Setup

MARCH MEETING 2019
BOSTON, MA MARCH 4-8

Continuing Search for the Origin of HTSC: DFT Studies of Selected CuO Proxy Structures

Were the Basic Physics Underlying HTSC Actually Revealed in 1941?

Paul Michael Patrick Grant

Aging IBM Pensioner

APS Senior Life Fellow

w2agz@w2agz.com

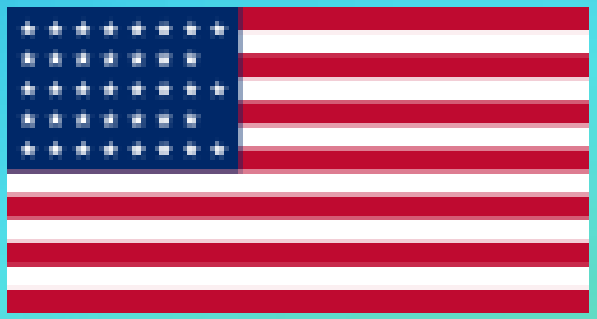
RESEARCH JOINTLY SUPPORTED UNDER THE IBM AND SSA RETIREMENT FUNDS

St. Patrick's Day - 2019 (In 13 Days!)

-2014-

PMPG Accepted as a Dual National by the Republic of Ireland

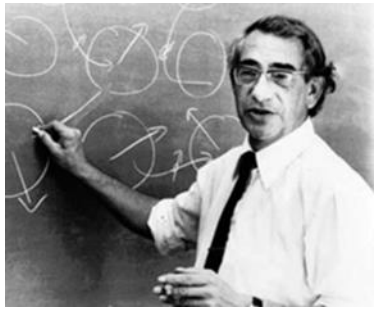
Bridget Ann Mullen-Whalen



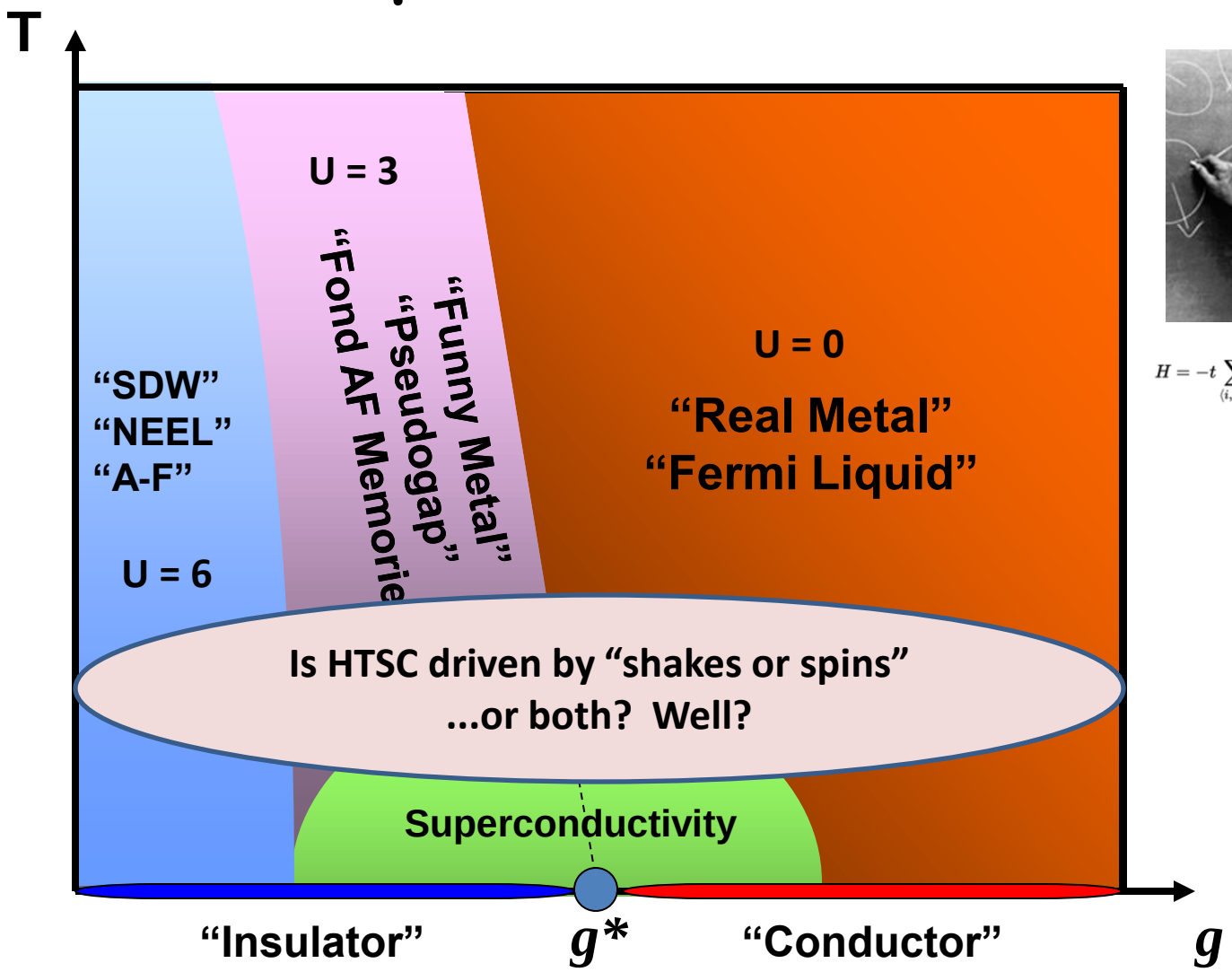
Paul Michael Patrick Grant

A Grandson of Two Proud Lands

The Great Colossal Quantum Conundrum of HTSC in Cuprates, Ferrous Oxides, etc.



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

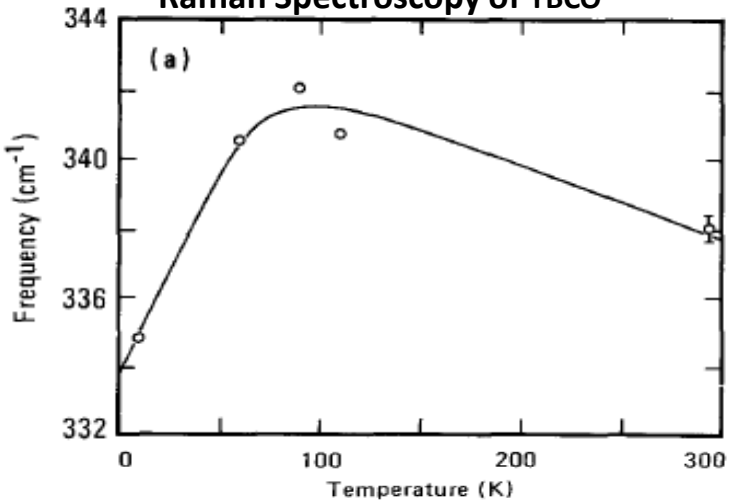


"Order Parameter"

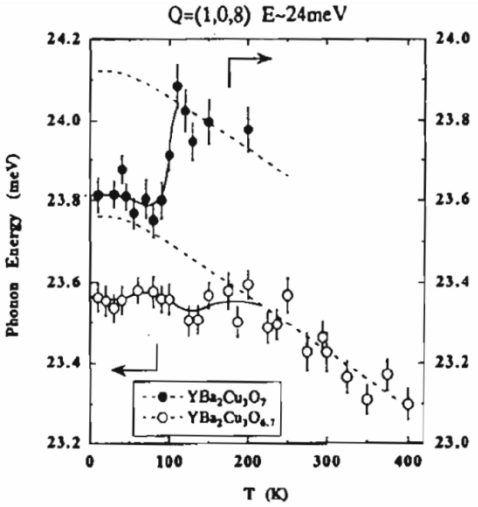
(charge, magnetic field, pressure...whatever)

The Story Since 1987

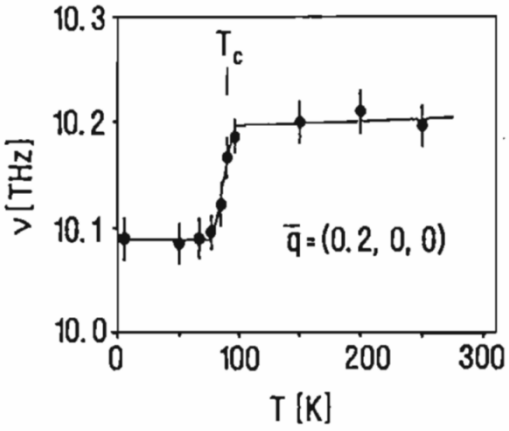
Macfarlane, Rosen, Seki, SSC 63, 831 (1987)
Raman Spectroscopy of YBCO



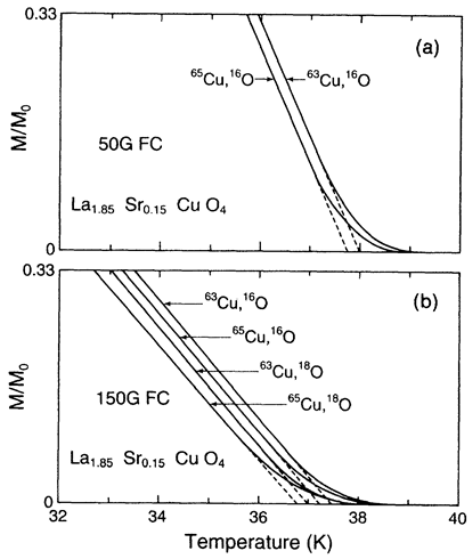
Harashima, et al., Physica C263, 257 (1996)



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



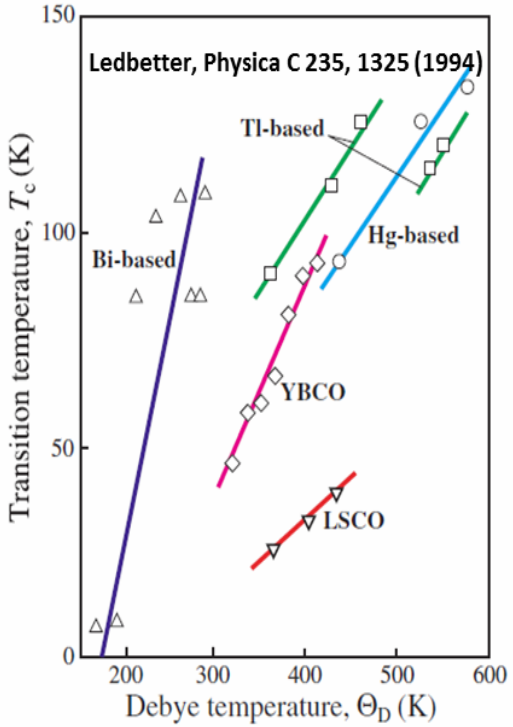
Franck, Harker, Brewer, PRL 71, (1993)
Cu and O Isotope Effects in $La_{2-x}Sr_xCuO_4$



We can see Shakes have been there ever since the Creation of HTSC!

...But so have Spins! (Cu3+/Cu2+)

Ledbetter, Physica C 235, 1325 (1994)



Well...Maybe It Takes Two to Tango!

So Might the "Other Partner" Be Spins?

So Perhaps the Past May Indeed be Prologue!

Attributed to Bill S.,
edited by Paul G.

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.

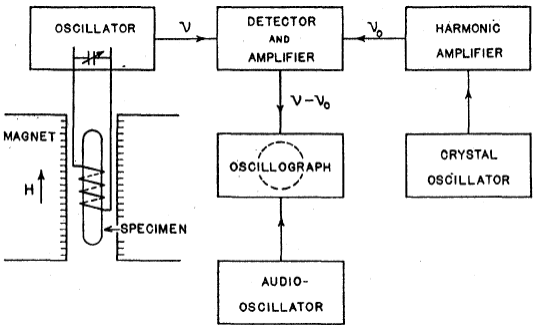


TABLE I. *Spin system data determined from dispersion measurements.*

	$10^{-6}a/c$					
	STARR 77°	TSU-NISSEN 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

Did this former Harvard/MIT postdoc guess the mechanism of HTSC 78 years ago? !

Chauncey Starr

1912 - 2007

The Physics Years (1936 - 1943)
Birth of the Nuclear Age (1944 - 1965)
UCLA & Risk Analysis (1966 - 1971)
The EPRI Years (1972 - 2007)

Please Visit Chauncey's Page at www.w2agz.com

Relevant Sreen Shots from Chauncey's 1941 PR Paper

THEORY

The theory of Casimir and du Pre is based upon the thermodynamics of two coupled systems, the magnetic spin system and the lattice vibration system. **CduP, Physica V, 507 (1938)**

The heat content of the spin system changes according to the equation

$$dq = dU - Hd\sigma = -\alpha\Theta dt,$$

where U is the internal energy of the spin system. With the assumption of adiabatic conditions for the paramagnetic compound as a whole, the resulting change of the spin system temperature $dT = d\Theta + \alpha\Theta L^{-1}dt$. Application of the fundamental thermodynamic relations of magnetization[10] (T and H independent variables) gives the solution for the above field suddenly applied:

$$\Theta = \Theta_0 e^{-t/\tau} - T_S\left(\frac{\partial\sigma}{\partial T}\right)_H \frac{he^{i\omega t}}{C_H} \frac{i\omega\tau}{1+i\omega\tau},$$

where the relaxation time $\tau = C_H/\alpha(1+C_H L^{-1})$. The first term of this equation represents a transient temperature change due to the sudden application of H_0, causing the spin temperature to increase isentropically[11] by an amount Θ_0. The second term is the steady-state condition, and shows the frequency dispersion.

Read and search the content and references in Starr's paper, especially the selection on the left. Decide what the relative contributions of lattice and spin fluctuations are to thermodynamic equilibrium temperatures such as the Debye and Neel constant values in the presence (and absence) of an applied external magnetic field. And then, how do we incorporate all this into the creation of a new general BCS pairing **formalism** to replace/augment the current Migdal-Eliashberg-Allen-Dynes-Bardeen algorithims for fermion-boson-fermion coupling, with relevant adjustment/replacement of lamba and mu*star?

So What's Needed Next?

A DFT + U package (Elk? Quantum-Espresso? VASP?) that will allow the simultaneous calculation of electron-phonon interactions as well as spin-spin excitations, and thus enable an estimation of the Casimir/du Pre coupling…and maybe...MAYBE... a combined phonon-spin pairing λ plus $\mu*$ calculation tool?

What a Great PhD Thesis Project!

I. Thoroughly review the 1941 Starr paper and all its references.

II. Configure an appropriate PSD setup with a cryogenic sample chamber between 10 T dipoles.

III. Check out a few of the Starr measurements on paramagnetic compounds of Fe, Mn and/or Cr.

IV. Then grind up some Y-123 (with various oxgyen levels), and measure...if results mimic Chauncey 1941...

V. Derive an alternative to McMillan-Eliashberg fermion-fermion coupling which contains spins as well as phonons, and apply. If it "works," then...

VI. Buy a new suit...or dress...for your upcoming trip to Stockholm!

“You can’t always get what you want…”

“…you get what you need!”