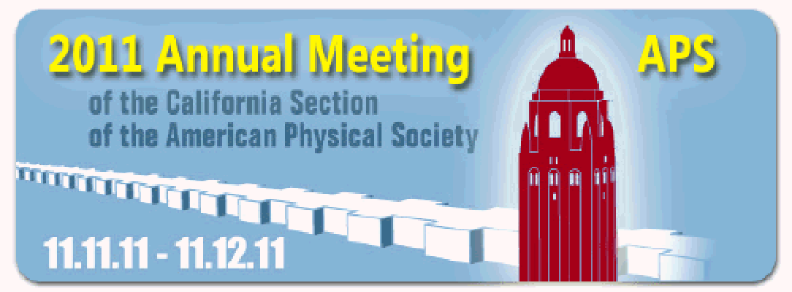

SLAC NATIONAL ACCELERATOR LABORATORY

The Great Quantum Conundrum

Paul M. Grant
W2AGZ Technologies
www.w2agz.com

AGING IBM PENSIONER

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Menlo Park, CA 94025 USA

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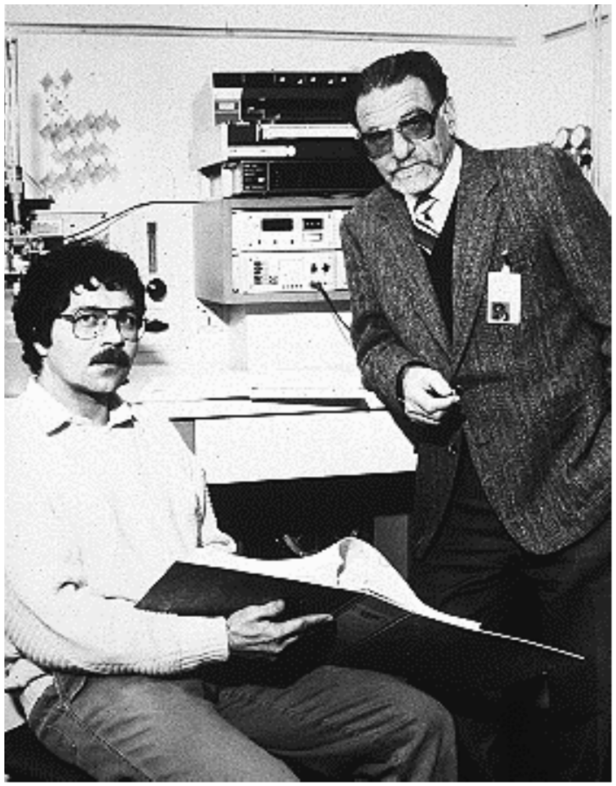
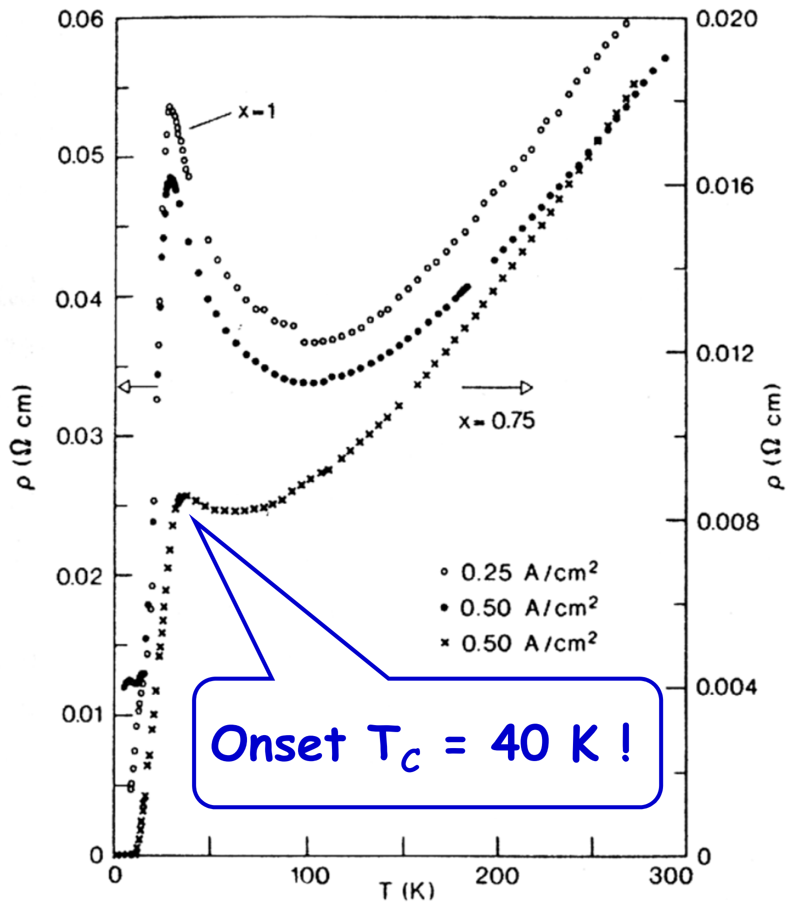
Menlo Park, CA

1986
Another Big Surprise!



Bednorz and Mueller
IBM Zuerich, 1986

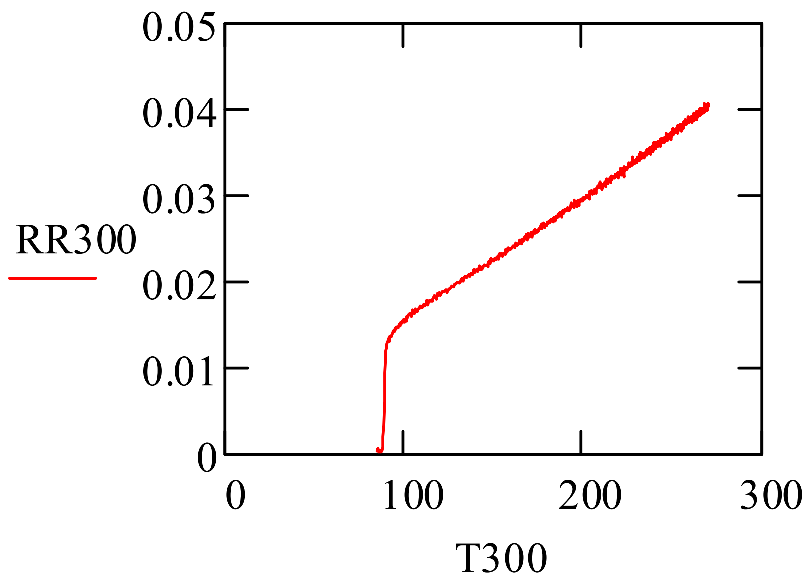


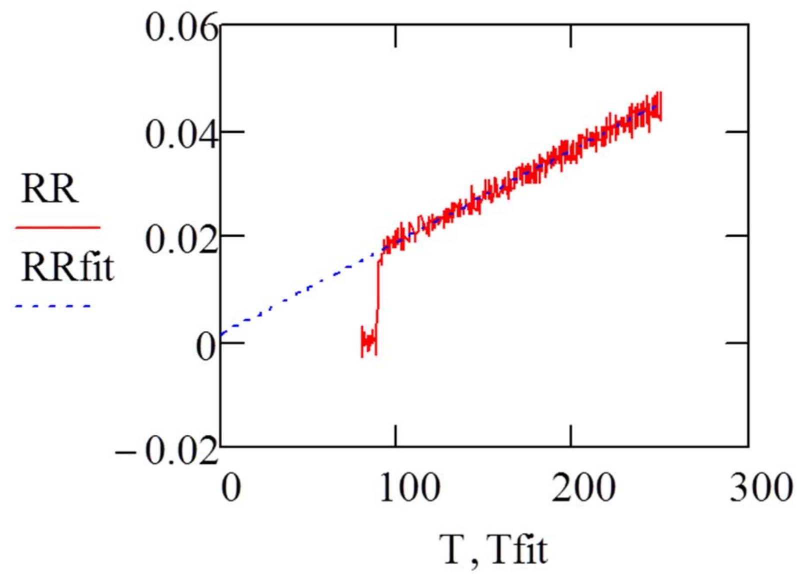
1987
"The Prize!"

Associated Press

J. Georg Bednorz, left, and K. Alex Müller after learning they had won the Nobel Prize in physics.

2 Get Nobel for Unlocking Superconductor Secret





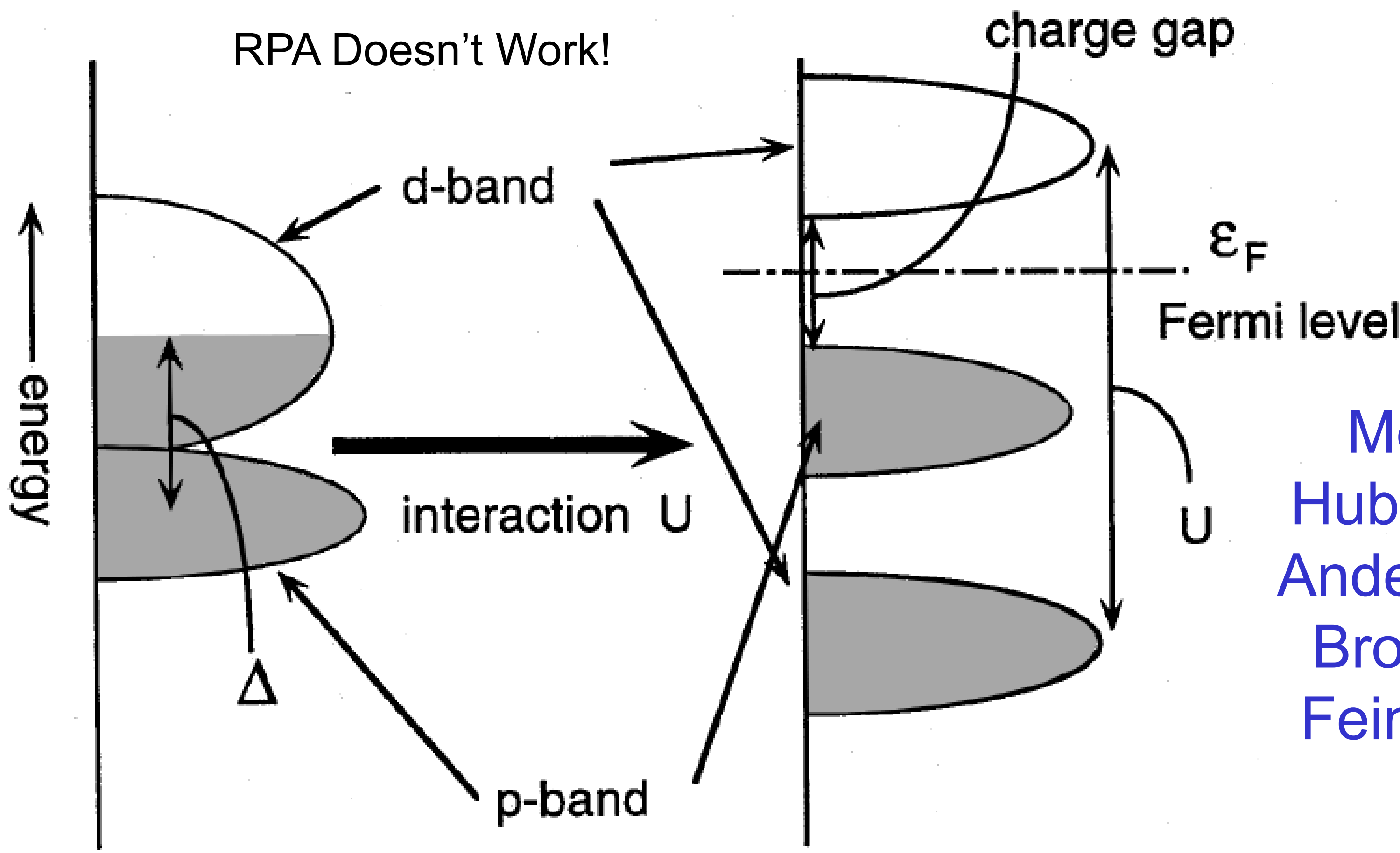
A quarter-centrury after Bednorz-Mueller, it is still not clear why:

1) Tc is so high
2) The normal state appears non-Fermi liquid-like

That is the Great Quantum Conundrum

Transition Metal Oxides
“Should be Metals, But Aren’t”
(Charge Transfer Insulators, Instead)

RPA Doesn’t Work!

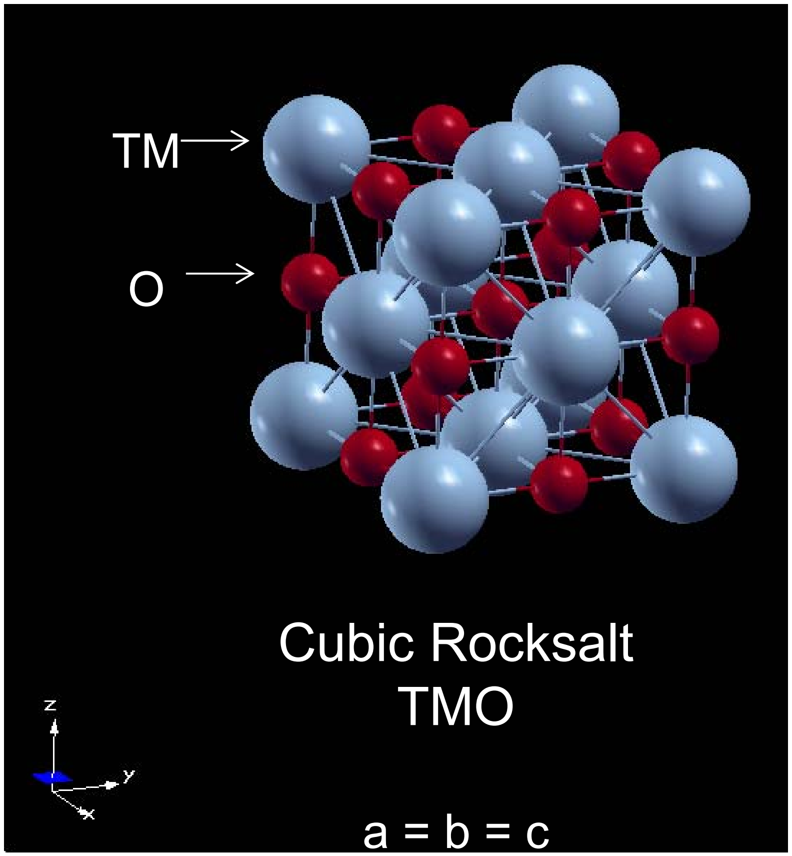


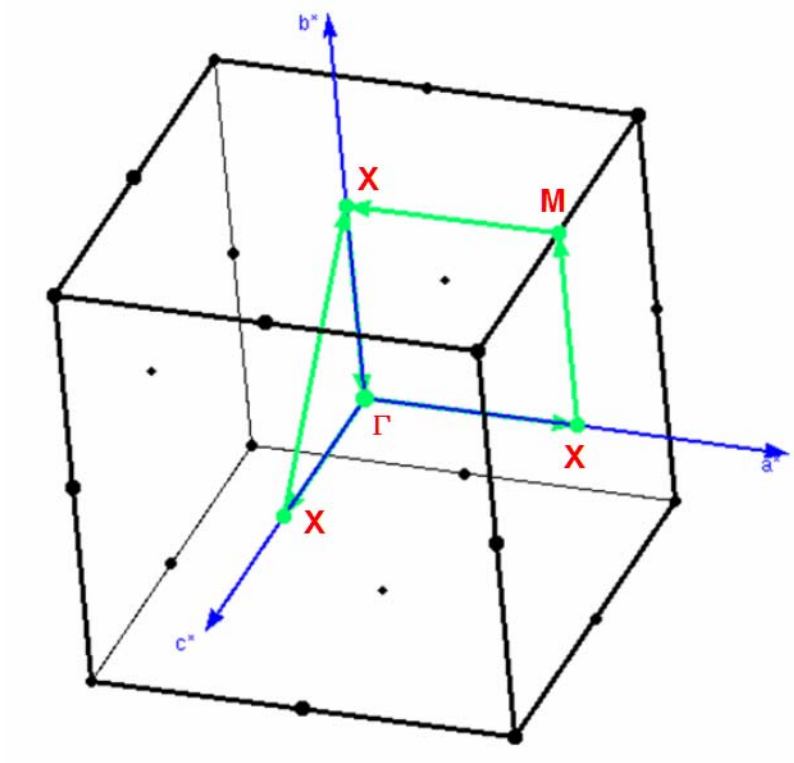
Mott
Hubbard
Anderson
Brooks
Feinlieb

After Imada, et al, RMP 70, 1039 (1998)

Cubic Rocksalt TMOs

Direct and Reciprocal Lattices





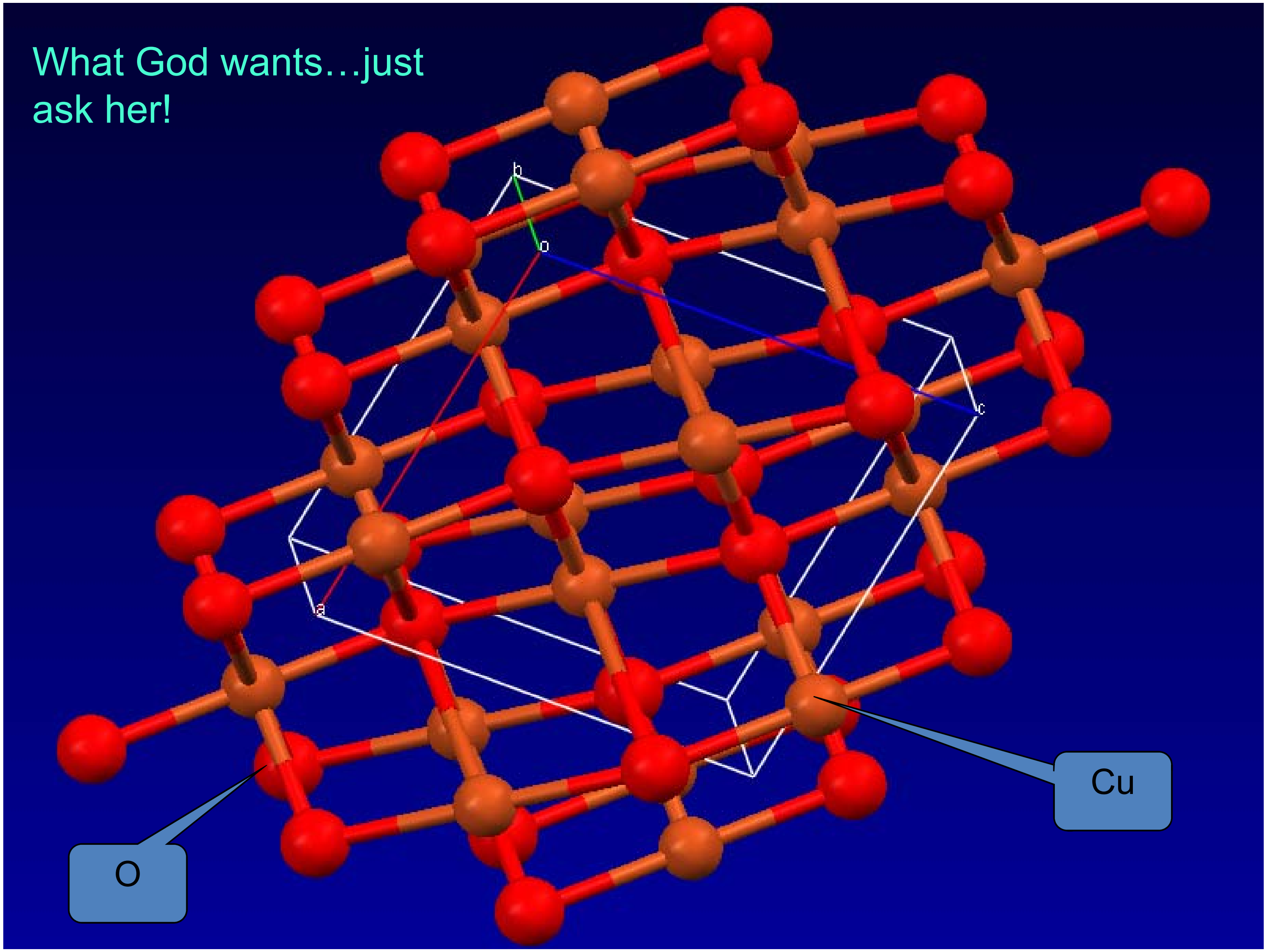
Cubic Rocksalt Divalent TMOs

TMO	3d Config	Properties
MnO	5	MH-CTI (5.6)
FeO	6	MH-CTI (5.9)
CoO	7	MH-CTI (6.3)
NiO	8	MH-CTI (6.5)
CuO	9	**XX *Doesn't Exist!***

See Imada, Fujimore, Tokura, RPM 70 (1988)

Why Not?

Tenorite (Monoclinic CuO)



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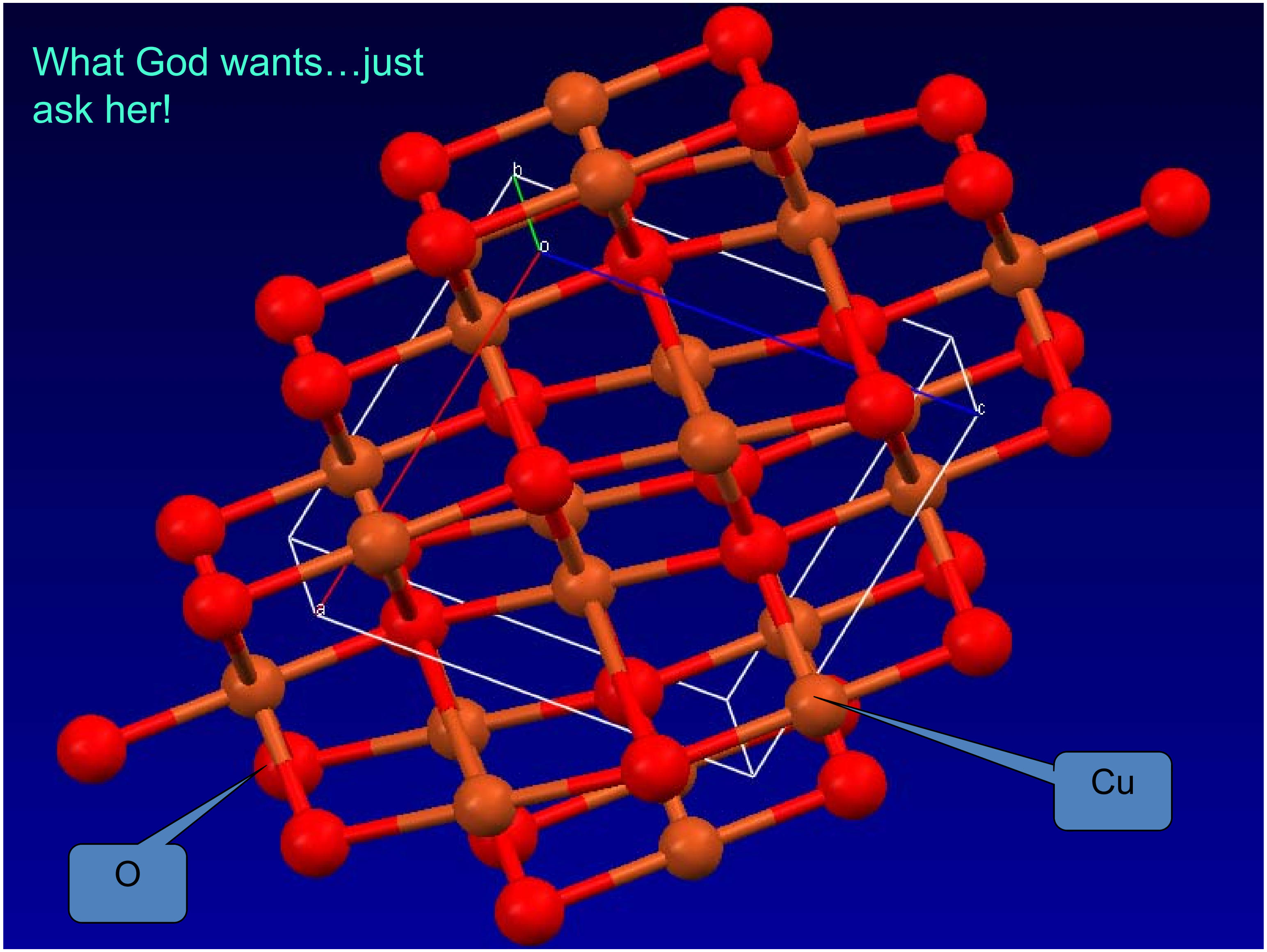
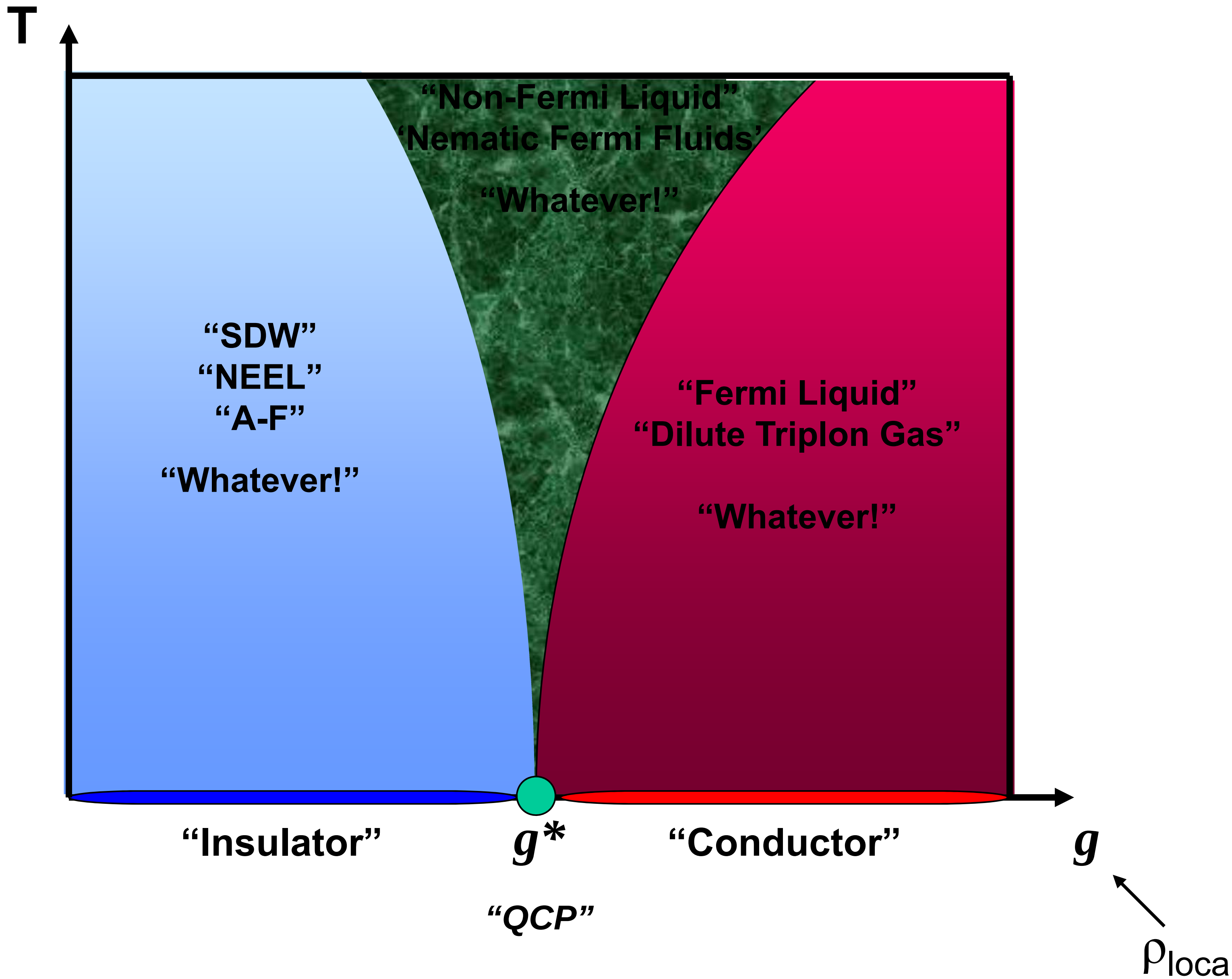
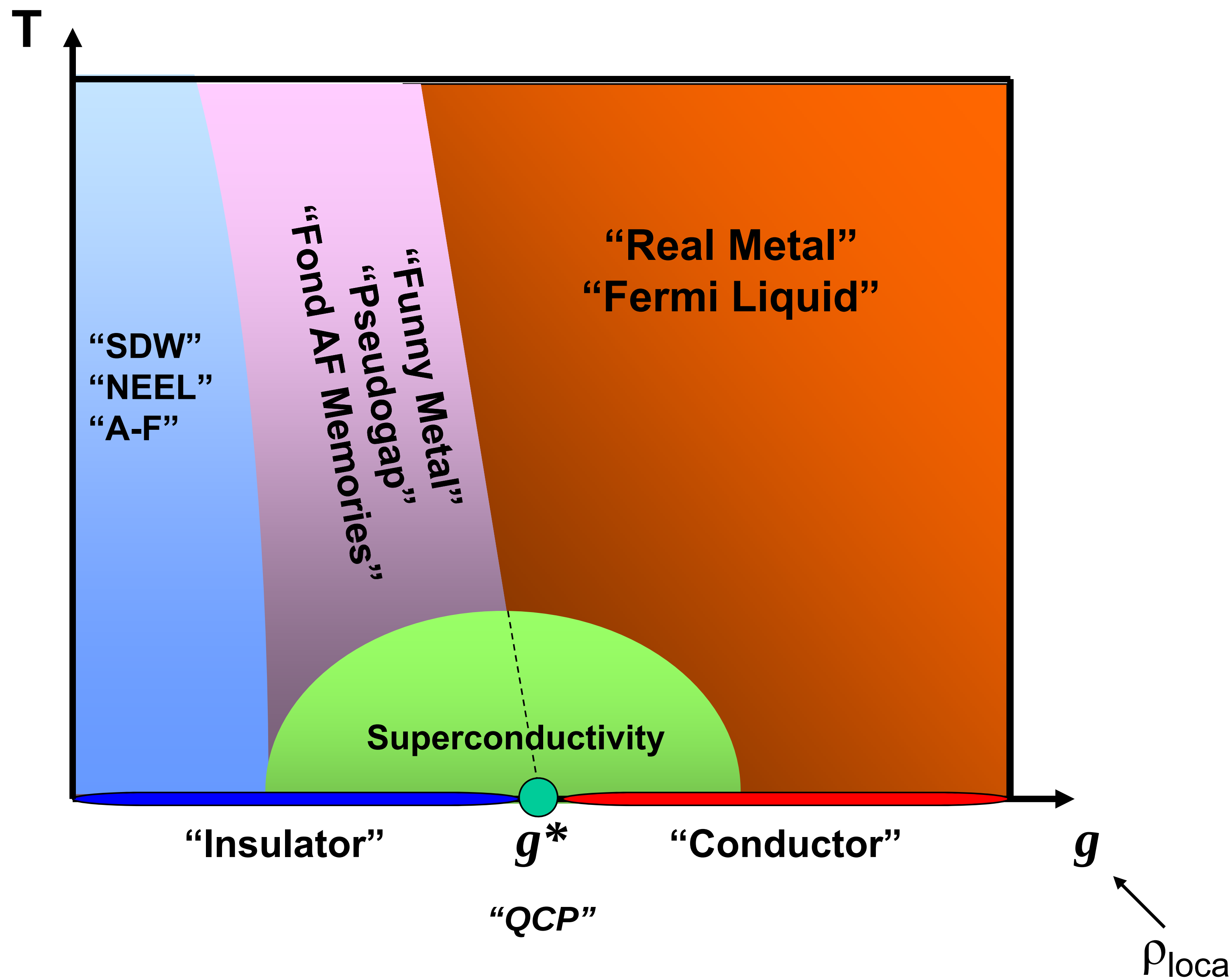


The Great Quantum Conundrum



The Colossal Quantum Conundrum



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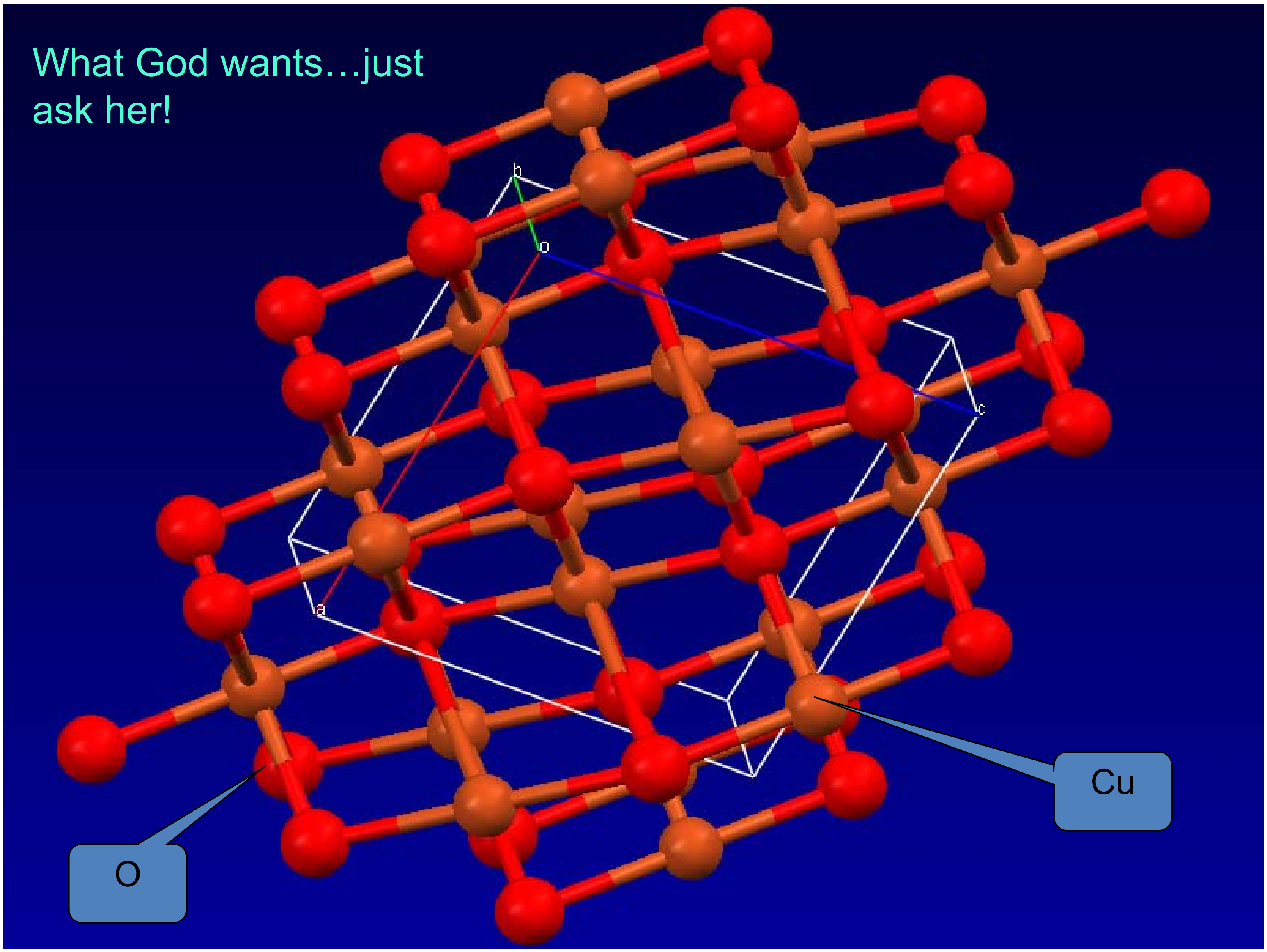
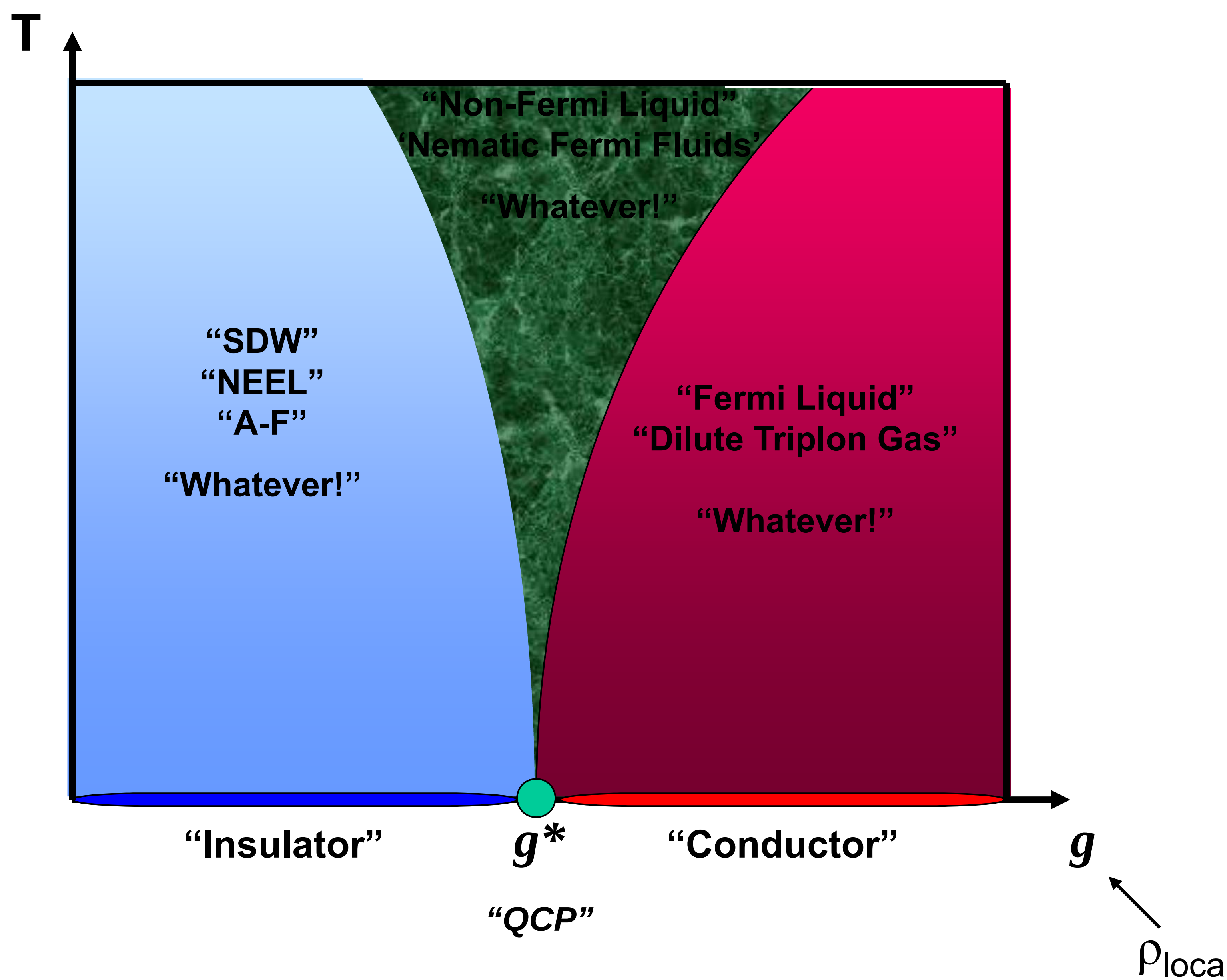
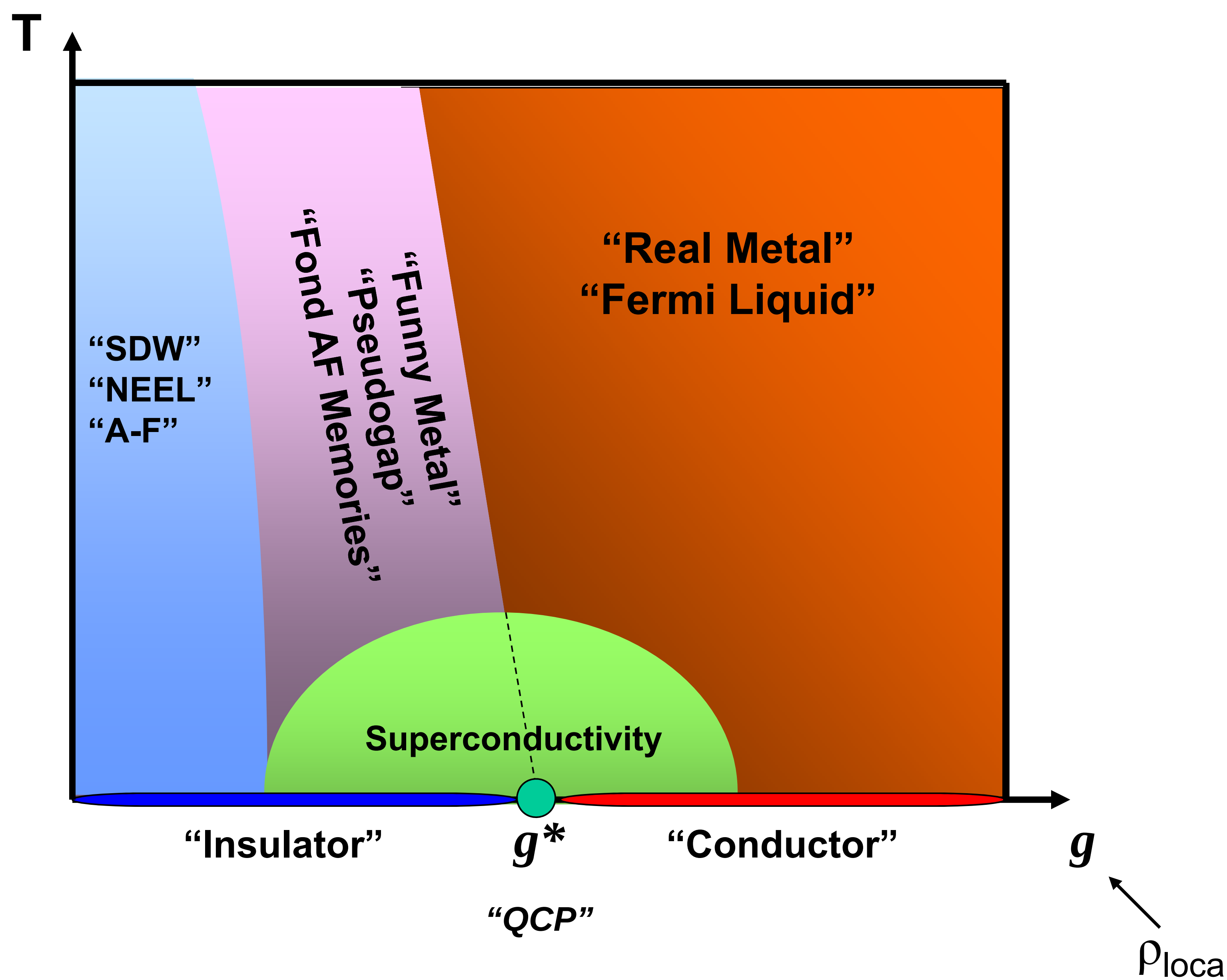
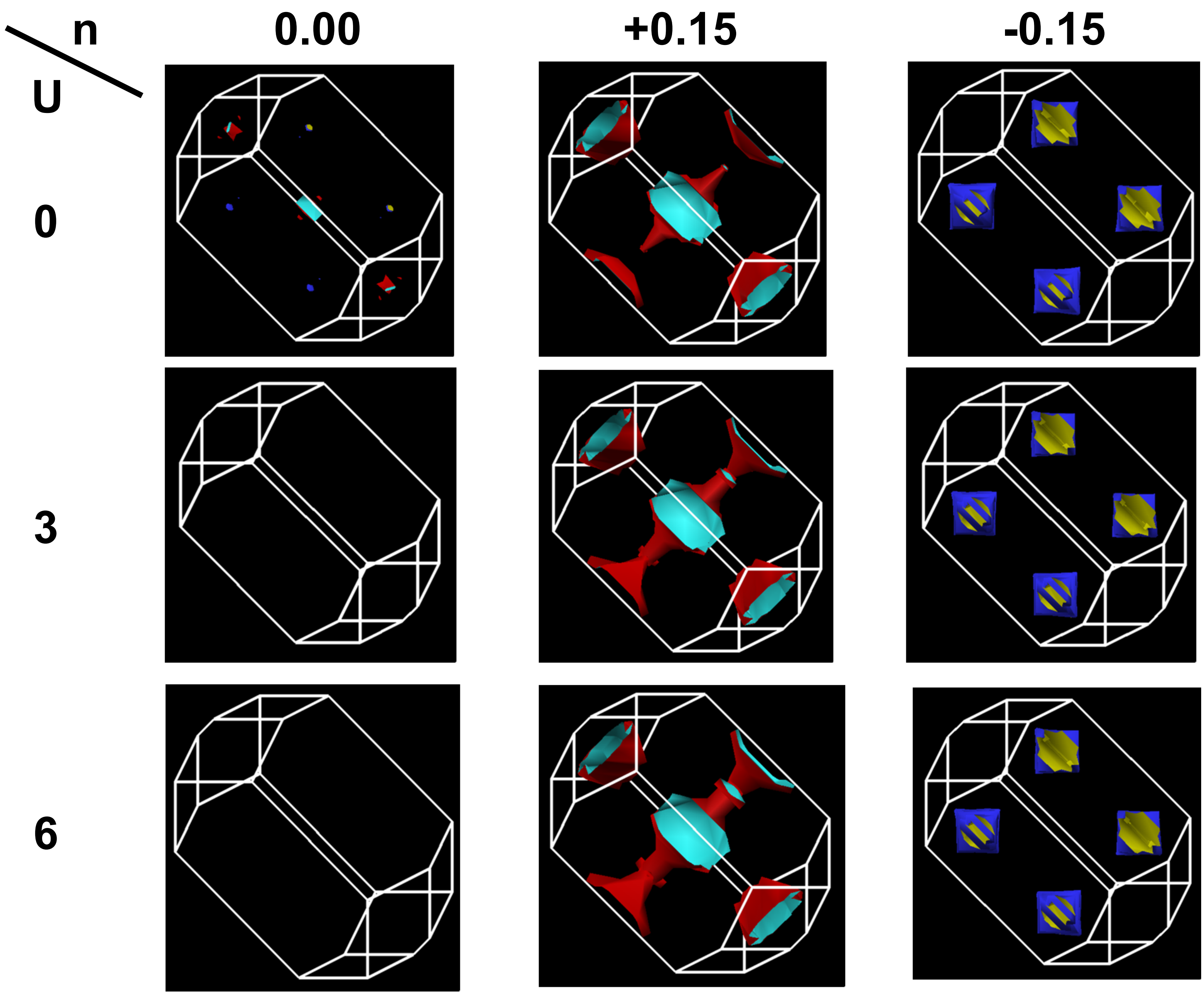


The Great Quantum Conundrum



The Colossal Quantum Conundrum




n
U
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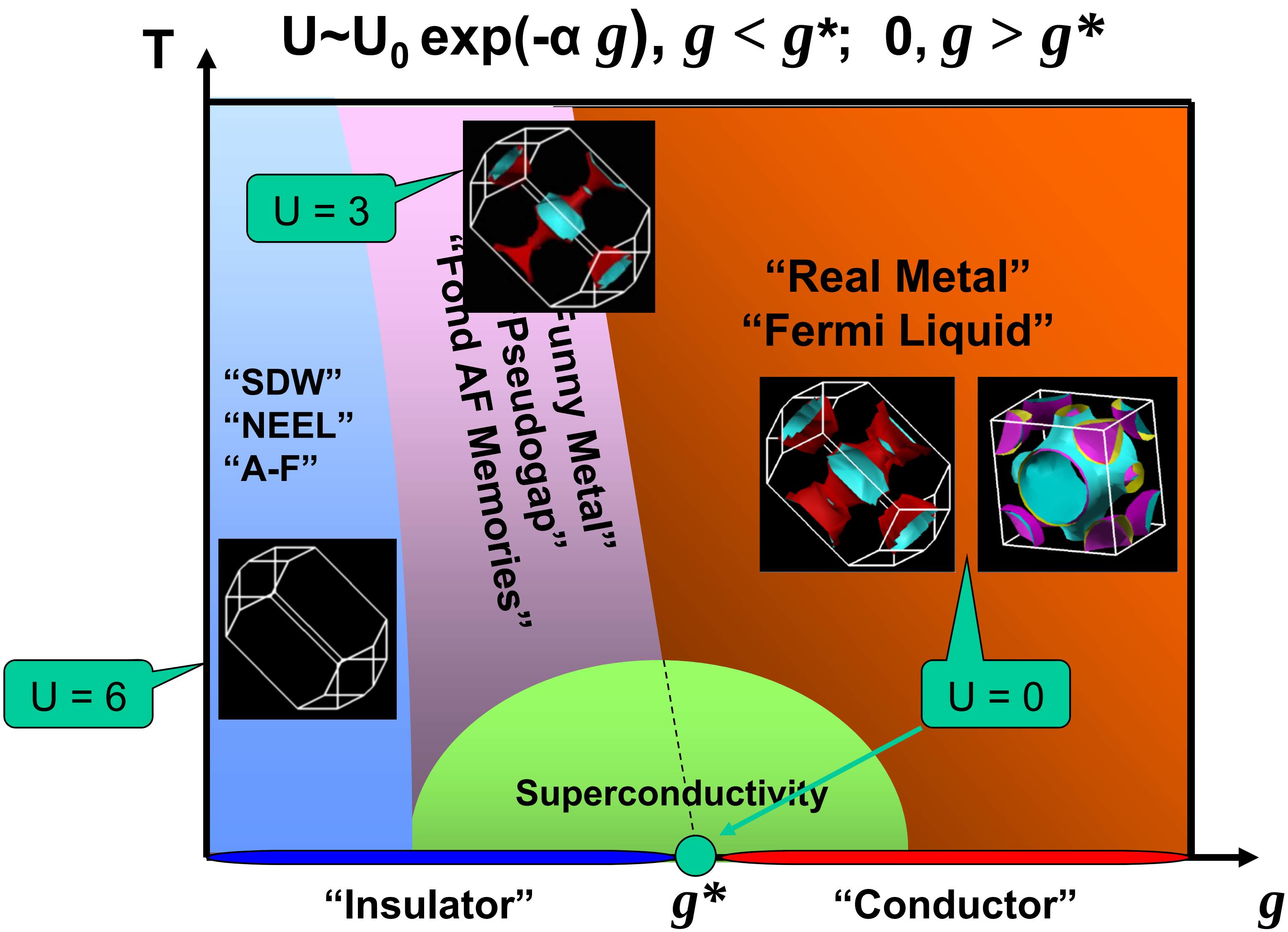
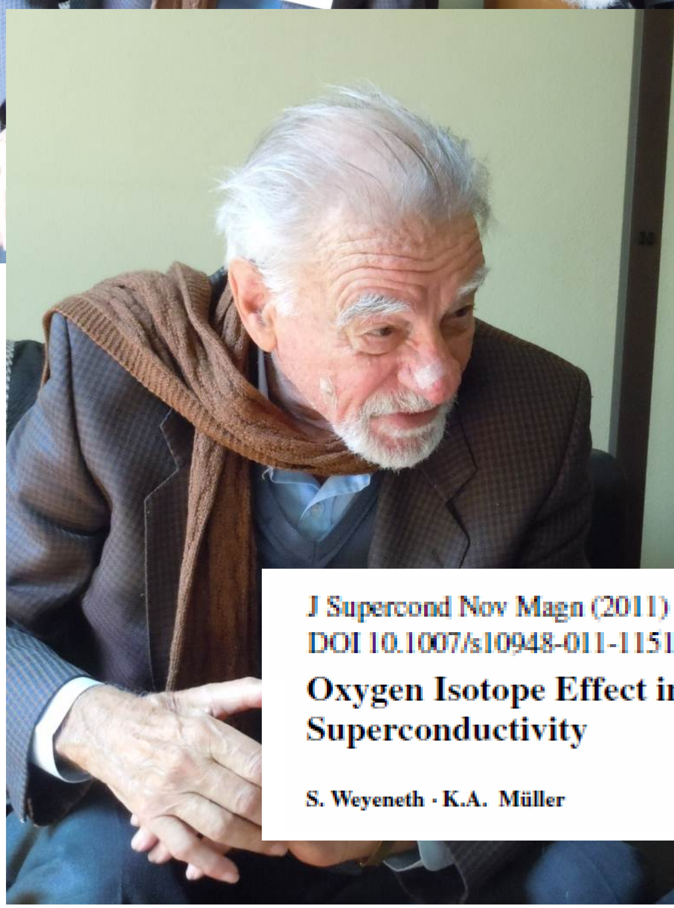
+0.15
-0.15
0
3
6

The Colossal Quantum Conundrum



Somewhere in here there has to be "BCS-like" pairing!



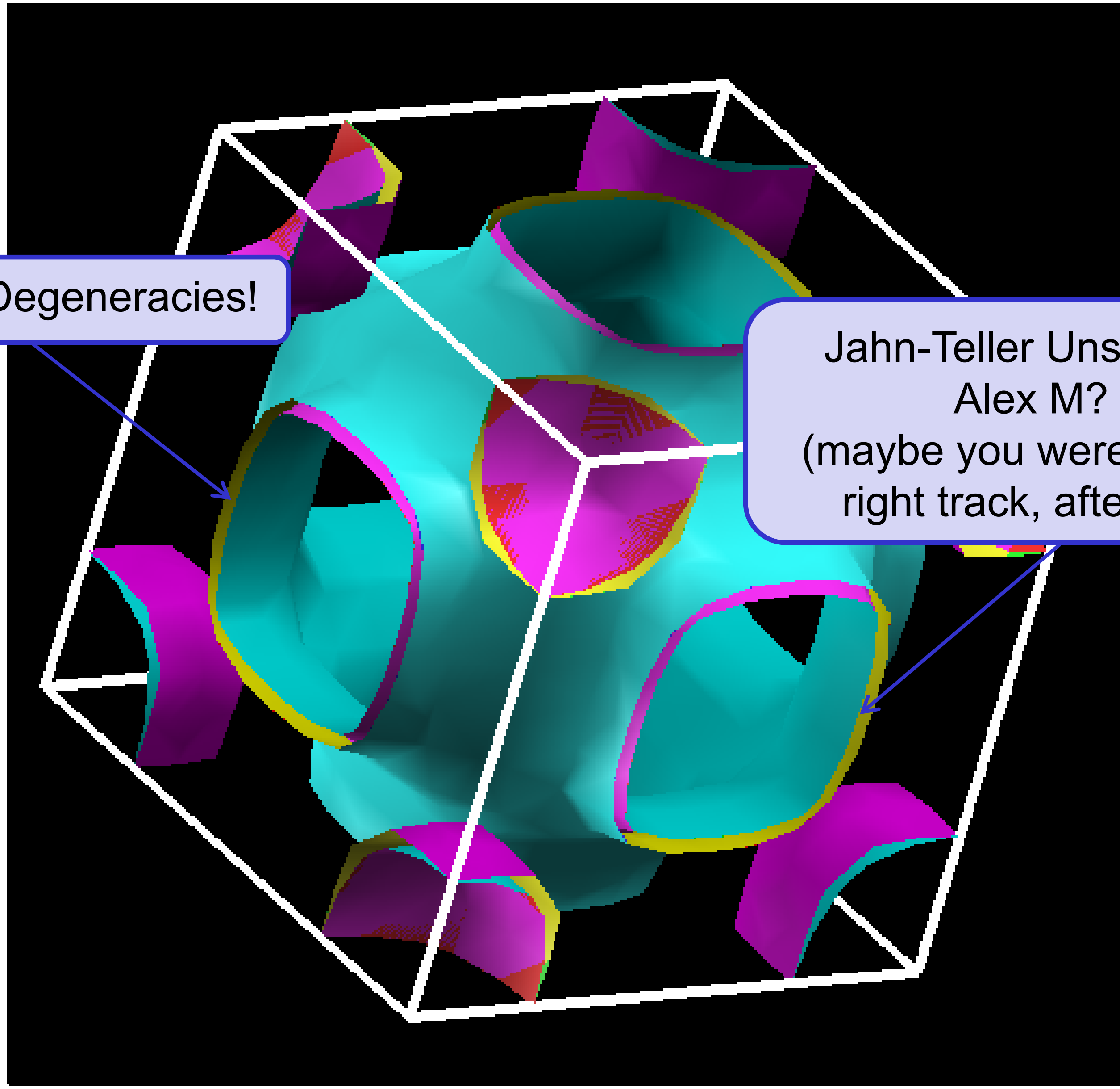



J Supercond Nov Magn (2011) 24: 1235–1239
DOI 10.1007/s10948-011-1151-3

Oxygen Isotope Effect in Cuprates Results from Polaron-induced Superconductivity

S. Weyeneth · K.A. Müller

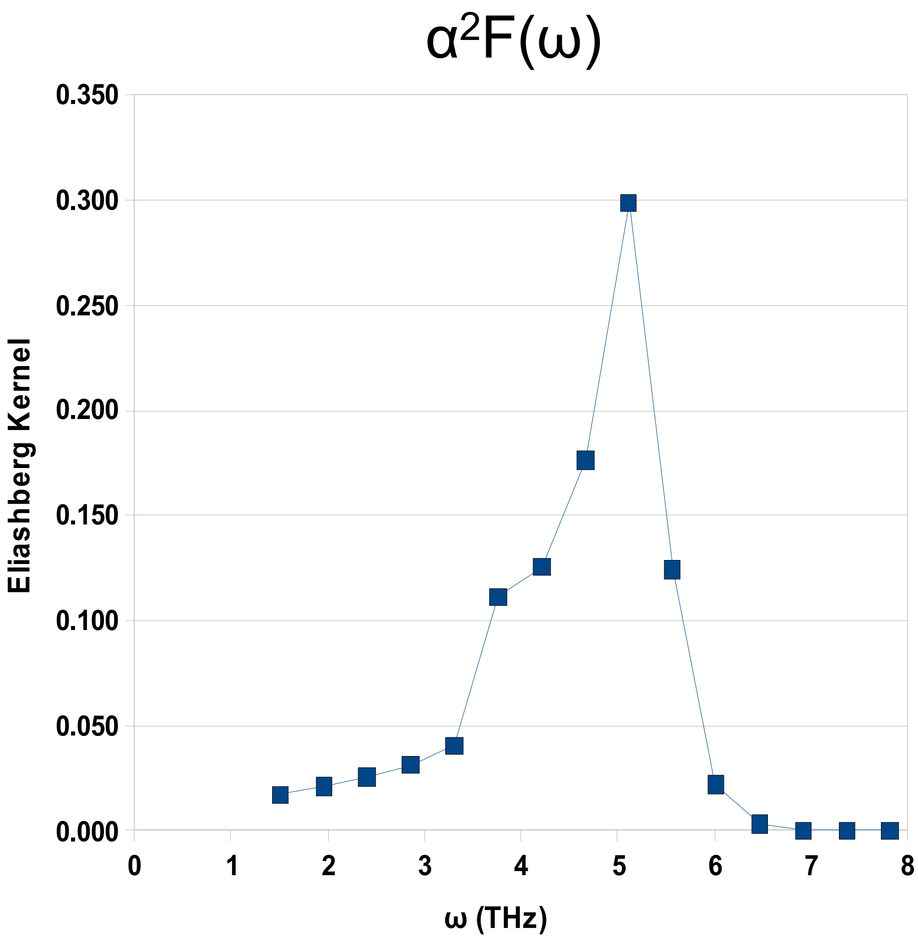
Rocksalt CuO Fermiology (U = 0 eV)
(8 Bands Combined)



Note (Near) Degeneracies!

Jahn-Teller Unstable?
Alex M?
(maybe you were on the right track, after all!)

Non-Magnetic (U = 0) Cubic Rocksalt CuO -- Electron-Phonon Properties --



σ = 0.04

- λ ~ 0.6 – 0.7
- Consistent with other non-magnetic "HTSCs"

$$T_C = a\Theta e^{-\frac{1}{\lambda-\mu^*}} \qquad \lambda k\Theta \ll E_F$$

	T_C (K)	λ	μ*
K_3C_{60}	16.3	0.51	-
Rb_3C_{60}	30.5	0.61	-
Cs_3C_{60}	47.4	0.72	-

Shakes or Spins or Both?

Are They Copacetic, Competitive…or…

…just another Conundrum?

What formalism is the HTSC analogy to Migdal-Eliashberg-McMillan?

(In other words, how do I calculate the value of the BCS gap?)

- Original Strong Coupling, Eliashberg *(JETP, 1960), McMillan (PR, 1968)*
- Generalized Linhard Response Function (RPA + fluctuations) *Hu and O'Connell (PRB 1989)*
- Dielectric Response Function *Kirznits, Maximov, Khomskii (JLTP 1972)*

McMillan Strong Coupling

(Computationally implemented by Wierzbowska, et al., cond-mat/0504077, 2006)

What's the HTSC equivalent?

$$\alpha^2(\omega)F(\omega) = \int_S \frac{d^2p}{v_F}\int_{S'}\frac{d^2p'}{(2\pi\hbar)^3 v_F'}\sum_\nu g_{pp'\nu}{}^2\delta(\omega-\omega_{p-p'\nu}) \Big/ \int_S \frac{d^2p}{v_F}\,, \tag{19}$$

where the integral $\int d^2p$ is taken over the Fermi surface and the electron-phonon matrix elements are given by[14]

$$g_{pp'\nu} = (\hbar/2MNV\omega_{p-p'\nu})^{1/2}\mathcal{I}_\nu(p,\,p')\,, \tag{20}$$

where $\mathcal{I}_\nu(pp')$ is the electronic matrix element of the change in the crystal potential $\mathcal{U}$ as one atom is moved:

$$\mathcal{I}_\nu(pp') = \int \psi_p{}^*(\boldsymbol{\varepsilon}_{p-p'\nu}\cdot\nabla\mathcal{U})\psi_{p'}d\mathbf{r}. \tag{21}$$

Generalized Linhard Function

$$\chi^0(\mathbf{q},\omega)=\sum_{\mathbf{k},\sigma}\frac{f(\mathbf{k})-f(\mathbf{k}+\mathbf{q})}{\hbar\omega-(\varepsilon_{\mathbf{k}+\mathbf{q}}-\varepsilon_{\mathbf{k}})+iDq^2}$$

$$D=\lim_{t\to\infty}\frac{1}{2t}\overline{\delta\mathbf{R}^2(t)}$$

$$V(\mathbf{q})=4\pi e^2/q^2$$

$$\epsilon(\mathbf{q},\omega)=1-V(\mathbf{q})\chi^0(\mathbf{q},\omega)$$

$$\epsilon_1(x,y)=1+\frac{q_{\mathrm{TF}}^2}{8k_F^2x^2}\left[1+\frac{1}{8x}\left[(1+b^2x^2-\nu_+^2)\ln\left[\frac{(1+\nu_+)^2+b^2x^2}{(1-\nu_+)^2+b^2x^2}\right]+(1+b^2x^2-\nu_-^2)\ln\left[\frac{(1+\nu_-)^2+b^2x^2}{(1-\nu_-)^2+b^2x^2}\right]\right]\right.$$
$$\left.-\frac{b}{2}\left\{\nu_+\left[\arctan\left[\frac{1-\nu_+}{bx}\right]+\arctan\left[\frac{1+\nu_+}{bx}\right]\right]+\nu_-\left[\arctan\left[\frac{1-\nu_-}{bx}\right]+\arctan\left[\frac{1+\nu_-}{bx}\right]\right]\right\}\right]$$

where

$$x=\frac{q}{2k_F},\quad y=\frac{\hbar\omega}{4\varepsilon_F},\quad q_{\mathrm{TF}}^2=\frac{4me^2k_F}{\pi\hbar^2},\quad b=\frac{2mD}{\hbar},\quad \nu_\pm=x\pm y/x\ ,$$

“Fluctuations?”
“Empirical?”

HO (1989)

Dielectric Response Function

$$G(\mathbf{k}, i\omega_n) = 1/(i\omega_n - \xi_k)$$

$$F(\mathbf{p}, i\omega_n) = -G(\mathbf{p}, i\omega_n)G(-\mathbf{p}, -i\omega_n)T_c \sum_{\mathrm{m}} \int [d^3k/(2\pi)^3]$$

$$\times V(\mathbf{p} - \mathbf{k}, i\omega_n - i\omega_{\mathrm{m}})F(\mathbf{k}, i\omega_{\mathrm{m}})$$

$$V(\mathbf{q}, i\omega_n) = \frac{4\pi e^2}{q^2}\left[1 - \int_0^\infty \frac{dE^2 \rho(\mathbf{q}, E)}{\omega_n^2 + E^2}\right]$$

In principle, KMK can calculate the BCS gap for general “bosonic” fields, be they phonons, magnons, spin-ons, excitons, plasmons…or morons!

KMK (1972)

So...

- Let's "Shut up and start calculating."
  - David Mermin, Cornell, as quoted by yours truly, in Nature 4 August 2011.
- I'd like to help...
  - Then,

Bottom Line

Can studying CuO proxies with DFT
+ LDA+U
+ phonons
+ spins
provide insight into the origins of High-T_C?

I say "Yes," but…
As Bob Laughlin says, "Size Matters…!"
…and I need a…
BIGGER COMPUTER!