Psi_{R1}^\dagger(k_1) \Psi_{R1}(k_2) \Psi_{L1}^\dagger(k_3) \Psi_{L1}(k_4) + c_2(1 \leftrightarrow 2) \\
 & + f_{12}(\Psi_{R1}^\dagger(k_1) \Psi_{R1}(k_2) \Psi_{L2}^\dagger(k_3) \Psi_{L2}(k_4) + 1 \leftrightarrow 2) \\
 & + c_{12}(\Psi_{R1}^\dagger(k_1) \Psi_{R2}(k_2) \Psi_{L1}^\dagger(k_3) \Psi_{L2}(k_4) + 1 \leftrightarrow 2)].
 \end{aligned}$$

$$\frac{dc_1}{dl} = -\frac{1}{2\pi v_2} c_{12}^2$$

$$\frac{dc_2}{dl} = -\frac{1}{2\pi v_1} c_{12}^2$$

$$\frac{df_{12}}{dl} = \frac{1}{\pi(v_1 + v_2)} c_{12}^2$$

$$\frac{dc_{12}}{dl} = \frac{c_{12}}{\pi} \left( \frac{2f_{12}}{v_1 + v_2} - \frac{c_1}{2v_1} - \frac{c_2}{2v_2} \right)$$

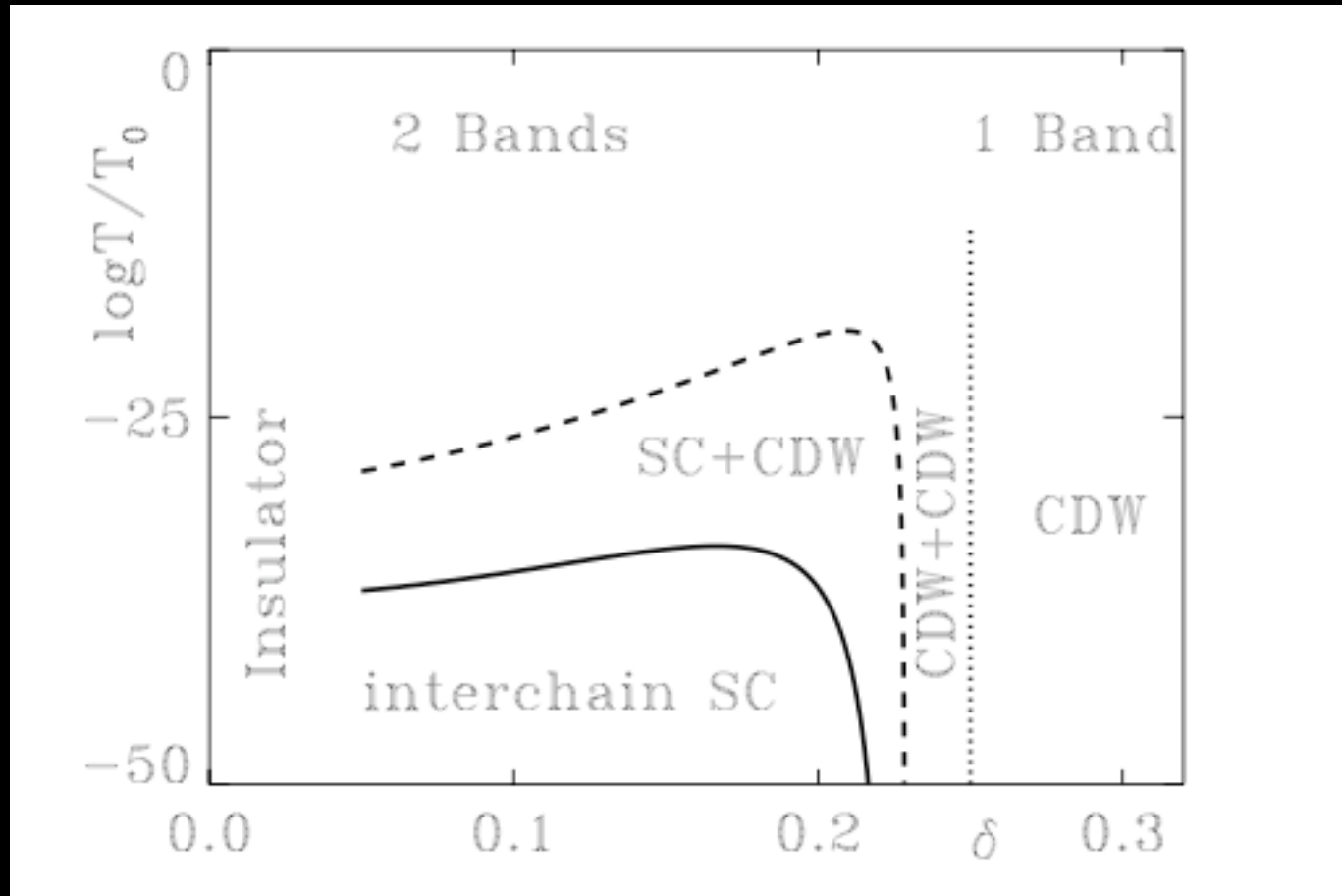
$$D' \sim t e^{-l}$$

$$v_1 - v_2 = \frac{2t_\perp}{\tan(\pi n)}$$

**$c_{12}$ :**  
phase coherence  
between bands

Solvable set of differential equations + strong coupling treatment

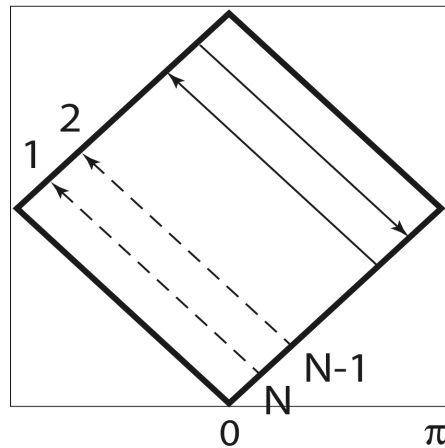
# Phase Diagram



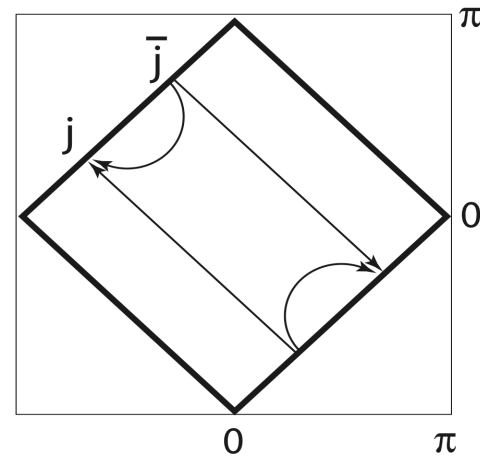
Urs Ledermann & K. Le Hur, PRB 61, 2497 (2000)

# Extension to 2D...

AFM channels



D-wave Cooper channel



- Antiferromagnetism at half-filling
- D-wave superconducting phase
- Fermi liquid phase for large dopings

Karyn Le Hur and T. Maurice Rice, arXiv:0812.1581 (98 pages)  
Annals of Physics, Special Issue (2009)

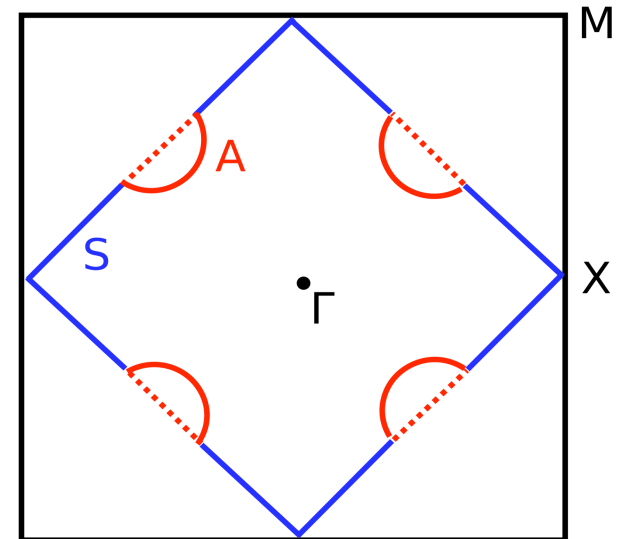
# Close to half-filling

- New phase (D-Mott)

antinodal incompressible RVB regions

nodal regions: metallic

proximity effect of the Fermi arcs with the RVB region = Andreev scattering (?)



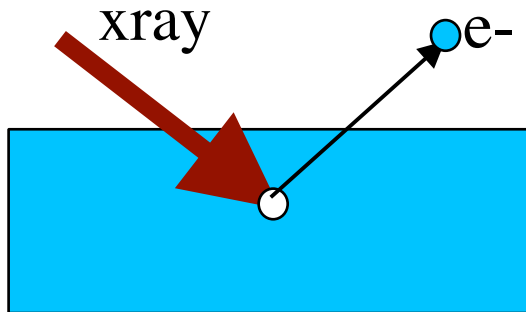
Only the Fermi arcs become  
superconducting below  $T_c$ : “2 gaps”

Karyn Le Hur and T. Maurice Rice, arXiv:0812.1581 (98 pages)  
Urs Ledermann, Karyn Le Hur, T. Maurice Rice, PRB **62**, 16383 (2000)  
J. Hopkinson and K. Le Hur, PRB **69**, 245105 (2004)



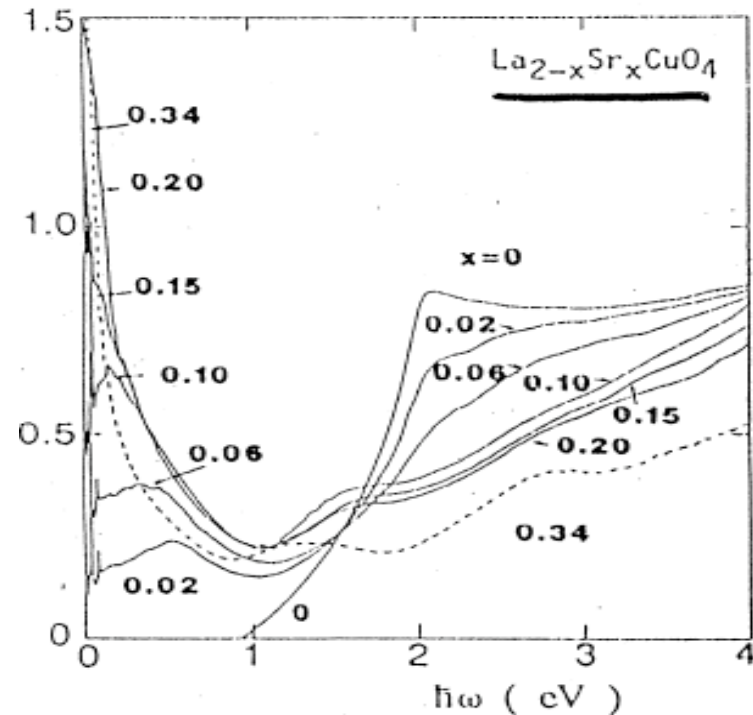
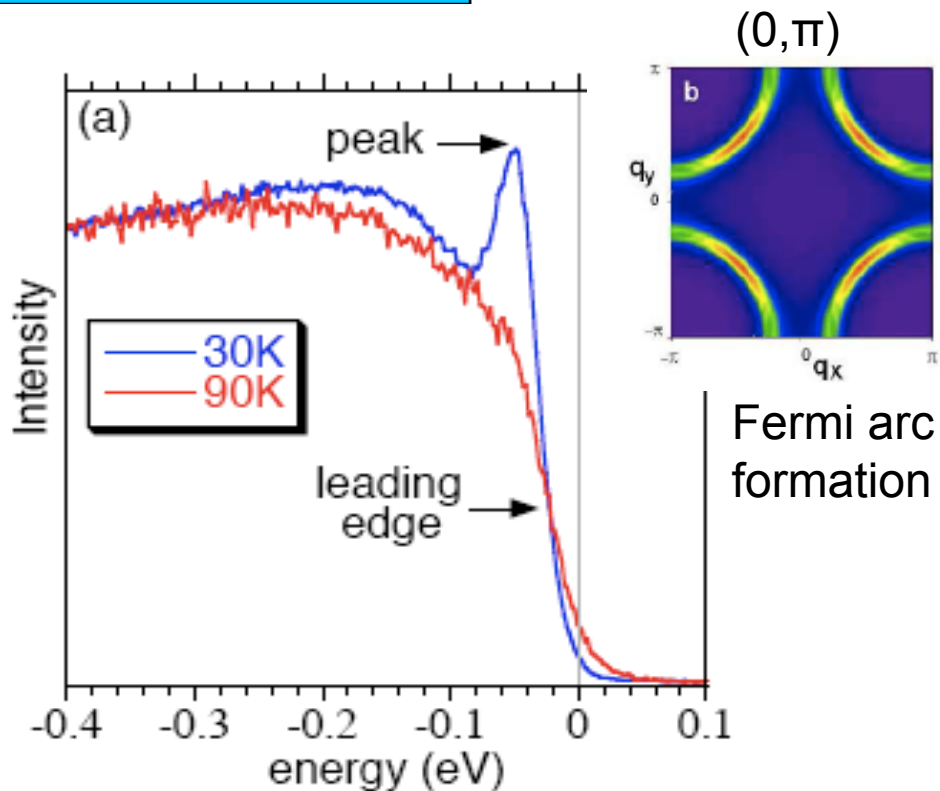
# Pseudogap: RVB-like

Also spin gap in  $\chi(T)$ , and  $\rho_c$  increases  
(Orsay: Alloul, Friedel, 1989)



Photoemission:

Optical conductivity  $\sigma$



Mott gap versus Drude:  
Drude weight  $\propto \delta$

Kaminski-Campuzano

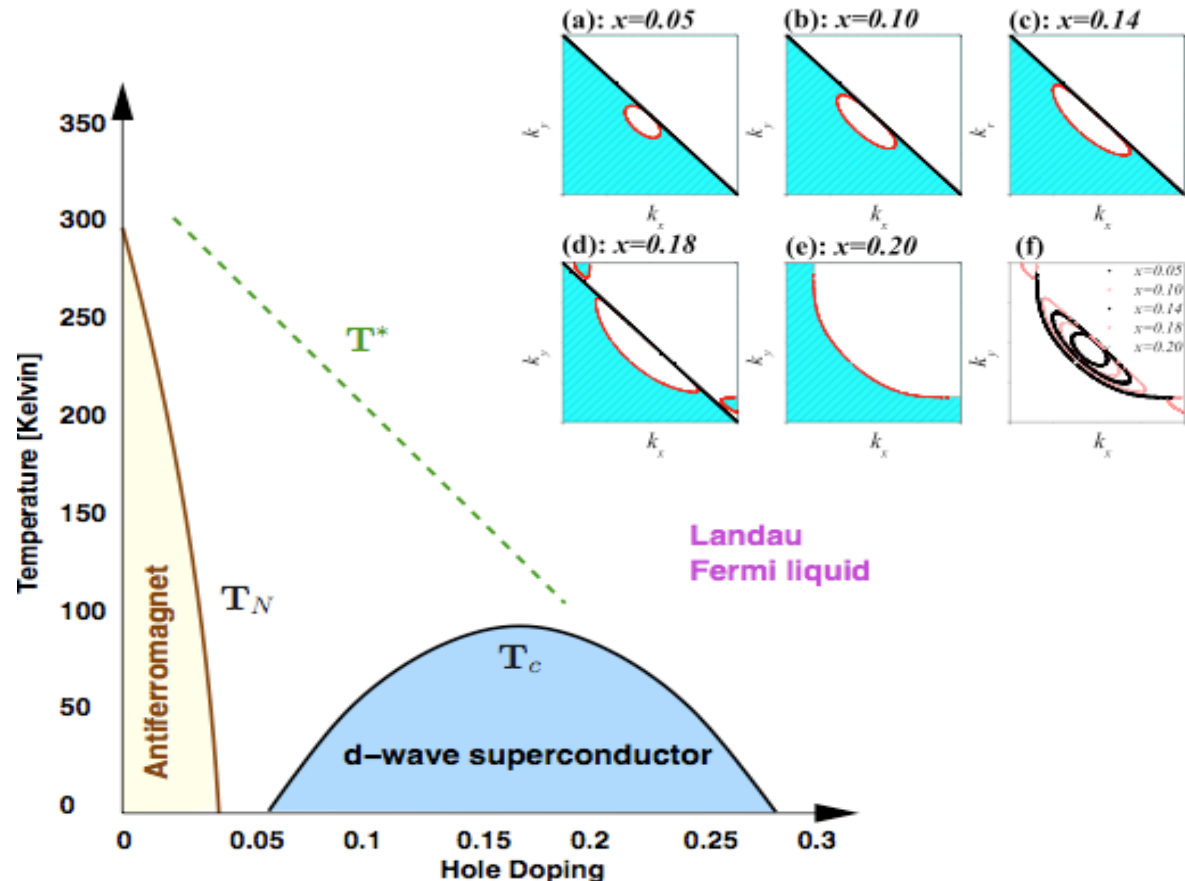
# Conclusion

Increase  $T_c$ ?  
bilayer?

Fe-based systems

Sc in graphene  
Bergman/Le Hur (2009)

Applications to cold atomic  
Gases: “phonons” can be  
engineered by a BEC



2 distinct gaps: D-Mott gap ( $T^*$ ) & SC gap ( $T_c$ )  
(SUPPORTED BY ARPES EXPERIMENTS, ANDREEV REFLECTION, AND RAMAN SCATTERING)

Thank you for your Attention!

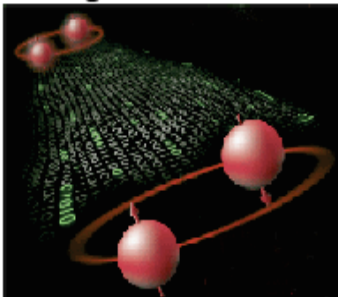
# Interests of my group

## Research

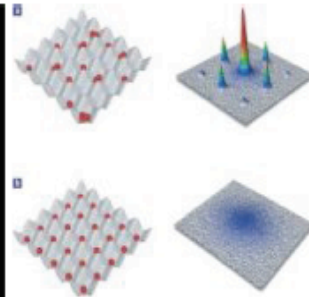
### Quantum Phenomena, Simulators and Computing

- I am a theorist aiming to answer important fundamental questions in physics-related interdisciplinary research areas engaging condensed-matter, many-body systems, quantum information theory, quantum field theory, statistical physics, cold atomic systems, and nanoelectronics.
- **Keywords**
  - Many-Body Theory
  - Quantum Computation
  - Novel Quantum Phenomena: Fractionalization, Superconductivity
  - Quantum Simulators: Cold Atomic gases, NanoSystems, Photons
  - Non-equilibrium Transport

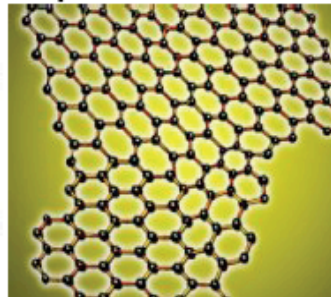
Entanglement



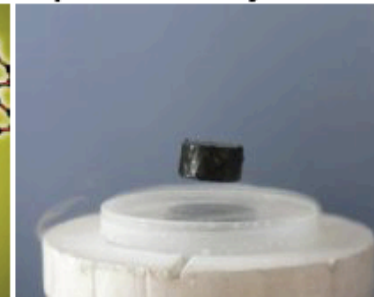
Quantum Simulators



Graphene



Superconductivity



Topological Superconductors/Insulators

