Superconductivity in the Hubbard Model

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Outline

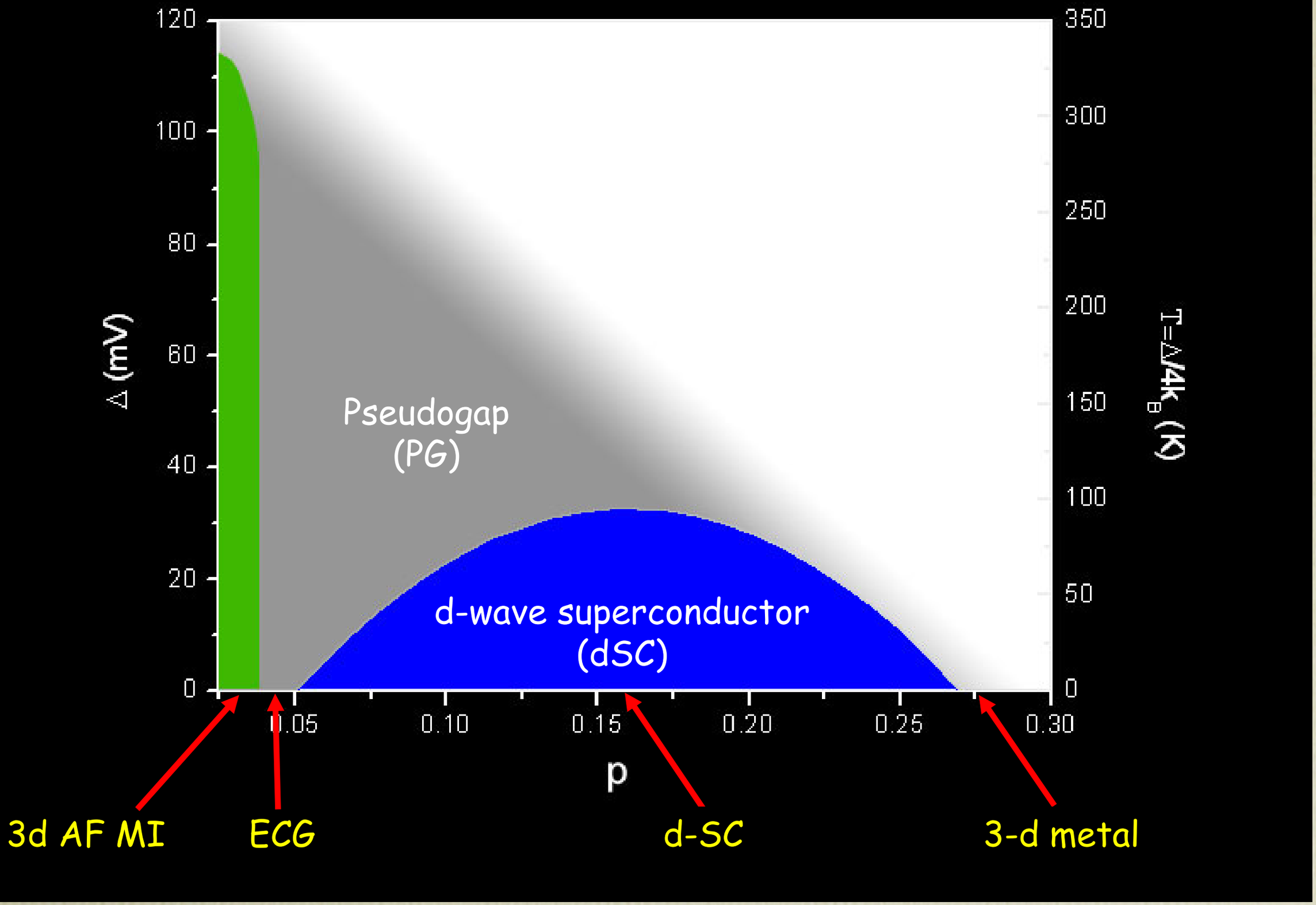
based on: arXiv:1007.1195, 1008.5116, July, August 2010

Outline

- High Tc phenomenology and the usual paradigm
- Hubbard Model
- Exact Cooper-Pair potential
- Thermodynamics: Fermi Surfaces
- Solutions to the gap equation
- Conclusions

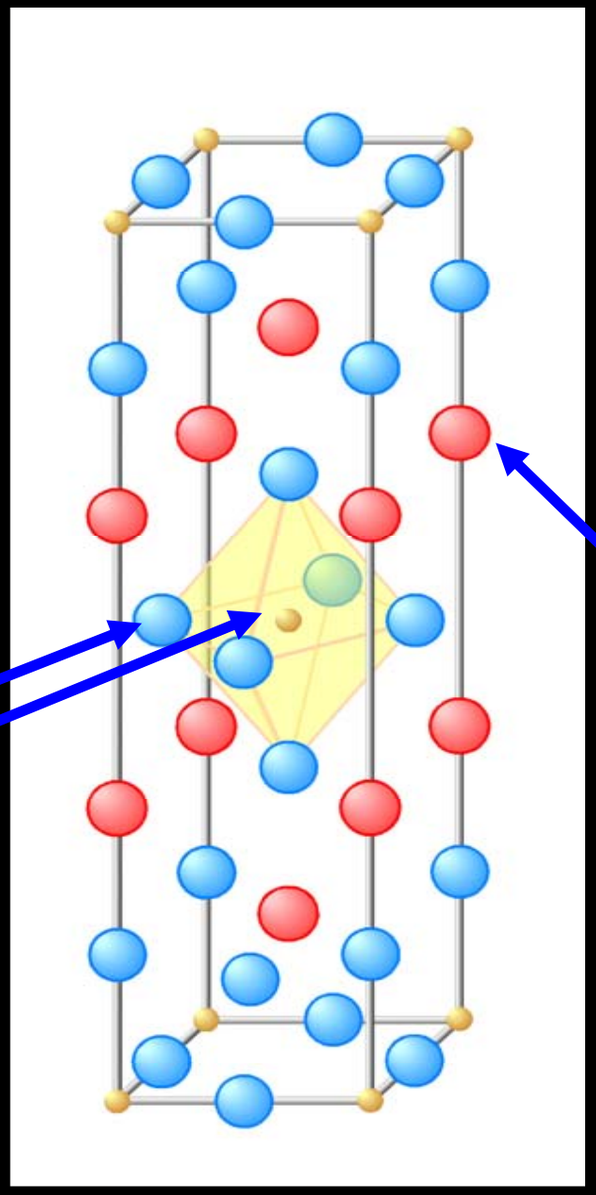
based on: arXiv:1007.1195, 1008.5116, July, August 2010

Schematic phase diagram of hole-doped cuprates



(these slides courtesy of Seamus Davis)

$La_{2-x}Ba_xCuO_4$



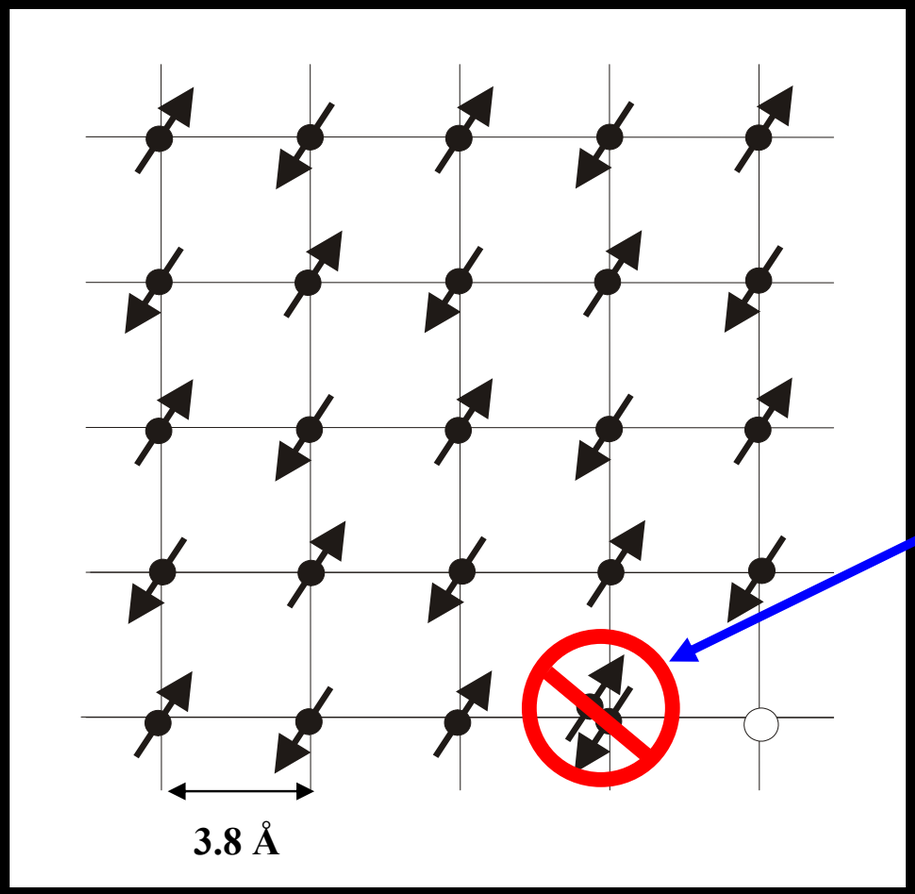
Antiferromagnetic

Mott Insulator

Z. Phys. Rev. **B 64** 189 (1986)

The common paradigm

Mott Insulator: Repulsive Coulomb U~3eV

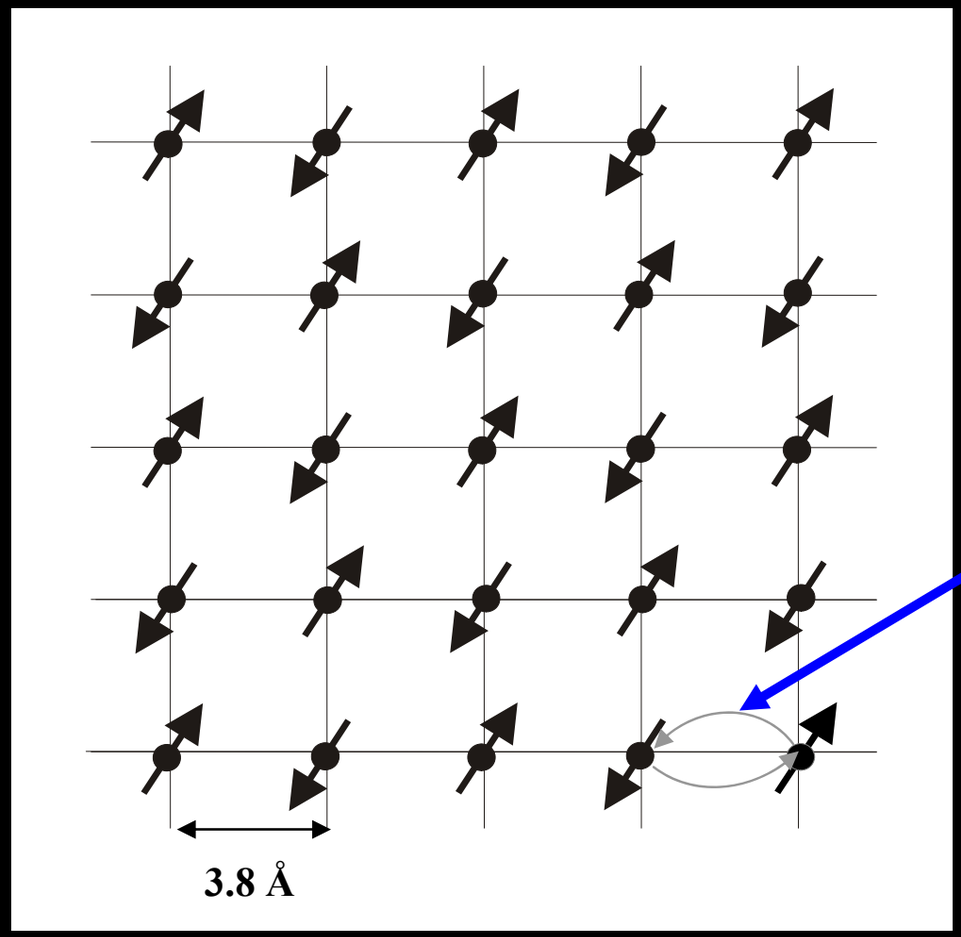


No double occupancy allowed..

N.F. Mott, *Proc. Phys. Soc A62*, 416 (1949)

This AF phase is well understood.

Antiferromagnetic: Superexchange J~0.14eV



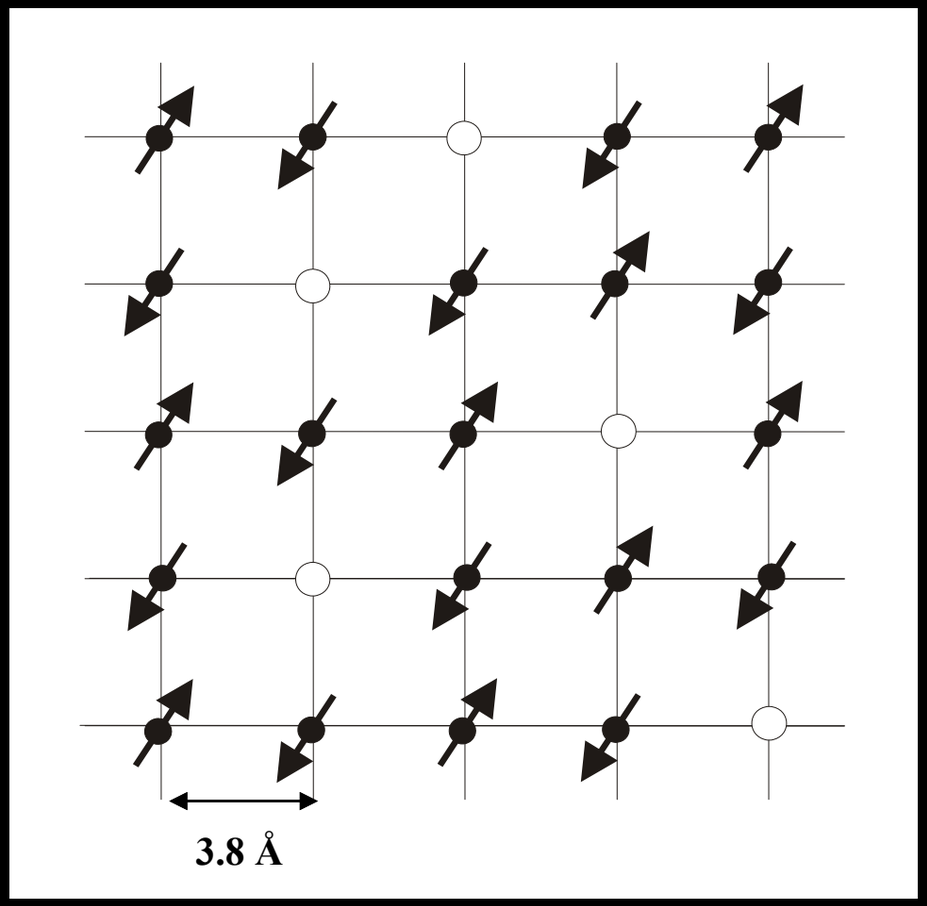
..except as a virtual process.

$$H = \frac{4t^2}{U} \sum_{<i,j>} \vec{S}_i \bullet \vec{S}_j - \frac{1}{4} n_i n_j$$

P. W. Anderson, ***Phys. Rev. 115***, 2 (1959)

AF order preferred since it allows virtual hopping, which lowers the energy.

Holes introduced $\Longrightarrow$ carriers become mobile



Dopant density p
= number of holes
per CuO_2 plaquette

$$H = -t\sum_{<i,j>}(c^{\dagger}_{i\sigma}c_{j\sigma} + h.c.) \quad + \quad U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

J. Hubbard, ***Proc. Roy. Soc A276***, 238 (1963)

Holes rapidly destroy the AF order.

How can this state become superconducting?

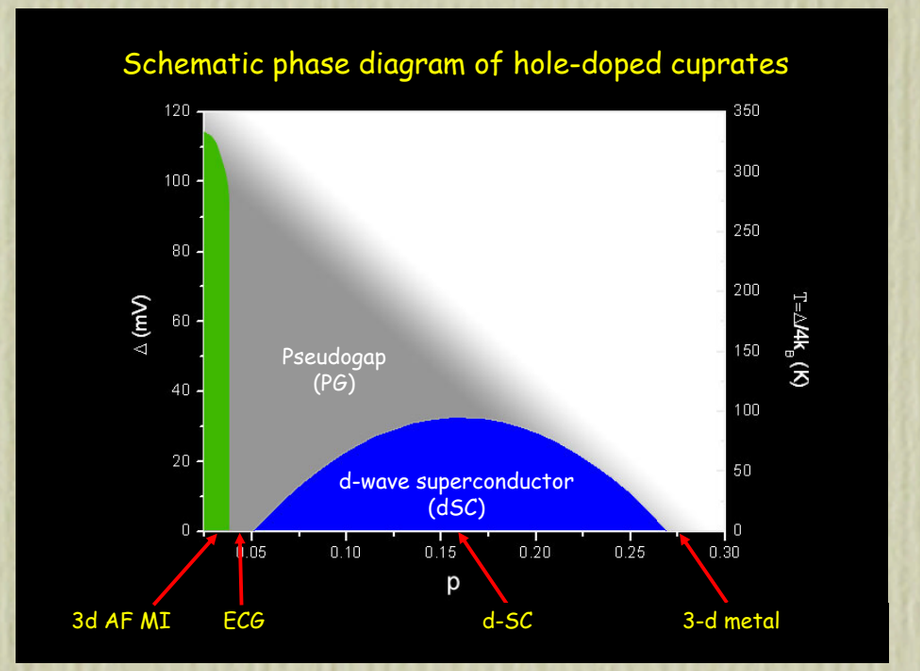
Fundamental, unanswered questions, we will address:

- What is the attractive "glue" that binds the electrons into Cooper pairs? The Hubbard model is defined with attractive interactions. Lattice phonons do not play a role.

- What is the pseudogap? Is it a distinct phenomenon from superconductivity?

- What is the origin of the anisotropy of the gap? Is it exactly d-wave? Fermi arcs, etc.

Where to begin?



AF is spatial, whereas SC order is delocalized.

* on overdoped side, perhaps dilute enough to treat as a gas.
* far away from competing orders.
* attempt to understand the attractive mechanism in a pure form, then track it down to lower doping.

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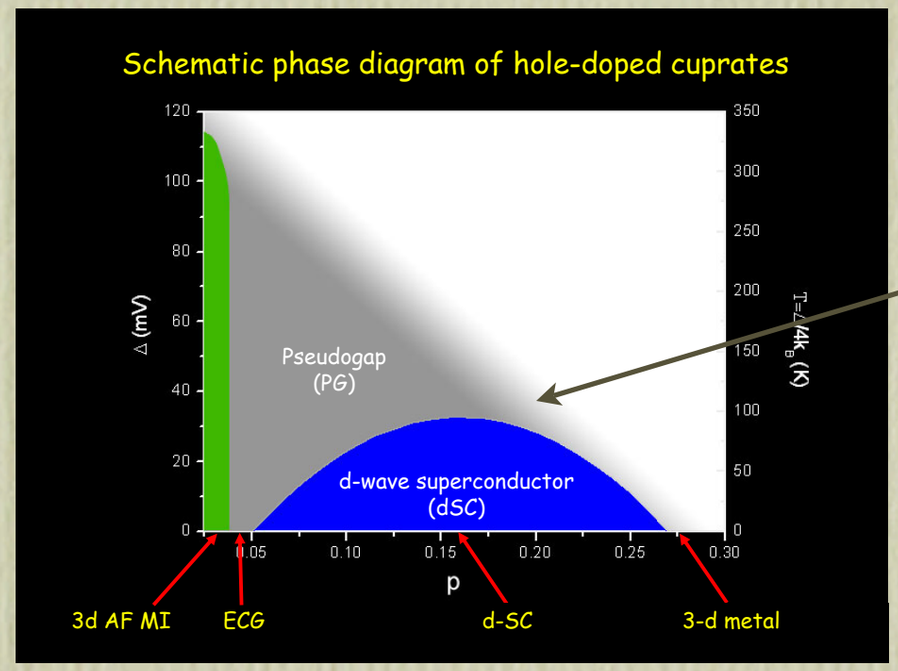

Here.....

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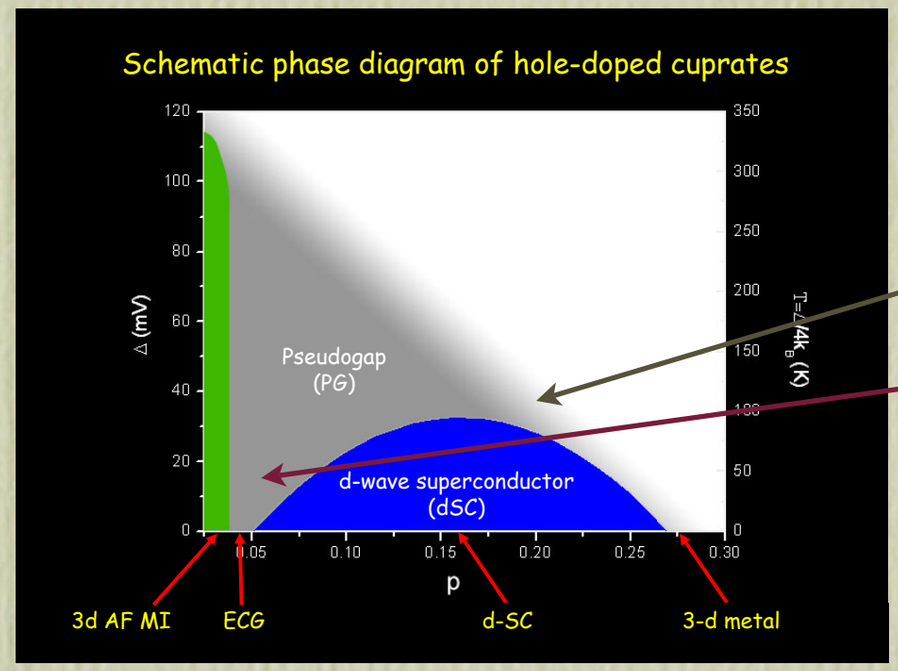

Here.....

Not here

AF is spatial, whereas SC order is delocalized.

* on overdoped side, perhaps dilute enough to treat as a gas.
* far away from competing orders.
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Hubbard Model

$$H = -t \sum_{<i,j>,\alpha=\uparrow,\downarrow} \left(c^\dagger_{\mathbf{r}_i,\alpha} c_{\mathbf{r}_j,\alpha}\right) - t' \sum_{<i,j>',\alpha=\uparrow,\downarrow} \left(c^\dagger_{\mathbf{r}_i,\alpha} c_{\mathbf{r}_j,\alpha}\right) + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow}$$

* t, t' = nearest and next nearest neighbor hopping on 2d square lattice. t' will be important!

* U>0, large Coulomb repulsion

* Hopping term easily diagonalized:

$$H_{\text{free}} = \int d^2\mathbf{k}\, \omega_{\mathbf{k}} \sum_\alpha c^\dagger_{\mathbf{k},\alpha} c_{\mathbf{k},\alpha}$$

$$\omega_{\mathbf{k}} = -2t\left(\cos(k_x a) + \cos(k_y a)\right) - 4t' \cos(k_x a)\cos(k_y a)$$

Introduce continuum fields: $\psi_\alpha(\mathbf{r}) = \int \frac{d^2\mathbf{k}}{(2\pi)^2}\, c_{\mathbf{k},\alpha}\, e^{i\mathbf{k}\cdot\mathbf{r}}$

Interaction is local with density:

$$\mathcal{H}_{\text{int}} = \frac{u}{2}\, \psi^\dagger_\uparrow \psi_\uparrow \psi^\dagger_\downarrow \psi_\downarrow$$

Scaling out lattice spacing a and t, dimensionless coupling:

$$g = \frac{u}{a^2 t} = \frac{2U}{t}$$

Henceforth, all energy scales in units of t

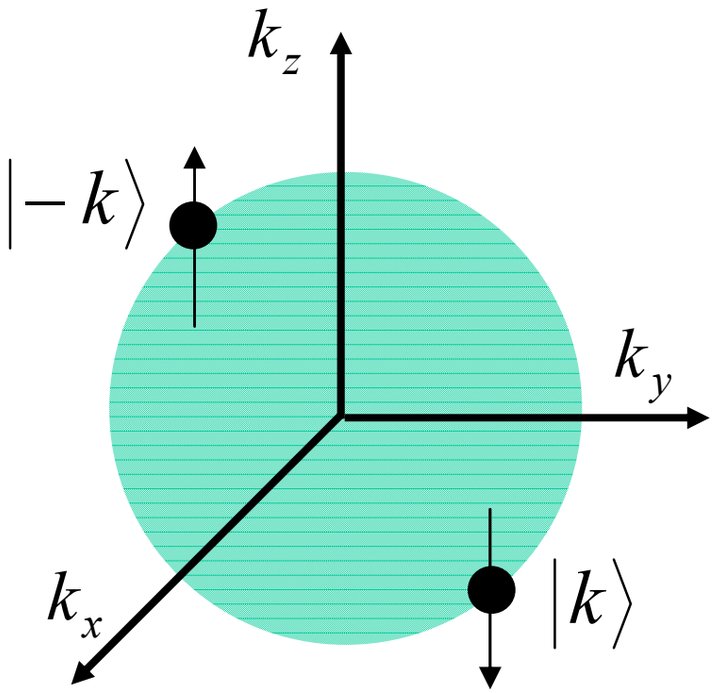
BSCO cuprate: U/t = 13, t'/t = -0.3, t=3000K

Conventional BCS theory of SC

Bardeen Schrieffer Cooper

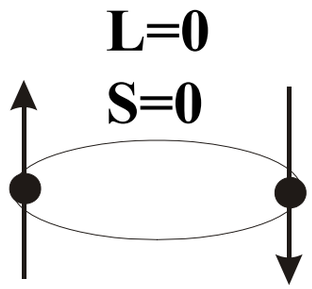
BCS theory of the superconducting state

Normal State (Metal)



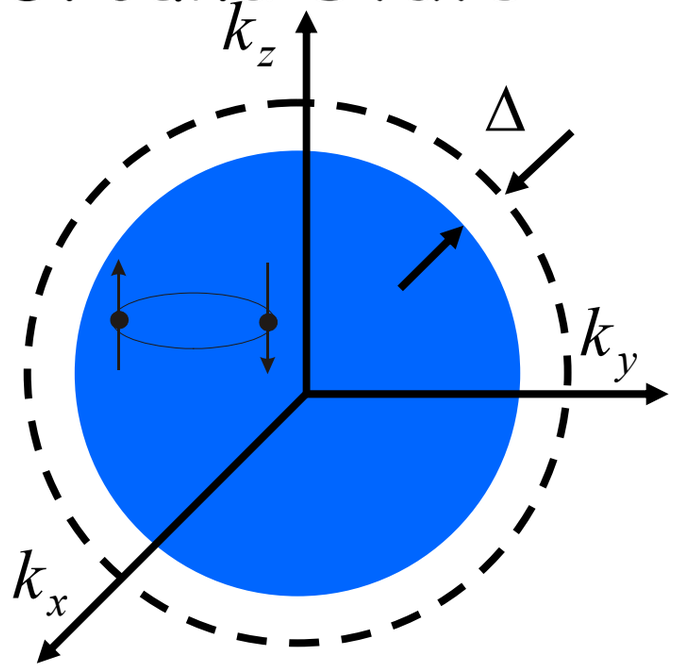
- Degenerate Landau/Fermi Liquid

Low Temp. Cooper Pairing



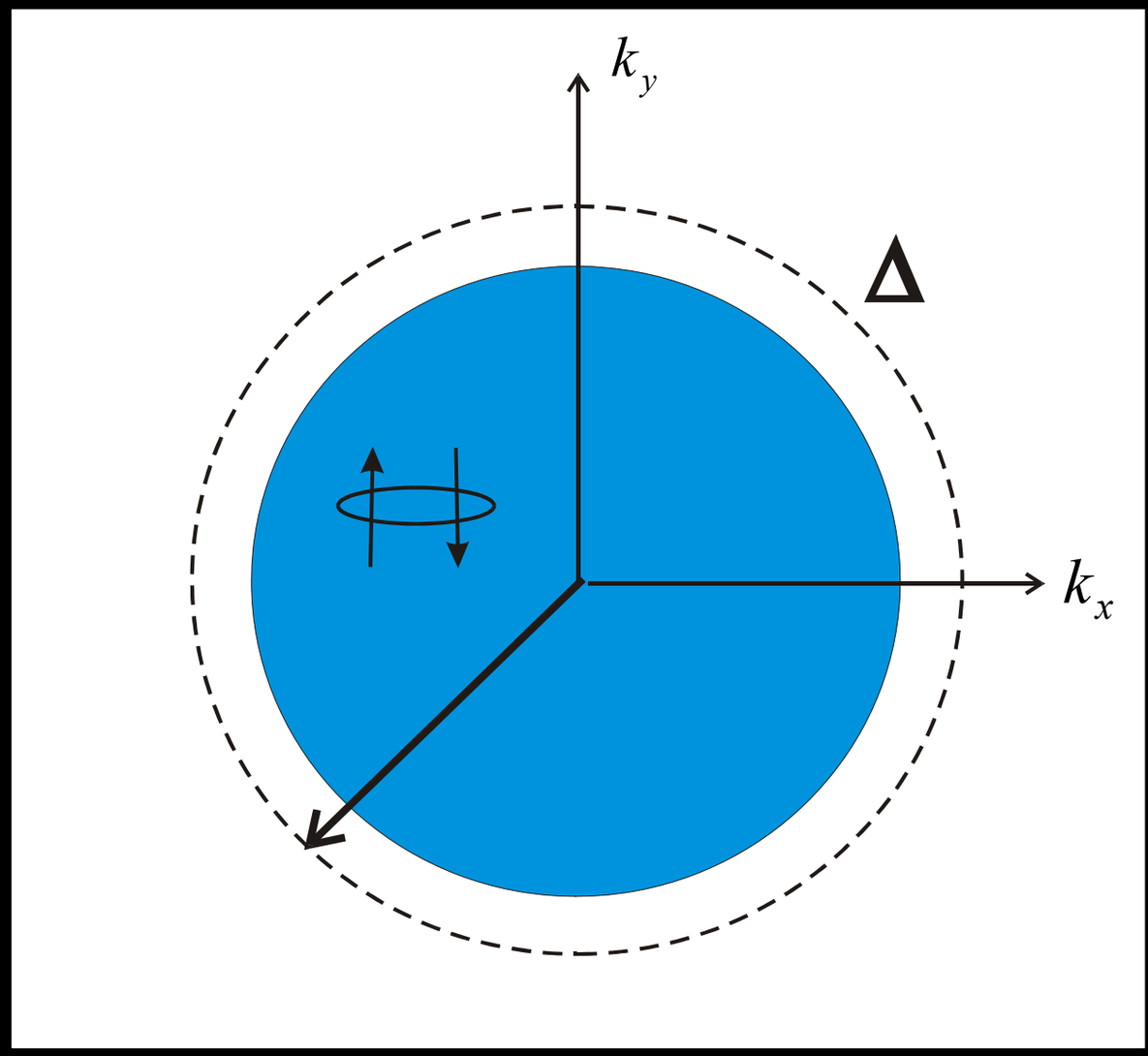
- Pair-binding energy Δ
- Pair COM motion in $\vec{k}$ -space

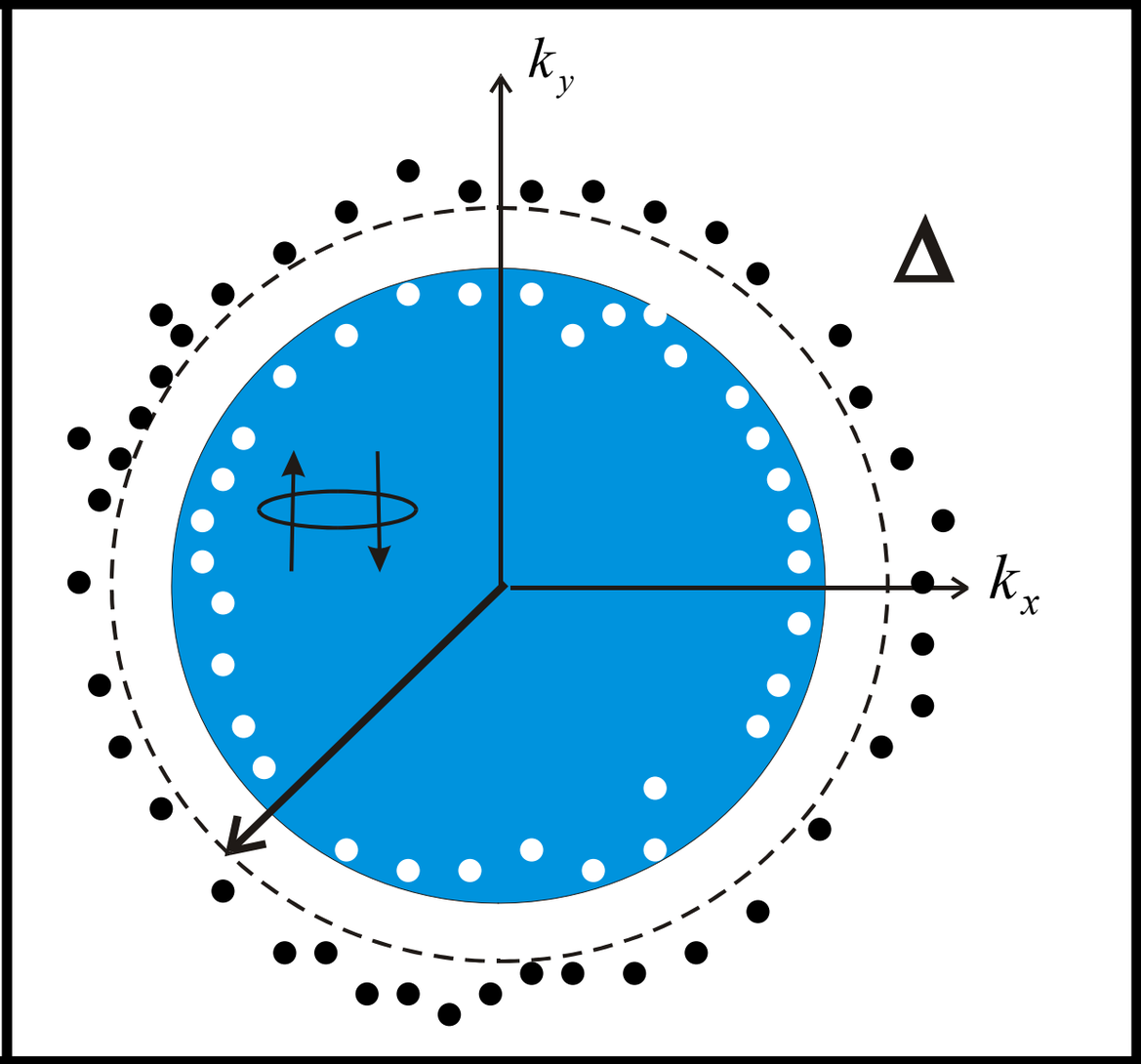
Superconducting Ground State



- Gas Cooper-pairs
- Energy Gap Δ

SC Excited States: Quasiparticles





SC Ground State

$$\Psi_{BCS} = \prod_k \left(u_k + v_k c^*_{k\uparrow} c^*_{-k\downarrow} \right) | 0 >$$

BCS, Phys Rev 108, 1175 (1957)

SC Excited States

$$\gamma^*_{k\uparrow} = u_k c_{k\uparrow} + v_k c^*_{-k\downarrow}$$

Bogoliubov, Nuovo Cimento 7, 794 (1958)

Gap equation for superconductivity

It is known that Cooper pairs of charge 2e exist. We thus assume that the BCS construction of the ground state goes through, leading to the well-known gap equation:

$$\Delta(\mathbf{k}) = -\int \frac{d^2\mathbf{k}'}{(2\pi)^2}\, V(\mathbf{k},\mathbf{k}')\frac{\Delta(\mathbf{k}')}{2E(\mathbf{k}')}\,\tanh(E(\mathbf{k}')/2T), \qquad E(\mathbf{k}) \equiv \sqrt{\xi(\mathbf{k})^2 + \Delta(\mathbf{k})^2}$$

Specialize to the Hubbard Model:

$V(\mathbf{k},\mathbf{k}')$ = Cooper pair potential, we calculate exactly

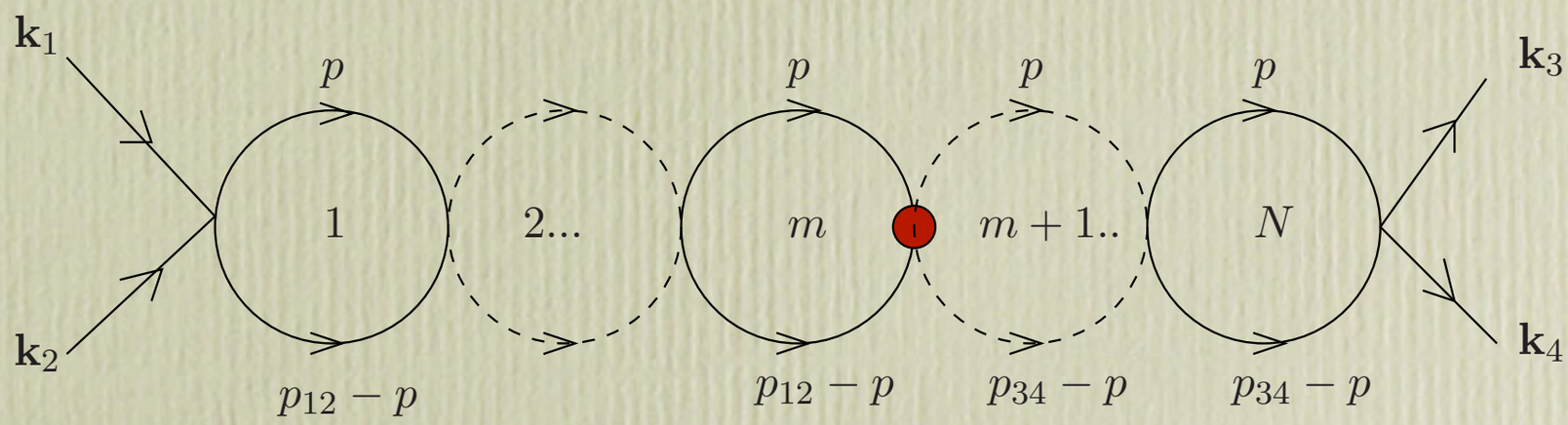
$\xi(\mathbf{k})$ = quasiparticle energy of normal state, determines the Fermi surfaces, $\xi(\mathbf{k}) = 0$, we calculate approximately, or fit to data.

Cooper pair potential

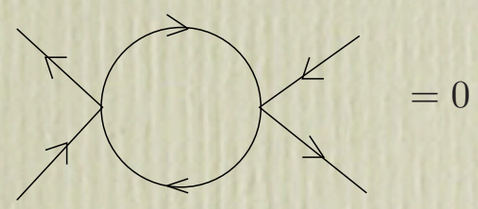
The pair potential is the "form-factor":

$$V(\mathbf{k},\mathbf{k}') = \int d^2\mathbf{r}\ \langle \mathbf{k}'\uparrow, -\mathbf{k}'\downarrow |\mathcal{H}_{\rm int}(\mathbf{r})|\mathbf{k}\uparrow, -\mathbf{k}\downarrow\rangle$$

It is given exactly by the sum of Feynman diagrams:



since:



These multi-loop Feynman diagrams factorize, with the result:

$$V(\mathbf{k},\mathbf{k}') = \frac{g/2}{1 + ig(\mathcal{L}(\mathbf{k}) + \mathcal{L}(\mathbf{k}'))/4}$$

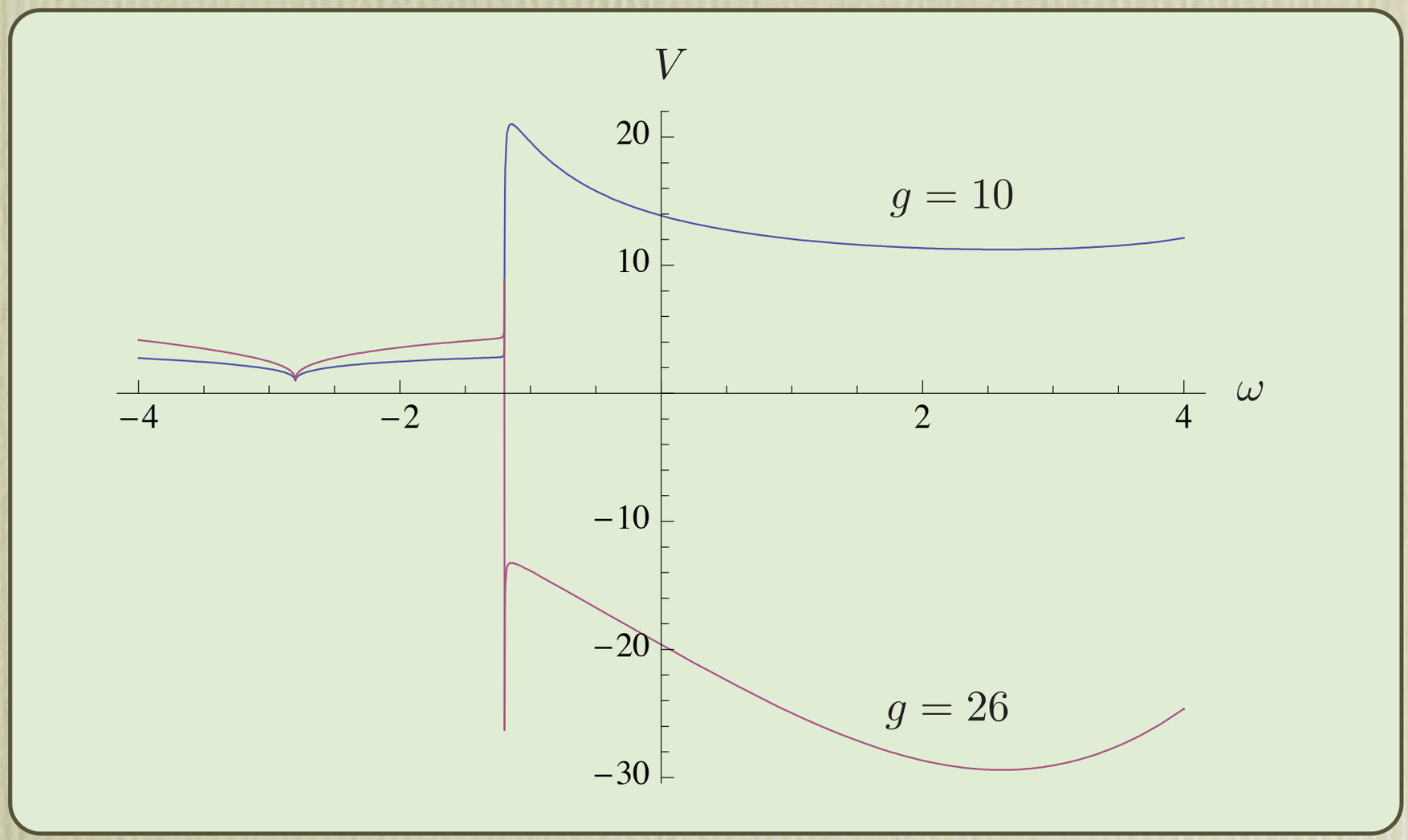
L is a 1-loop integral, can be expressed in terms of elliptic functions K

$$\mathcal{L}(\mathbf{k}) = \frac{1}{\pi}\left(\frac{(\omega_{\mathbf{k}} - 4t')}{(\omega_{\mathbf{k}} + 4 + 4t')(\omega_{\mathbf{k}}(4 - \omega_{\mathbf{k}}) + 16t'(t' - 1)}\right)^{1/2} K\left(\frac{16(\omega_{\mathbf{k}}t' - 1)}{(\omega_{\mathbf{k}} + 4t')^2 - 16}\right)$$

Allows a 1/g expansion!

"What is the glue?"

The main point: When g is large enough, the pair potential can change sign, i.e. become negative, signifying attractive interactions. Only when V is negative are there solutions to the gap equation.



Here, the glue comes from quantum loop corrections

Thermodynamics: the Fermi surfaces

Based on a new approach to the thermodynamics of gases based on the S-matrix. (with Pye-Ton How) The following represents a consistent resummation of 2-body scattering processes. Higher N-body processes are neglected.

Occupation numbers:

$$f(\mathbf{k}) = \frac{1}{\mathrm{e}^{\varepsilon(\mathbf{k})/T} + 1}$$

pseudo-energy satisfies the integral equation:

$$\varepsilon(\mathbf{k}) = \omega_{\mathbf{k}} - \mu - \int \frac{d^2\mathbf{k}'}{(2\pi)^2}\, G(\mathbf{k},\mathbf{k}') \frac{1}{\mathrm{e}^{\varepsilon(\mathbf{k}')/T} + 1}$$

Free energy density:

$$\mathcal{F} = -T \int \frac{d^2\mathbf{k}}{(2\pi)^2} \left[\log(1 + e^{-\beta\varepsilon}) + \frac{\beta}{2} \frac{1}{e^{\beta\varepsilon} + 1} (\varepsilon - \omega + \mu) \right]$$

The kernel G is related to log of the 2-body S-matrix, can calculate exactly.

Technical details on the kernel G:

$$L(\mathbf{k}_1,\mathbf{k}_2) = i\int \frac{d^2\mathbf{p}}{(2\pi)^2}\,\frac{1}{\omega_{\mathbf{k}_1}+\omega_{\mathbf{k}_2}-\omega_{\mathbf{p}}-\omega_{\mathbf{k}_1+\mathbf{k}_2-\mathbf{p}}+2i\epsilon} \quad \equiv \quad \mathcal{I}+i\gamma$$

$$G = -\frac{i}{2\mathcal{I}}\log\left(\frac{1/g_R - i\mathcal{I}/2}{1/g_R + i\mathcal{I}/2}\right)$$

S-matrix

$$g_R \;=\; g/(1-g\gamma/2)$$

gR is a renormalized coupling, I a phase space factor.

The kernel G also reflects the flip in sign of the effective interaction. Positive G corresponds to attractive interactions.

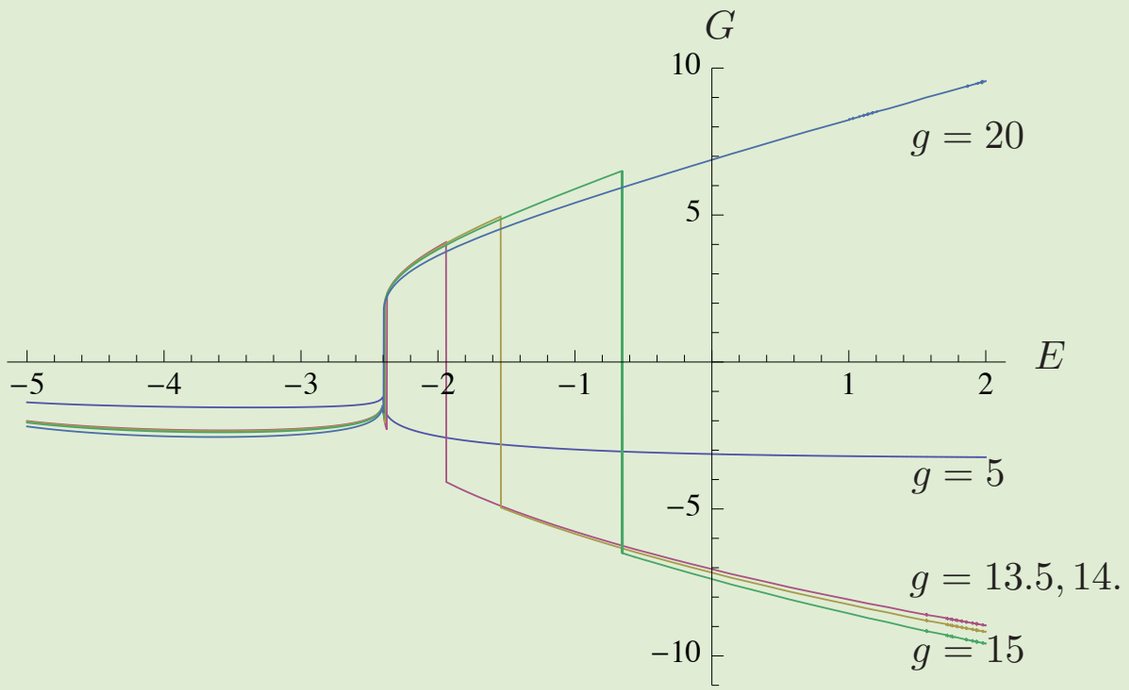
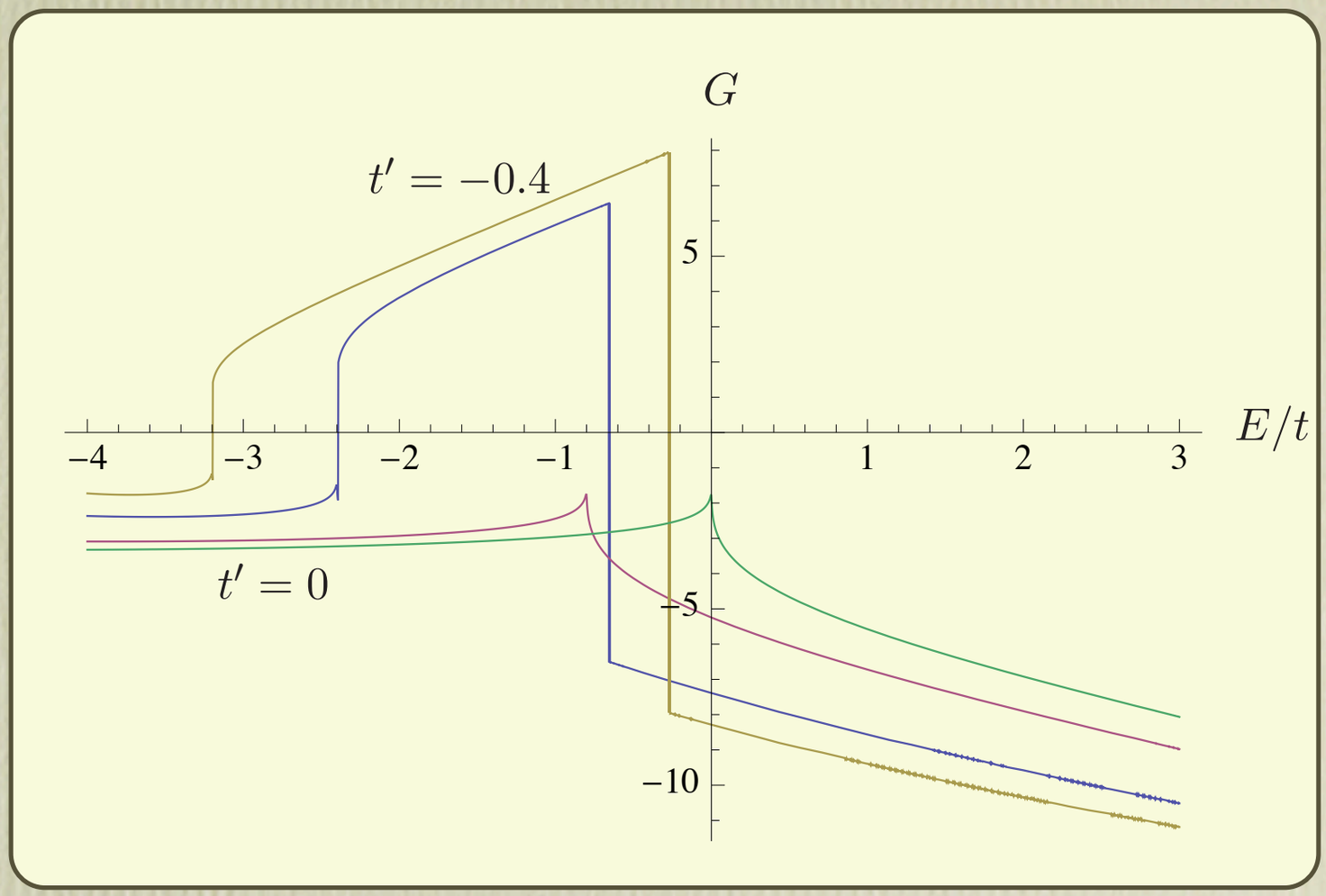


FIG. 3: The kernel G as a function of total energy E for $g = 5, 13.5, 14, 15, 20$, and $t'/t = -0.3$ (Color figures on-line.)

The role of t'

Fixed g=13, various t'



For g=13, no attractive region for t'=0.
prediction: no superconductivity for t'=0.
There is experimental evidence for this.
Simonelli et. al. 2005.

Hole doping h and chemical potential

density: $$n = 2\int \frac{d^2\mathbf{k}}{(2\pi)^2}\,\frac{1}{e^{\varepsilon(\mathbf{k})/T}+1} = \frac{1-h}{a^2}$$ (h=holes per plaquette)

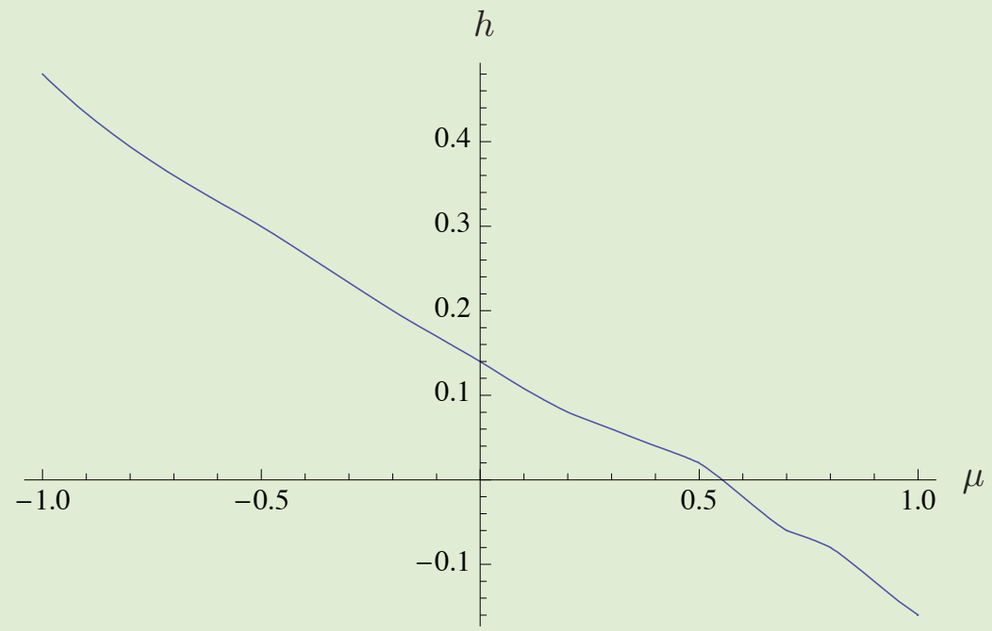
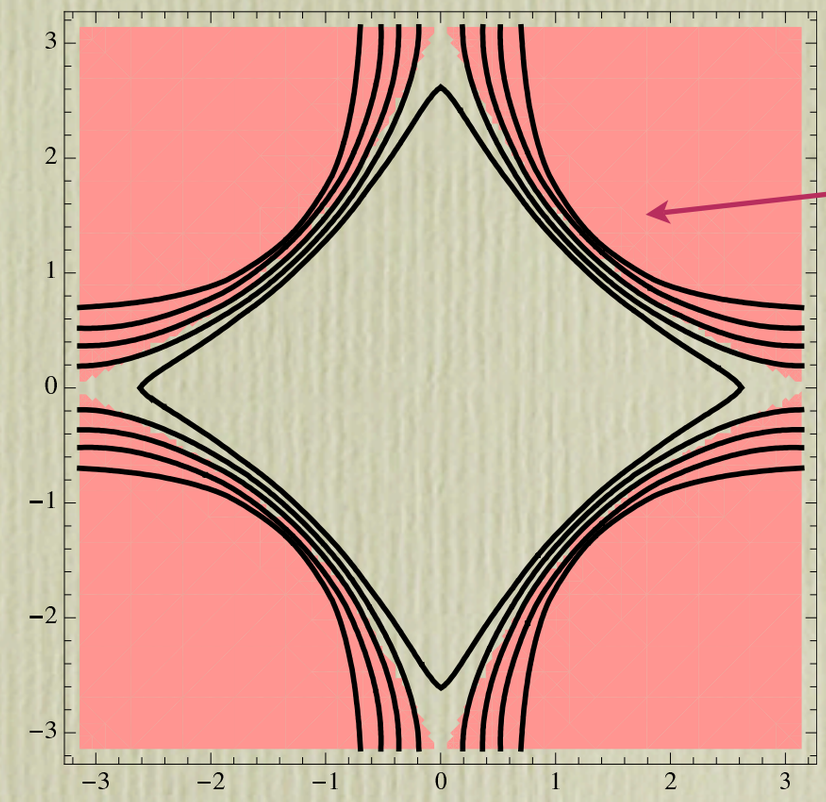


FIG. 5: Hole doping h as a function of chemical potential μ at the reference temperature $T_0 = 0.1$. $(g = 26, t' = -0.3.)$

Calculated Fermi surfaces

$\xi(\mathbf{k})$ = pseudo-energy = 0

node



Attractive region in pink

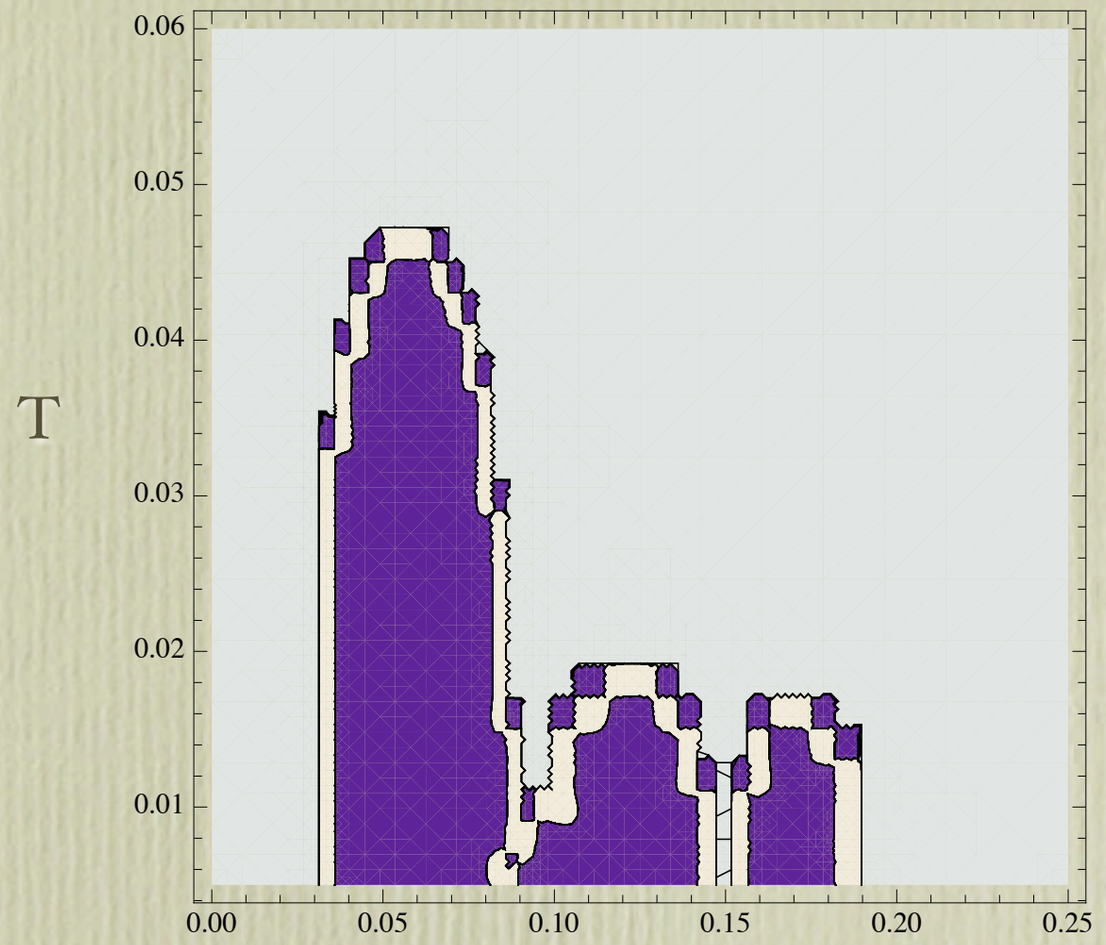
anti-node

hole dopings: 0, .1, .2, .3, .4

prediction: no superconductivity for h> 0.35

prediction: gap will be anistropic, largest in the anti-nodal directions

Regions in density/temperature with no solution to the pseudo-energy integral equation are interpreted as instabilities toward the formation of new phases.

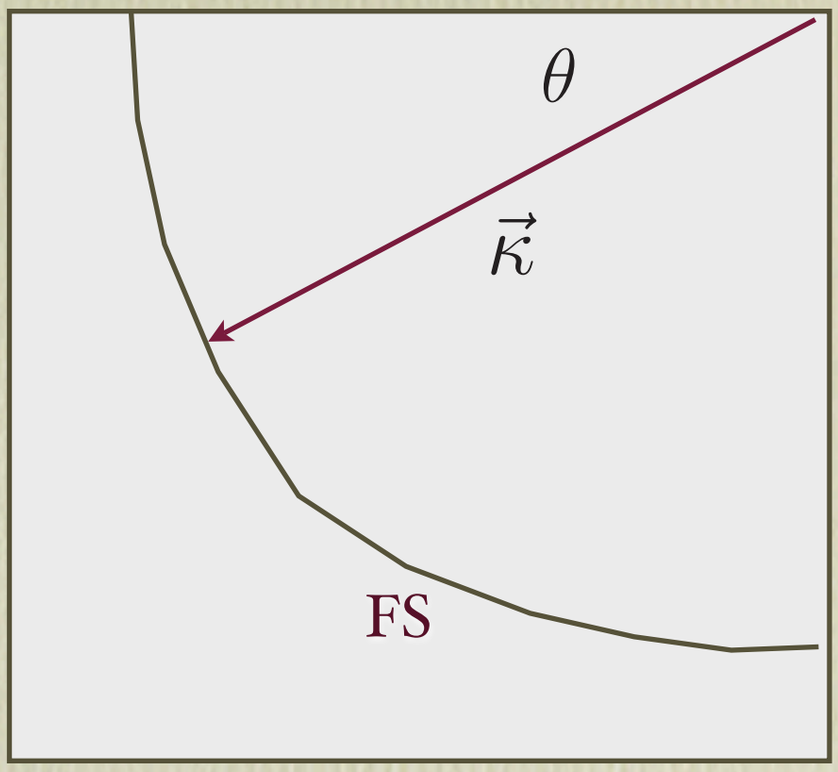


(g=13)

predictions: * 60K < Tc < 120K
at h=0.15 (exp: Tc/t = 0.025)
*instability continues to low doping, suggestive of pseudo-gap.

Solutions to the gap equation

first quadrant of
Brillouin zone:

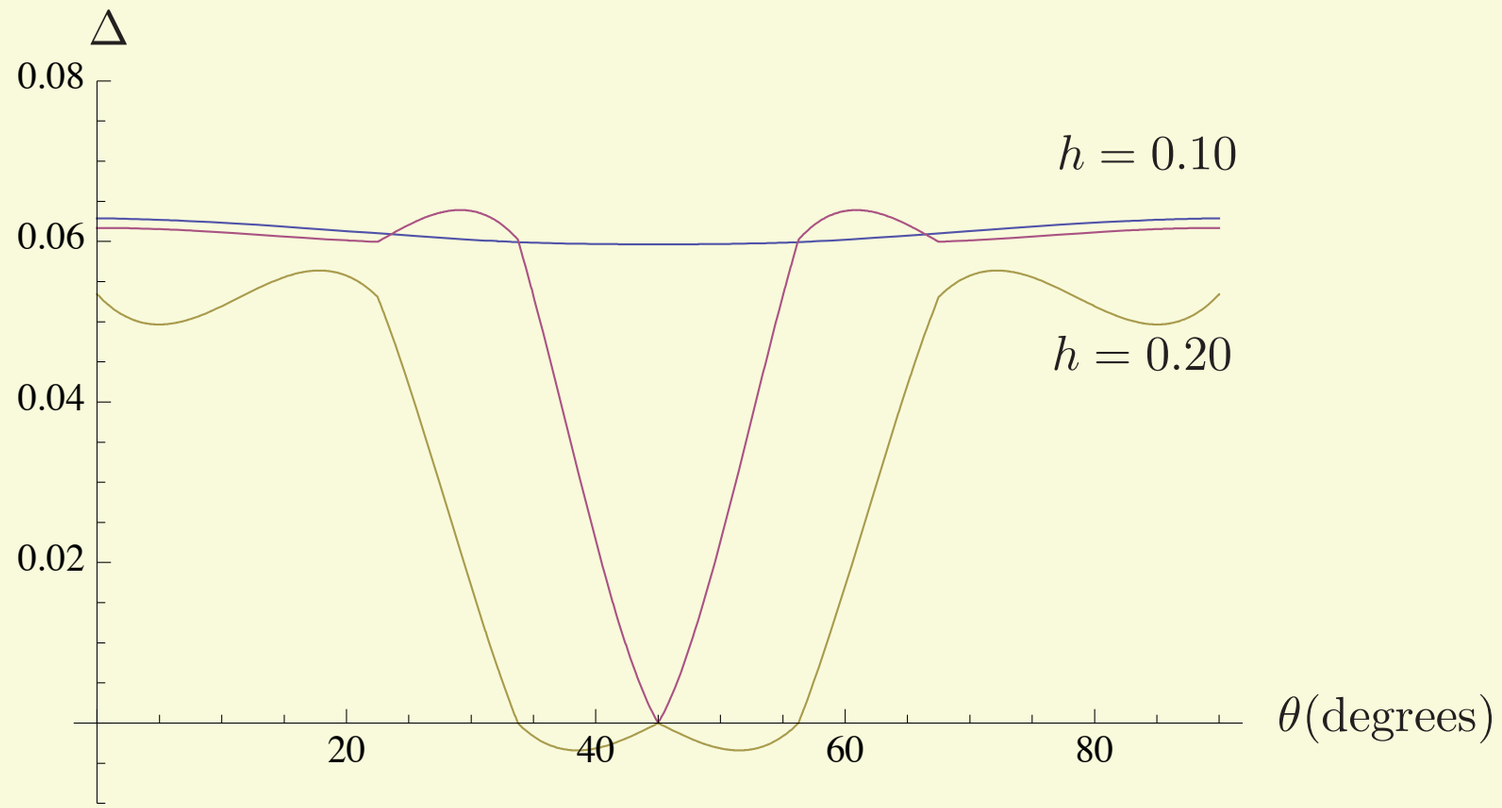


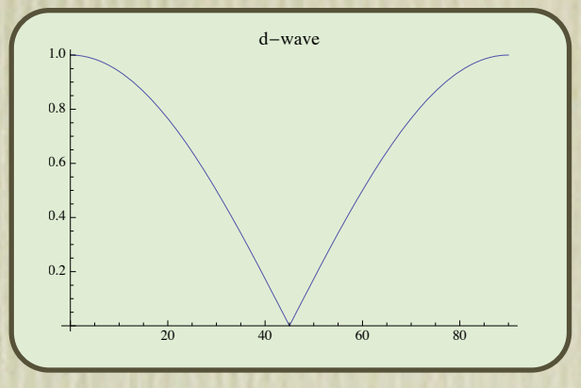
$$\Delta(\kappa,\theta) = -\frac{1}{8\pi^2}\int_0^{\pi/2} d\theta' \int_{\kappa_F(\theta')-\delta\kappa}^{\kappa_F(\theta')+\delta\kappa} d\kappa'\kappa'\ V_-(\kappa,\theta;\kappa',\theta')\frac{\Delta(\kappa',\theta')}{E(\kappa',\theta')}\tanh\left(\frac{E(\kappa',\theta')}{2T}\right)$$

$$E = +\sqrt{\xi^2+\Delta^2},$$

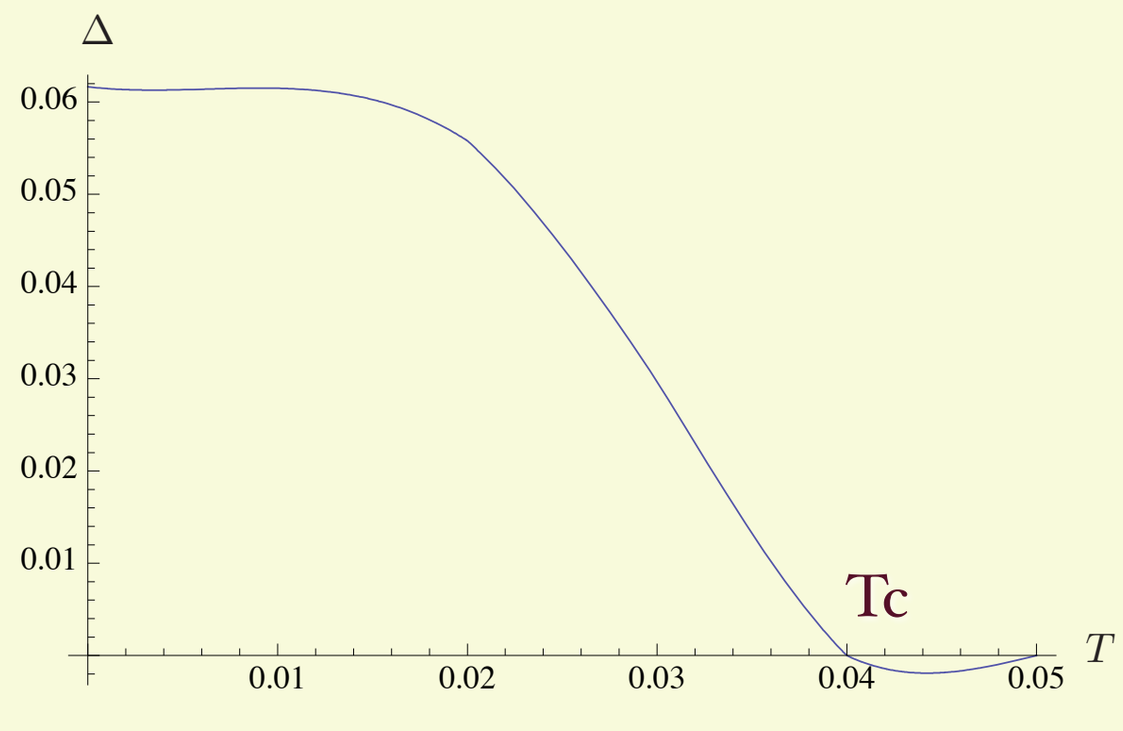
$\delta\kappa$ = cut-off = 0.04 (based on distance between FS and attractive region.

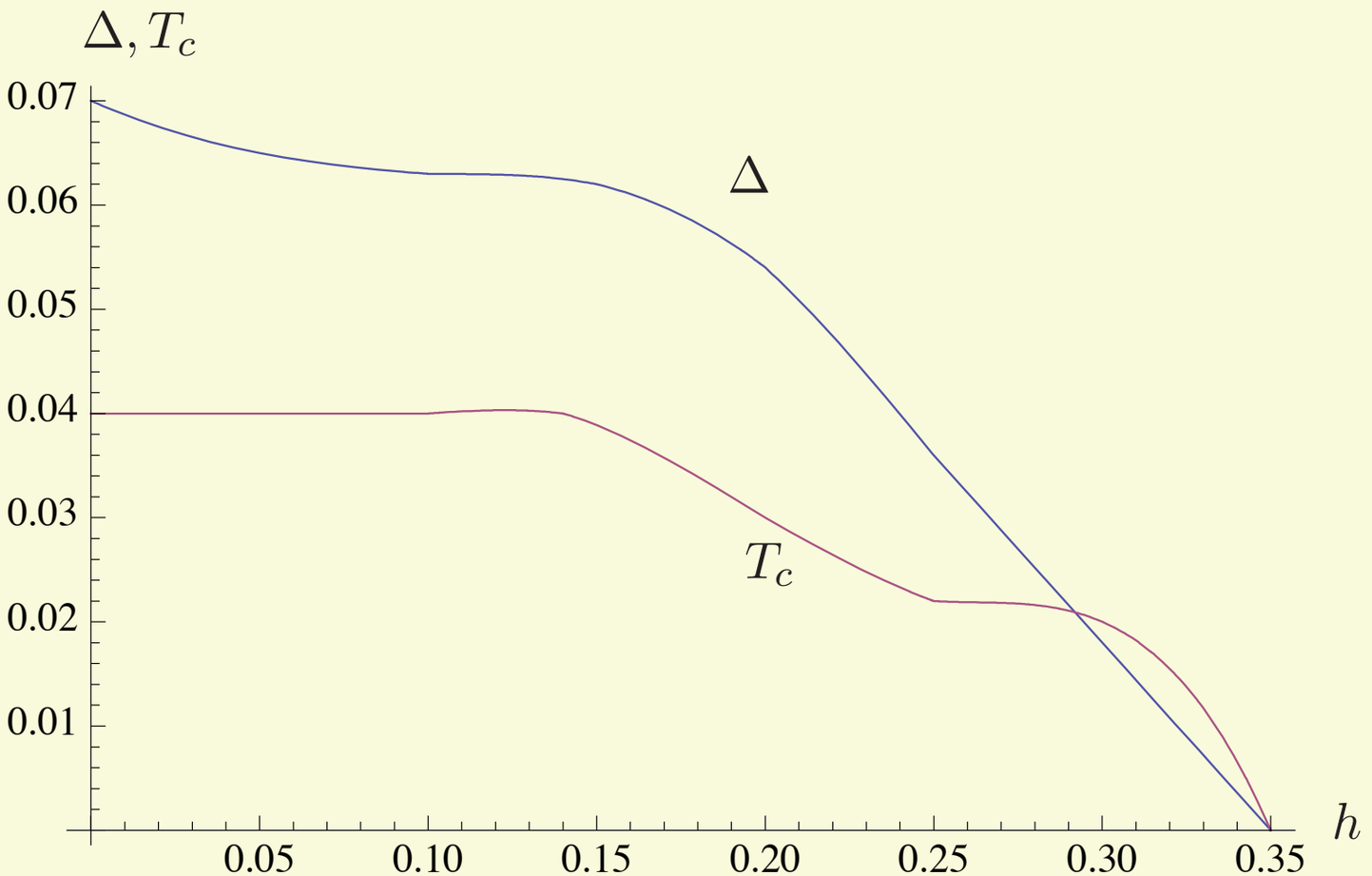
RESULTS

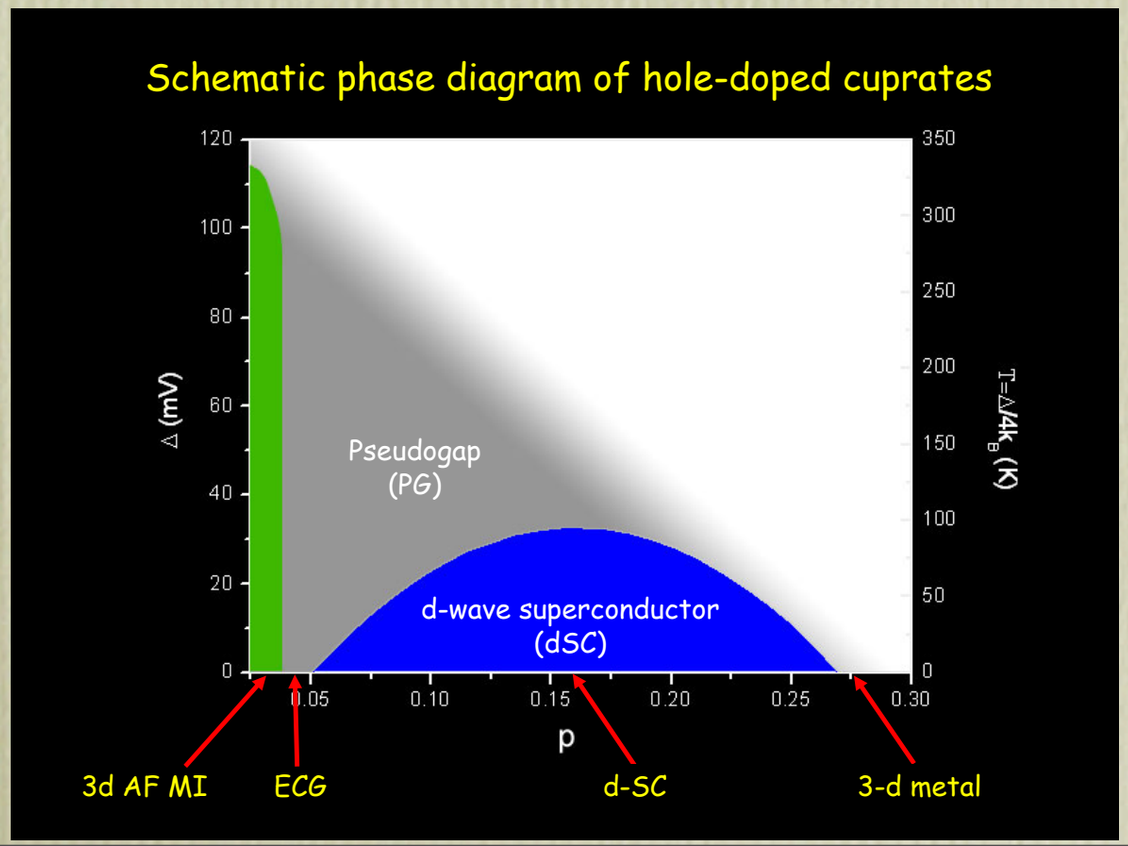




d-wave

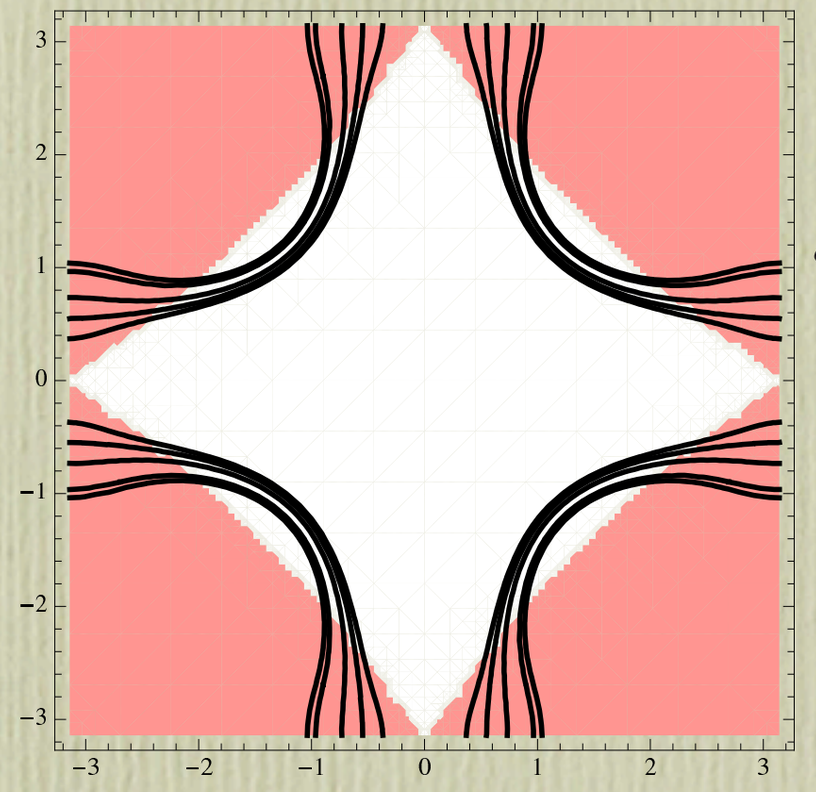




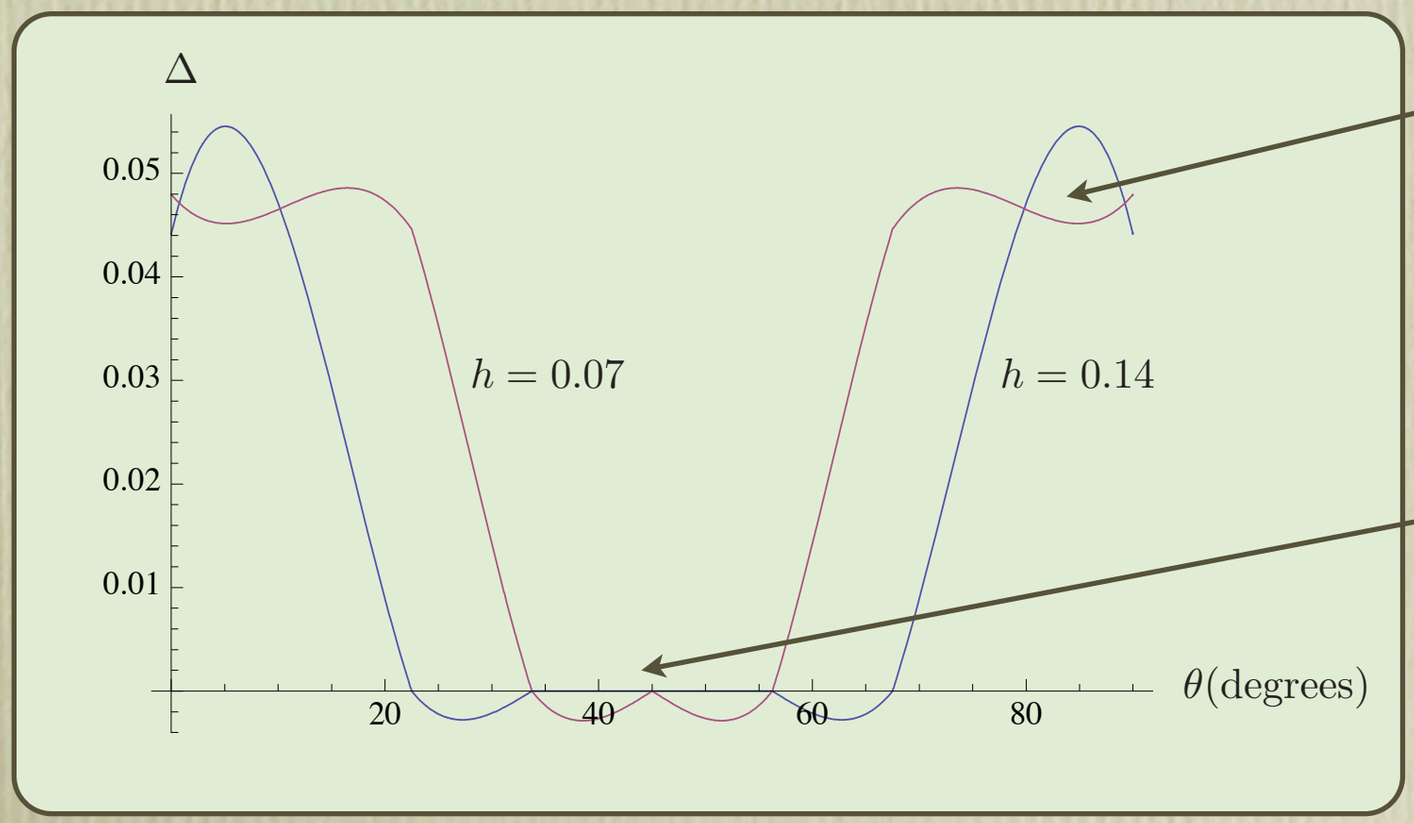


At h=0.15,
Tc= 120K (exp. = 90K)
Delta = 20meV (exp=30)

Solutions for phenomenological fit to the Fermi surfaces



$$\xi(\mathbf{k}) = -\widehat{\mu} - 2\left(\cos k_x + \cos k_y\right) + 0.6513 \cos k_x \cos k_y - 0.4455\left(\cos 2k_x + \cos 2k_y\right)$$
$$- 0.1716\left(\cos 2k_x \cos k_y + \cos k_x \cos 2k_y\right) + 0.6357 \cos 2k_x \cos 2k_y \qquad (2$$



Extinction?

Fermi arc
(flat region)

Summary of the main features

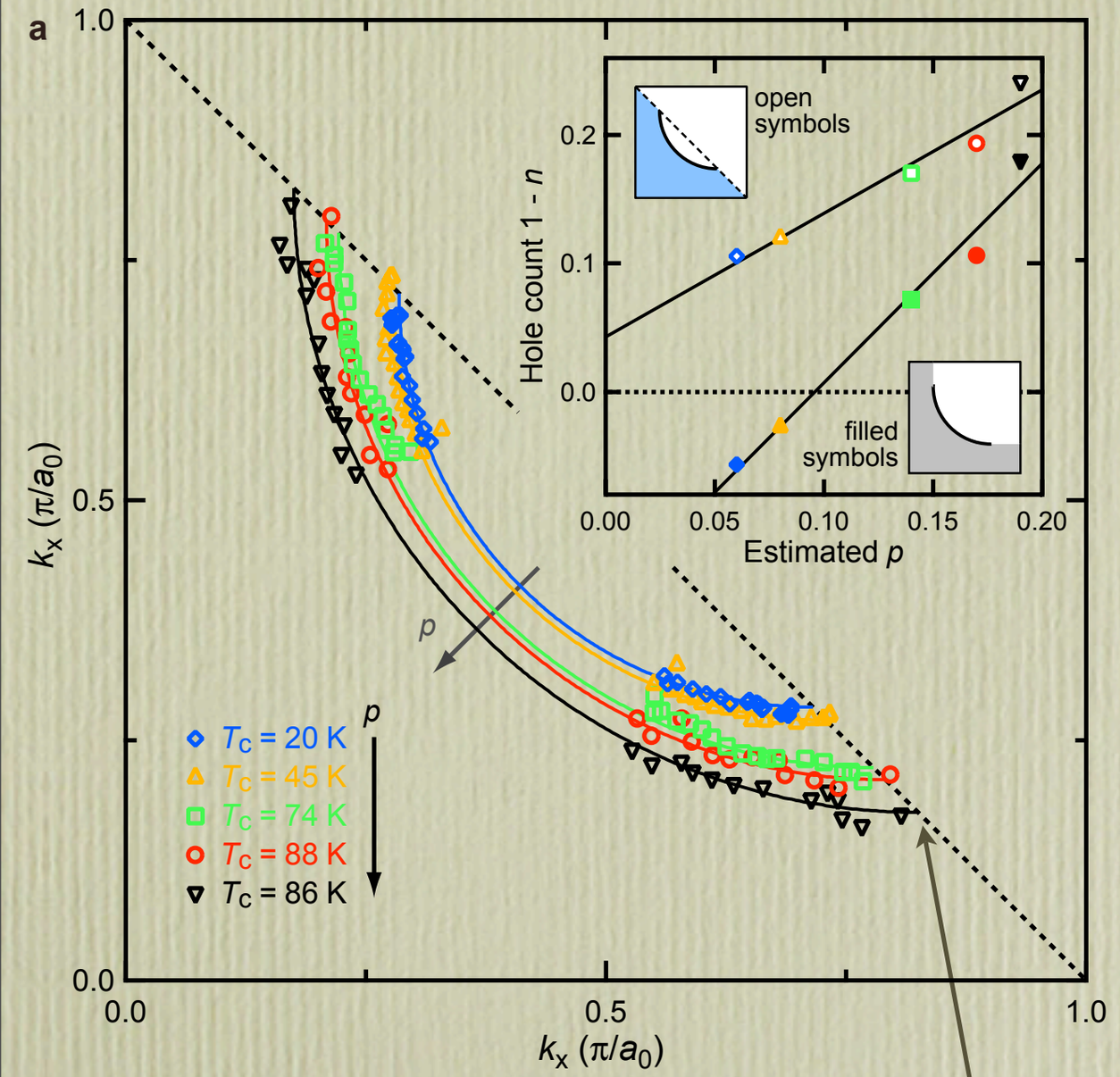
- Energy scales are roughly correct: Tc/t = 0.04 (exp: Tc/T = 0.025), Gap = 30 meV, at optimal doping.

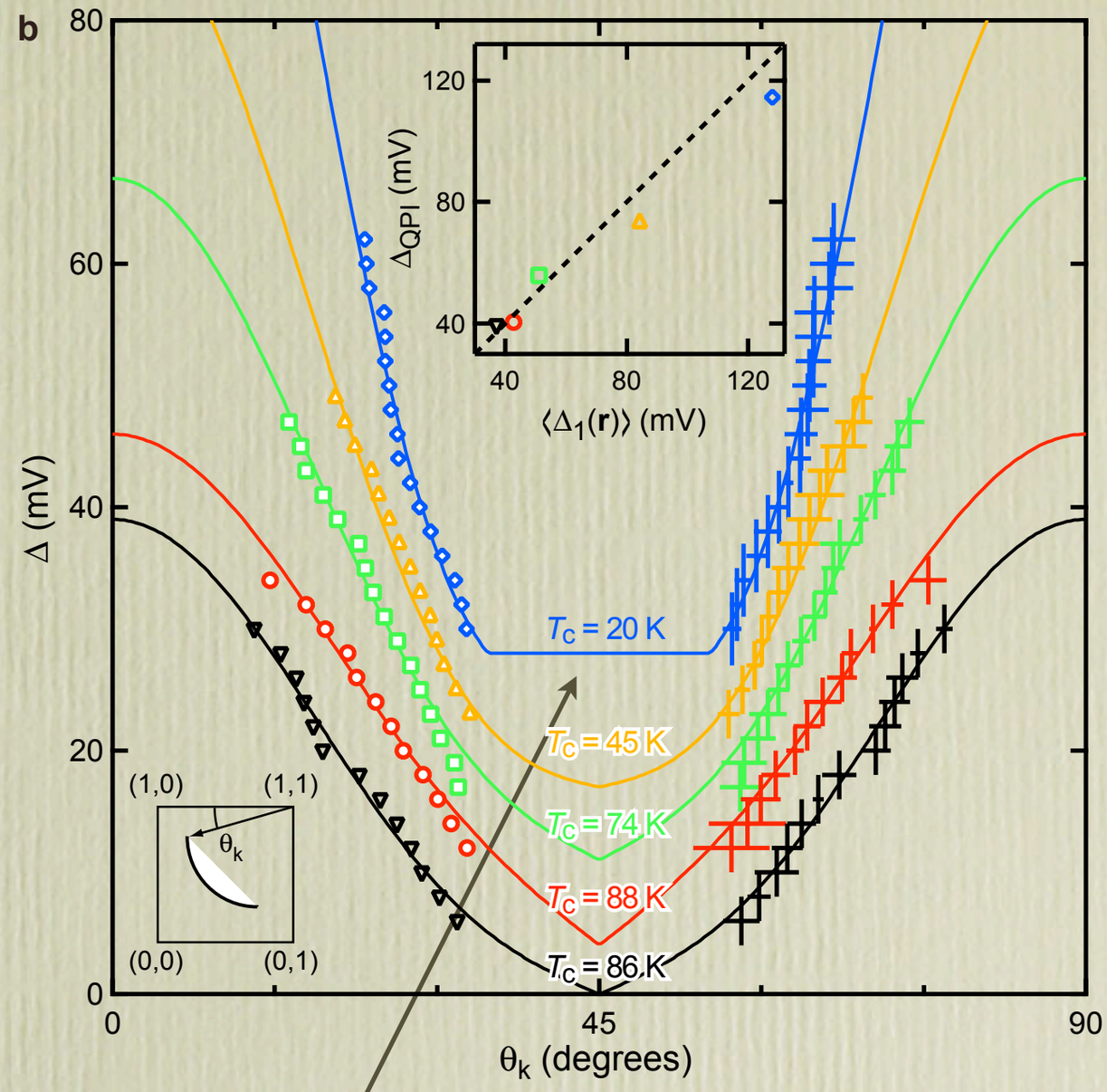
- The gap has a flat region around 45 deg. These are the Fermi arcs, and they exist at zero T. Gap is not d-wave, i.e. not $\Delta \propto |\cos k_x - \cos k_y|$

- The gap increases all the way down to zero doping, suggesting that the SC gap and pseudo-gap arise from the same mechanism. (There is growing experimental evidence for this.)

Norman et. al. Nature (1998), Chatterjee et. al. Nature Phys. 2010, Kohsaka et. al. Nature (2008).

Comparison with recent STM experiments





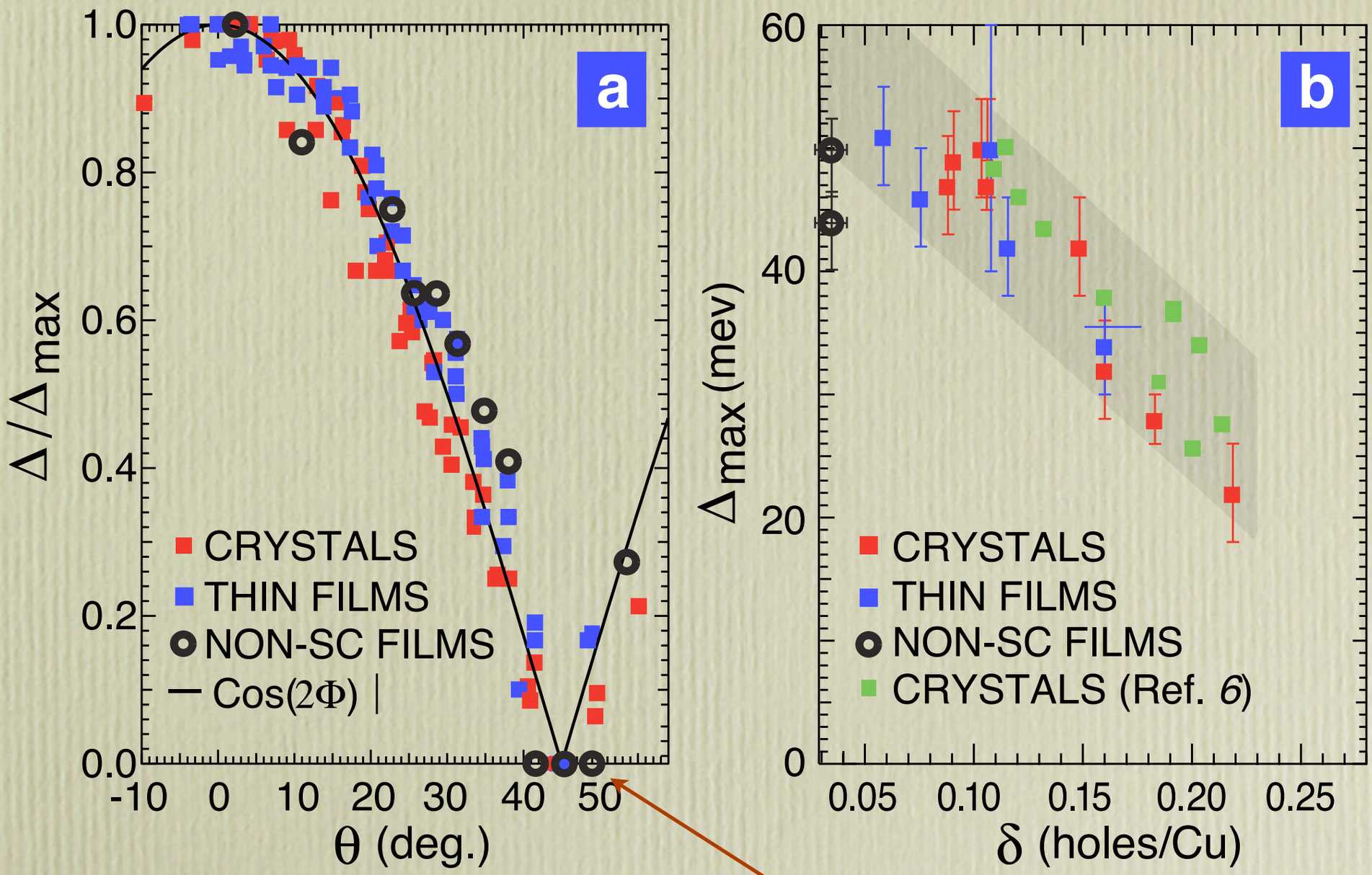
Extinction

Fermi arc

S. Davis group
Nature 454 (2008)

Our results are evocative of what is seen in STM at low doping, i.e. a Fermi arc that persists to zero temperature. ARPES sees more of a d-wave gap everywhere.

ARPES sees more of a d-wave gap:



Flat arc?

Chatterjee et. al. Nature Phys. 2010

Conclusions

- Main idea explored: quantum loop corrections to the pair potential leads to an attractive mechanism. Energy scales for Tc and the gap come out right.

- Results strongly suggest the pseudogap and SC gap arise from this same attractive mechanism.

- Calculated gap reflects some features recently seen in STM, zero temperature Fermi arc, at low doping, etc. At higher doping, agreement is not as good, and disagrees with the d-wave gap seen by ARPES. (needs to be resolved.)

The End