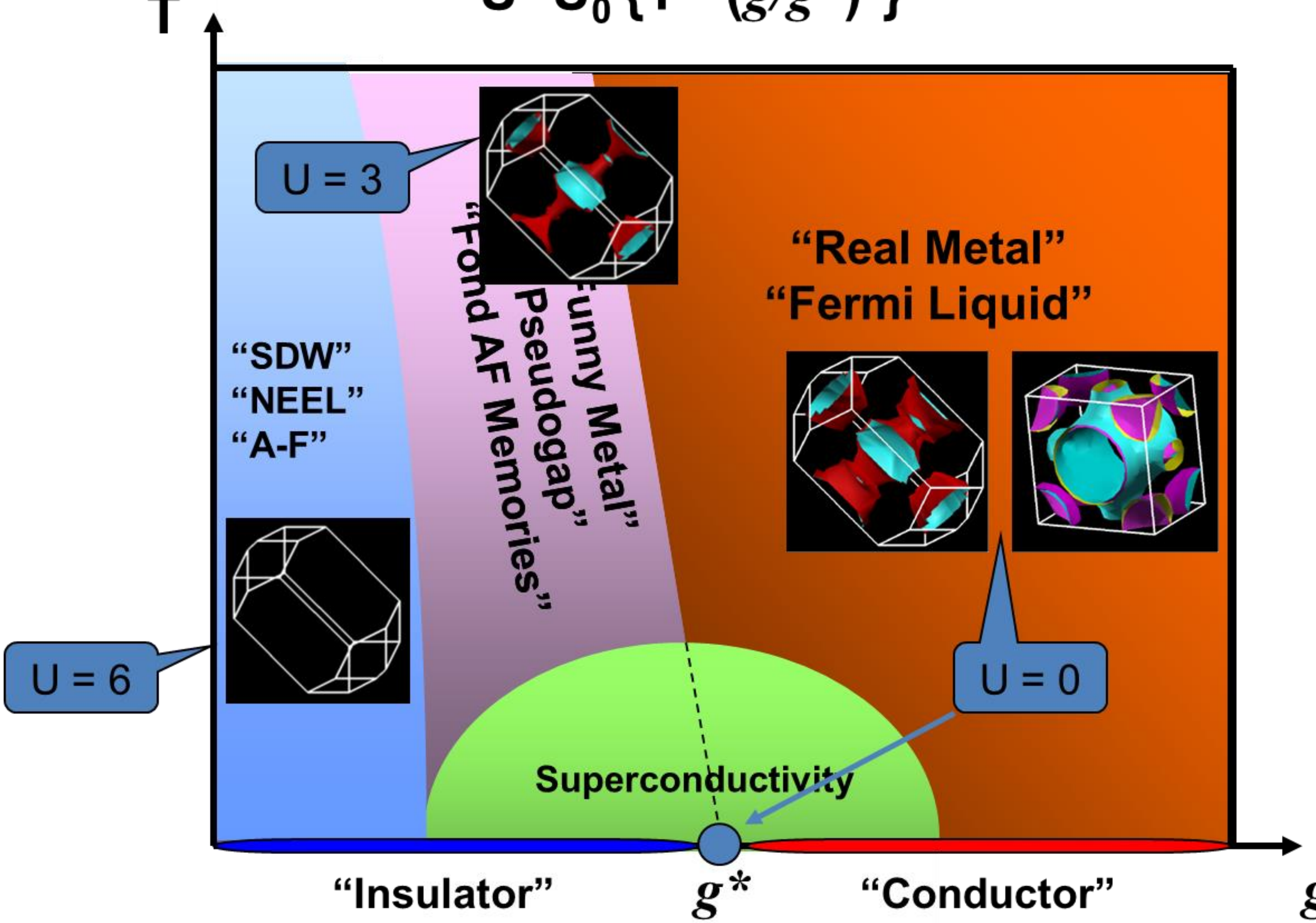
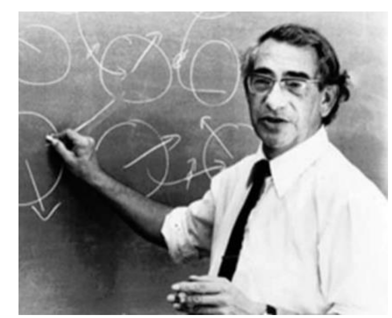
# The Colossal Quantum Conundrum

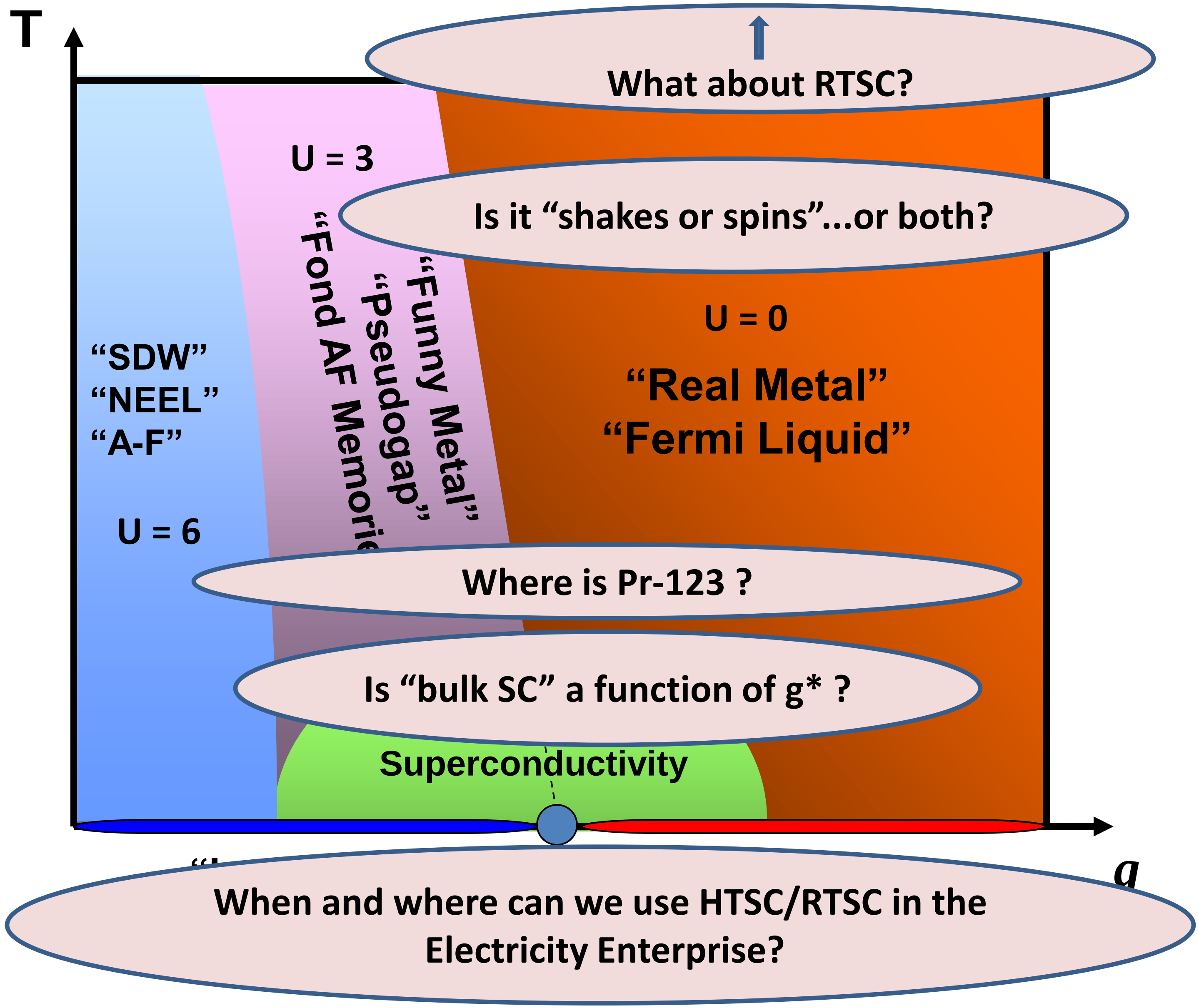
$$U \sim U_0 \{1 - (g/g^*)^2\}^{1/2}$$



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

# Five HTSC "In Your Face" Questions



# Shakes or/and Spins?

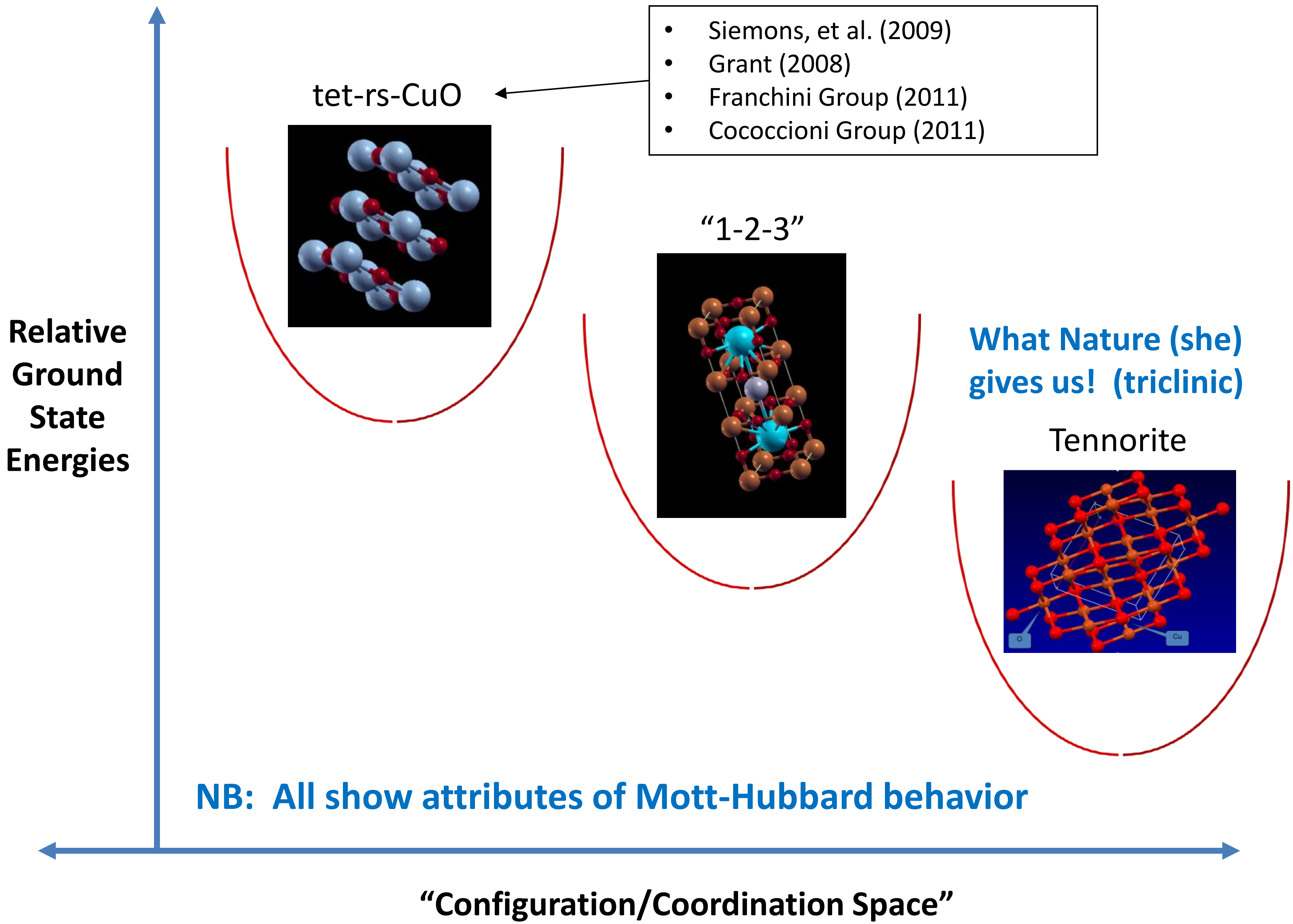
# The Pairing Glue

**"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”

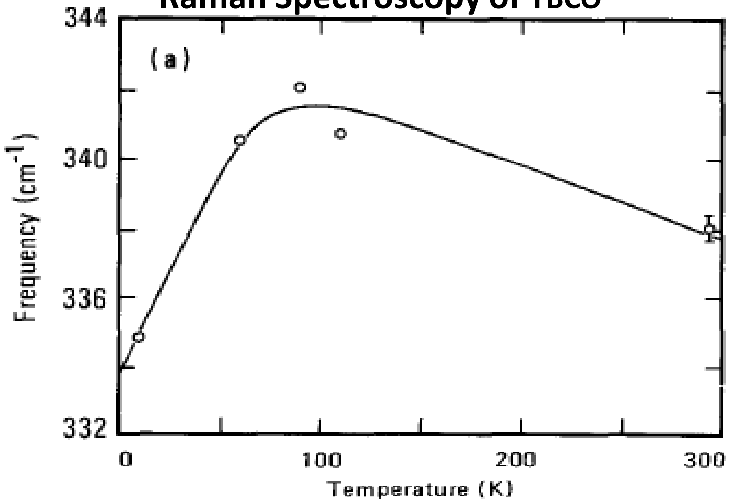


# *Interesting...*

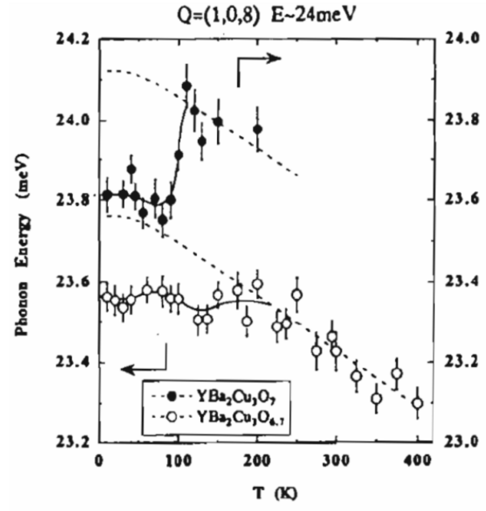
- Lowest symmetry yields lowest ground state energy.
- Higher...at least in a computer...gives greater (localized around given "optimal lattice" constants).
- Why?  Jahn-Teller "degeneracies"!  Nature abhors them (Aristole).
- Were Bednorz-Mueller (Chakravarty & Hoecht) on the right path in 1986 after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

# The Lattice is Shaking

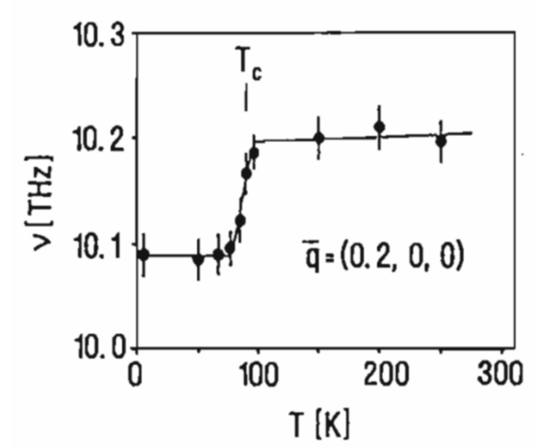
**Macfarlane, Rosen, Seki, SSC 63, 831 (1987)**
**Raman Spectroscopy of YBCO**



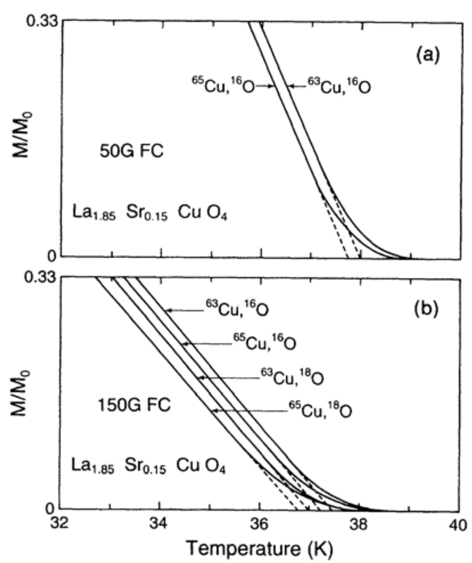

**Harashima, et al., Physica C263, 257 (1996)**




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

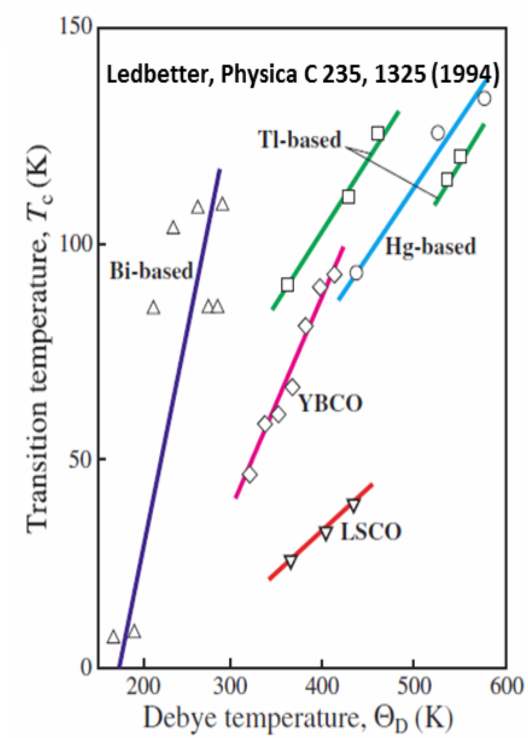



**Franck, Harker, Brewer, PRL 71, (1993)**
**Cu and O Isotope Effects in $La_{2-x}Sr_xCuO_4$**

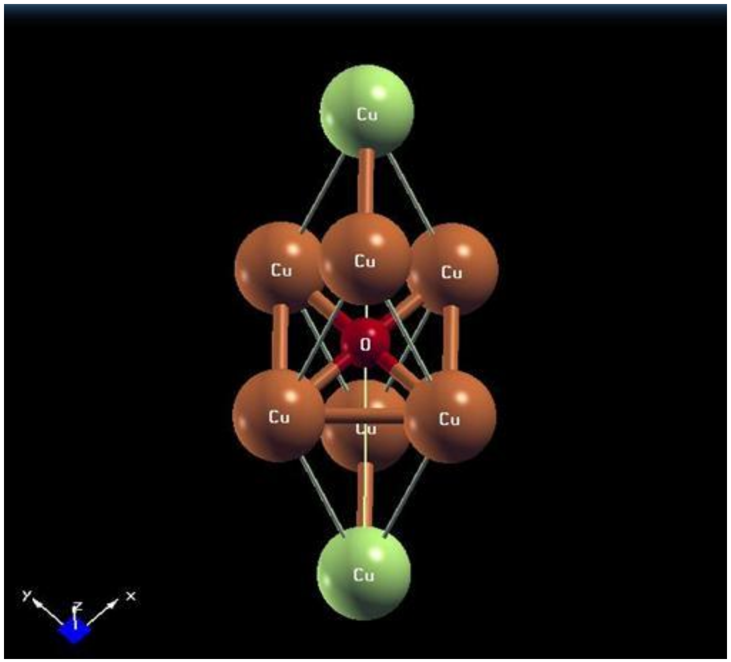


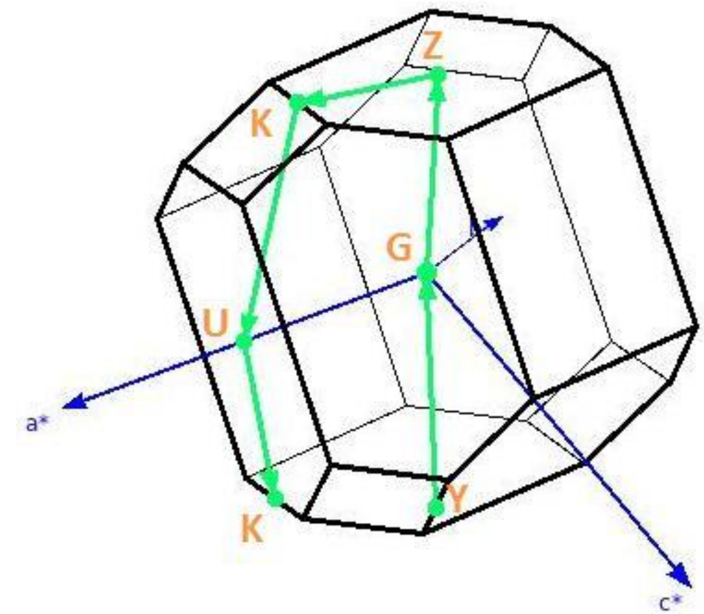

***We can see Phonons have been there ever since the Creation!***

**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

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

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

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

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

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 $g_{\mathbf{k+q},\mathbf{k}}$ !

# e-p Interaction in the DFT/LDA Formalism

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

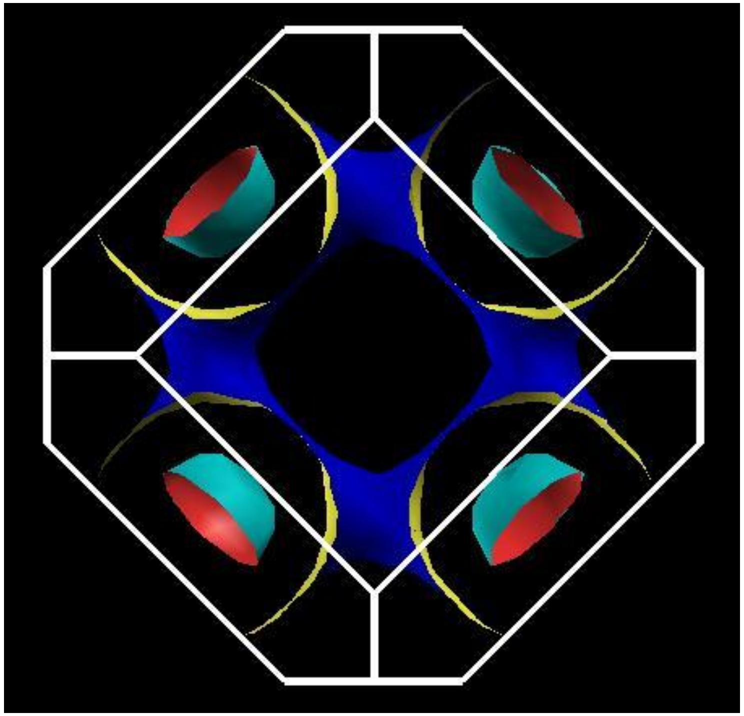
$$\Delta V_{KS}^{\mathbf{q},\nu} = \sum_{\mathbf{R}} \sum_{s} \frac{\partial V_{KS}}{\partial \vec{u}_{s,\mathbf{R}}} \cdot \vec{u}_s^{\mathbf{q},\nu} \frac{e^{i\mathbf{q}\cdot\mathbf{R}}}{\sqrt{N}}$$

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

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

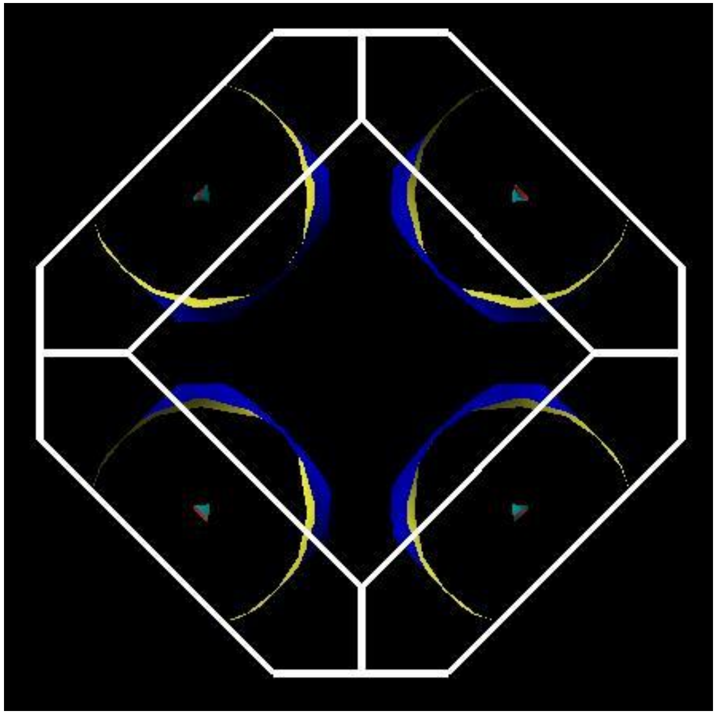
(*we use the Quantum-Espresso & Gibbs2 DFT packages)

**q = 0.15 |e|/CuO (holes)**



**≈ 43 °K**

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



**≈ 25 °K**

**Apply DFT to obtain $g^{\mathbf{q}_{\nu,mn}}_{\mathbf{k+q},\mathbf{k}}$ 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*

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*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.

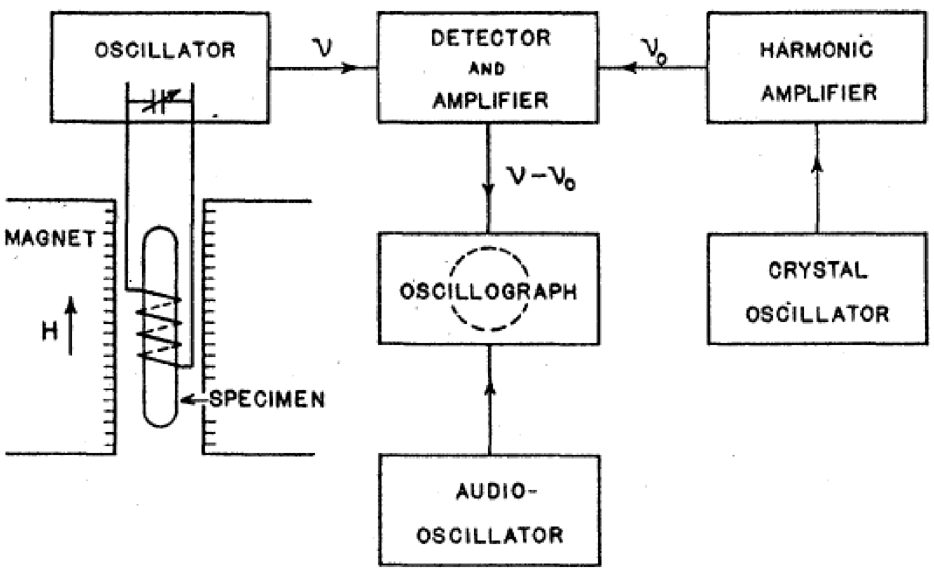


TABLE I. *Spin system data determined from dispersion measurements.*

| | $10^{-6}a/c$ Starr 77° | Teunissen and Gorter 77° | du Pre 1°–4° | $10^{-6}a$ | $\eta$ | $\delta$ |
|---|---|---|---|---|---|---|
| $FeNH_4(SO_4)_2\cdot 12H_2O$ | 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* $\lambda$ *?*