

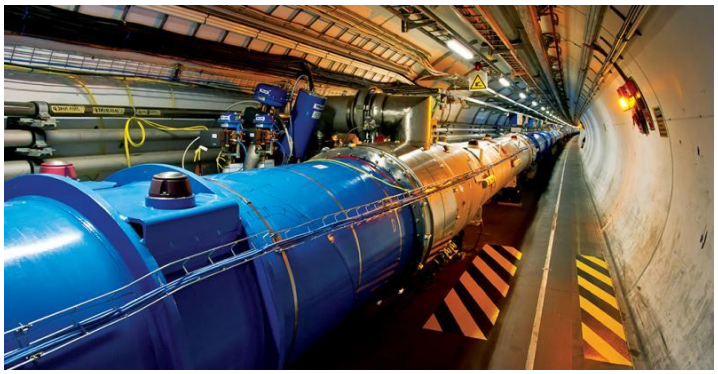

Whither High-Tc 30 Years Following Its Discovery?

-Challenges Facing the Path Forward for High Temperature Superconductivity from Its Fundamental Understanding to Eventual Societal Deployment-

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EPRI Science Fellow (Retired)

IBM Research Staff Member/Manager Emeritus

(etc, etc...& so forth and so on)

W2AGZ Technologies, (w2agz@w2agz.com)

Aging IBM Pensioner

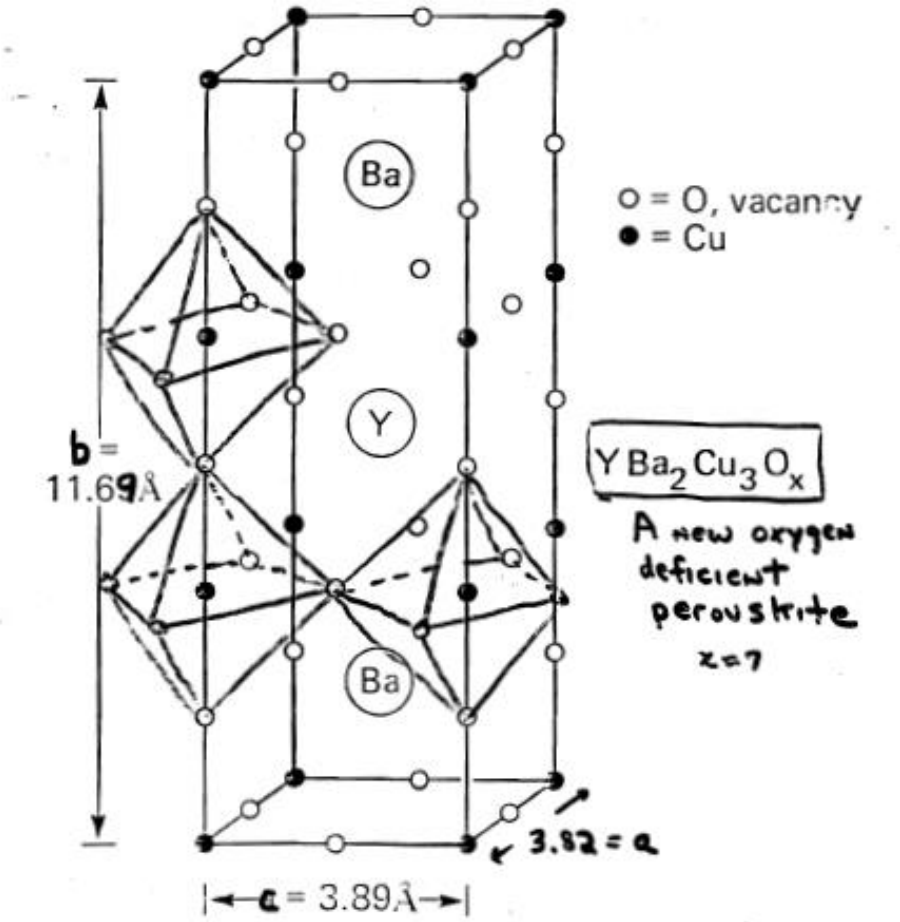
2016 Annual Meeting of the APS Far West Section

UC Davis

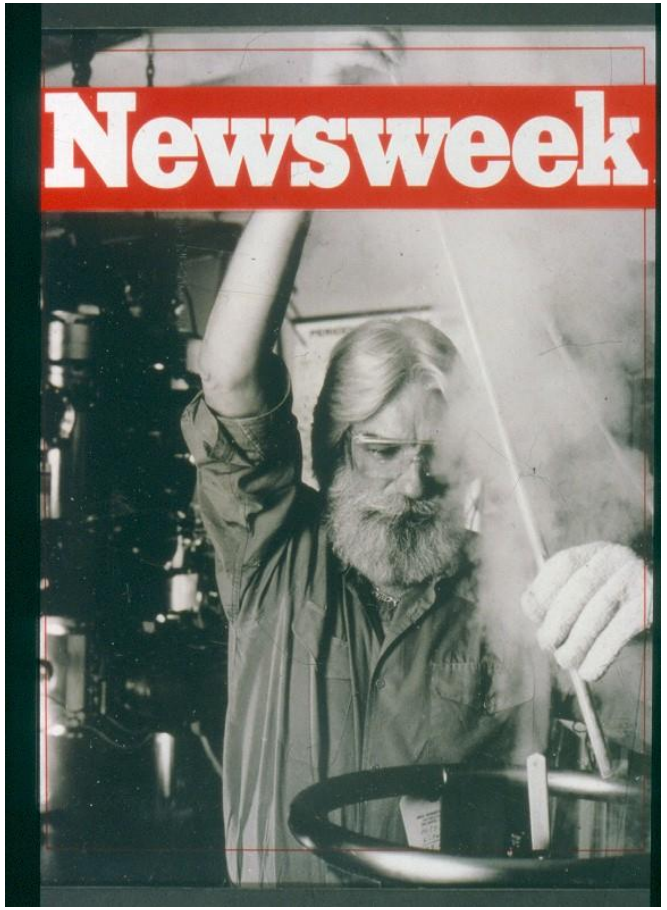
October 28-29, 2016

Physics at IBM Almaden (3 March 1987)

A Band of Brothers...and a Sister!
(IBM Almaden – 1986-87)



It's as Simple as 1-2-3!



All Night Session, APS March Meeting, NYC, 18 March1987

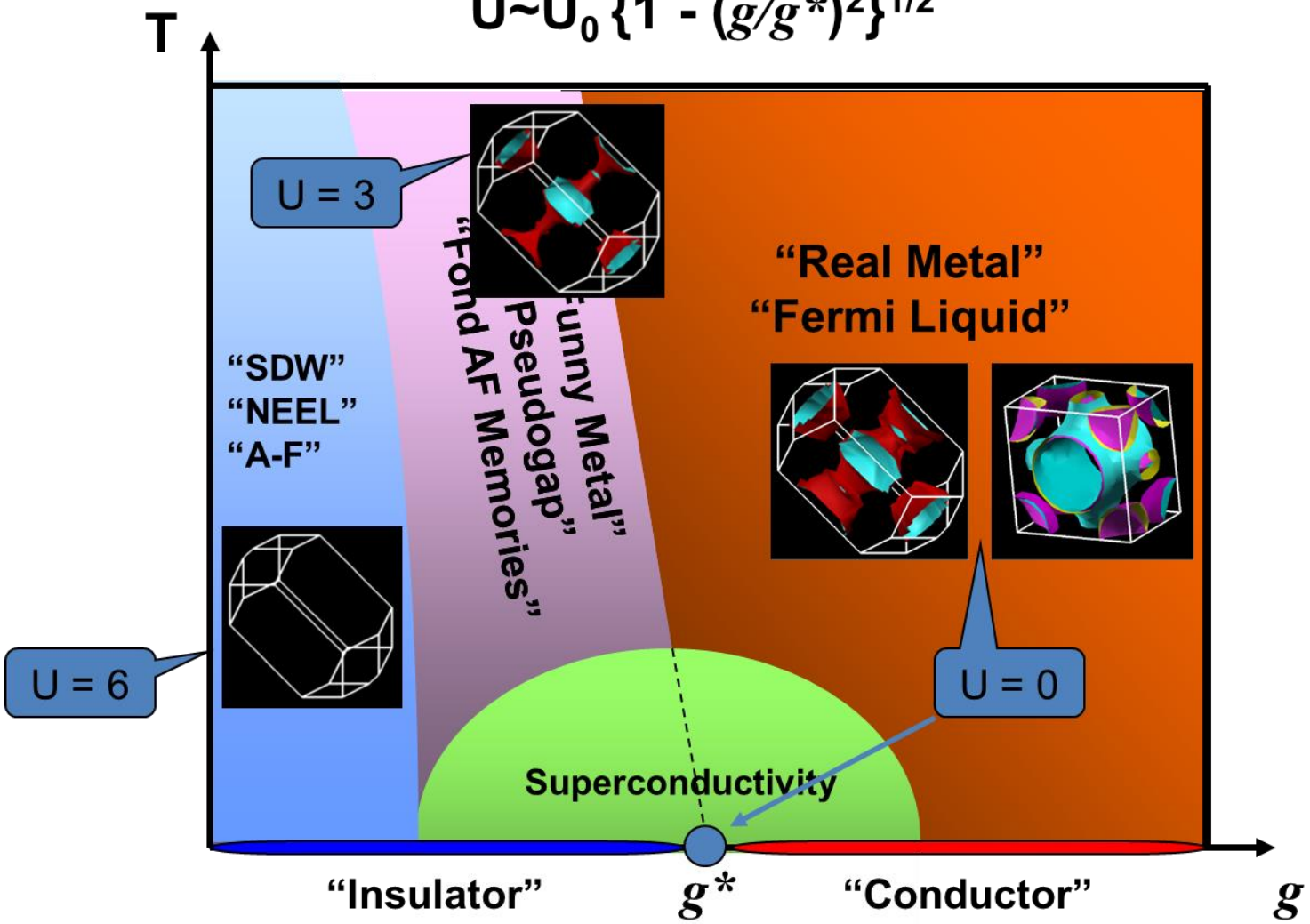
"The Woodstock of Physics"

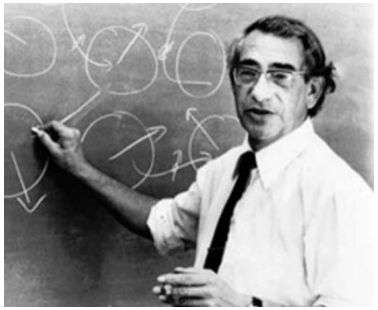
HTSC Symposium, MRS Spring Meeting, Anaheim, 23-24 April 1987

"The Altamont of Materials"

The Colossal Quantum Conundrum

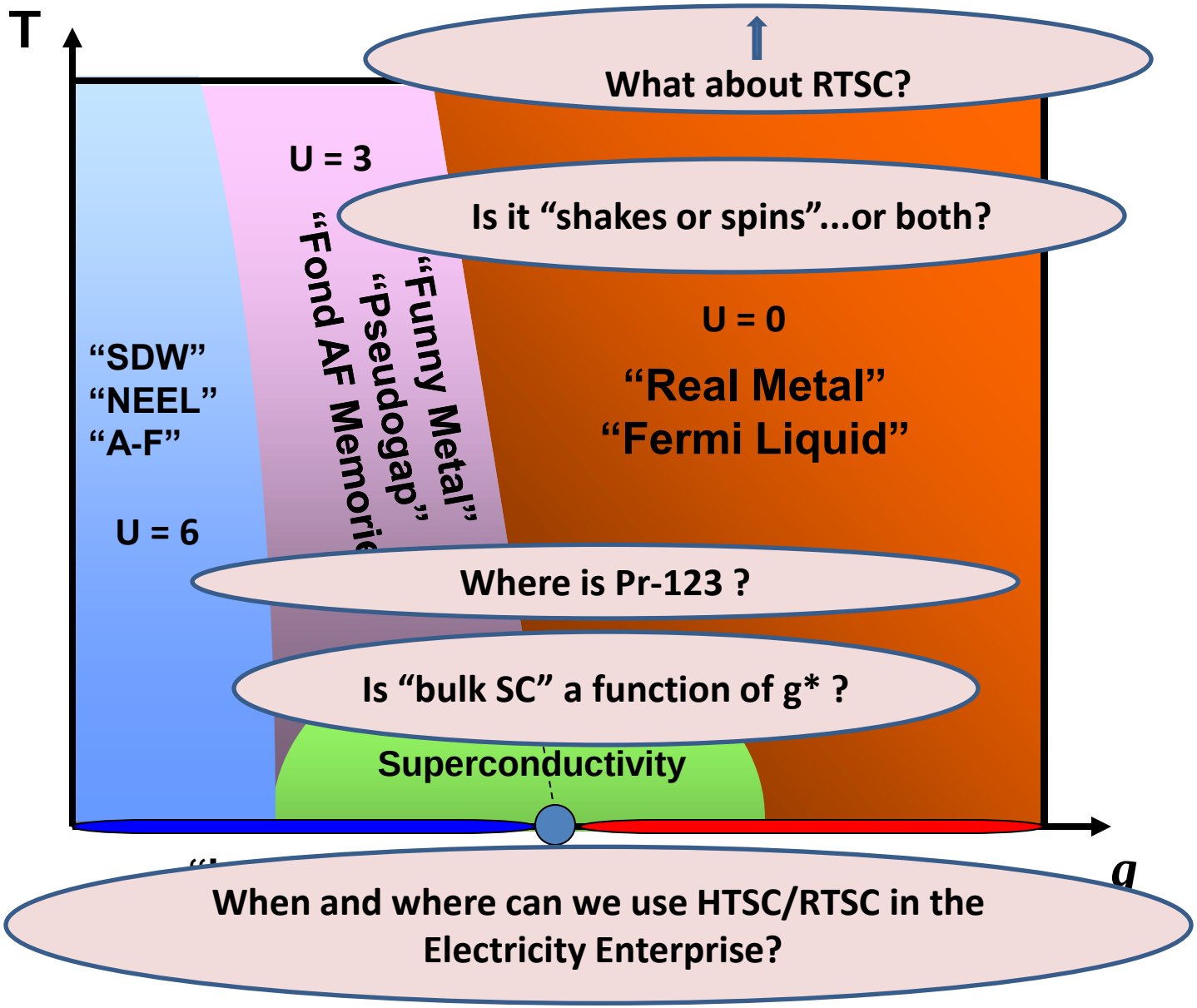
$U \sim U_0 \{1 - (g/g^*)^2\}^{1/2}$





$$H = -t \sum_{\langle i,j \rangle, \sigma} (c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma}) + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow}$$

Five HTSC "In Your Face" Questions



Shakes or/and Spins?

The Pairing Glue

“Alex says it’s phonons”

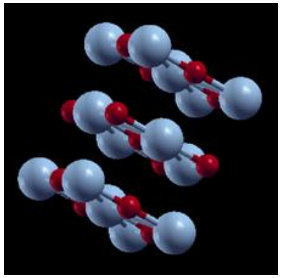
OK, OK...J-T polarons and/or bipolarons (after Chakravarty/Hoest)

Could he be right after all?

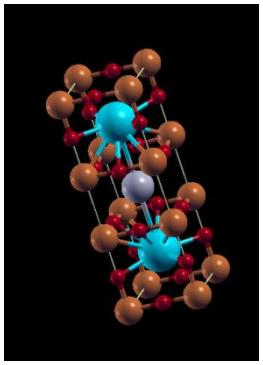
The Various Flavors of Copper "Monoxide"

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

tet-rs-CuO

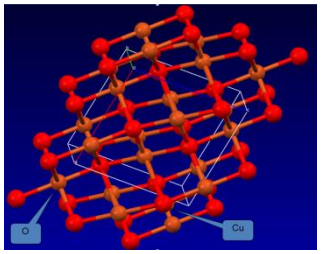


"1-2-3"



What Nature (she) gives us! (triclinic)

Tennorite



Relative Ground State Energies

NB: All show attributes of Mott-Hubbard behavior

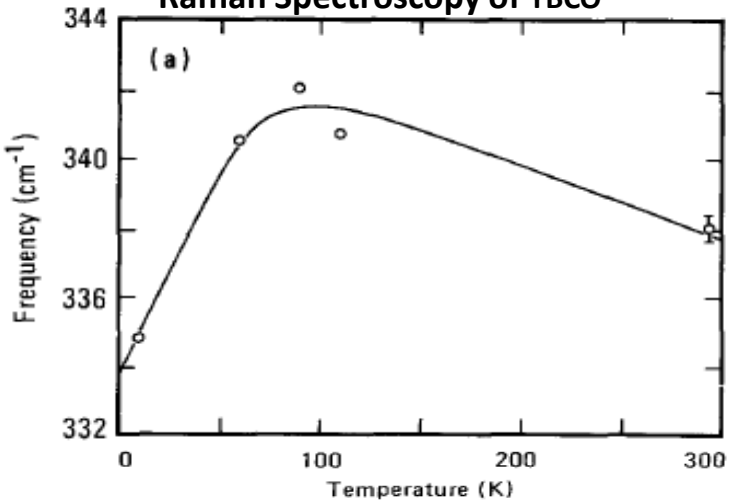
"Configuration/Coordination Space"

Interesting...

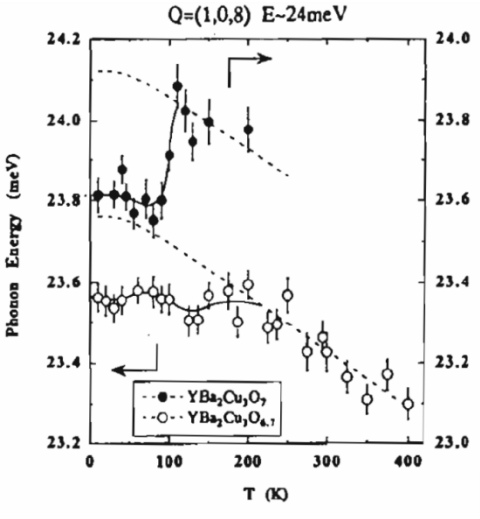
- Lowest symmetry yields lowest ground state energy.
- Higher...at least in a computer...gives greater (localized around given “optimal lattice” constants).
- Why? Jahn-Teller “degeneracies”! Nature abhors them (Aristole).
- Were Bednorz-Mueller (Chakravarty & Hoecht) on the right path in 1986 after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

The Lattice is Shaking

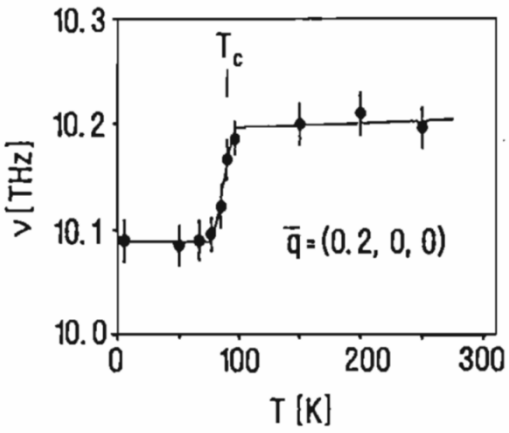
Macfarlane, Rosen, Seki, SSC 63, 831 (1987)
Raman Spectroscopy of YBCO



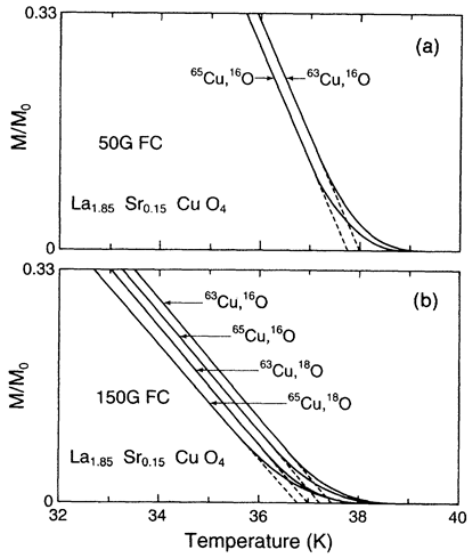
Harashima, et al., Physica C263, 257 (1996)



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

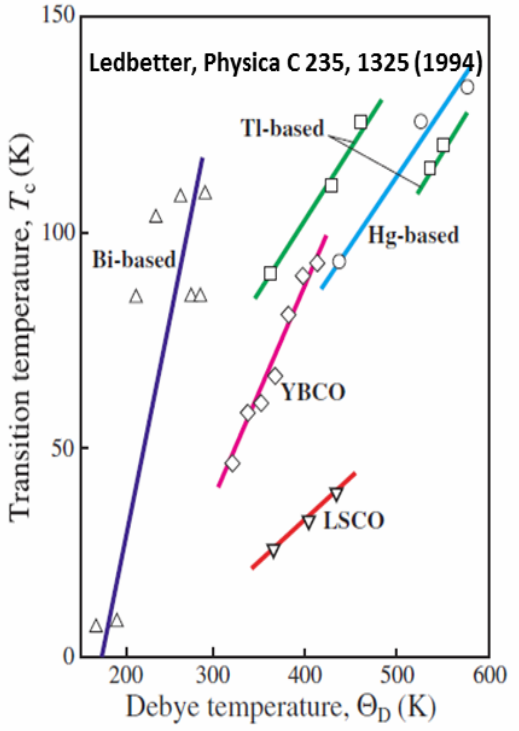


Franck, Harker, Brewer, PRL 71, (1993)
Cu and O Isotope Effects in $La_{2-x}Sr_xCuO_4$

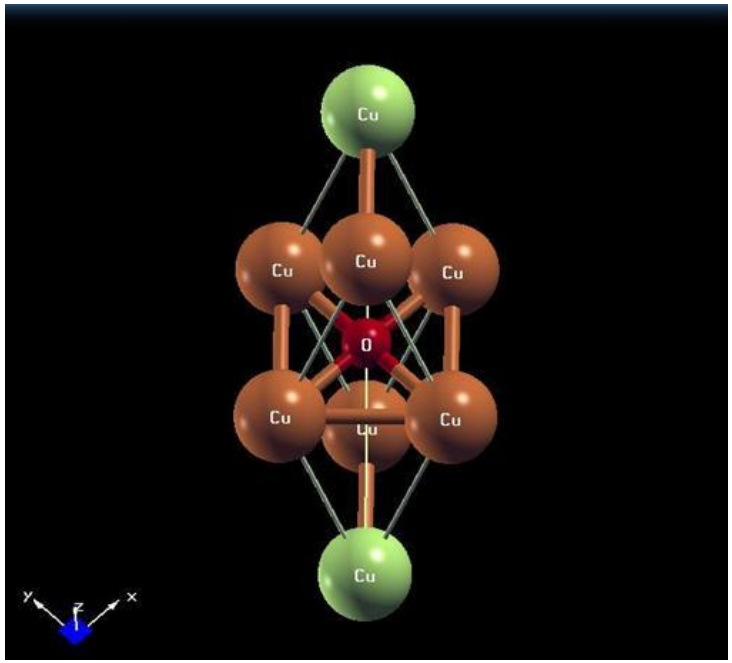


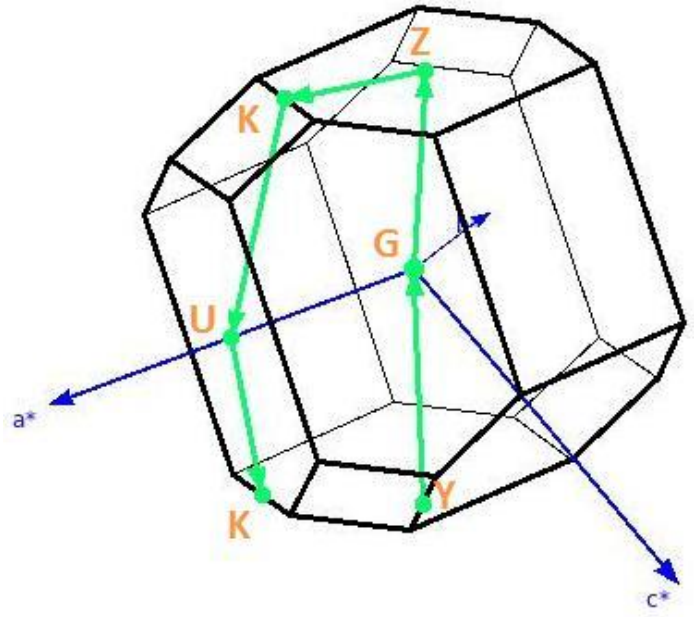
We can see Phonons have been there ever since the Creation!

Ledbetter, Physica C 235, 1325 (1994)



So how about 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

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

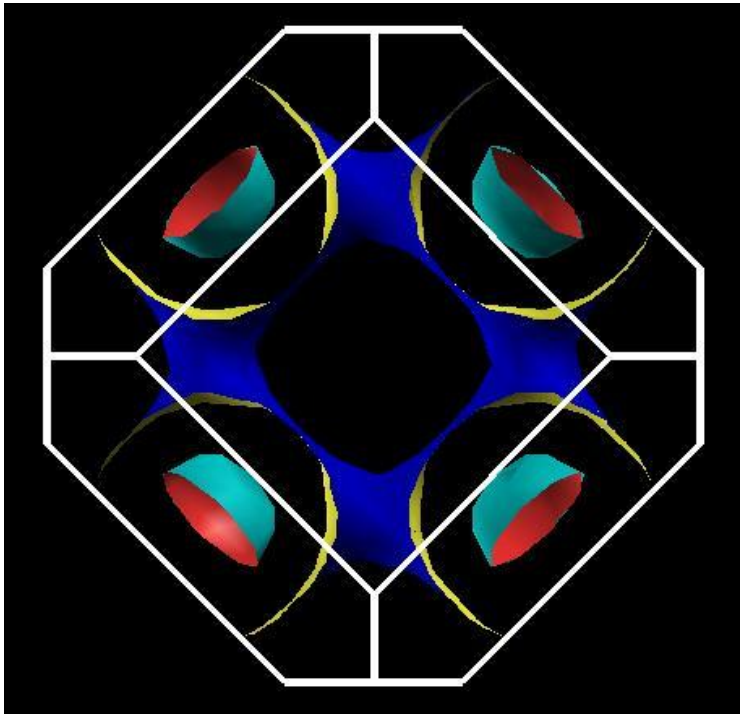
$$\Delta V^{\mathbf{q},\nu}_{KS} = \sum_{\mathbf{R}} \sum_{s} \frac{\partial V_{KS}}{\partial \vec{u}_{s,\mathbf{R}}} \cdot \vec{u}^{\mathbf{q},\nu}_{s} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{\sqrt{N}}$$

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

So let's do it and "compute*" what happens!

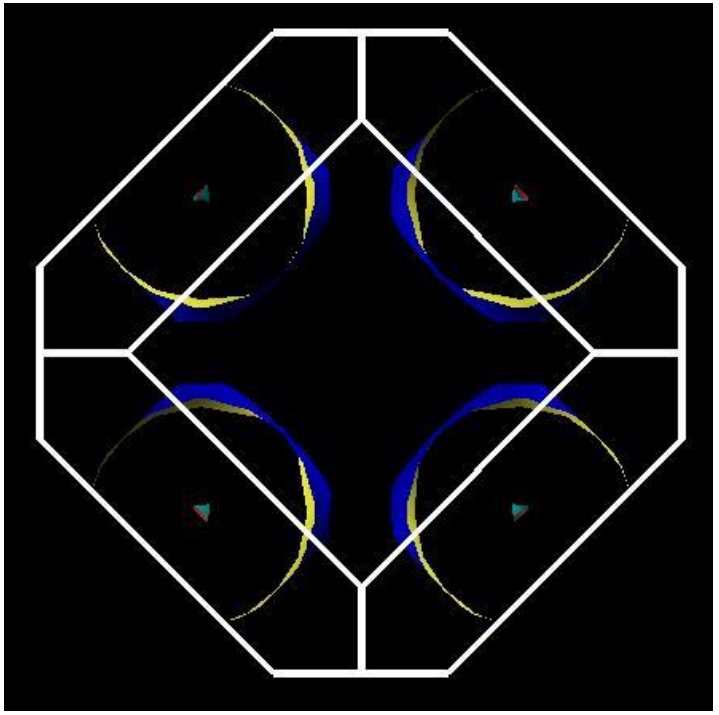
(*we use the Quantum-Espresso & Gibbs2 DFT packages)

q = 0.15 |e|/CuO (holes)



≈ 43 °K

q = -0.15 |e|/CuO (electrons)



≈ 25 °K

Apply DFT to obtain $g^{\mathbf{q}\nu,mn}_{\mathbf{k}+\mathbf{q},\mathbf{k}}$ between electrons and phonons, followed by application of the Eliashberg-McMillan-Allen-Dynes formalism to find Tc:

But...maybe it takes Two to Tango!

Has the Clue been There all Along?

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.

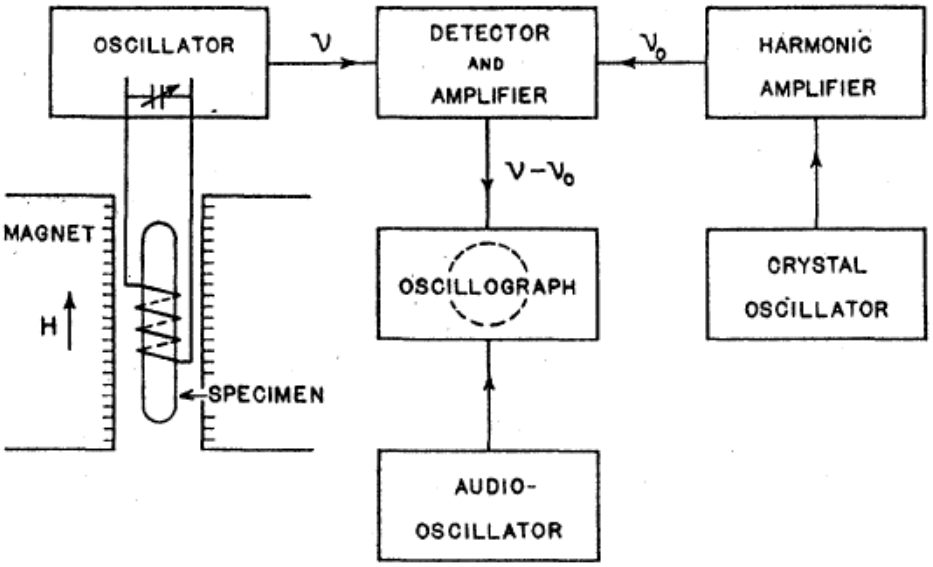


TABLE I. *Spin system data determined from dispersion measurements.*

	$10^{-6}a/c$ 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?

What's Needed

A DFT + U package that will allow the simultaneous calculation of electron-phonon interactions as well as spin-spin excitations, and thus enable an estimation of the Casimir/de Pre coupling…*and maybe a combined phonon-spin pairing λ ?*

Lessons from
“Four Aging British Philosophers”

...for engineers and physicists under 50...

“You can’t always get what you want…”

“…you get what you need!”