Electron pairing mechanism in high-transition temperature superconductors

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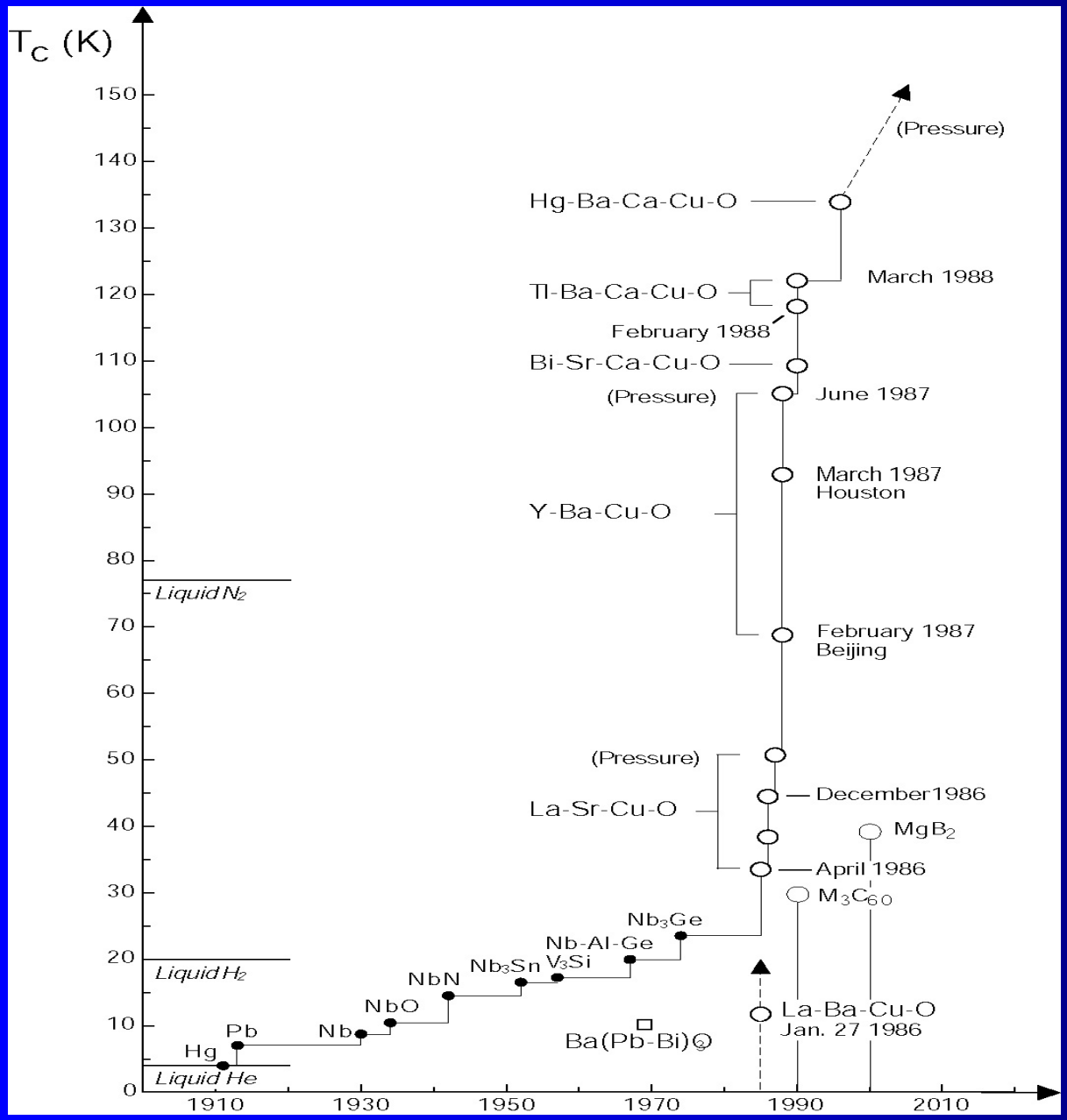
Overview of Superconductivity



- Metals:
  - Hg, Al, Pb, Nb, Nb_3Sn
- Doped copper oxides: $La_{2-x}Sr_xCuO_4$, $YBa_2Cu_3O_{6+x}$ …
- Other materials:
  - Heavy Fermion
  - M_3C_{60}
  - MgB_2

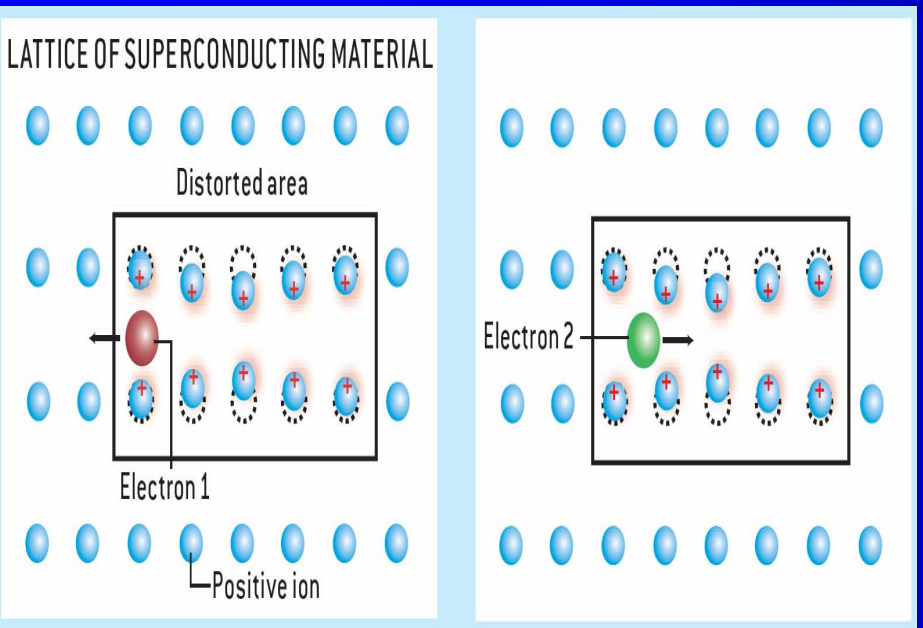
Exciting possibilities in studying the new class of high-T_c cuprates

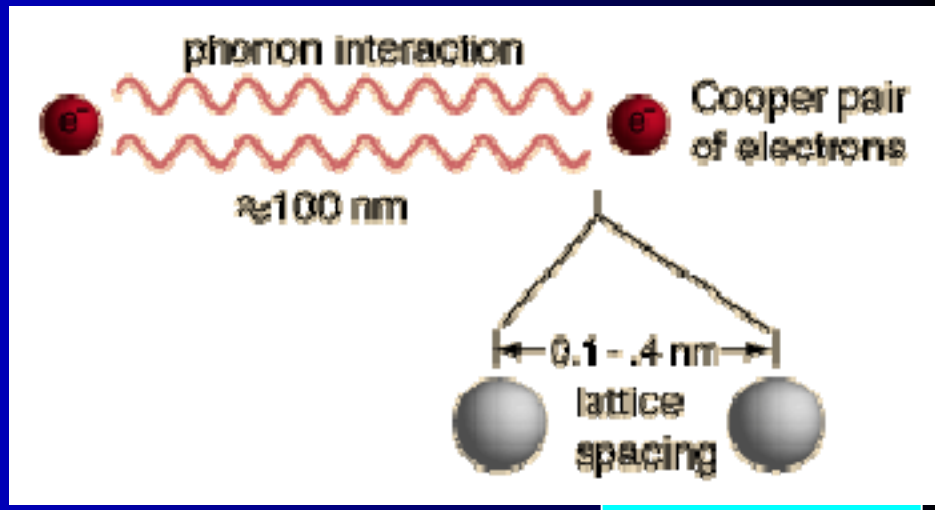
BCS theory of superconductivity

- **The binding of electrons into Cooper pairs is essential.**

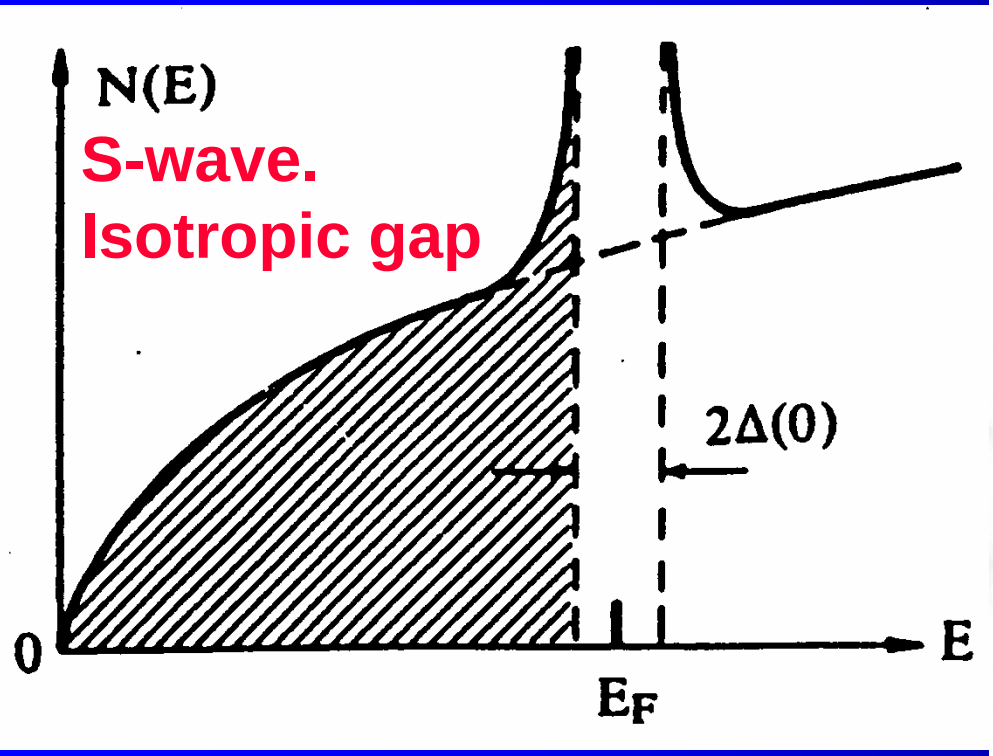
Two Fermions form a spin singlet boson: $\Psi = (k_x^2 - k_y^2)(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$; $\langle \mathbf{S} \rangle = \uparrow + \downarrow = 0$

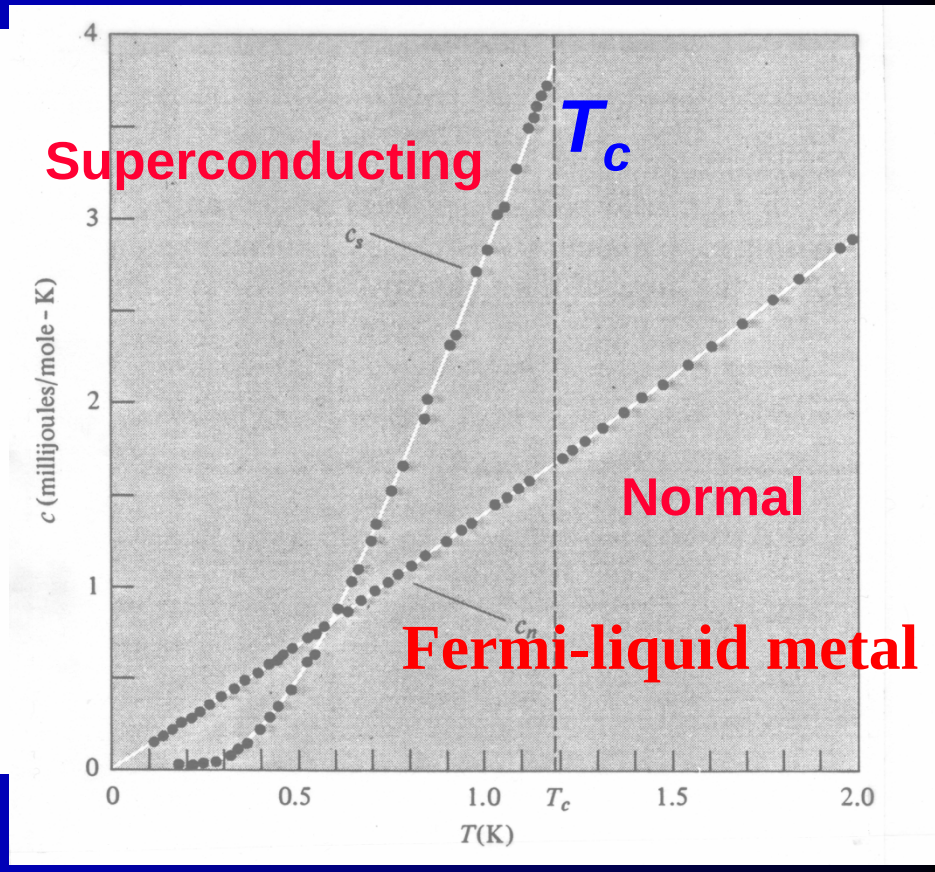
- **Long-range phase coherence among the pairs is also required to have superconductivity.**
- **Electron pairing is mediated by electron-phonon interaction.**
- **Electron pairing and phase coherence are established at T_c.**





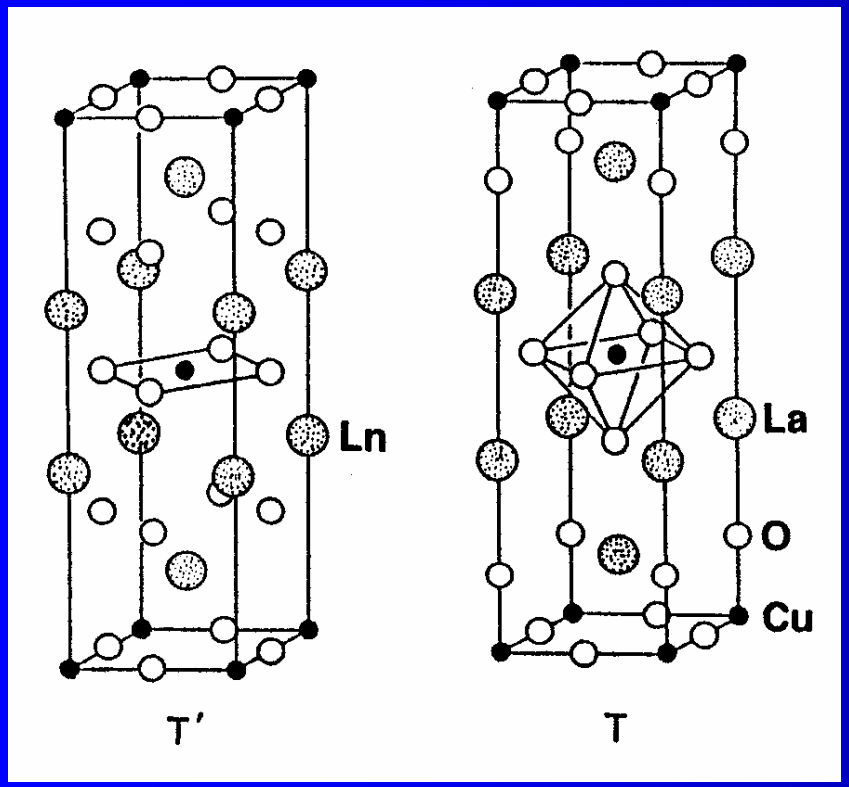
Density of states in a BCS superconductor





The BCS pairing is driven by a gain in the attractive potential at the expense of kinetic energy.
Kinetic energy gain due to frustration
A much large potential energy drop

Structures of copper oxides

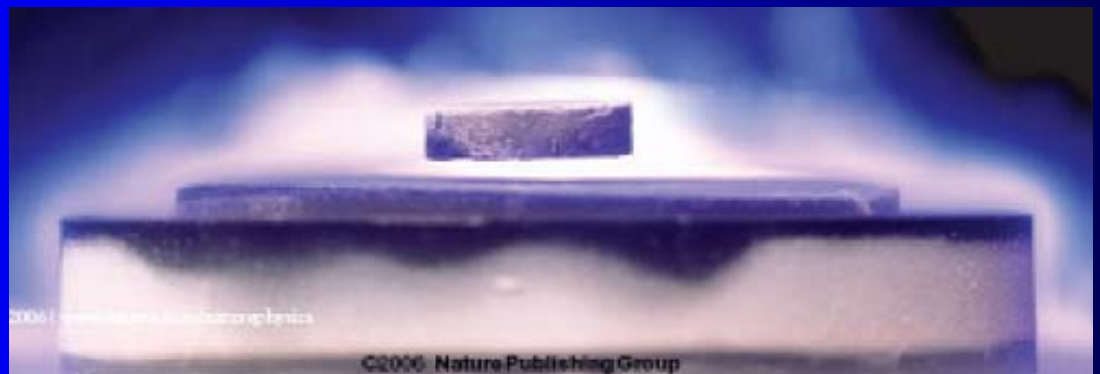


Single CuO_2 layer/unit cell

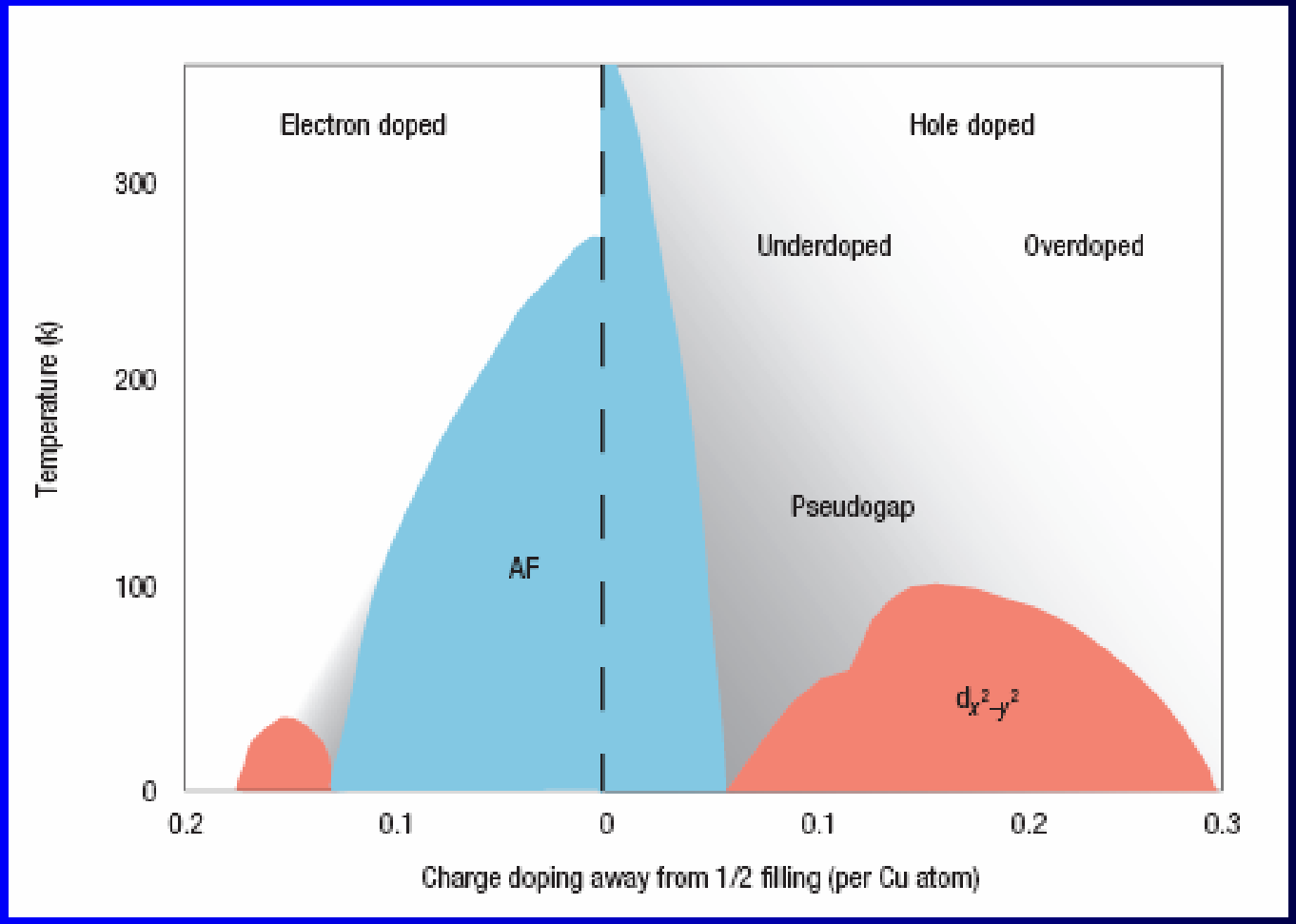
Hole-doping:
$La_{2-x}^{3+}Sr_x^{2+}CuO_4$ (T_c~40 K)

$Tl_2Ba_2CuO_{6+\delta}$ (T_c~90 K)

Electron-doping:
$Nd_{2-x}^{3+}Ce_x^{4+}CuO_4$ (T_c~25 K)
$Pr_{1-x}LaCe_xCuO$ (T_c~25 K)



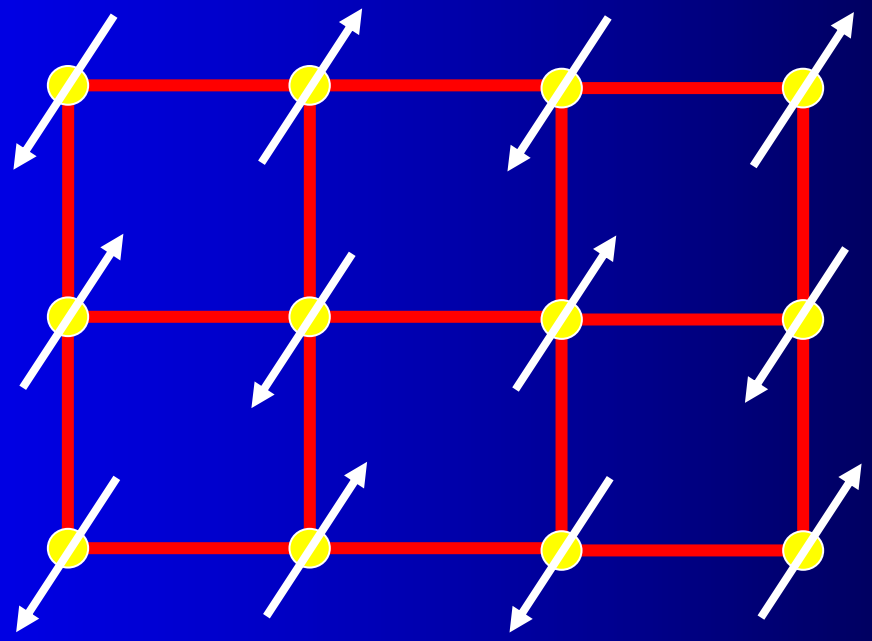
Phase diagram of cuprates



CuO_2 layers, AF order in parent compounds, doped either by holes or electrons to make SC.

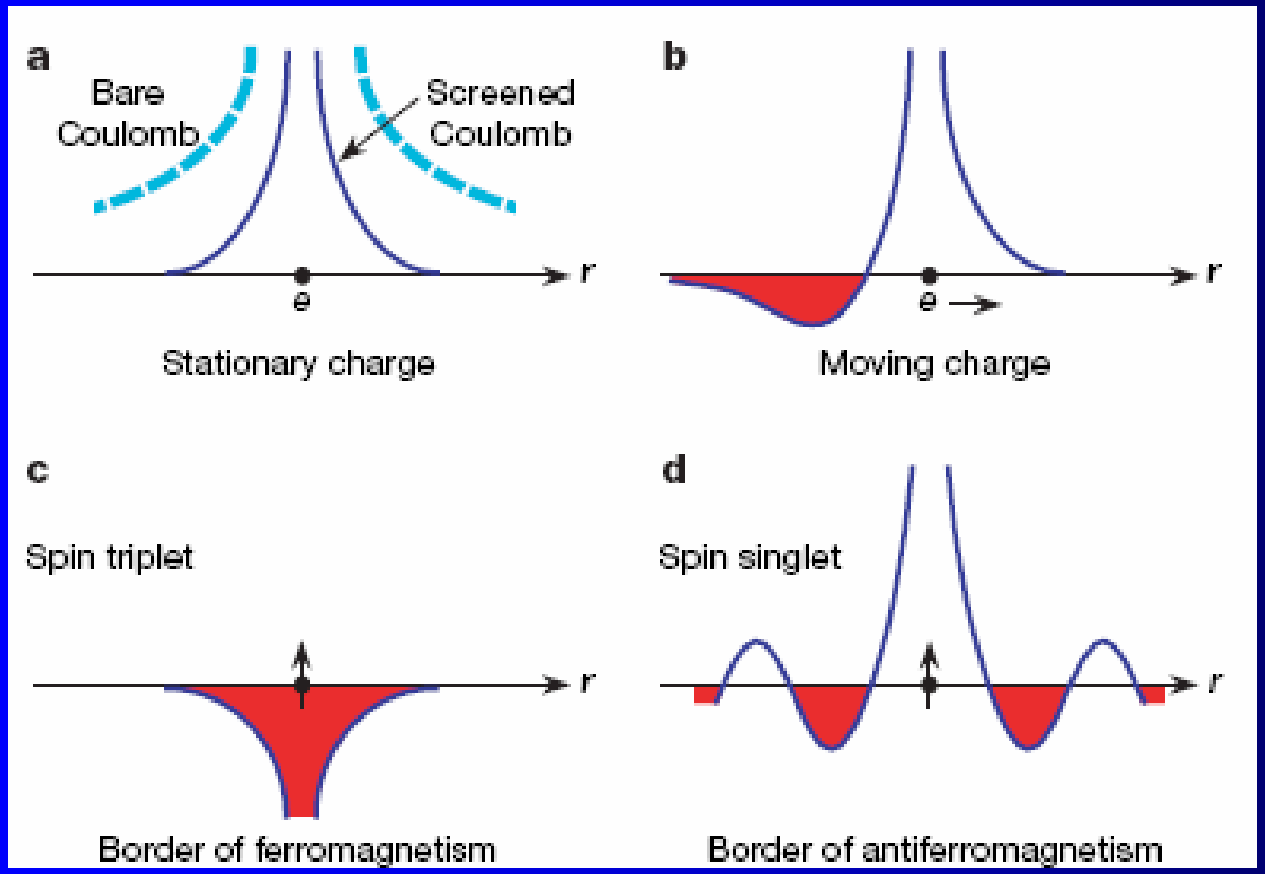
Statement of the problem

$$H = \sum_{<ij>} J_{ij} \, \vec{S}_i \cdot \vec{S}_j$$



Are high-T_c superconductors another BCS-like superconductor with additional features or something fundamentally different?

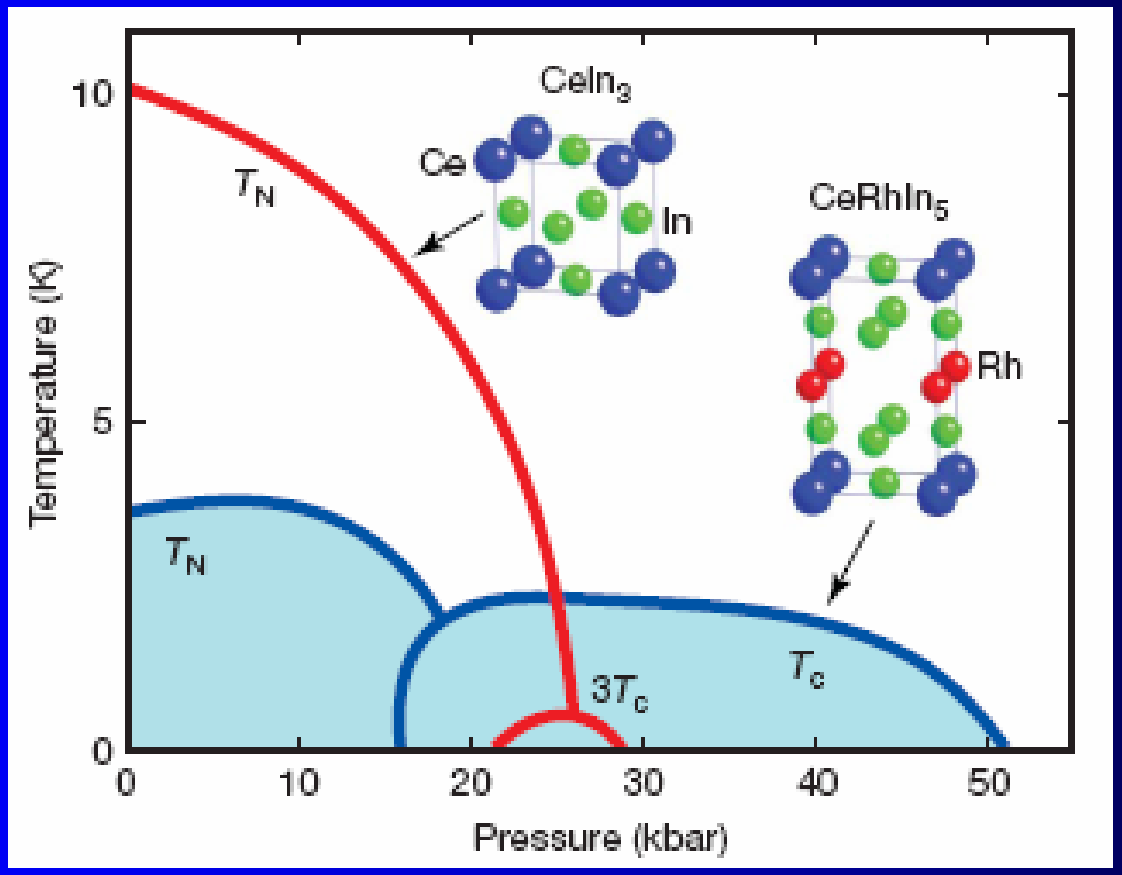
Is it possible to have superconductivity without phonons?



This attraction is caused by the polarization of the positively charged and heavy ions that lie behind the moving charge and its electron screening cloud.

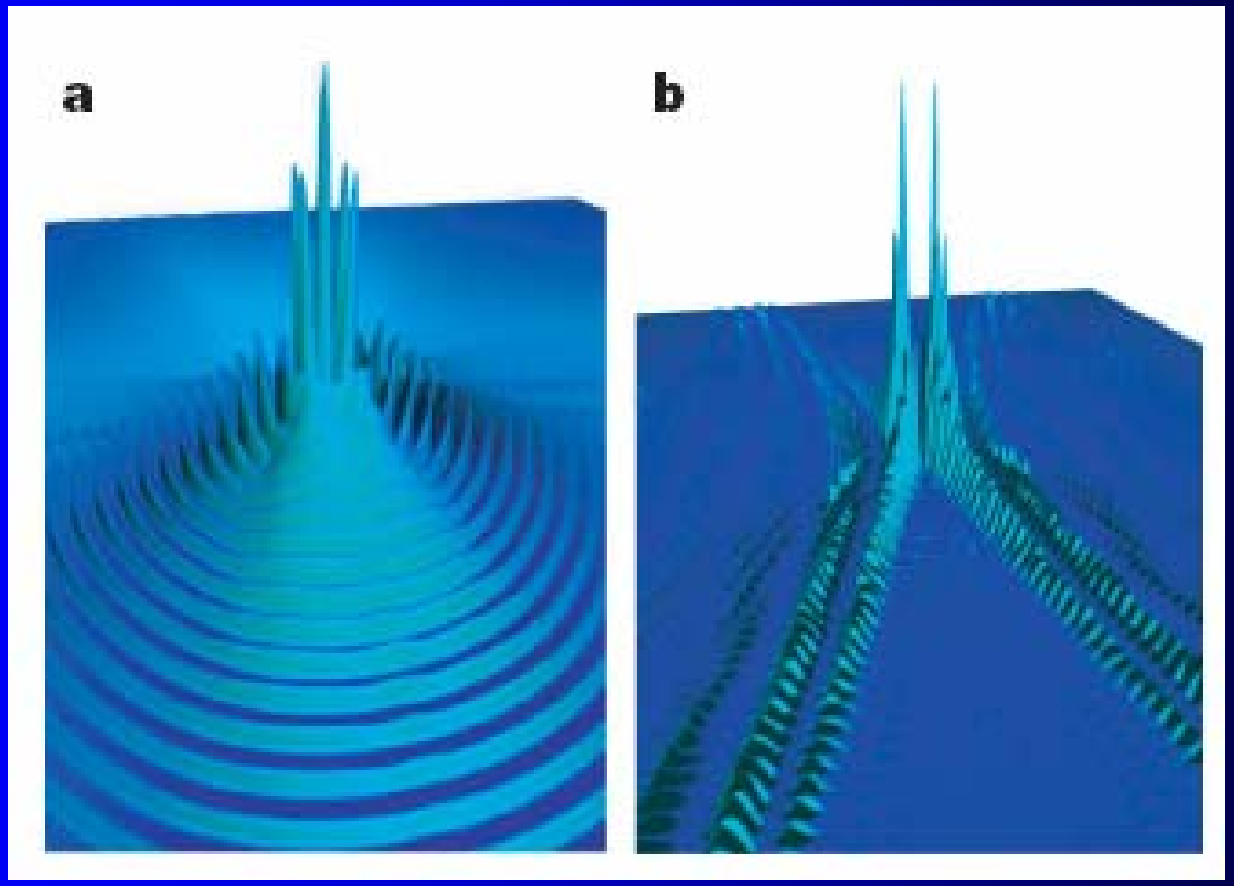
Monthoux, Pines & Lonzarich, Nature (2007)

For heavy Fermions, isotropic pressure can drive the system from AF phase to superconducting phase.



- Pairing exchange is likely to be magnetic in origin.

Anisotropic magnetic interaction induces *d*-wave electron pairing, as found in high-Tc cuprate superconductors.



- *S*-wave.
- *d*-wave.

How do we prove whether magnetism has sufficient energy to induce electron pairing and superconductivity in high-Tc superconductors?

Total Energy = KE + PE

PE or exchange energy is directly related to the spin-spin correlation function, which can be measured by inelastic neutron scattering.

However, this determination requires the knowledge of the normal state spin-spin correlation function at Zero temperature, a quantity that is difficult to obtain because the presence of superconductivity.

$$\Delta E_{ex} = 2J(\left\langle \vec{S}_i \cdot \vec{S}_j \right\rangle_N - \left\langle \vec{S}_i \cdot \vec{S}_j \right\rangle_S)$$

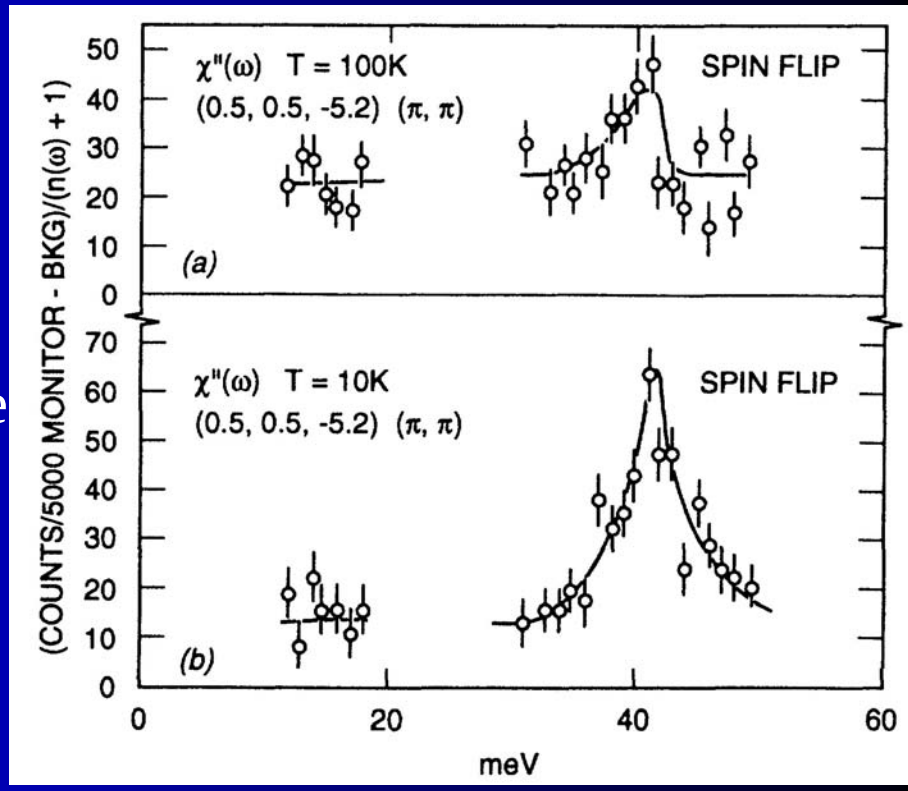
- Scalapino and White, PRB 58, 8222 (1998).

Spin behavior in parent compounds

- Parent long-range AF order
  - AF Bragg reflections at (0.5, 0.5) positions
- La_2CuO_4
  - Spin wave excitations
  - 2D Heisenberg AF on square lattice

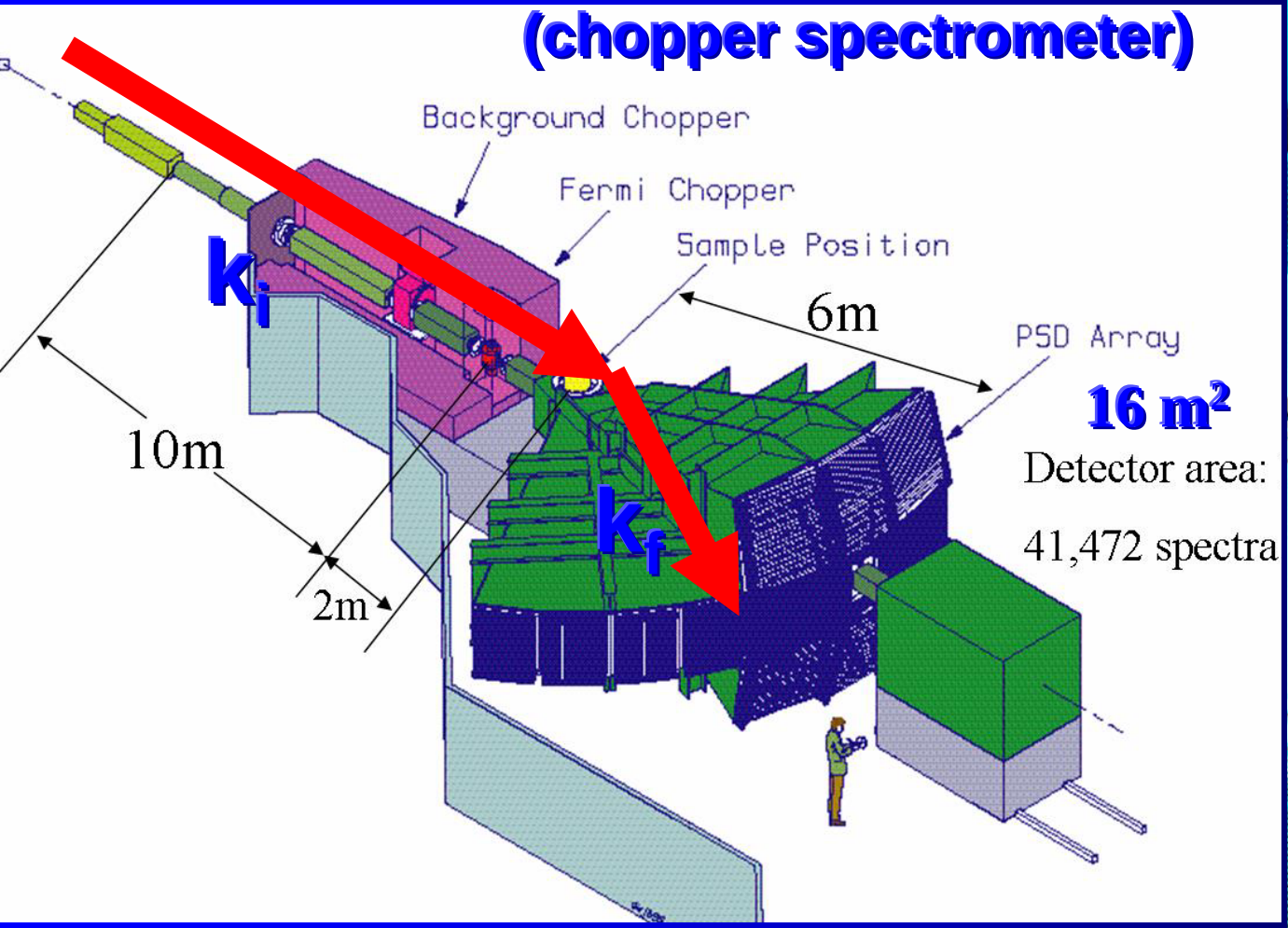
$$H = \sum_{<ij>} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

  - $J_{ab} \sim 104$ meV (nn), $J_{ab} >> J_c$
- Nd_2CuO_4 and Pr_2CuO_4 qualitatively same behavior
- How do dynamics change when carriers doped into CuO_2 layers?



YBCO7, T_c = 92.4 K, H. A. Mook *et al.*, PRL 70, 3490 (1993).

Experiment on MAPS, ISIS Facility

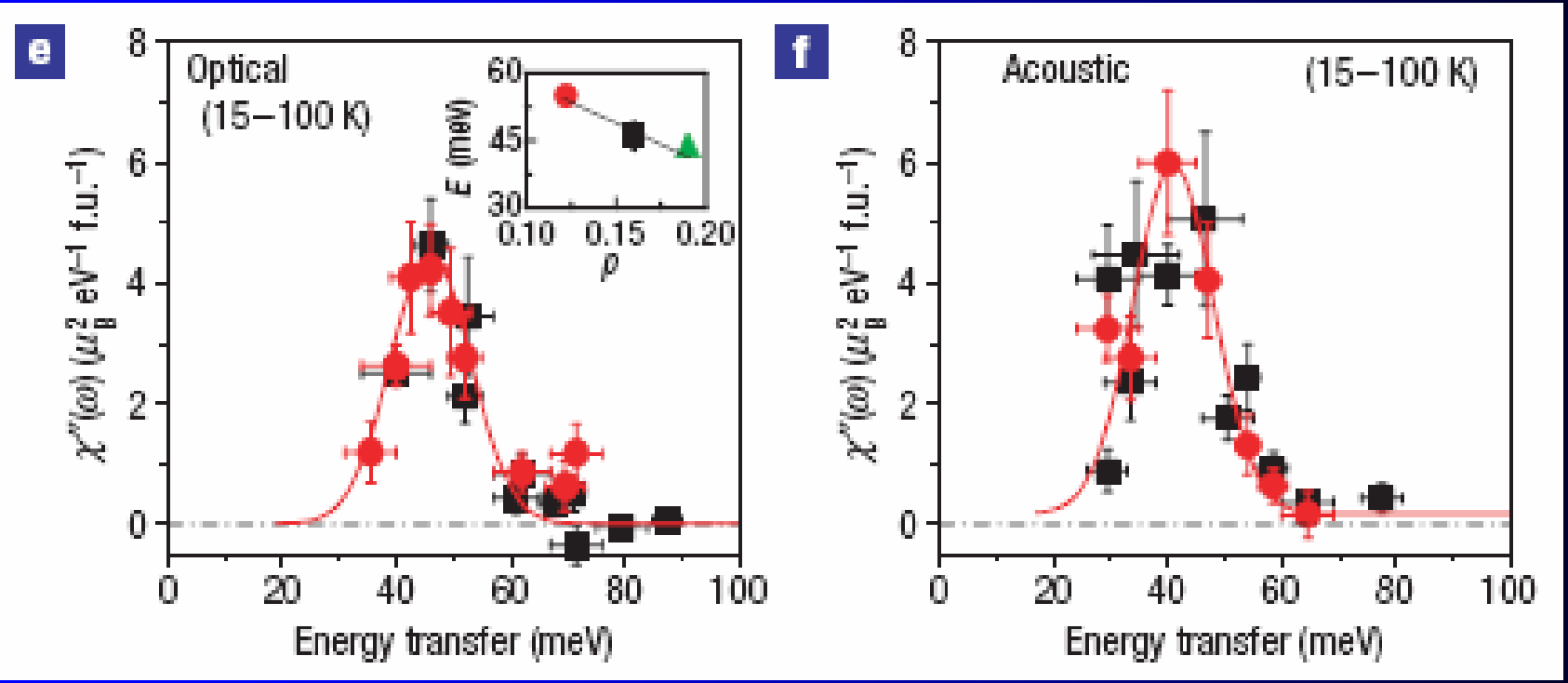


- Used incident energies from ~ 15 meV to ~ 2 eV.
- Crystal aligned with c* (chain) perpendicular to ki.

Energy resolution (Ei, f):

hω / *Ei* = 2 – 5% FWHH at elastic line (hω = 0); 1.5% FWHH at full energy transfer (hw = *Ei*)

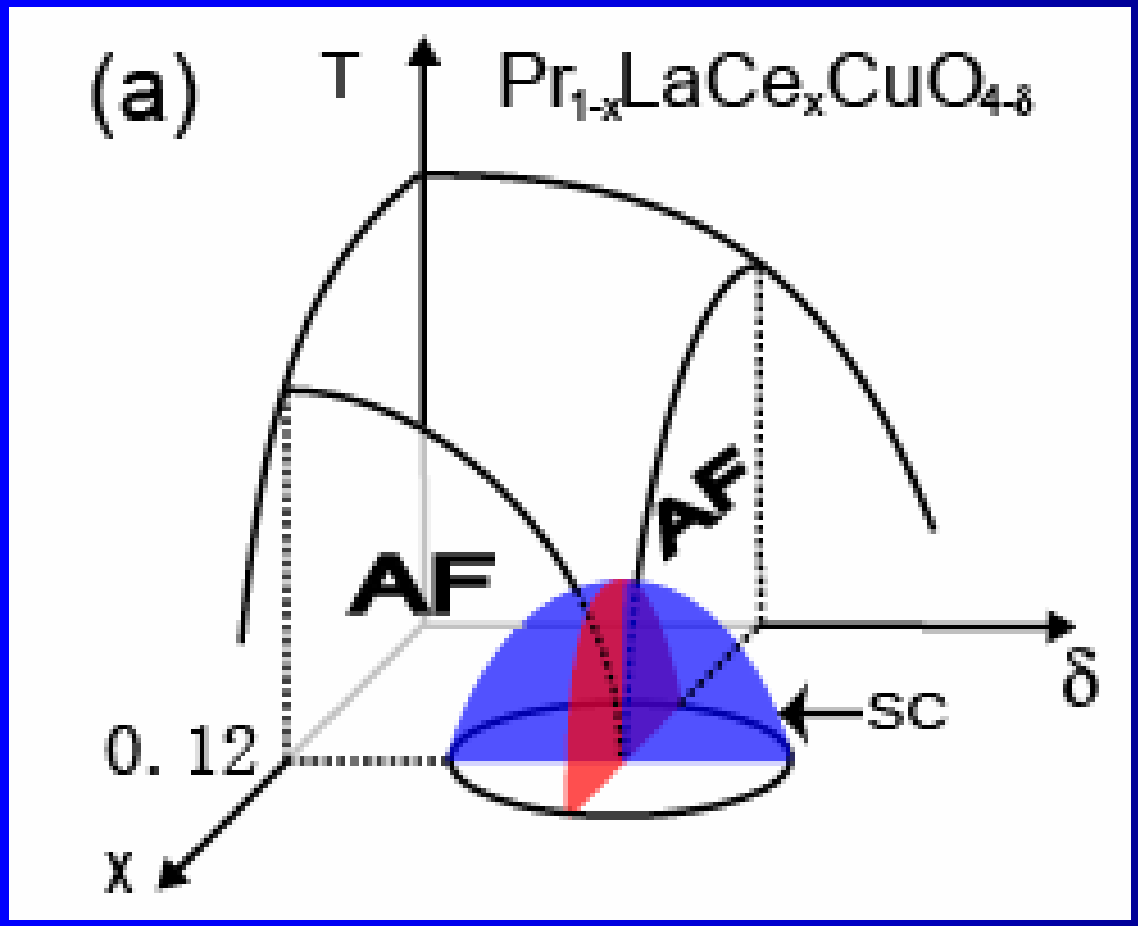
The changes in dynamic susceptibility from the normal to the superconducting state is large enough to account for the superconducting condensation energy in YBCO.



Problem: low-T normal state susceptibility is unknown.

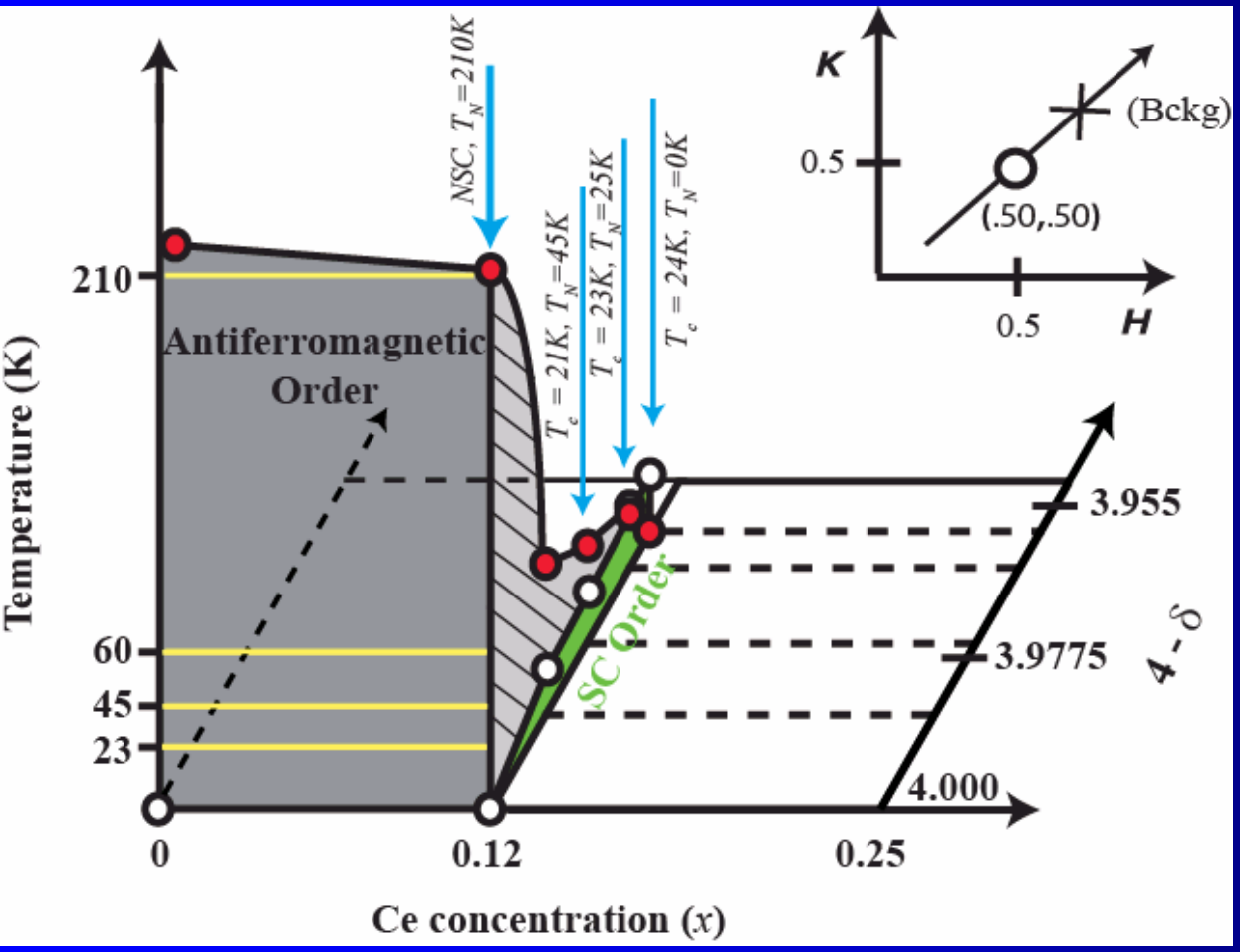
Woo et al., Nature Phys. (2006)

Phase diagram of $Pr_{1-x}LaCe_xCuO_{4-\delta}$ as a function of Ce concentration and annealing process



Superconductivity in PLCCO requires finite Ce-doping and annealing at high-temperatures in oxygen poor condition to remove a small amount of excess oxygen.

Phase diagram of PLCCO as a function of Ce doping and O content



One can control annealing temperature and thus T_c and T_N of the crystal.

Wilson *et al.*, PRB 74, 144514 (2006).

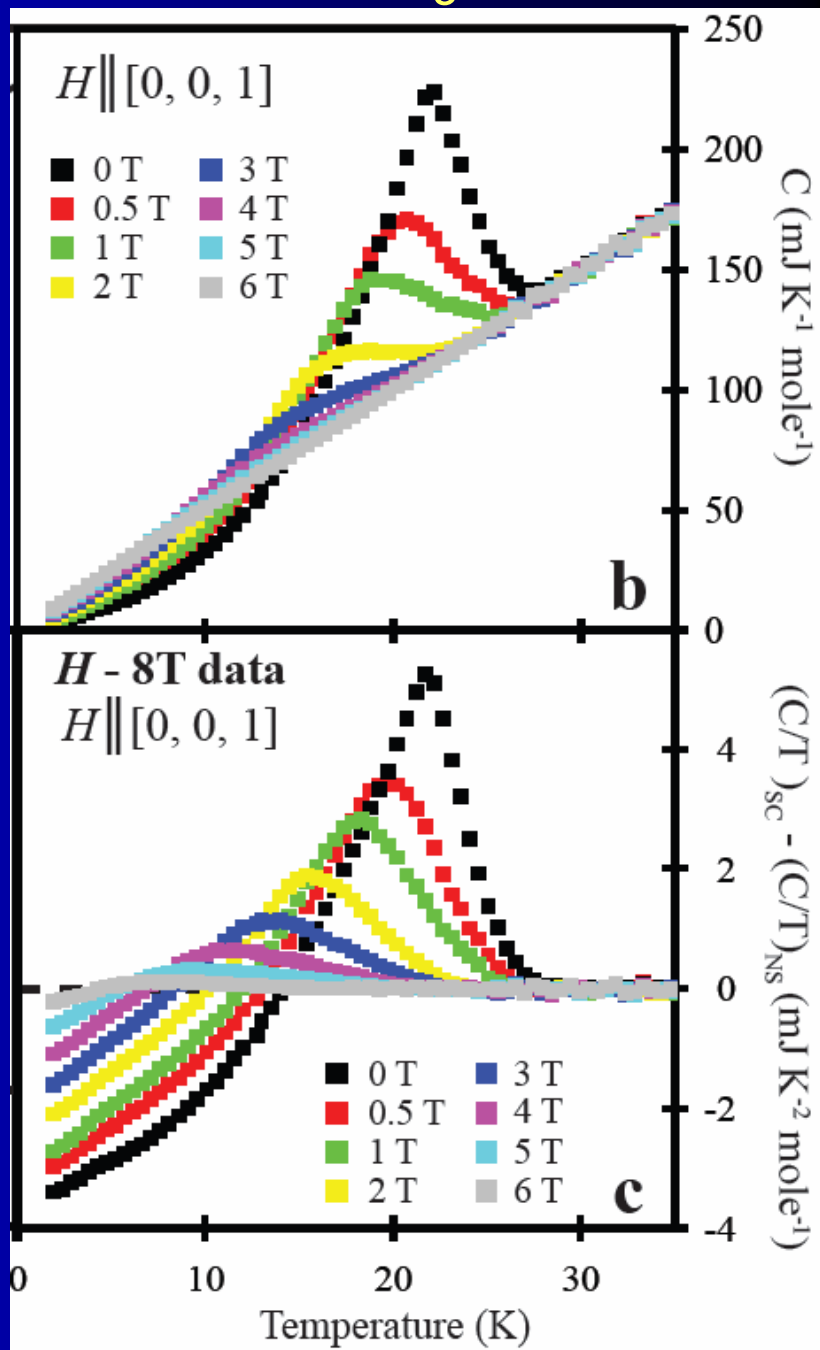
Transport measurements for PLCCO T_c= 24K

SC can now be completely suppressed for neutron experiments!

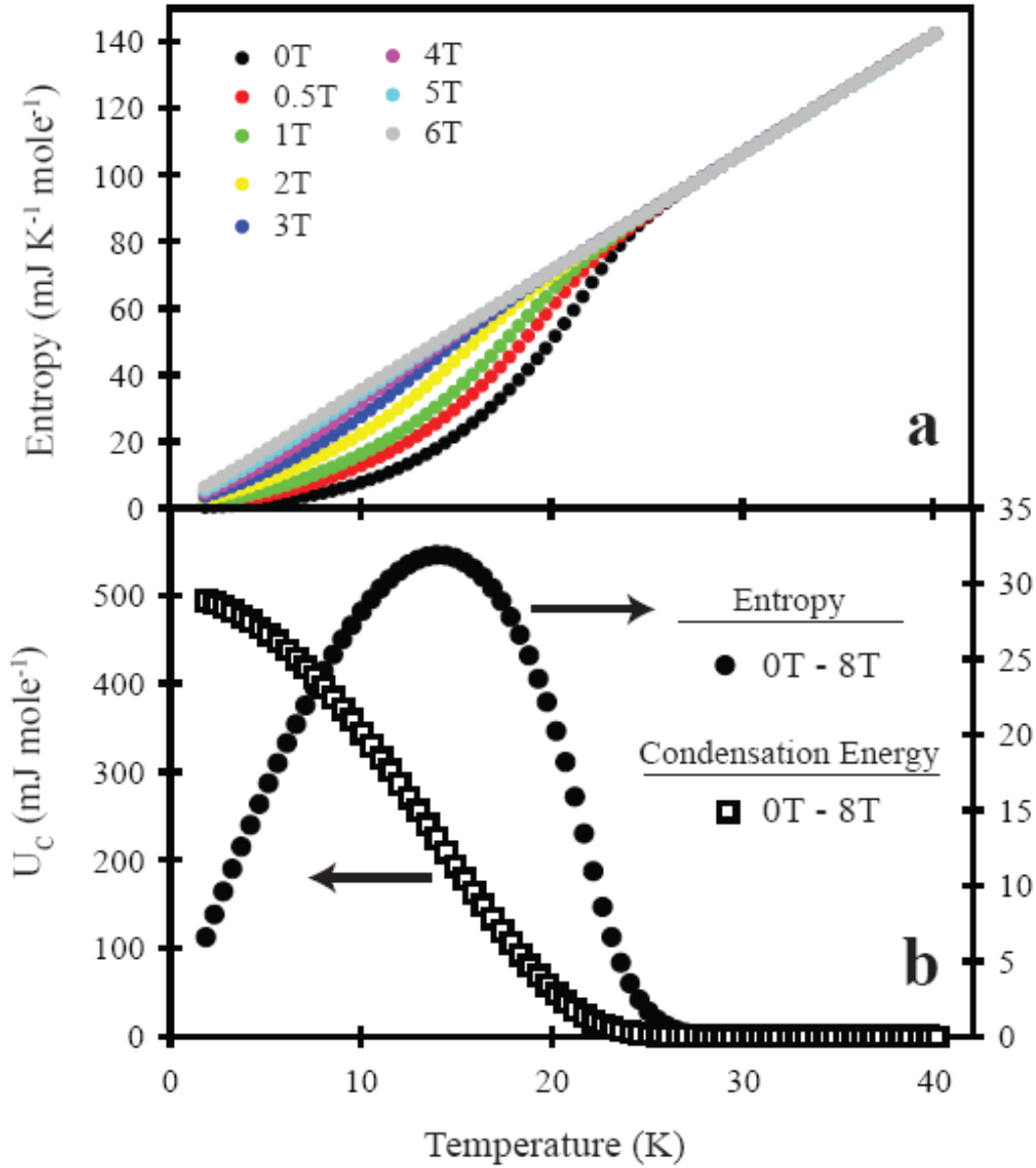
H_{c2}~8T for PLCCO (T_c=24K)

$$S_N(T) - S_{SC}(T) = \int_0^T (C_N - C_{SC}) dT' / T'$$

$$U_c(T) = \int_T^{T_c+15K} [S_N(T') - S_{SC}(T')] dT'$$

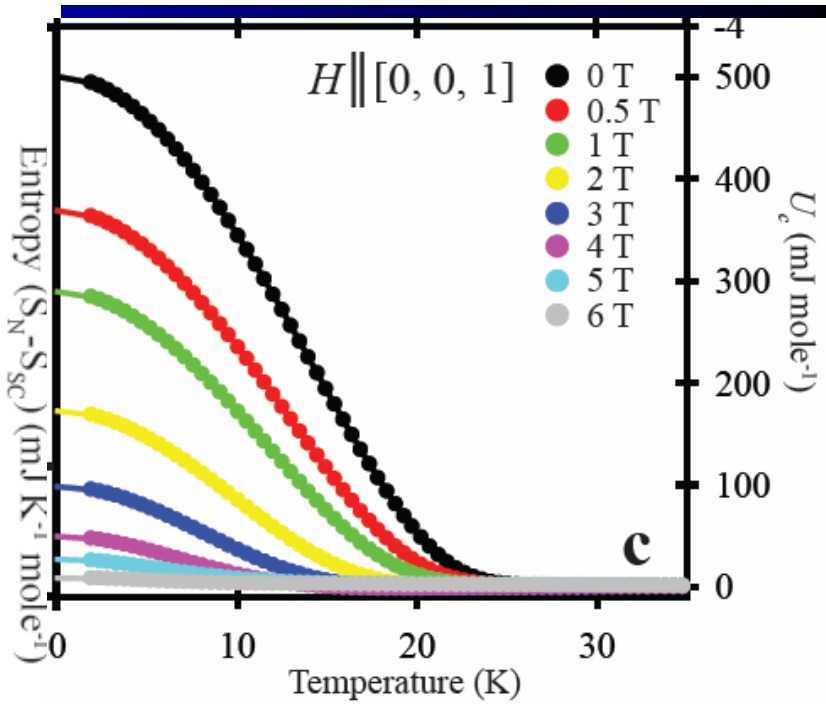


Calculating the entropy and superconducting condensation energy in PLCCO at IOP.

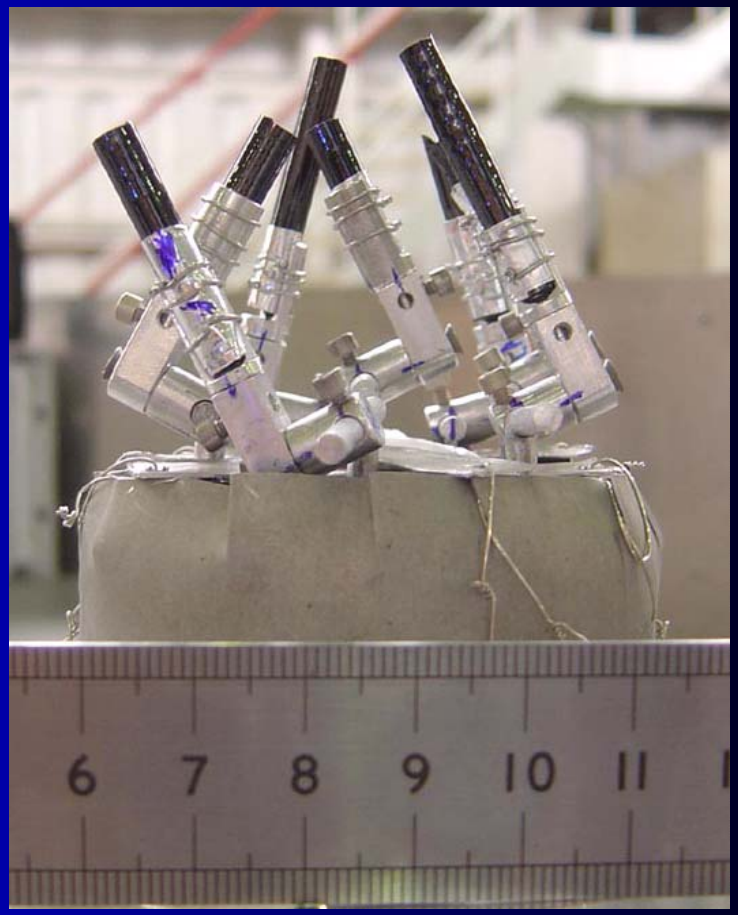


$$S_N(T) - S_{SC}(T) = \int_0^T (C_N - C_{SC})dT'/T'$$

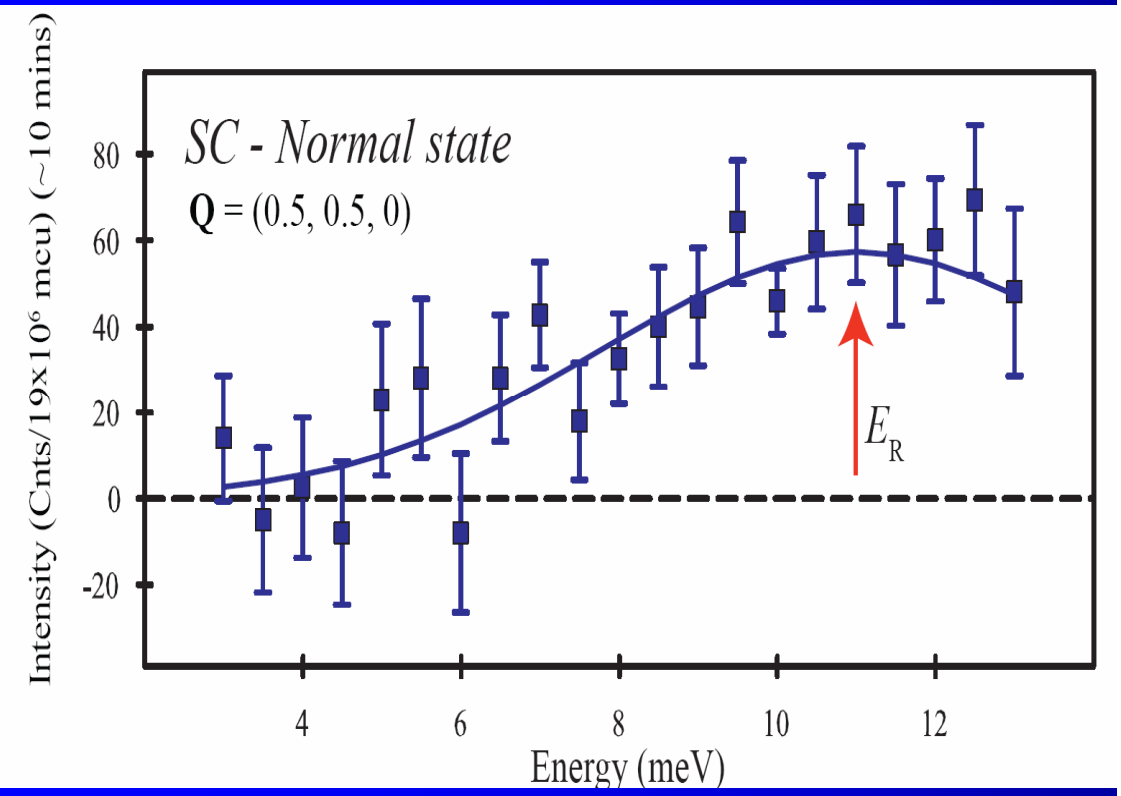
$$U_c(T) = \int_T^{T_c+15K} [S_N(T') - S_{SC}(T')]dT'$$

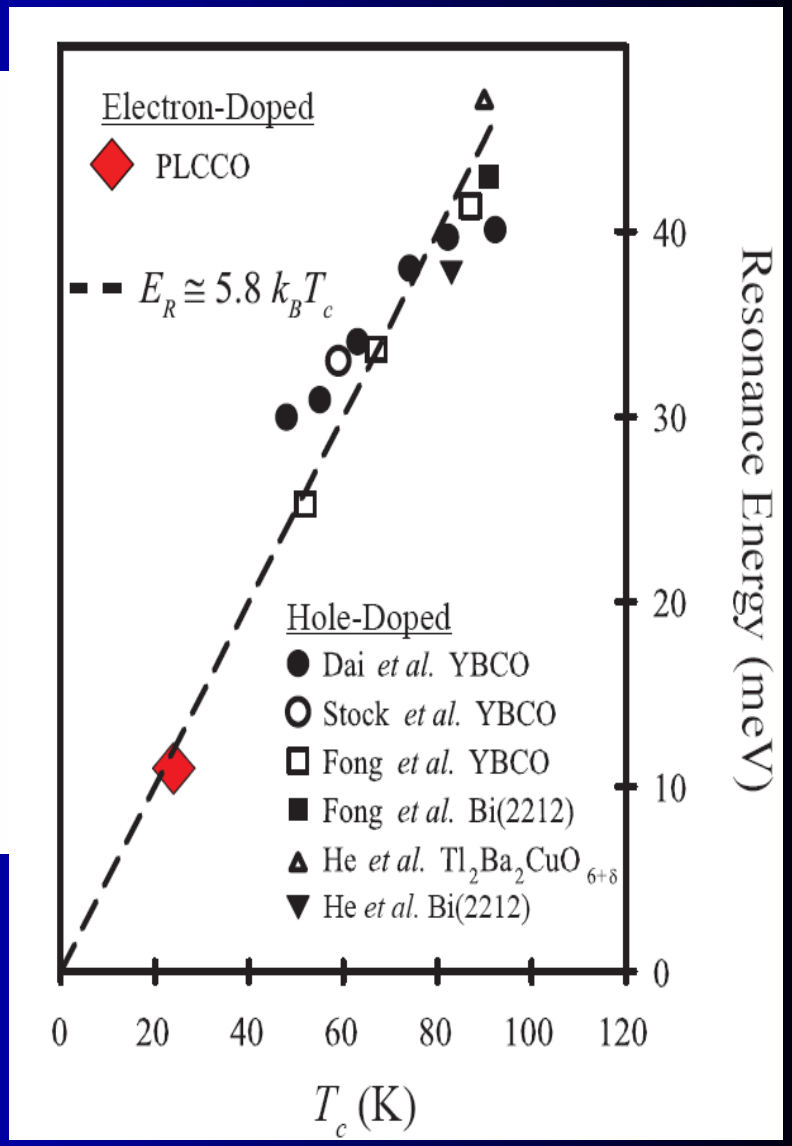


We grow single crystals $Pr_{0.88}LaCe_{0.12}CuO_{4-\delta}$ at the University of Tennessee and this allow us to have sufficient sample volume for inelastic neutron scattering experiments at SNS.



Resonance in *N*-type PLCCO

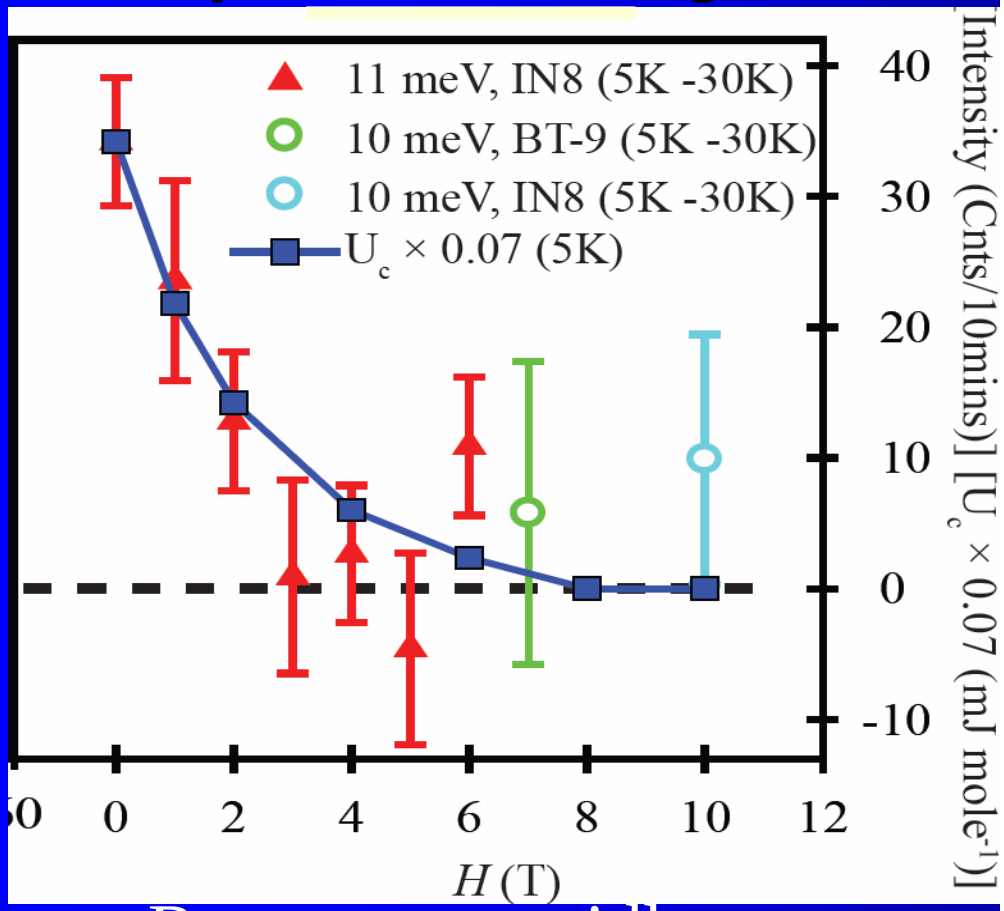


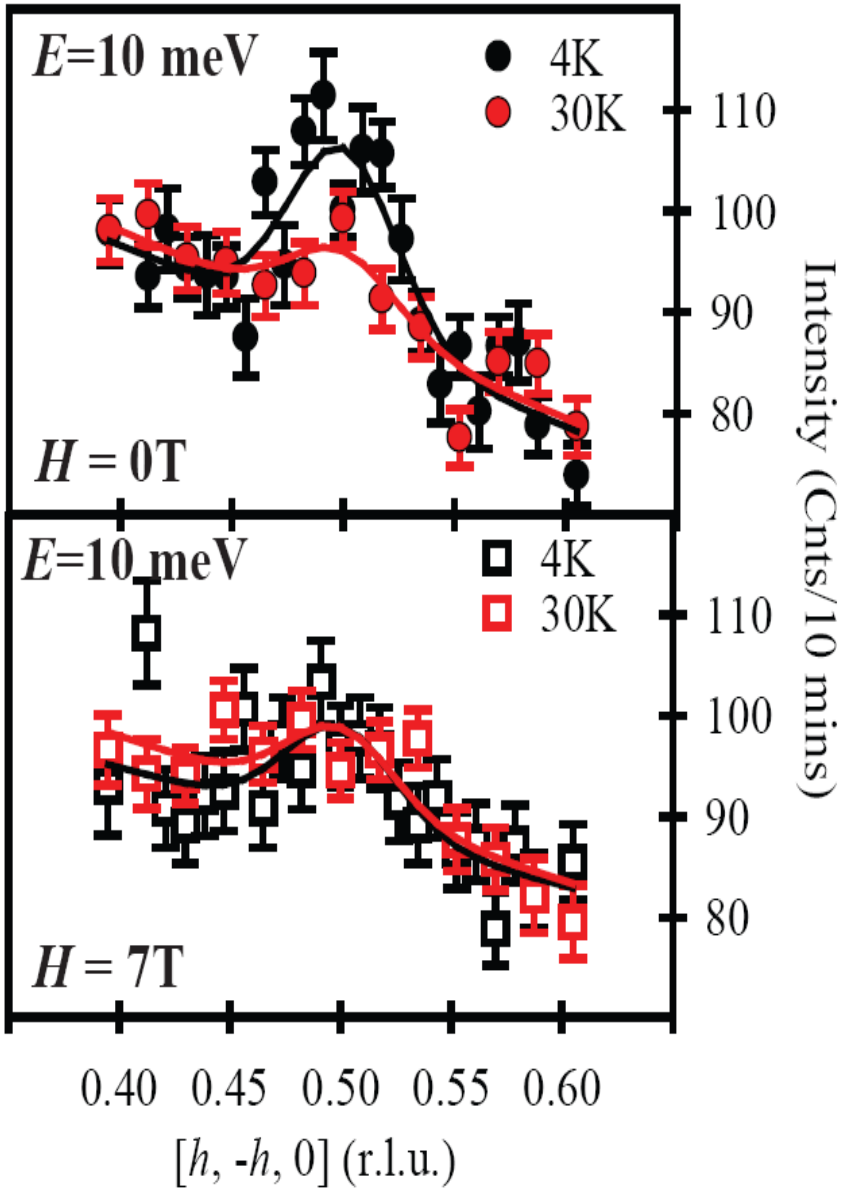


- Follows E_R=5.8$k_B T_c$
- Commensurate excitations dispersing into it
- Observed above gapless magnetic spectrum

Wilson et al., Nature (2006); Wilson et al., PNAS (2007).

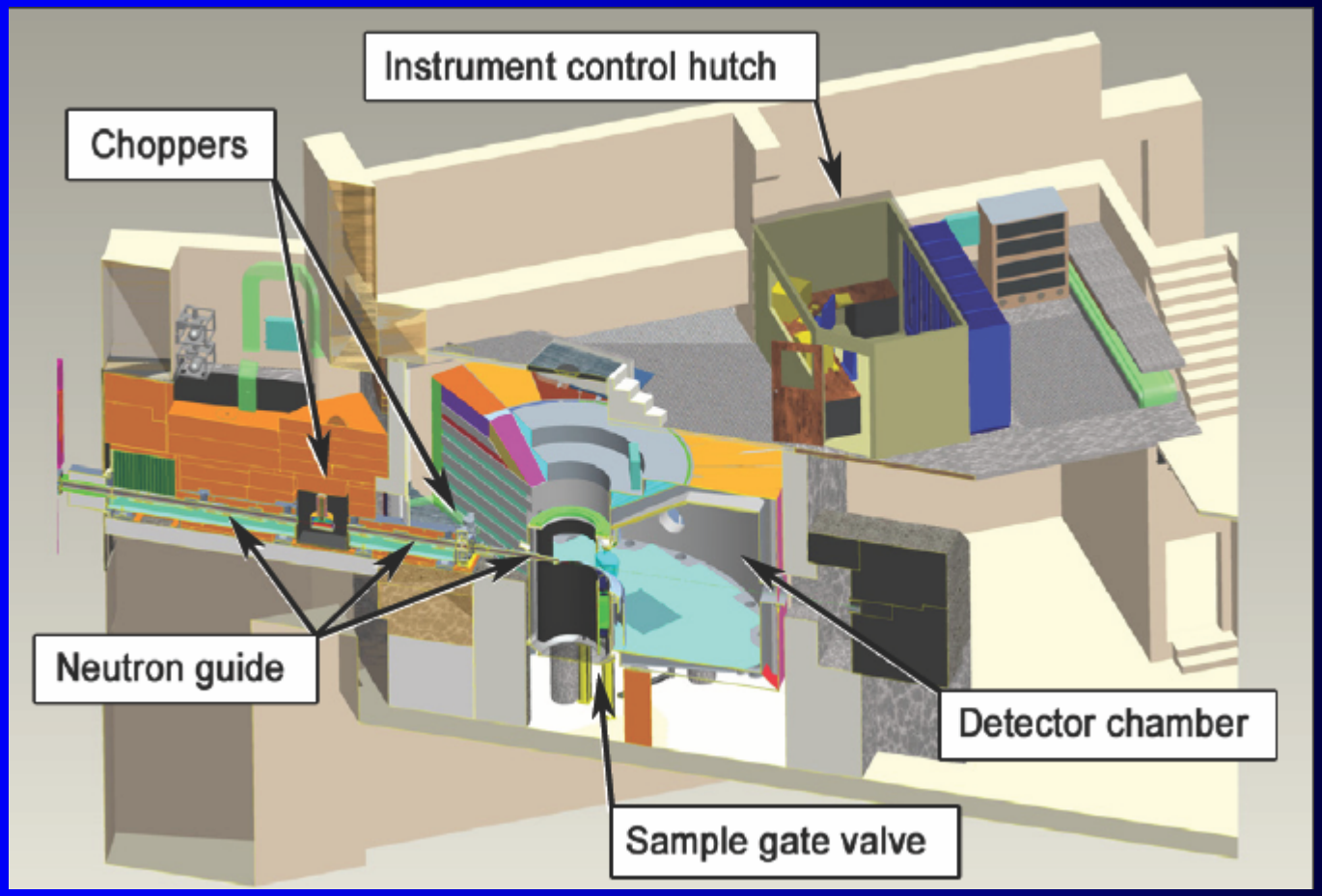
Using magnetic field as a probe to tune the superconducting-normal phase transition





- Resonance rapidly suppressed under field
- Intensity tracks condensation energy

We are going to use ARCS spectrometer at SNS to carry out measurements to determine dynamic susceptibility over a wide energy/wavevector space



The purpose of our experiment and its relationship with computing science

To measure magnetic susceptibility in absolute units using ARCS spectrometer at SNS over a wide (from 1 to 300 meV) energy and momentum space S(Q, ω) in the superconducting state and superconductivty suppressed normal state (using either a magnetic field or Ni/Zn impurities) at low temperature.

Using experimentally obtained susceptibility from neutron scattering and band structure from photo-emission as input for the Hubbard model to calculate the superconducting transition temperature. This can then be compared with experimentally measured Tc and condensation energy. Therefore determining the electron pairing mechanism.