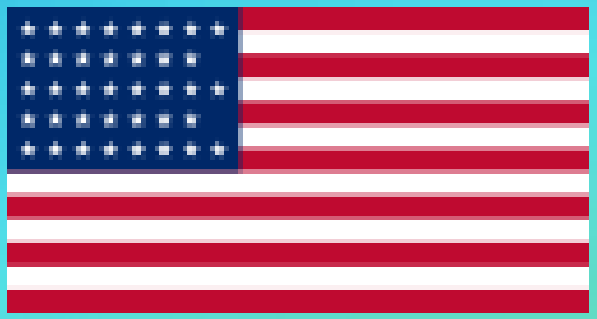
St. Patrick's Day - 2016

-2014-

PMPG Accepted as a Dual National by the Republic of Ireland

Bridget Ann Mullen-Whalen

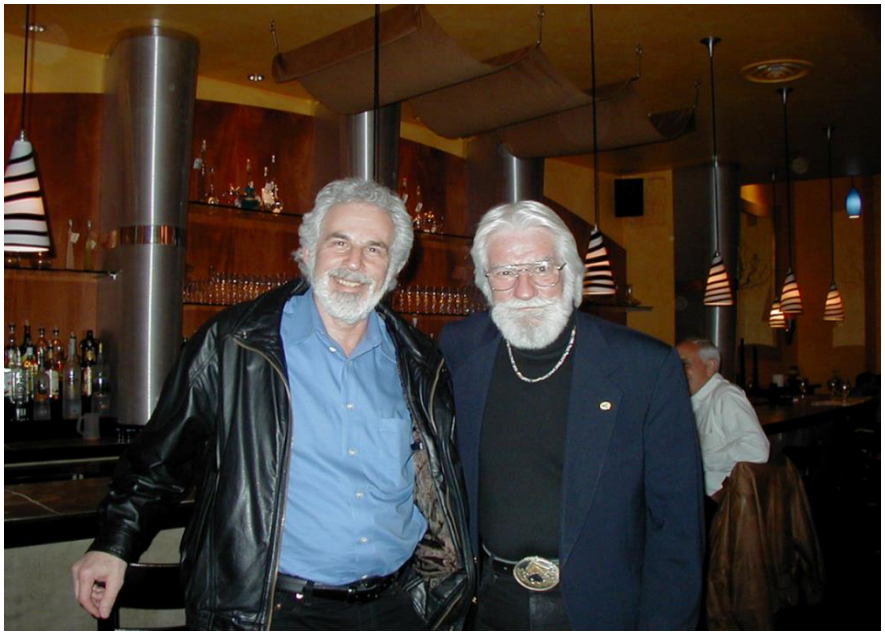


Paul Michael Patrick Grant

Grandson of
Two Proud Lands

“Woodstock” (#30 Upcoming)

“Band of Brothers (and a Sister!)”
- IBM Almaden, March 1987 -



“Infamous Irish-Jewish
Catskill Borscht-Belt Comedy Team”

MARCH 14 - 18

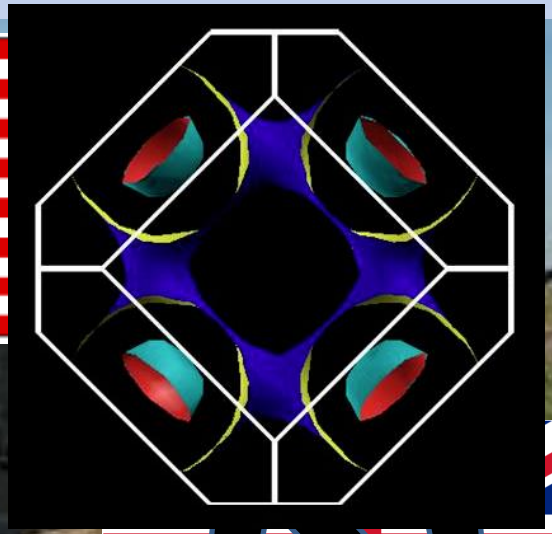
MARCH MEETING 2016

BALTIMORE, MD

A DFT Study of Electron-Phonon Mediated Superconductivity in Doped Mott-Hubbard Proxy Cubic-Tetragonal Copper Monoxide

Paul M. Grant
W2AGZ Technologies

AGING IBM PENSIONER
RESEARCH SUPPORTED UNDER
THE IBM RETIREMENT FUND



er 8
9:24 A 9:36 A
Roo

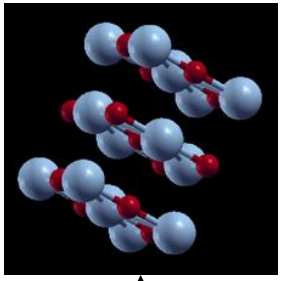
– Our Computational Tool Box –

- DFT
  - Quantum Espresso
    - Fermiologies, States (DOS), Phonons, e-p “Lambda”
  - Gibbs2
    - Debye Statistics
  - ELK
    - LDA + U
- Graphics
  - Xcrysden, XMGRACE
    - Fermi Surfaces, Projected DOS
- Modeling
  - Then e-p Superconductivity via Eliashberg/McMillan!

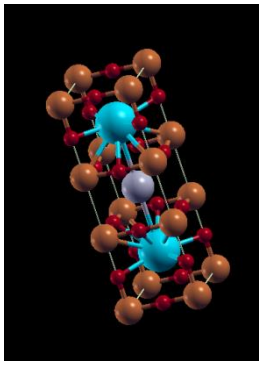
The Various Flavors of Copper "Monoxide"

- Siemons, et al. (2009)
- Grant (2008)
- Franchini Group (2011)
- Cococcioni Group (2011)

tet-rs-CuO

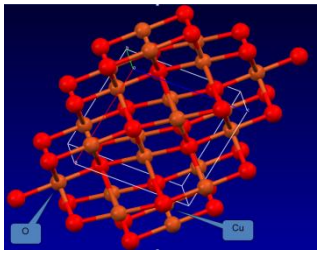


"1-2-3"



What Nature (she) gives us! (triclinic)

Tennorite



Can we <u>compute/synthesize</u> its physical properties wrt magnetism and superconductivity?

Relative Ground State Energies

NB: All show attributes of Mott-Hubbard behavior

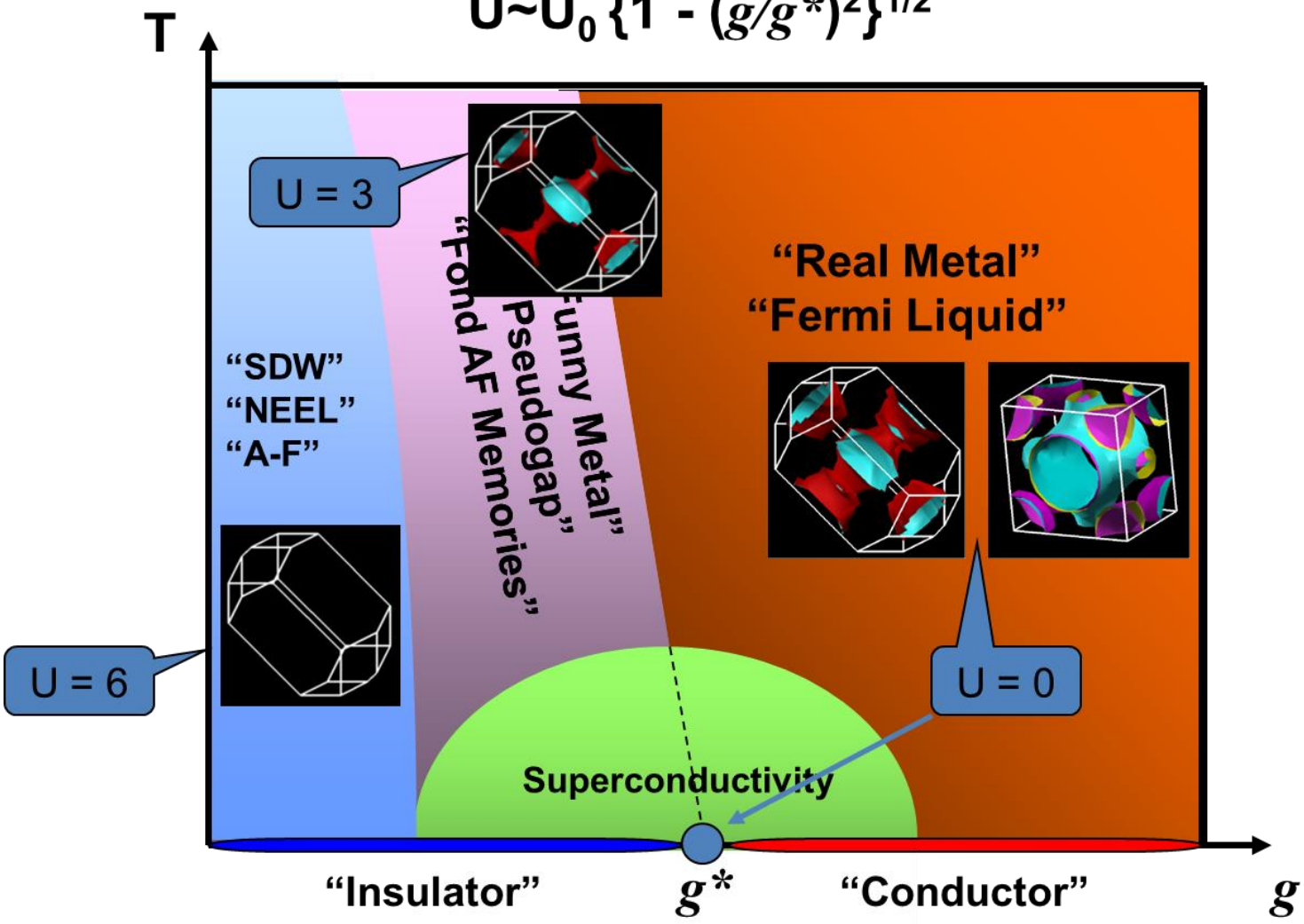
"Configuration/Coordination Space"

Interesting...

- Lowest symmetry yields lowest ground state energy.
- Higher...at least in a computer...gives greater (localized around given “optimal lattice” constants).
- Why? Jahn-Teller “degeneracies”! Nature abhors them (Aristole).
- Were Bednorz-Mueller (Chakravarty & Hoecht) on the right path in 1986 after all?

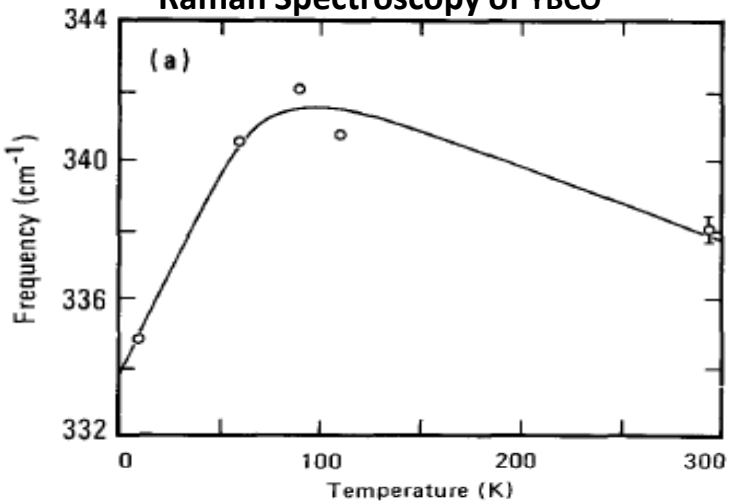
The Colossal Quantum Conundrum

$U \sim U_0 \{1 - (g/g^*)^2\}^{1/2}$

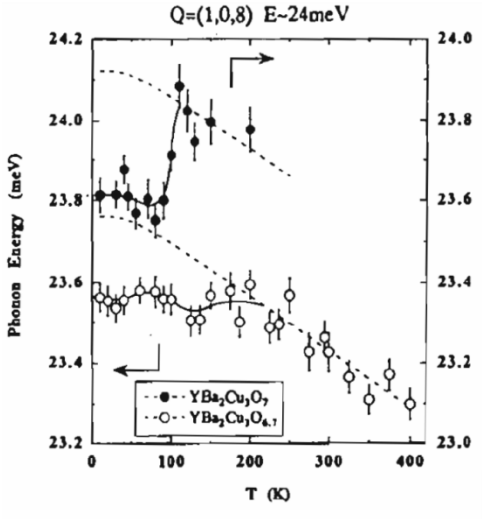


Phonons are there!

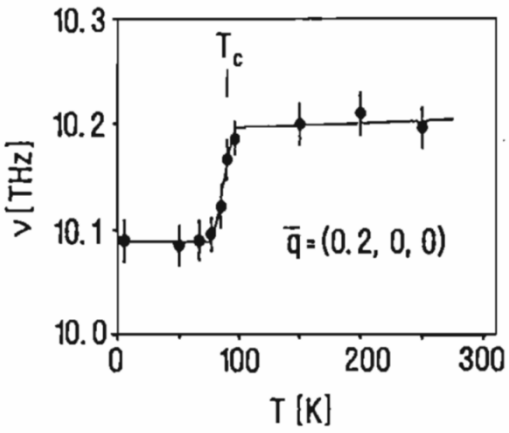
Macfarlane, Rosen, Seki, SSC 63, 831 (1987)
Raman Spectroscopy of YBCO



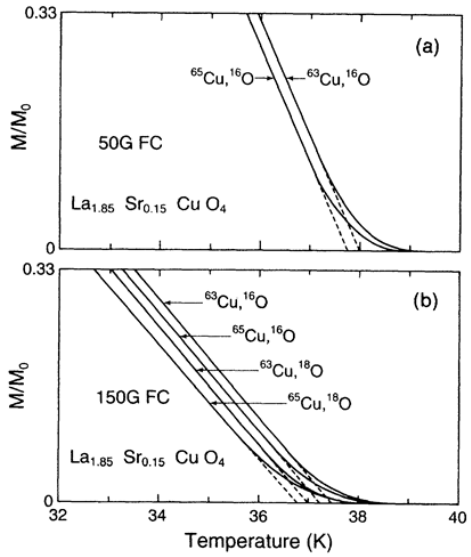
Harashima, et al., Physica C263, 257 (1996)



Pyka, et al., PRL 70, 1457, (1993)

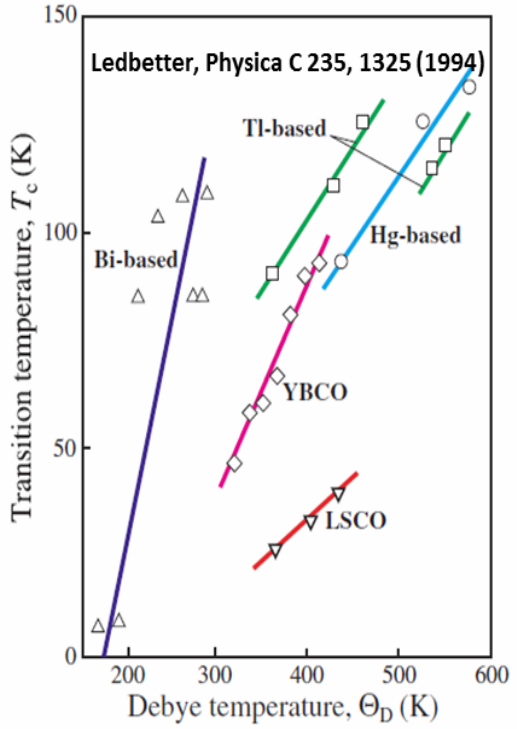


Franck, Harker, Brewer, PRL 71, (1993)
Cu and O Isotope Effects in $La_{2-x}Sr_xCuO_4$

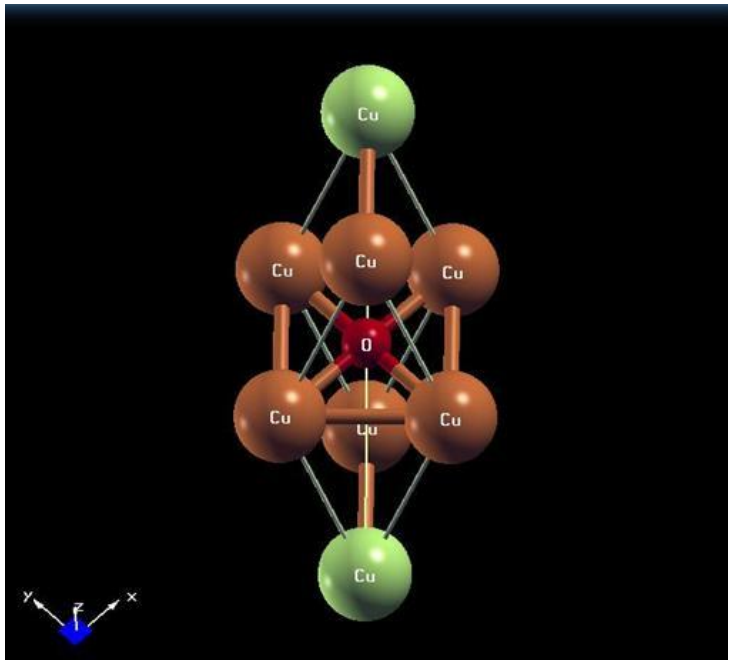


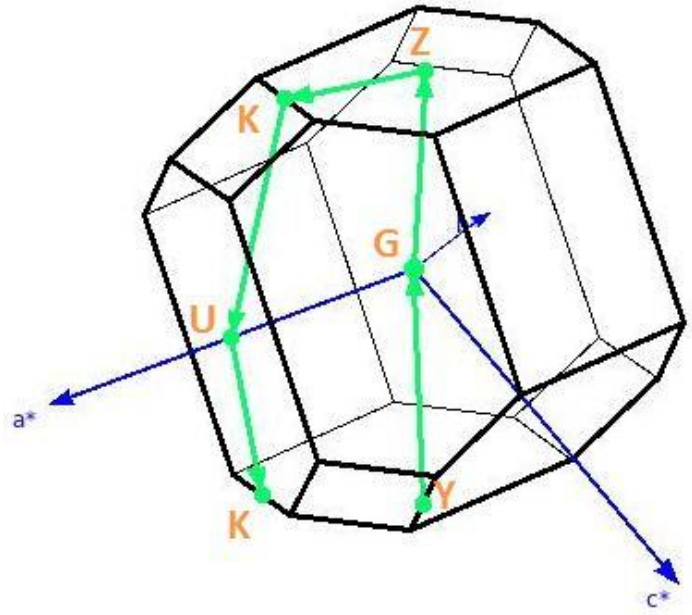
But maybe spins too?

Ledbetter, Physica C 235, 1325 (1994)



Let's look at the "U = 0, Fermi Liquid" limit for doped proxy tet-CuO!





Electronic properties of rocksalt copper monoxide:
A proxy structure for high temperature superconductivity

The International Conference on Theoretical Physics 'Dubna-Nano2008'
IOP Journal of Physics: Conference Series 129 (2008) 012042
doi:10.1088/1742-6596/129/1/012042

Superconductivity and Phonons

BCS via Eliashberg-McMillan

$$H_{el-ph} = \sum_{\mathbf{k},\mathbf{q},\nu} g^{\mathbf{q}_{\nu,mn}}_{\mathbf{k}+\mathbf{q},\mathbf{k}} c^{\dagger m}_{\mathbf{k}+\mathbf{q}} c^{n}_{\mathbf{k}} (b^{\dagger}_{-\mathbf{q},\nu} + b_{\mathbf{q},\nu})$$

$$\lambda_{\mathbf{q},\nu} = \frac{2}{N(\varepsilon_F)\omega_{\mathbf{q},\nu}} \sum_{mn}\sum_{\mathbf{k}} \left| g^{\mathbf{q}_{\nu,mn}}_{\mathbf{k}+\mathbf{q},\mathbf{k}} \right|^2 \delta(\varepsilon_{\mathbf{k}+\mathbf{q},m} - \varepsilon_F)\delta(\varepsilon_{\mathbf{k},n} - \varepsilon_F)$$

$$\alpha^2 F(\omega) = \frac{1}{N(\varepsilon_F)} \sum_{mn}\sum_{\mathbf{q},\nu} \delta(\omega - \omega$$

$$\lambda = 2\int_0^{\infty} \frac{\alpha^2 F}{\omega}$$

NB! The "double deltas" will be approximated by two Gaussians of width "sigma (σ)" whose numerical convergence is governed by imposed precision limits and basis set symmetry. Con Quidado!

To get λ, need to compute $g_{\mathbf{k}+\mathbf{q},\mathbf{k}}$!

e-p Interaction in the DFT/LDA Formalism

$$g^{\mathbf{q}_\nu,mn}_{\mathbf{k}+\mathbf{q},\mathbf{k}} = \sqrt{\hbar / 2\omega_{\mathbf{q},\nu}} \left\langle \psi_{\mathbf{k}+\mathbf{q},m} \left| \Delta V^{\mathbf{q},\nu}_{KS} \right| \psi_{\mathbf{k},n} \right\rangle$$

$$\Delta V^{\mathbf{q},\nu}_{KS} = \sum_{\mathbf{R}} \sum_{s} \frac{\partial V_{KS}}{\partial \vec{u}_{s,\mathbf{R}}} \cdot \vec{u}^{\mathbf{q},\nu}_{s} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{\sqrt{N}}$$

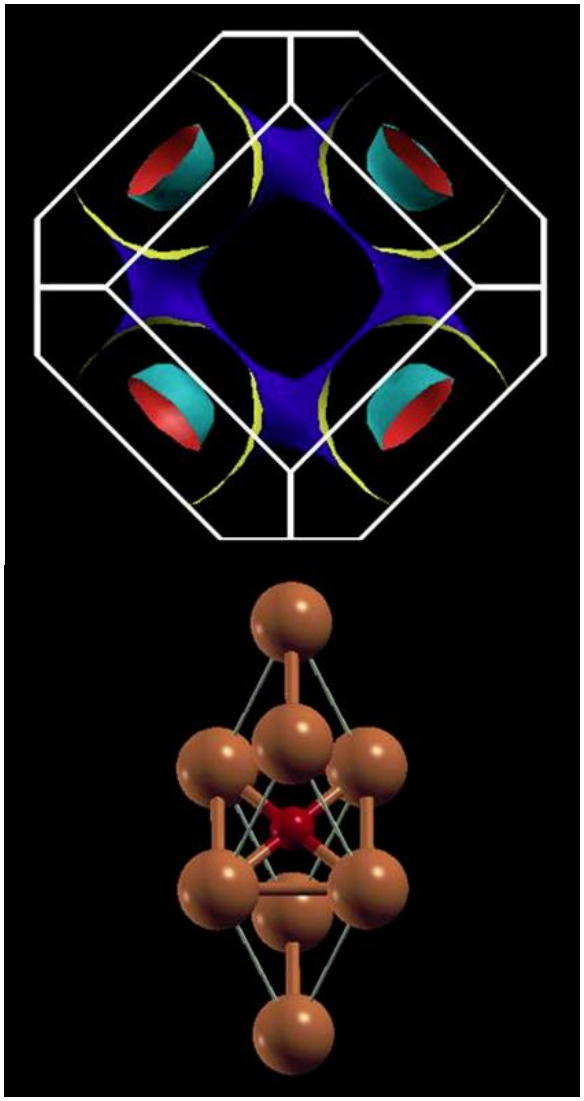
$$T_C = \frac{\Theta_D}{1.45} \exp\left(-\frac{1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)} \right)$$

CuO

(tetragonal)

q = 0.15/CuO

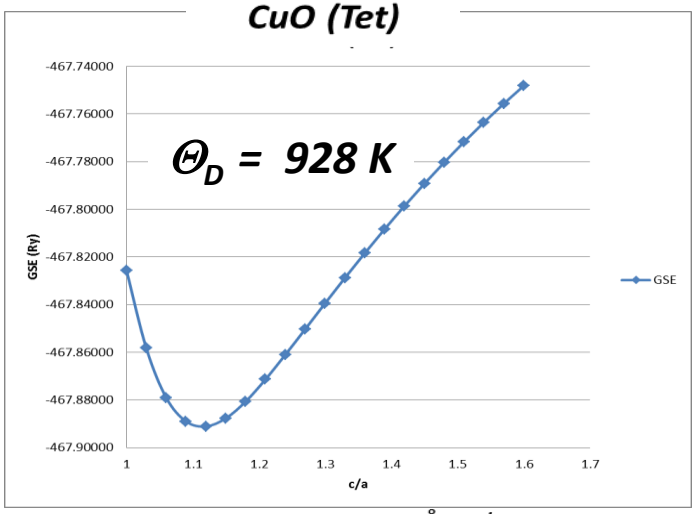
T_c



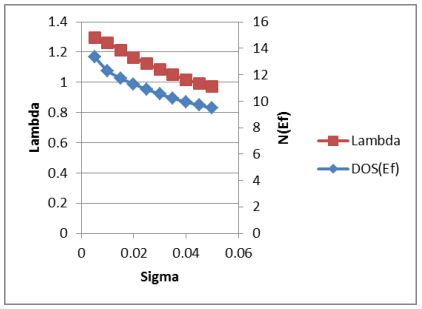
Ipso Facto...
At least at optimum doping...

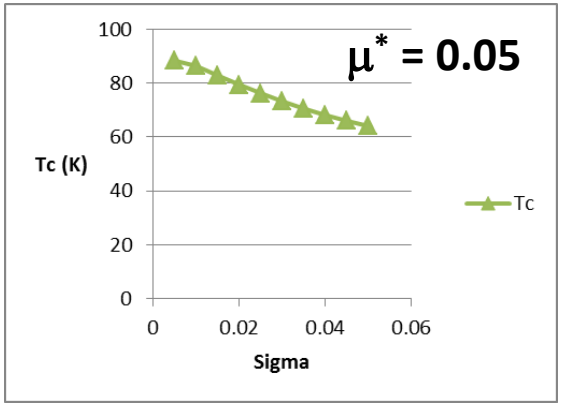
the holes are paired by lattice shakes...

with maybe a little help from their spins?



Min GSE at a0 = 3.9 Å, c/a = 1.15





T_c(avg) ~ 75 K

Voice from the Past!

AUGUST 1, 1941 PHYSICAL REVIEW VOLUME 60

Paramagnetic Dispersion Measurements at 77.3°K*

C. STARR
Massachusetts Institute of Technology, Cambridge, Massachusetts
(Received June 7, 1941)

The dispersion of the magnetic susceptibility of some paramagnetic compounds of Fe, Mn, and Cr, was studied at 77.3°K over a frequency range of 2 to 10 megacycles/sec. with magnetic fields up to 60,000 gauss. The results substantiate the theory of Casimir and du Pre, which is based upon the thermal coupling between the magnetic spin system and the lattice vibrations.

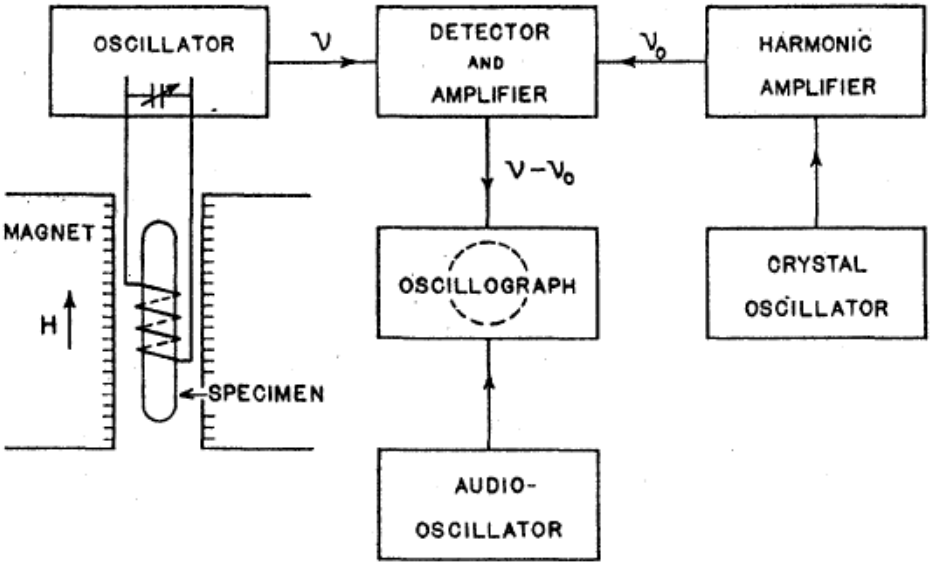


TABLE I. *Spin system data determined from dispersion measurements.*

	$10^{-6}a/c$ STARR 77°	TEUNISSEN AND GORTER 77°	DU PRE 1°–4°	$10^{-6}a$	η	δ
$FeNH_4(SO_4)_2 \cdot 12H_2O$	0.263	0.248	0.256	1.14	0.0472°	0.193°
$CrK(SO_4)_2 \cdot 12H_2O$	0.64	0.7	0.80	1.19	0.0204	0.231
$CrNH_4(SO_4)_2 \cdot 12H_2O$	2.68			4.99	0.0200	0.486
$MnSO_4 \cdot 4H_2O$	4.2	6.2		18.2	0.126	0.903
$MnCl_2 \cdot 4H_2O$	19.8	19.5		85.9	0.135	2.11

Why not repeat this experiment on the CuO perovskites?

So is it Shakes and/or Spins?

Maybe it takes two to Tango!

Stay Tuned!

Five HTSC "In Your Face" Questions