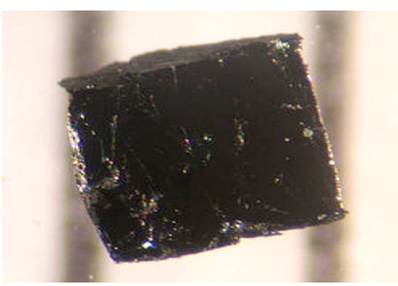
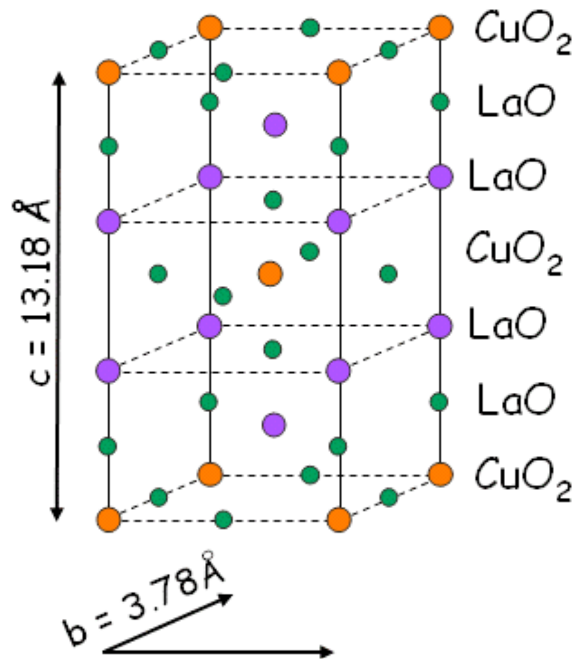
Physics behind High-Tc superconductors

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

Karyn Le Hur
Yale





collaborator

T. Maurice Rice

Outline of the Talk

- BCS superconductors
- Introduction to High-Tc superconductors

  What is understood? What is not…
- D-wave state: Gutzwiller-type wave-function

  Magnetic fluctuations mediate d-wave superconductivity

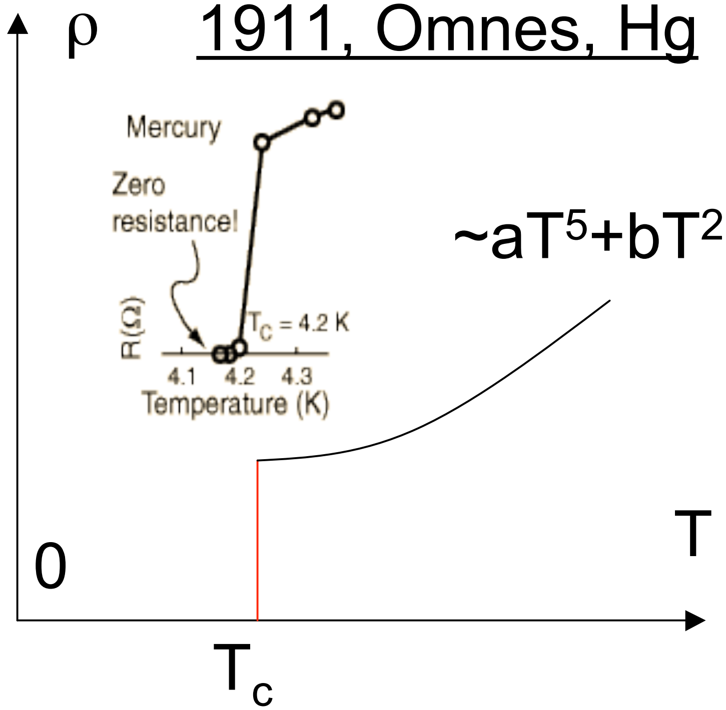
☒ Our approach(es) to the phase diagram and results for the pseudogap phase

Karyn Le Hur and T. Maurice Rice, arXiv:0812.1581 (97 pages)

published in Annals of Physics

(also: relevant applications in optical lattices and cold atoms)

1911, Omnes, Hg



(below H_c: type I Scs
below Hc_1: type II Scs)

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

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

Perfect diamagnetism

London & London (1935)

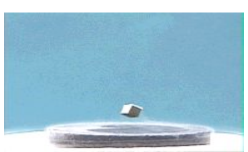
(transport without dissipation)

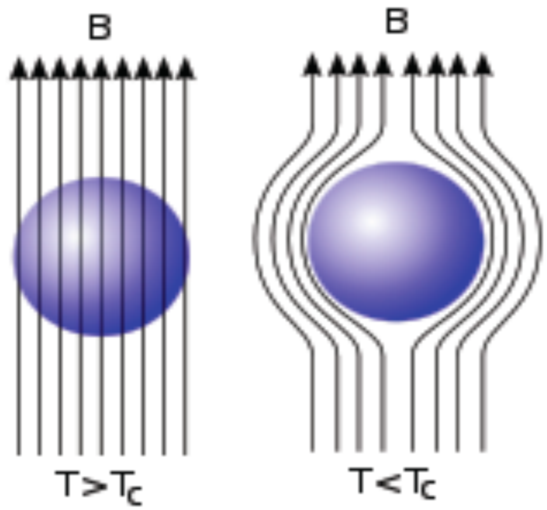
$$\vec{j}_s(\vec{r}) = -\frac{n_s e^2}{m} \vec{A}(\vec{r})$$

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

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

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





photon becomes
Massive
Anderson-Higgs
mechanism

Meissner-Ochsenfeld (1933)

Brief history of Superconductivity

1911: Kamerlingh Omnes

Hg becomes superconducting at 4K

1913: He won the Nobel price in physics

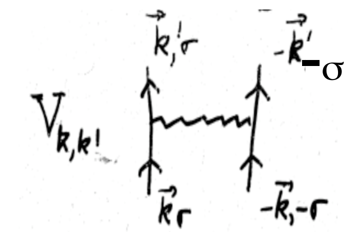
1933: Meissner effect

1941: niobium-nitride, T_c=16K

Ginzburg-Landau (1950)

2 types of superconductors: Abrikosov (1957)

Lattice Vibrations…



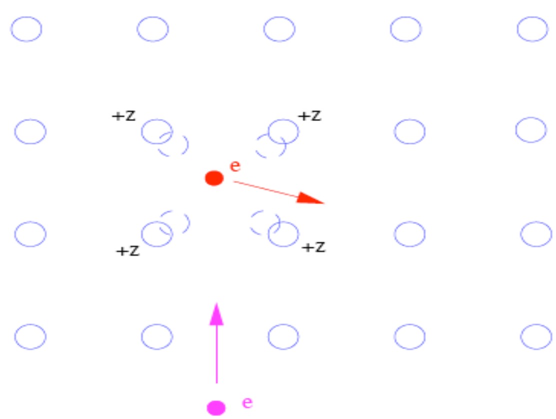
Simple model of screening: compute the full ε… (1950)

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

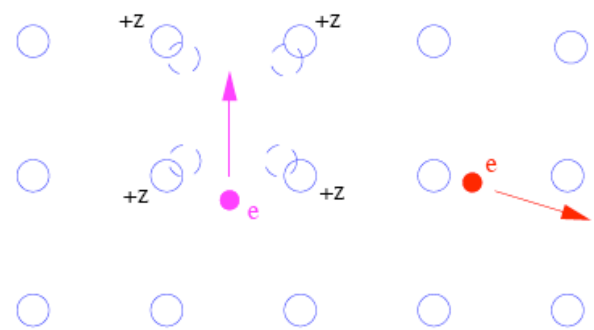
Thomas Fermi wave-vector

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,…

$$E_D = \hbar\omega_D$$

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

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

Determination of BCS coefficients through variational approach

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

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

Quasiparticle energy

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

Zero temperature evaluation of the gap

BCS Theory, 1957

Bogoliubov, 1958

BCS theory assumes some attraction between electrons

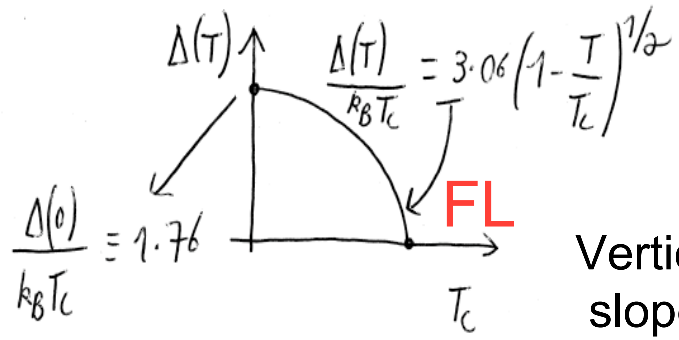
Coupling of electrons to the vibrating crystal lattice (phonons)

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

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

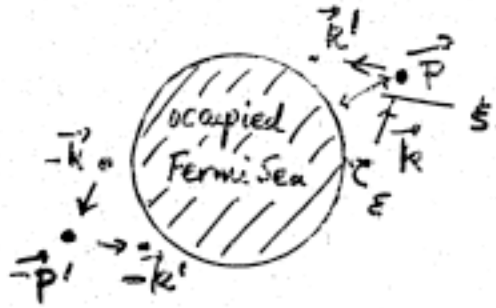
Gap at T=0 grows with T_c

Debye energy not high: 100K



Vertical slope!

Landau Theory



Matrix Element connecting initial and final states

$$\Gamma(\varepsilon) = V + \frac{V^2}{\Omega}\sum_{\vec{p}}^{\xi < D} \frac{2}{2(\varepsilon - \xi)} + \cdots$$

D: Energy Cutoff

Scaling Hypothesis

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

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

- attractive Interactions

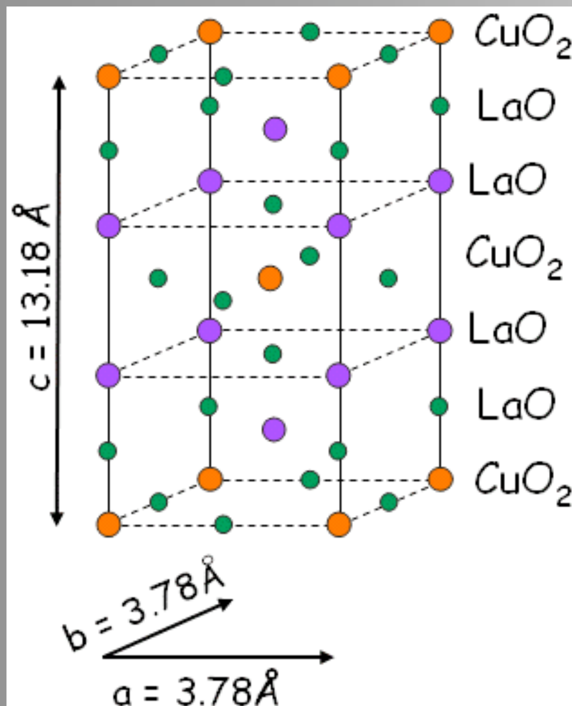
El-Phonon $D \sim \theta_D$ scale to $\underline{\underline{-\infty}}$

$\rightarrow$ BCS Theory based on Cooper Instability of an s-wave pair

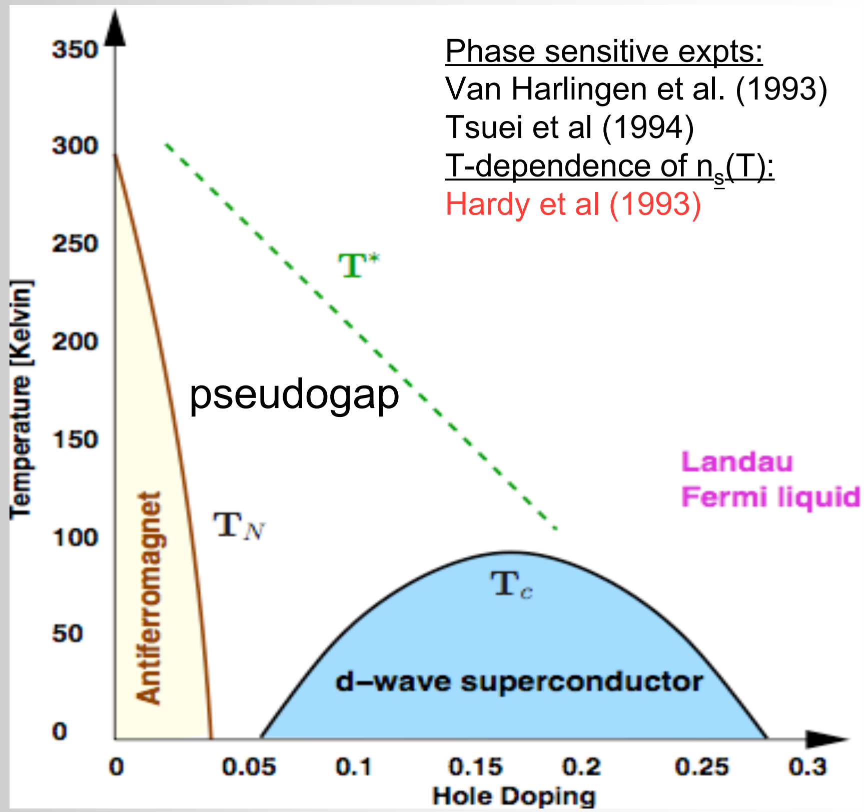
L. Cooper (1956)
RG formulation (Shankar colloquium)

Anderson-Higgs 1963,1964

High Temperature Superconductors

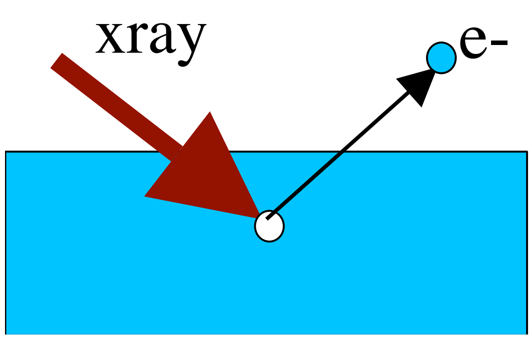


1986



- Coupled CuO_2 layers
- Doping with holes leads to SC
- Nonmonotonic Tc versus doping
- Maximum Tc ~ 150 K
- Electronic SC without phonons?
- Normal phase is not a Fermi liquid at low doping: gap doesnot follow Tc!

Pseudogap: RVB-like

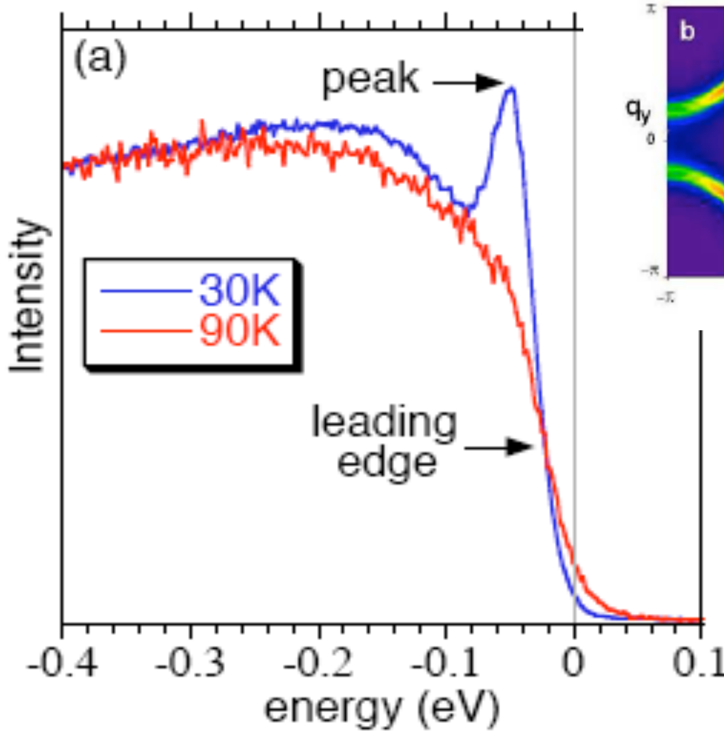


Also spin gap in $\chi(T)$, and ρ_c increases

(Orsay:Alloul, Friedel,1989)

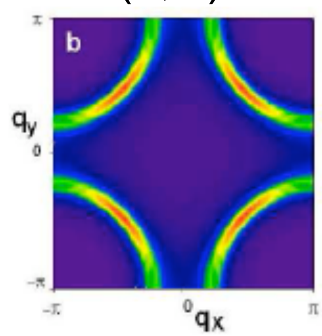
Photoemission:

Optical conductivity σ

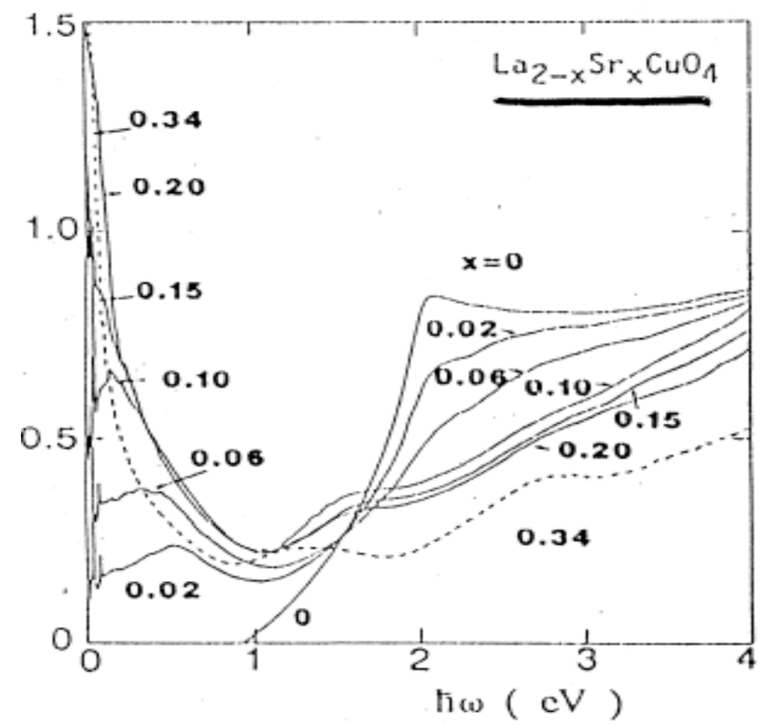


Kaminski-Campuzano

(0,π)



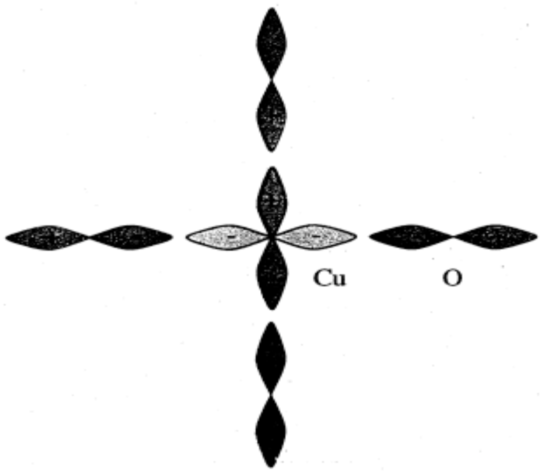
Fermi arc formation



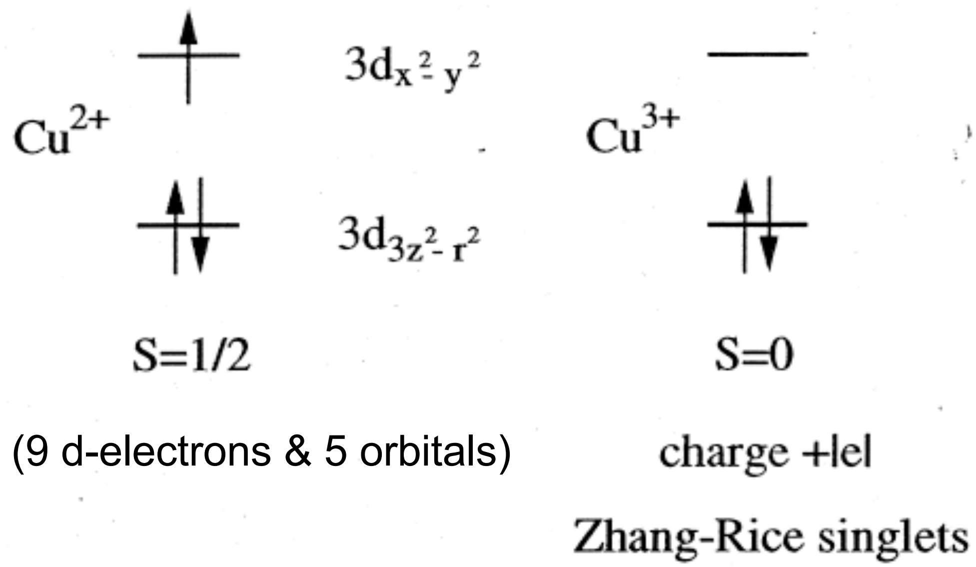
Mott gap versus Drude:
Drude weight $\propto \delta$

Planar cuprates

Octahedral crystal field: e_g
Square planar distortion

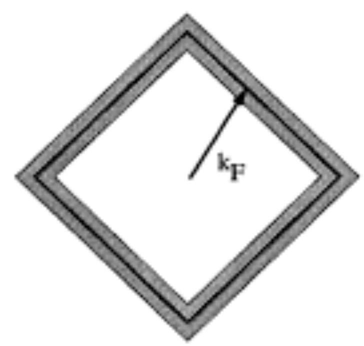


Oxidation States:



- Stochiometric Oxides:
  all $Cu^{2+} \rightarrow$ AF Mott Insulators.

$J \sim 4t^2/U$

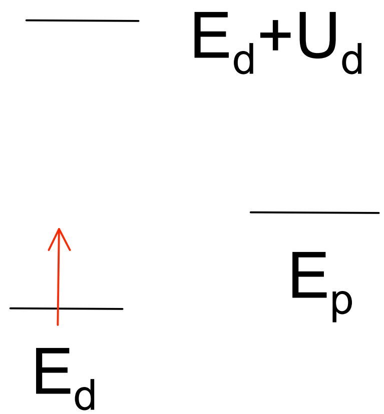


- Hole doped Oxides:
  $\sim 15\% Cu^{3+} \rightarrow$ High-T_c Superconductors.

t-J model or Hubbard model at large U

Zhang-Rice (1988)

Hole picture

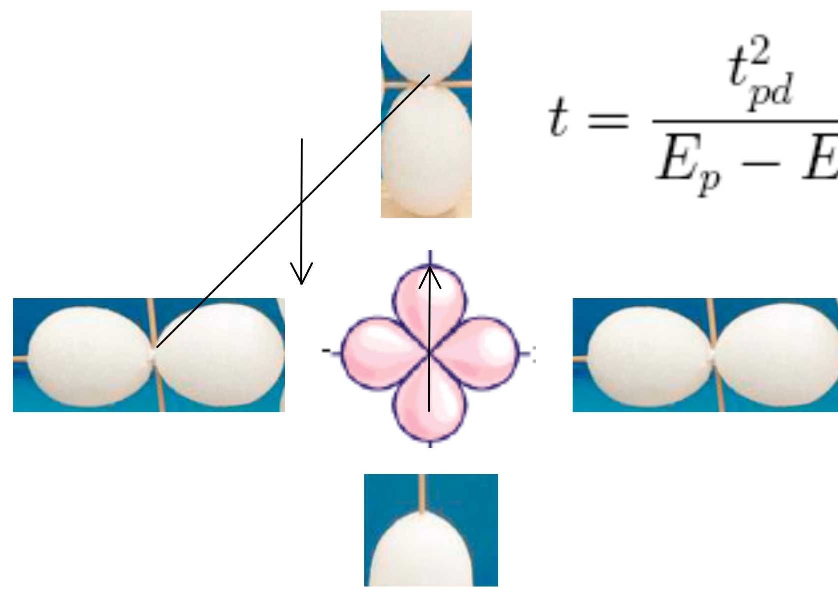


$$H_{eff} = J \sum_{\langle i;j \rangle} \left(\vec{S}_i \vec{S}_j - 1/4 \right)$$

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

U_d = 10.5eV
E_p-E_d ~3.6eV
t_{pd}~1.3eV

Schlüter et al



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

<u>Hubbard parameters:</u>

t ~ 0.4 eV

P. Fleury, Z. Fisk et al

<u>J~ 0.145eV (0.13-0.15eV)</u>

(Debye T for Cu ~315K)

U~ E_p-E_d (2-4 eV)

t-J model

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

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

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

Gutzwiller approximation (1963): statistical weighting factors

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

$$\boxed{\begin{array}{c} \langle d^\dagger_{is} d_{js} \rangle = g_t \langle d^\dagger_{is} d_{js} \rangle_0 \\ \langle \vec{S}_i \cdot \vec{S}_j \rangle = g_s \langle \vec{S}_i \cdot \vec{S}_j \rangle_0 \end{array}}$$

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

Renormalized mean-field theory

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

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

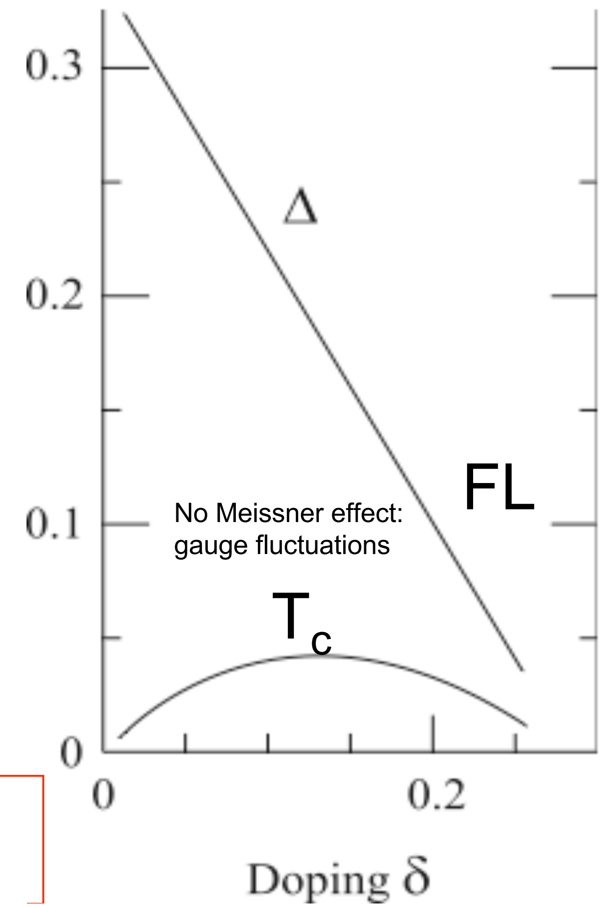
2 order parameters: $\chi_{ij} = (3g_sJ/4)\langle d^\dagger_{is}d_{js}\rangle$ and Δ_{ij}

$$\boxed{\begin{aligned}\Delta_{\vec{k}} &= \frac{3}{4}g_sJ\sum_{\vec{k}'}\gamma_{\vec{k}-\vec{k}'}\frac{\Delta_{\vec{k}'}}{2E_{\vec{k}'}}\\ \chi_{\vec{k}} &= \frac{3}{4}g_sJ\sum_{\vec{k}'}\gamma_{\vec{k}-\vec{k}'}\frac{\xi_{\vec{k}'}}{2E_{\vec{k}'}}\end{aligned}}$$

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

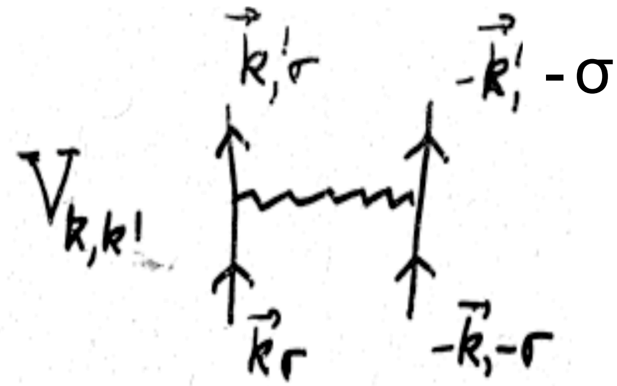
$\xi_{\vec{k}} = g_t\epsilon_{\vec{k}} - \mu - \chi_{\vec{k}}$ and $\epsilon_{\vec{k}} = -t\gamma_{\vec{k}}$

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



D-wave superconductivity…

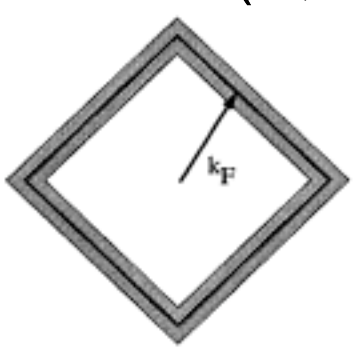
$$\Delta(\vec{p}) = -\sum_{\vec{p}'} V_S(\vec{p}-\vec{p}')\frac{\Delta(\vec{p}')}{2E_{\vec{p}'}}$$



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

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

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



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

Very general argument!

See also spin fluctuation model
Review D. Scalapino, 1999

“mean-field” theory of SC phase

- Superconducting $T_c = g_t.\Delta$

T_c must go to zero at zero doping: <u>insulator</u>

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

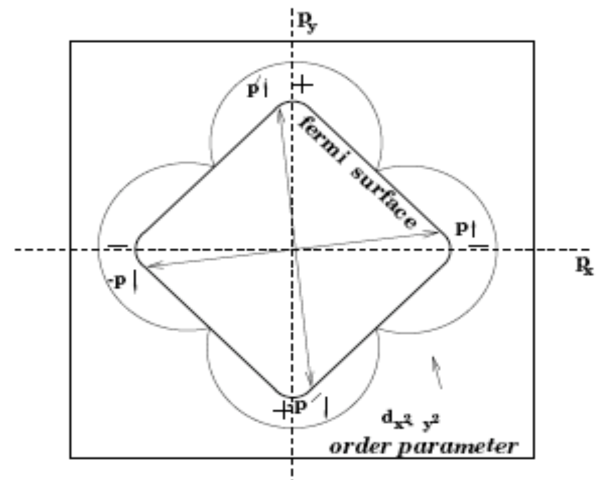
- <u>d-wave quasiparticles</u>: coherent spectral weight Z goes to zero as g_t but Fermi velocity is almost doping independent

$$\frac{n_s(T)}{m} = \frac{n_s(T=0)}{m} - aT$$

$$a = \frac{2\ln 2}{\pi}\alpha^2\frac{v_F}{v_\perp} \qquad \boxed{\alpha^2 = 0.5}$$

T_c follows $n_s(T=0) \sim g_t$ and Δ

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



$$\vec{j}(\vec{k}) = -e\alpha\vec{v}_F$$

Brief Summary…

- Pairing glue in high-Tc cuprates: magnetic fluctuations (understood)

- Why high-Tc problem not declared as "solved"? pseudogap phase remains mysterious
  (phase/gauge fluctuations, many other competing channels)
  Attempt: gauge theories, Lee, Wen, Nagaosa (RMP, 2006)

- Challenges:

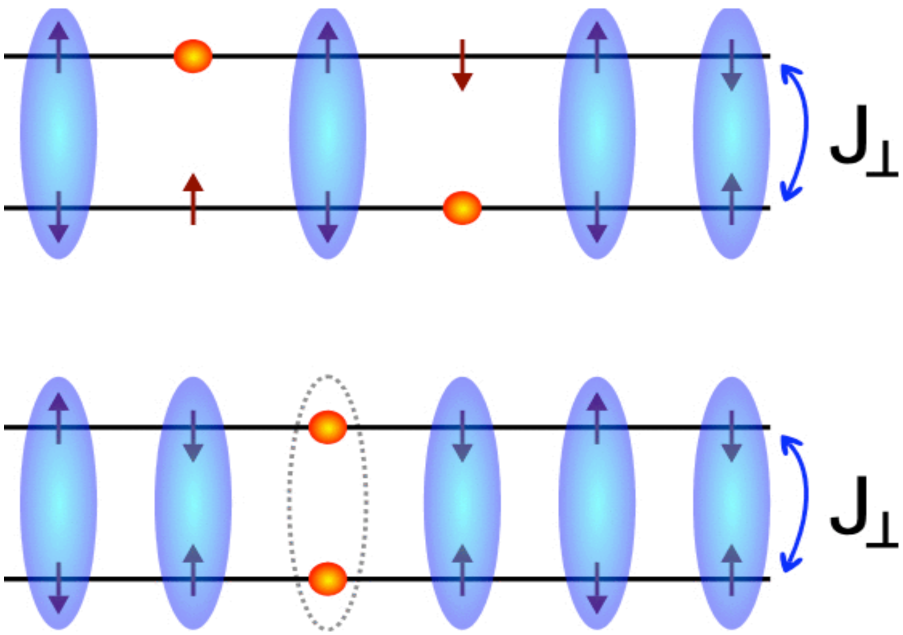
Pseudogap: friend or foe of SC? Rigorous theory of SC

Pseudogap phase (RVB physics) and Fermi arcs

Our idea: 1) Quasi-1D to 2D

(phase fluctuations treated rigorously)

Why quasi-1D: RVB and SC



Dagotto and Rice, Science **271**, 618 (1996)

Half-filling: exact wave-function

$$|RVB\rangle = P \sum_{i,j} F(i-j) \left(d^\dagger_{1i\uparrow} d^\dagger_{2j\downarrow} - d^\dagger_{1i\downarrow} d^\dagger_{2j\uparrow} \right)$$

Doping: superconductivity emerges

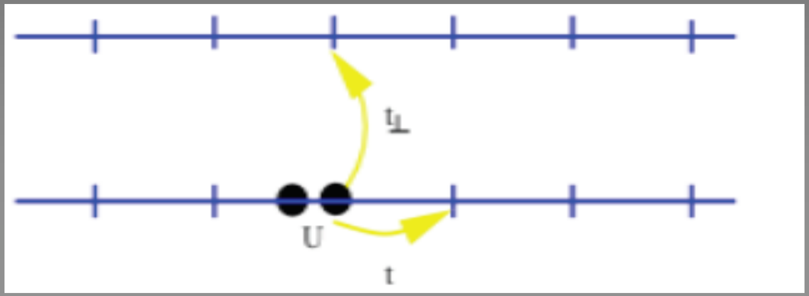
$$< \Delta(x) \Delta^\dagger(0) > \propto x^{-1/2}$$

(universal exponent
for a few holes)

Weak and Strong Interactions share the same physics

Weak coupling regime

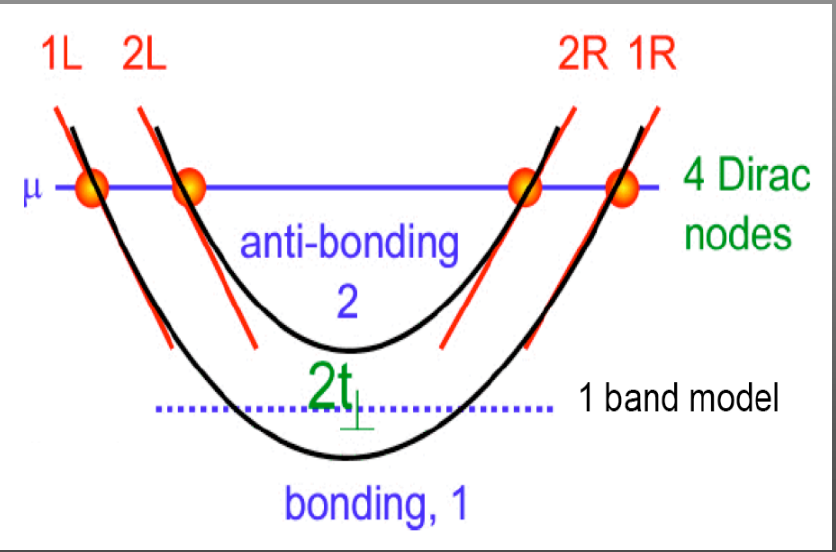
First, diagonalize the spectrum



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

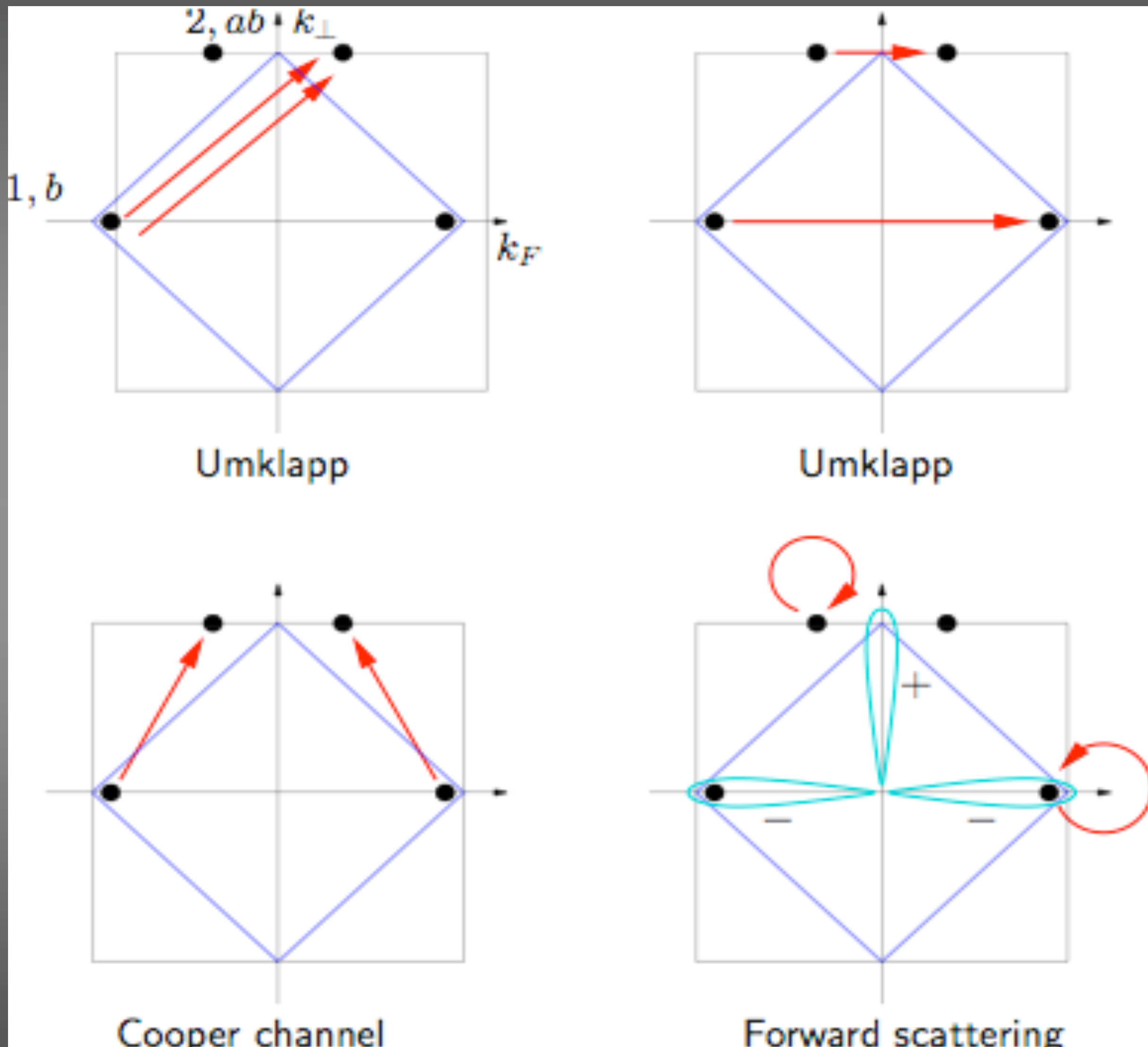
Half-filling: $\mathbf{v_1} = \mathbf{v_2}$
and $k_{F1} + k_{F2} = \pi$

Large Doping: $\mathbf{v_2} \ll \mathbf{v_1}$



Urs Ledermann & K. Le Hur, PRB **61**, 2497 (2000)
M. P. A. Fisher, Les Houches Notes, 1998

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

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

$$\frac{dc_1}{dl} = -\frac{1}{2\pi v_2} c_{12}^2$$
$$\frac{dc_2}{dl} = -\frac{1}{2\pi v_1} c_{12}^2$$
$$\frac{df_{12}}{dl} = \frac{1}{\pi(v_1 + v_2)} c_{12}^2$$
$$\frac{dc_{12}}{dl} = \frac{c_{12}}{\pi}\left(\frac{2 f_{12}}{v_1 + v_2} - \frac{c_1}{2v_1} - \frac{c_2}{2v_2}\right)$$

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

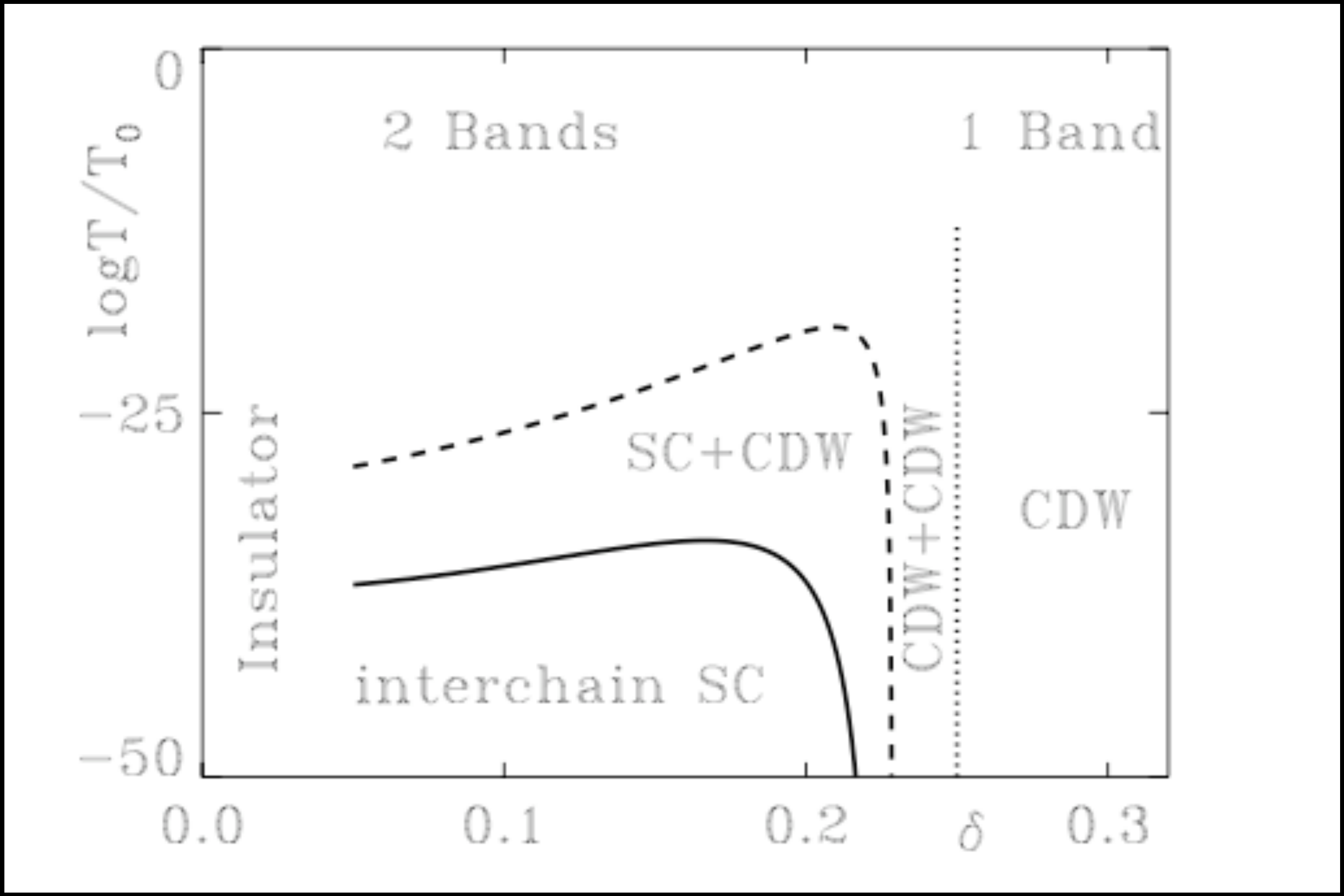
$$v_1 - v_2 = \frac{2t_\perp}{\tan(\pi n)}$$

C_{12}:
phase coherence between bands

Solvable set of differential equations + strong coupling treatment

Phase Diagram

(careful analysis of the strong-coupling theory)



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

(relevance to cold atom systems: noise correlations)

Extension to quasi-1D systems

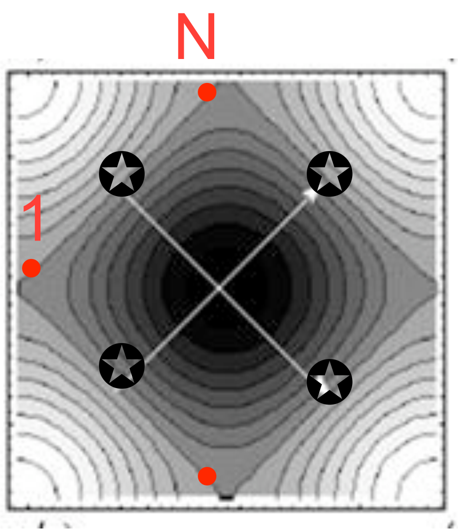
Urs Ledermann, Karyn Le Hur, T. Maurice Rice, PRB **62**, 16383 (2000)
J. Hopkinson and K. Le Hur, PRB **69**, 245105 (2004)

- Band/chain correspondence simple…

(chain) $$d_{is} = \sum_j \sqrt{\frac{2}{N+1}} \sin\left(\frac{\pi j i}{N+1}\right) \Psi_{js}$$ (band)

$$E_j(k) = -2t\cos k - 2t_\perp \cos(\pi j/(N+1))$$

$v_i = 2t\sin(k_{Fi})$ $$v_l = v_{\bar{l}} = 2\sqrt{t^2 - t_\perp^2 \cos(\pi l/(N+1))^2}$$



Band pair: $\bar{l} = N + 1 - l$ $\quad (k_{Fl} + k_{F\bar{l}}) = \pi$

μ=0 $\quad v_1 = v_N < v_2 = v_{N-1} < \ldots$

Large N limit

- Van Hove singularity similar to 2D:

$$t_\perp = t \longrightarrow v_1 = v_N \sim 2\pi t/N$$

- Quasi-1D approach is valid as long as energy difference between neighboring bands is larger than the largest energy scale: $te^{-t/U}$

$$U \ll t/\ln N, t_\perp/\ln N$$

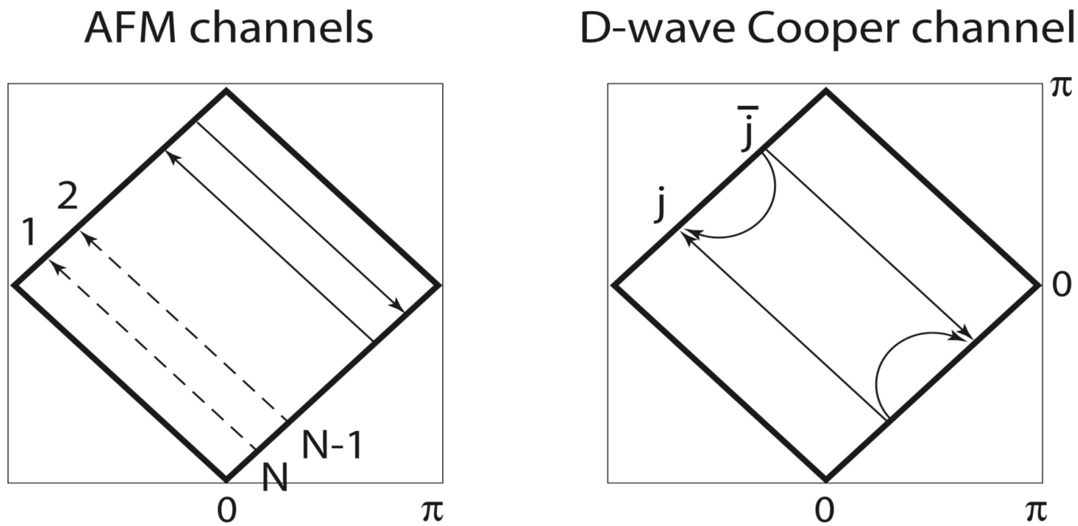
RG scheme: intra-band, inter-band scatterings (antiferromagnetic)

Proper classification of the different interaction channels

Strong coupling theory: pseudogap

Karyn Le Hur and T. Maurice Rice, arXiv: 0812.1581

Half-filling:
Antiferromagnetism



Uniform Mott gap and quasi-long range order: $T_M = te^{-\lambda t/U}$

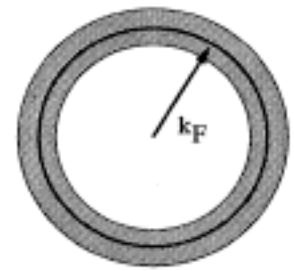
$$H = H_{Kin} - \frac{1}{2}\sum_{i,j}\int dx\, g_{ij}\vec{M}_i \cdot \vec{M}_j \qquad M_j^p = \Psi^\dagger_{Rjs}\tau^p_{ss'}\Psi_{L\bar{j}s'} + h.c.$$

Chain picture $\boxed{\langle \vec{S}_i(x) \cdot \vec{S}_j(0)\rangle = (-1)^{i+j}\cos(\pi x)/x^{1/N}}$

Extension of K. Le Hur, PRB 2001

Fermi liquid…

occurs when (4-band) AFM fluctuations and umklapp disappear completely



Forward scattering gives a contribution of order 1

Cooper processes, which favor the Fermi liquid, have a weight ~ N

$$\boxed{\frac{dV(\theta_1,\theta_2)}{dl} = -\frac{1}{v_F}\int d\theta V(\theta_1,\theta)V(\theta,\theta_2)}$$

Θ is the angle parametrizing the Fermi surface

Analogy to 2D: See Shankar

D-wave SC from RG

Intermediate regime

AFM processes irrelevant at low energy but
reinforce Cooper channels at high energy:
Important for 2D-like phase coherence

(example of Kohn-Luttinger attraction)

D-wave Superconductivity

$$\boxed{H = H_{Kin} + \sum_{i,j} \int dx V_{ij} \Delta_i^{\dagger} \Delta_j} \qquad \Delta_i \sim e^{i\theta_i}$$

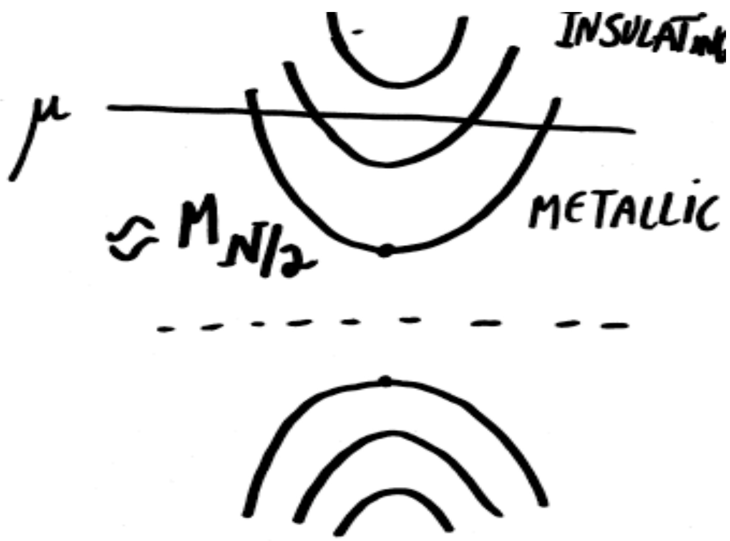
where $V_{ij}<0$ for $(i,j) \leq N/2$ and $(i,j)>N/2$ and $V_{ij}>0$ in all other cases

Strong-coupling theory: pseudogap

- 4-band interactions (antiferromagnetism) become cut-off by the chemical potential

For each band pair
SO(8) theory: Lin-Balents-Fisher

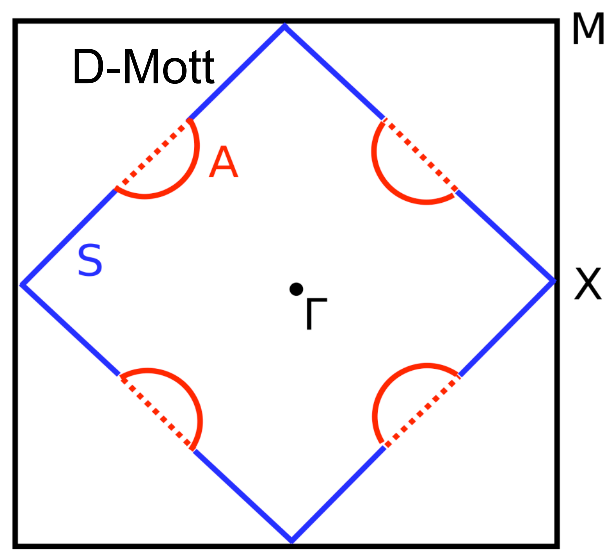
$$E_j(k) = \sqrt{M_j^2 + (v_j k)^2} \quad M_j \sim t e^{-v_j/U}$$



CHARGE SECTOR: SIMILAR TO SMALL N LIMIT

Urs Ledermann, Karyn Le Hur, T. Maurice Rice, PRB **62**, 16383 (2000)

D-Mott (RVB):
Spin gap
Charge gap
2-leg ladder



One can compute the electron Green's function exactly

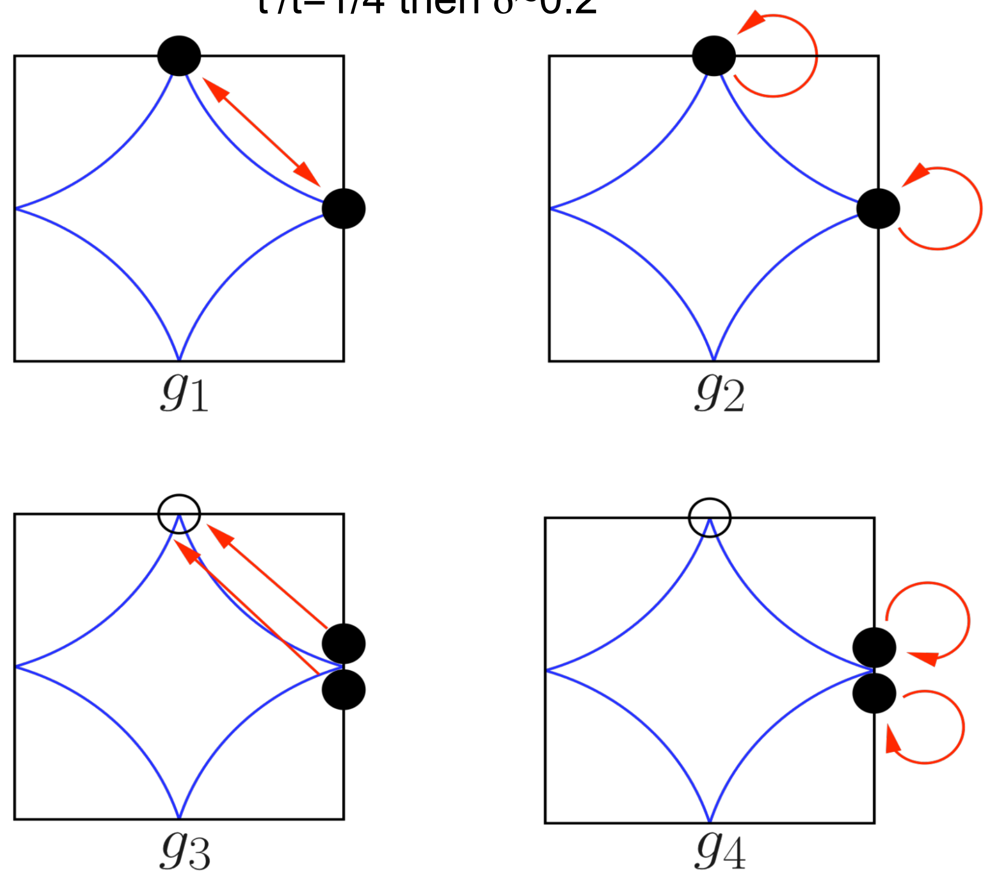
2) Two dimensions: 2-patch model

$$\epsilon(\vec{k}) = -2t(\cos k_x + \cos k_y) + 4t' \cos k_x \cos k_y$$

$$\begin{aligned}
\dot{g}_1 &= 2d(y) g_1 (g_2 - g_1) \\
\dot{g}_2 &= d(y)(g_2^2 + g_3^2) \\
\dot{g}_3 &= -2g_3 g_4 + 2d(y) g_3 (2g_2 - g_1) \\
\dot{g}_4 &= -\left(g_3^2 + g_4^2\right)
\end{aligned}$$

Schulz;Dzyaloshinskii;Lederer et al (1987)

t'/t=1/4 then δ~0.2



$$\dot{g}_i = dg_i/dy \quad y = \ln^2(T/D)$$

$$\chi^{pp}_{\vec{q}=0} \approx \ln^2 T$$

$$\chi^{ph}_{\vec{Q}} \approx \ln^2 T \text{ for } T > t'$$

$$\chi^{ph}_{\vec{Q}} \approx \ln T \text{ for } T < t'$$

Similar fixed point: g_3,g_4, and g_2 flow…

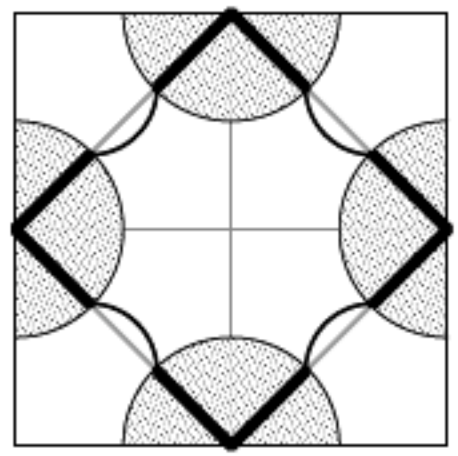
D-Mott state for $U>U_c = F(t/t')$ and $F(x)=1/\ln^2(x)$

T.M. Rice et al.: numerical strong coupling analysis (A. Läuchli)

Another proof: ladders with t' (J. Hopkinson and K. Le Hur, PRB **69**, 245105 (2004))

pseudogap & SC phase: Summary

Luttinger theorem



Insulating antinodal RVB directions:

Spin and Charge gap

At weak U, a unique energy scale

(quasi-1D theory & RG in 2-patch model)

Nodal directions: Fermi arcs

The (hole-like) Fermi surface consists of 4 arcs: Fermi liquid

Consistent with ARPES experiments, for example, on BSCCO

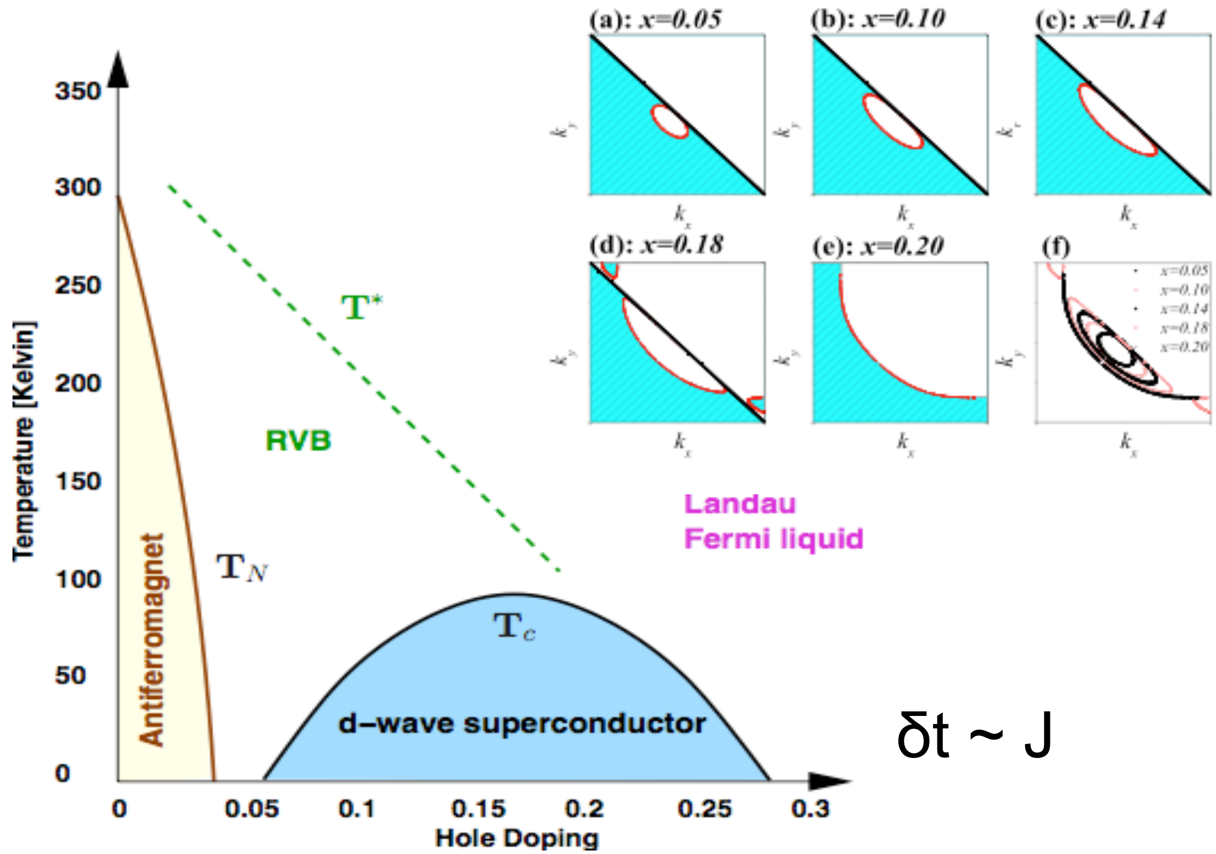
SC: proximity effects of the Fermi arcs with the RVB region

Andreev scattering (Geshkenbein, Larkin et al. 1998; KLH 2001)

Only the Fermi arcs become superconducting below Tc

$$H = \sum_q \varepsilon b_q^\dagger b_q + \sum_{p,q}' V_{p,q}(b_q^\dagger c_{p\uparrow} c_{q-p\downarrow} + h.c.) + \sum_p \xi_p c_{p,\sigma}^\dagger c_{p,\sigma}$$

Conclusion



$\delta t \sim J$

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!