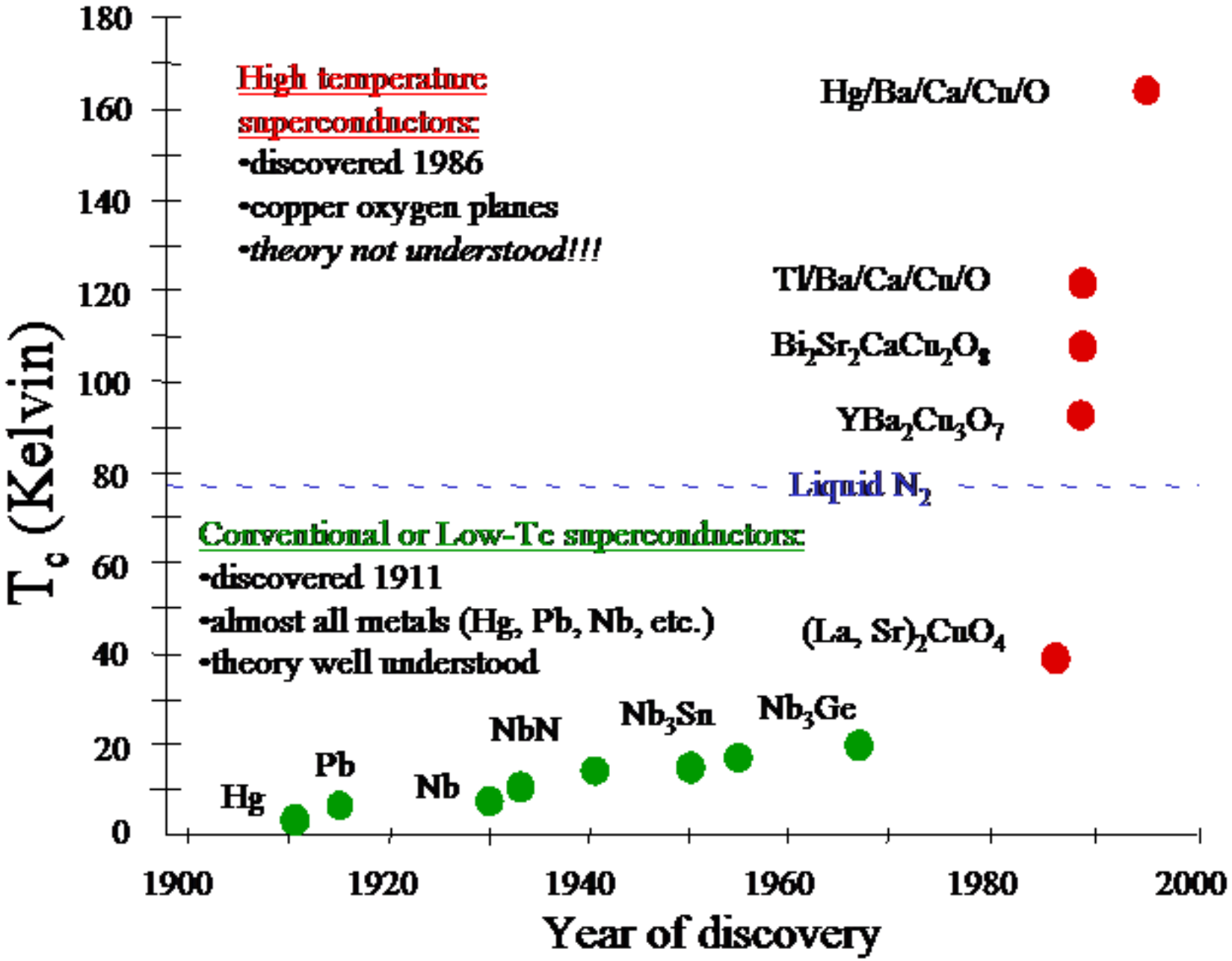
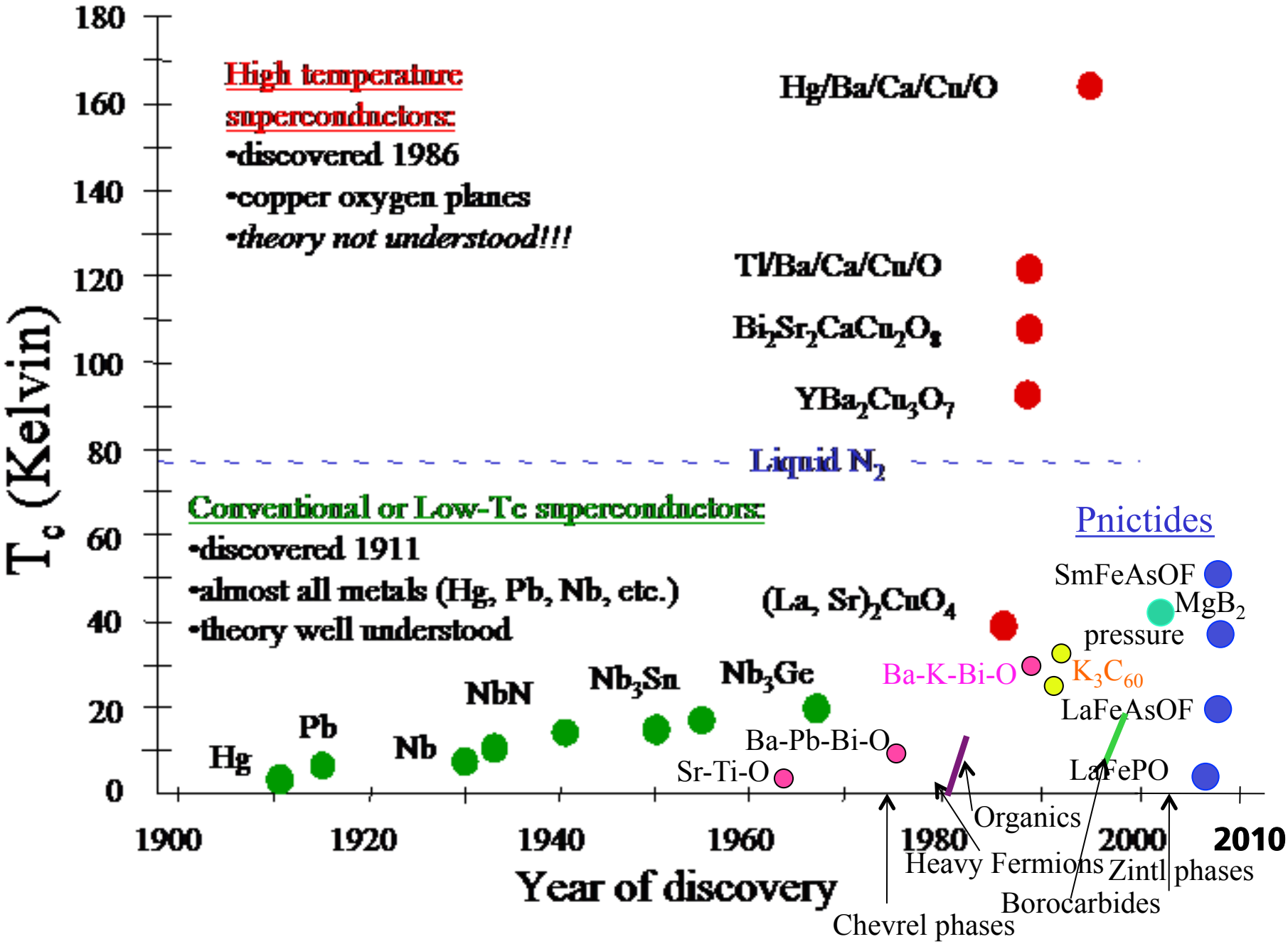
The Dynamic Hubbard Model: studies with DMFT and exact diagonalization

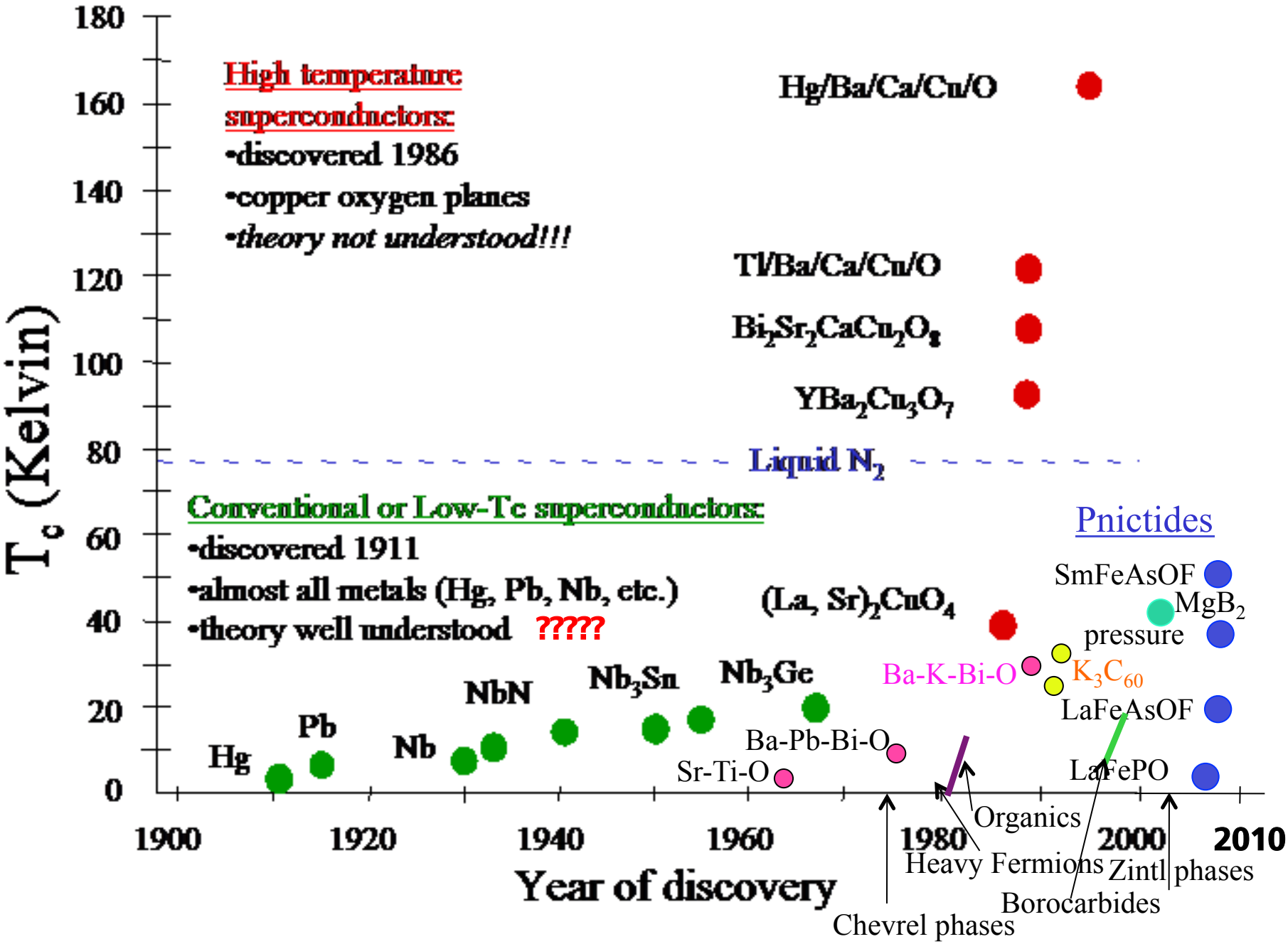
Frank Marsiglio
University of Alberta, Edmonton

20th Mardi Gras Conference
Petascale Many Body Methods for Complex Correlated Systems
Feb. 12-14 2015 Baton Rouge



http://spot.colorado.edu/~dessau/HighTc.shtml


High temperature superconductors:
•discovered 1986
•copper oxygen planes
•theory not understood!!!
Hg/Ba/Ca/Cu/O
Tl/Ba/Ca/Cu/O
$Bi_2Sr_2CaCu_2O_8$
$YBa_2Cu_3O_7$
Liquid N_2
Conventional or Low-Tc superconductors:
•discovered 1911
•almost all metals (Hg, Pb, Nb, etc.)
•theory well understood
Pnictides
$(La, Sr)_2CuO_4$
SmFeAsOF
MgB_2
pressure
Ba-K-Bi-O
K_3C_{60}
LaFeAsOF
Ba-Pb-Bi-O
Sr-Ti-O
LaFePO
Hg
Pb
Nb
NbN
Nb_3Sn
Nb_3Ge
T_c (Kelvin)
180
160
140
120
100
80
60
40
20
0
1900
1920
1940
1960
1980
2000
2010
Year of discovery
Organics
Heavy Fermions
Zintl phases
Borocarbides
Chevrel phases


High temperature superconductors:
•discovered 1986
•copper oxygen planes
•theory not understood!!!
Hg/Ba/Ca/Cu/O
Tl/Ba/Ca/Cu/O
$Bi_2Sr_2CaCu_2O_8$
$YBa_2Cu_3O_7$
Liquid N_2
Conventional or Low-Tc superconductors:
•discovered 1911
•almost all metals (Hg, Pb, Nb, etc.)
•theory well understood ????
Pnictides
SmFeAsOF
MgB_2
pressure
$(La, Sr)_2CuO_4$
Ba-K-Bi-O
K_3C_{60}
LaFeAsOF
Nb_3Ge
Nb_3Sn
NbN
Pb
Hg
Nb
Ba-Pb-Bi-O
Sr-Ti-O
LaFePO
Organics
Heavy Fermions
Zintl phases
Borocarbides
Chevrel phases
T_c (Kelvin)
Year of discovery
0
20
40
60
80
100
120
140
160
180
1900
1920
1940
1960
1980
2000
2010

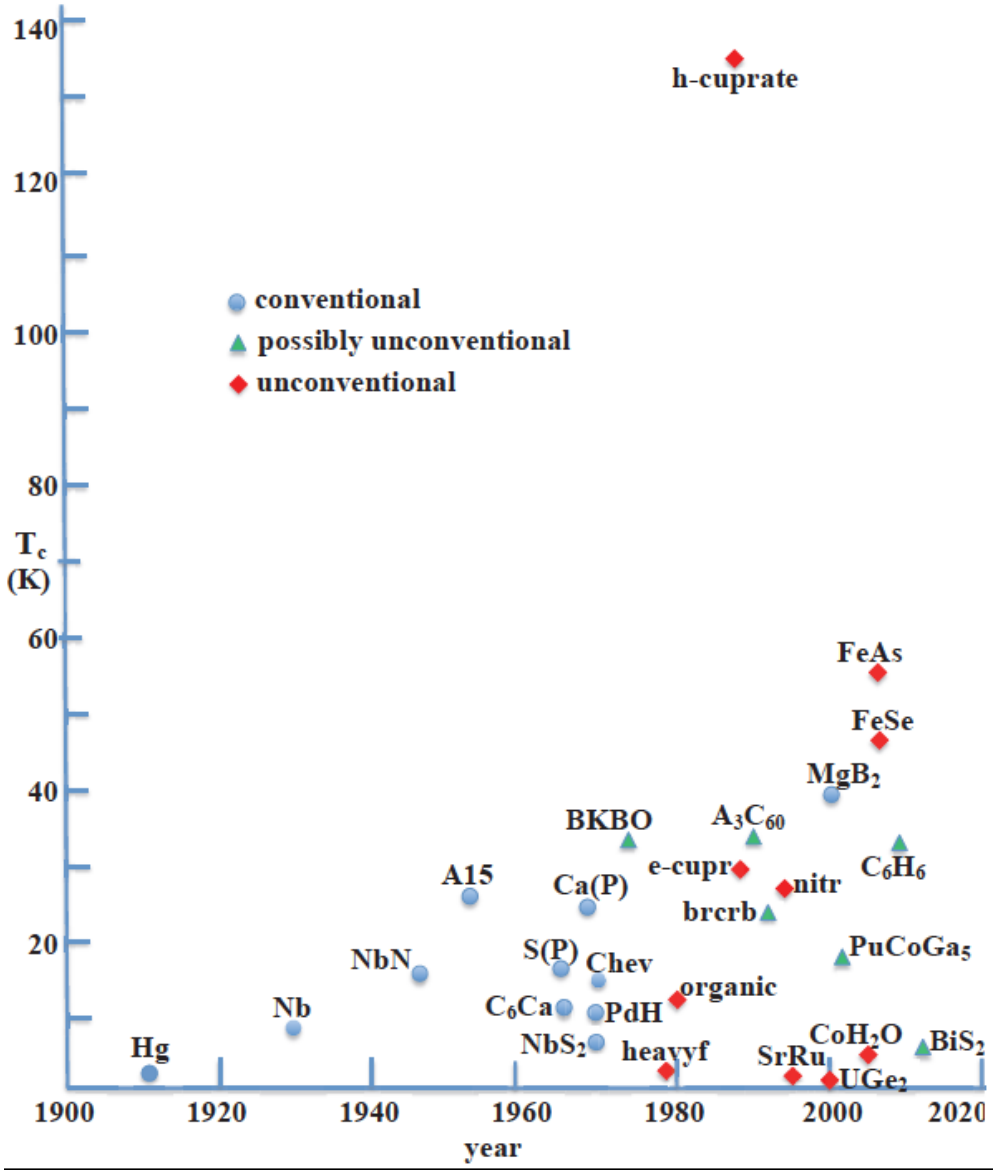
Physica C Special Issue on Superconducting Materials
Dedicated to Theodore H. Geballe on the year of his 95th birthday
Edited by J.E. Hirsch, M.B. Maple, and F. Marsiglio

Table of Contents

Physica C Special Issue on Superconducting Materials

Dedicated to Theodore H. Geballe on the year of his 95th birthday

Edited by J.E. Hirsch, M.B. Maple, and F. Marsiglio



What this talk is about

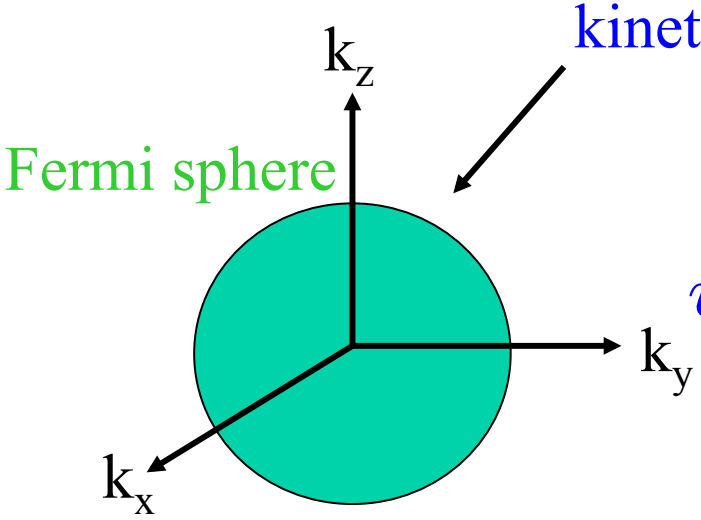
1) A `lightening-quick' overview of Eliashberg Theory, as I would teach in a graduate course, for example.

2) Is there more, at least for the cuprates, for example?

3) The Dynamic Hubbard model --- is there more to Coulomb repulsions than μ^* ?
   - (i) conceptual look
   - (ii) DMFT solution
   - (iii) 2-site model
   - (iv) relation to high-Tc experiments (optics)

The conventional scenario: BCS

Electrons in solids

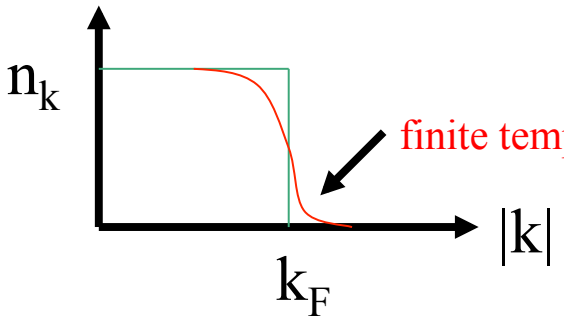


J. Bardeen L.N. Cooper J.R. Schrieffer

$$\psi_{BCS} = \prod_k (u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow})|0\rangle$$

all k's !! --- occupation is controlled by u_k and v_k.

order parameter (Δ_k) becomes non-zero, so, e.g.



$$v_k^2 = \frac{1}{2}(1 - \frac{\epsilon_k}{E_k}) \quad \text{where} \quad E_k = \sqrt{\epsilon_k^2 + \Delta_k^2}$$

$$\sim 1 \quad \text{for} \quad \epsilon_k < 0$$

$$\sim 0 \quad \text{for} \quad \epsilon_k > 0$$

$E_{kin} = 2\ \Sigma \varepsilon_k n_k$

It's all about pairs…

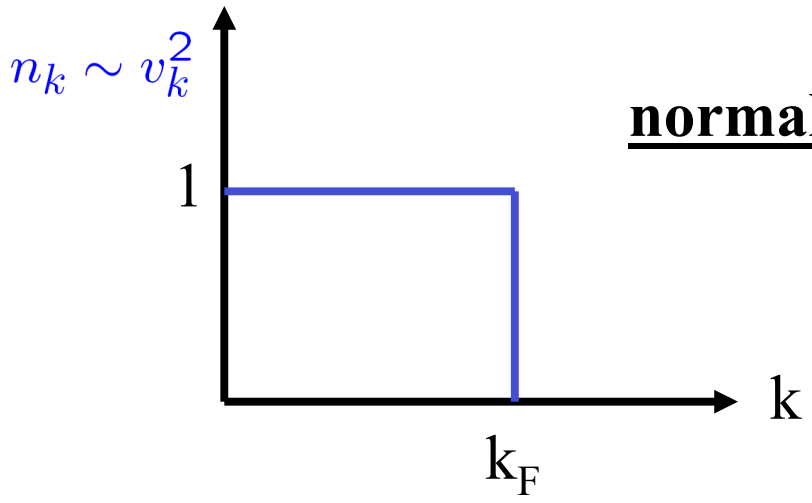
In Ogg's theory it was his intent
That the current keep flowing, once sent;
So to save himself trouble,
He put them in double,
And instead of stopping, it went.

George Gamow

Bose-Einstein Condensation of Trapped Electron Pairs. Phase Separation and Superconductivity of Metal-Ammonia Solutions

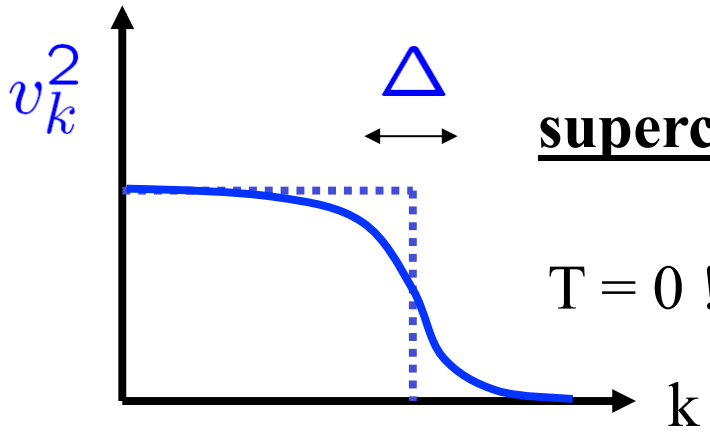
RICHARD A. OGG, JR.
Department of Chemistry, Stanford University, California
March 2, 1946

…Cooper pairs



normal state

why sacrifice kinetic energy ?



superconducting state

T = 0 !!

Ans: **gain potential energy**

remember, $v_k^2 = \frac{1}{2}(1 - \frac{\epsilon_k}{\sqrt{\epsilon_k^2 + \Delta_k^2}})$

BCS formalism vs. Pairing Mechanism

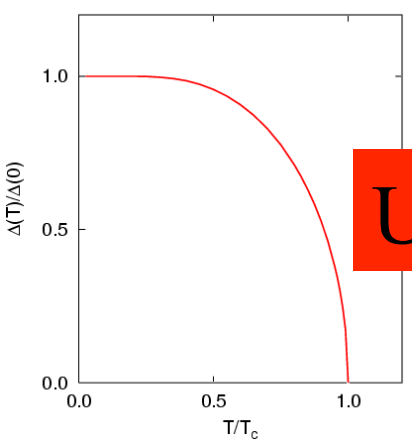
$$\Delta = |V| \frac{1}{N} \sum_k \frac{\Delta}{2E_k}$$

Tc equation (useless)

$$\frac{2\Delta}{k_B T_c} = 3.53$$

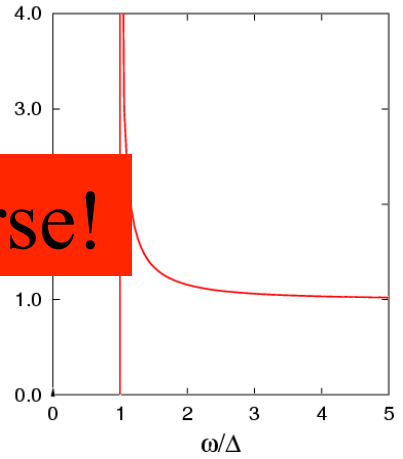
Universality

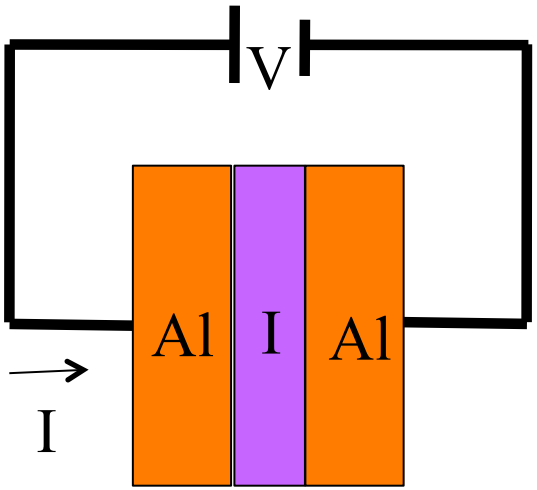
$$\frac{\Delta C}{\gamma T_c} = 1.43$$

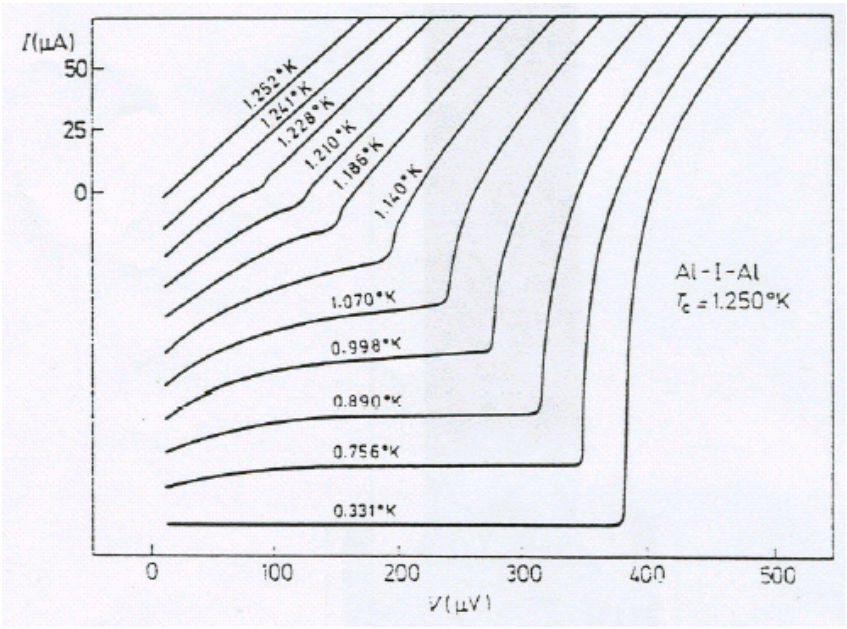


Universality is wonderful

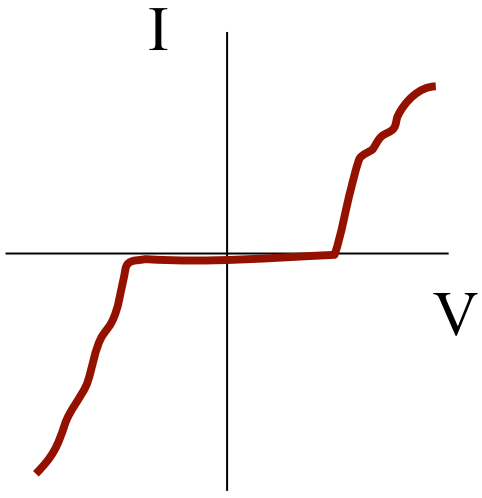
Universality is a curse!



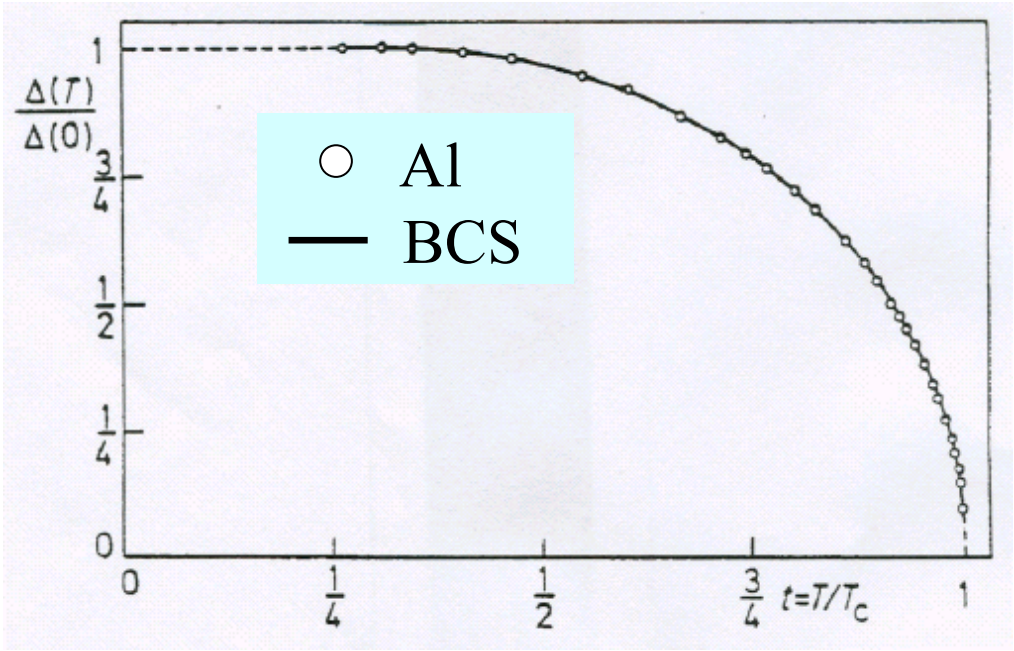




B.L. Blackford and R.H. March, Can. J. Phys. 46, 141 (1968)



$$\frac{dI}{dV} \propto N(V)$$



Eliashberg Theory

- Extension of BCS formalism to include

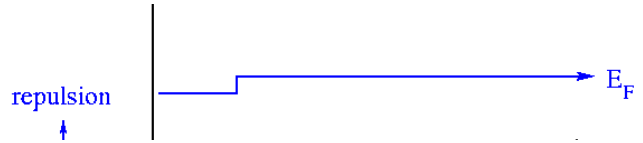
S-STATE INSTABILITIES FOR RETARDED INTERACTIONS†

C. S. OWEN‡ and D. J. SCALAPINO§

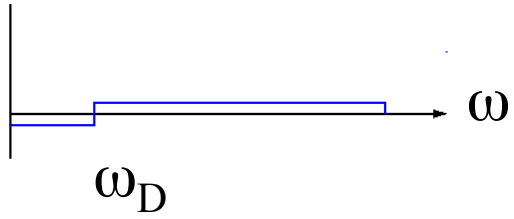
Physics Dept., University of Pennsylvania, Philadelphia, Pa., USA

- loc

Physica 55, 691 (1971)



$$\Delta(i\omega_n)Z(i\omega_n) = \pi T \sum_m \left[\lambda(i\omega_n - i\omega_m) - \mu^*\right] \frac{\Delta(i\omega_m)}{\sqrt{\omega_m^2 + \Delta^2(i\omega_m)}}$$



G. M. Eliashberg
Started graduate school in 1959
Wrote Eliashberg Theory paper in 1960
Graduated in 1963!

Eliashberg Theory

$$\Delta(k,\omega) = \mathcal{F}[V_{k,k'}(\omega,\omega')]$$

$$\downarrow$$

A functional of the interaction

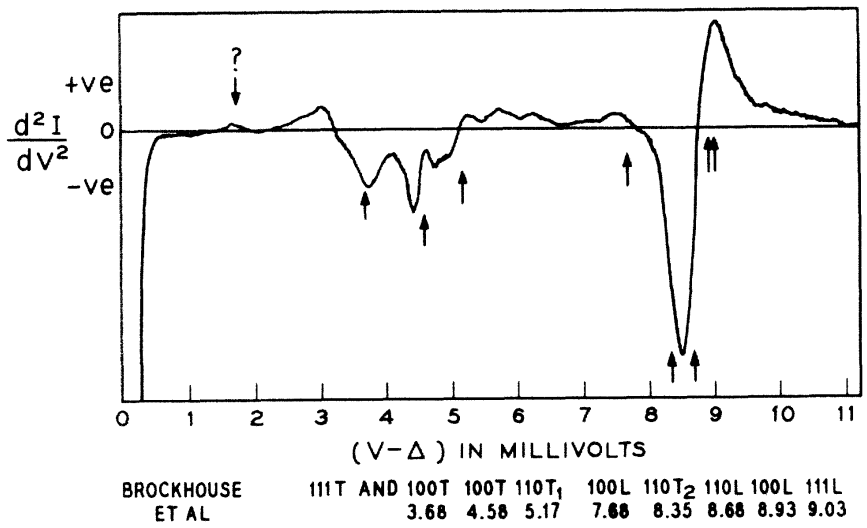
Question: Can we invert the theory to extract the potential uniquely from a knowledge of $\Delta(k,\omega)$?

G.
Sta
Wi
Gr

Answer is Yes!

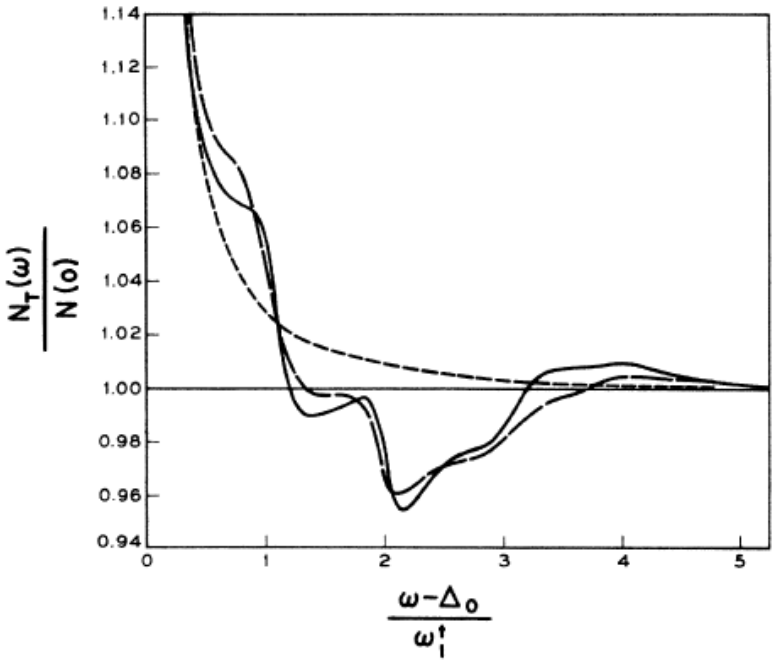
IMAGE OF THE PHONON SPECTRUM IN THE TUNNELING CHARACTERISTIC BETWEEN SUPERCONDUCTORS

J. M. Rowell, P. W. Anderson, and D. E. Thomas
Bell Telephone Laboratories, Murray Hill, New Jersey
(Received 14 March 1963)



EFFECTIVE TUNNELING DENSITY OF STATES IN SUPERCONDUCTORS*

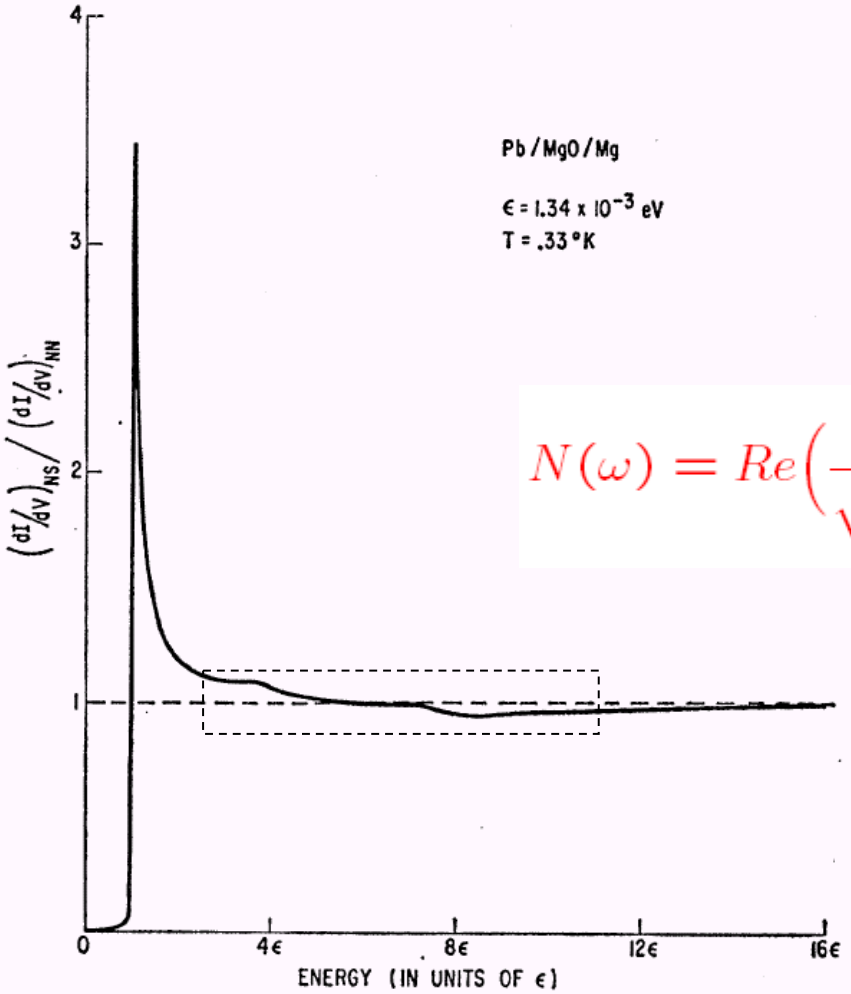
J. R. Schrieffer, D. J. Scalapino, and J. W. Wilkins
University of Pennsylvania, Philadelphia, Pennsylvania
(Received 15 March 1963)



Ivar Giaever

I. Giaever, H.R. Hart, Jr., and K. Megerle, PRB 126, 941 (1962)

$$\frac{dI}{dV} \sim N(\varepsilon)$$



$$N(\omega) = Re\left(\frac{\omega}{\sqrt{\omega^2 - \Delta^2(\omega)}}\right)$$

FIG. 10. The relative conductance of a Pb-MgO-Mg sandwich plotted against energy. At higher energies there are definite divergences from the BCS density of states as can be seen from the bumps in the experimental curve. Note that the crossover point corresponds in energy to the Debye temperature.

McMillan and Rowell, Superconductivity, ed. By R.D. Parks (1969)

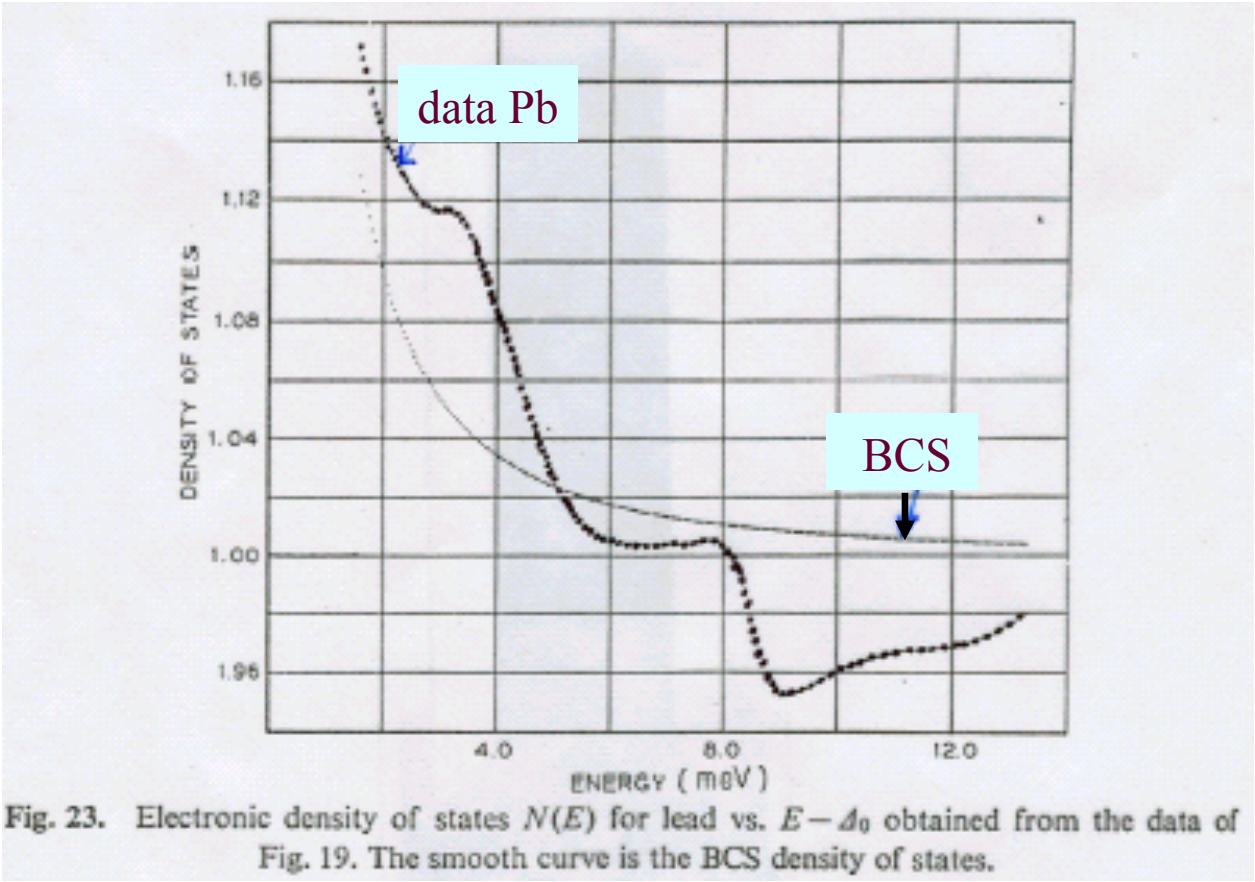


Fig. 23. Electronic density of states $N(E)$ for lead vs. $E-\Delta_0$ obtained from the data of Fig. 19. The smooth curve is the BCS density of states.

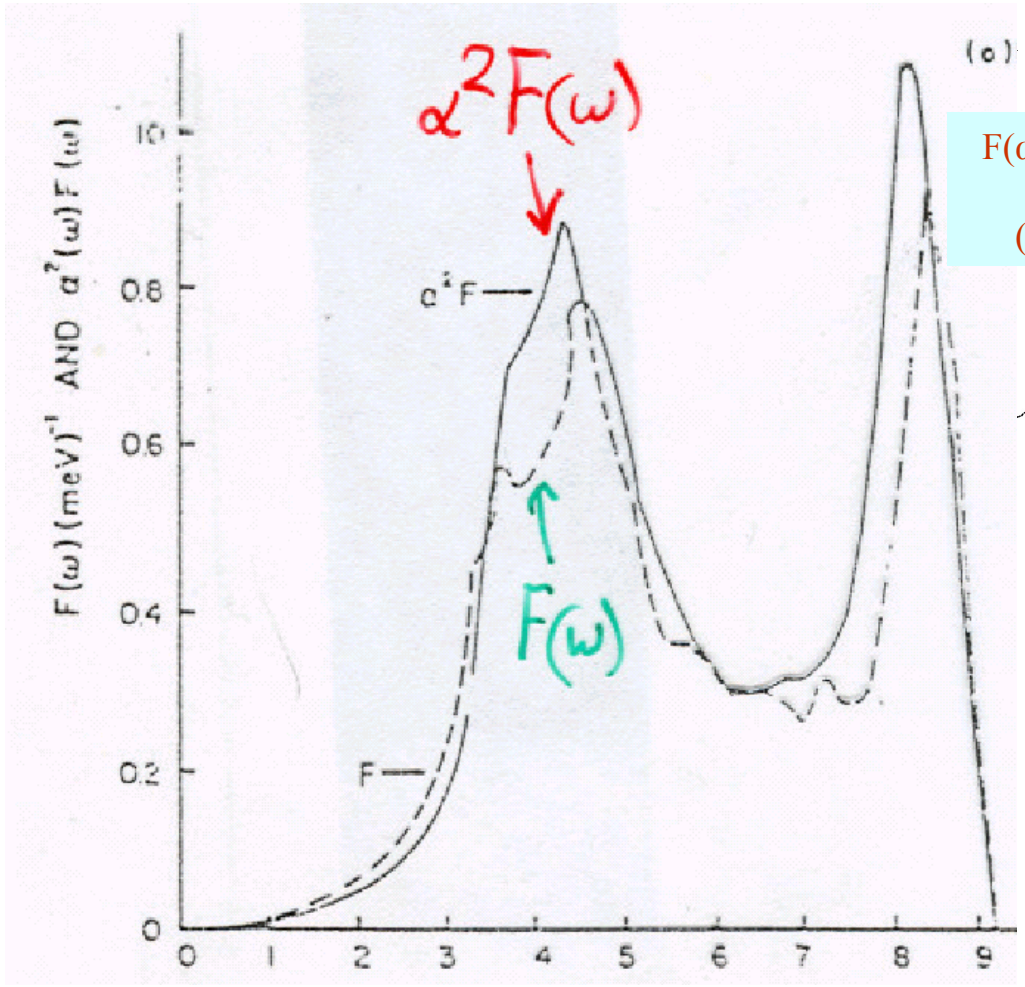
requires Eliashberg theory:

- phonon dynamics (retardation) taken into account $\alpha^2F(\Omega)$

$$\Delta(\omega) = \mathcal{F}[(\alpha^2F(\omega)), \mu^*]$$

  - gap is a function of frequency

  - density of states is modified: $\frac{dI}{dV} \propto N(\omega) = N(\epsilon_F)\mathrm{Re}\left(\frac{\omega}{\sqrt{\omega^2-\Delta^2(\omega)}}\right)$



F(ω): density of phonon states from neutron scattering (Brockhouse at Chalk River)

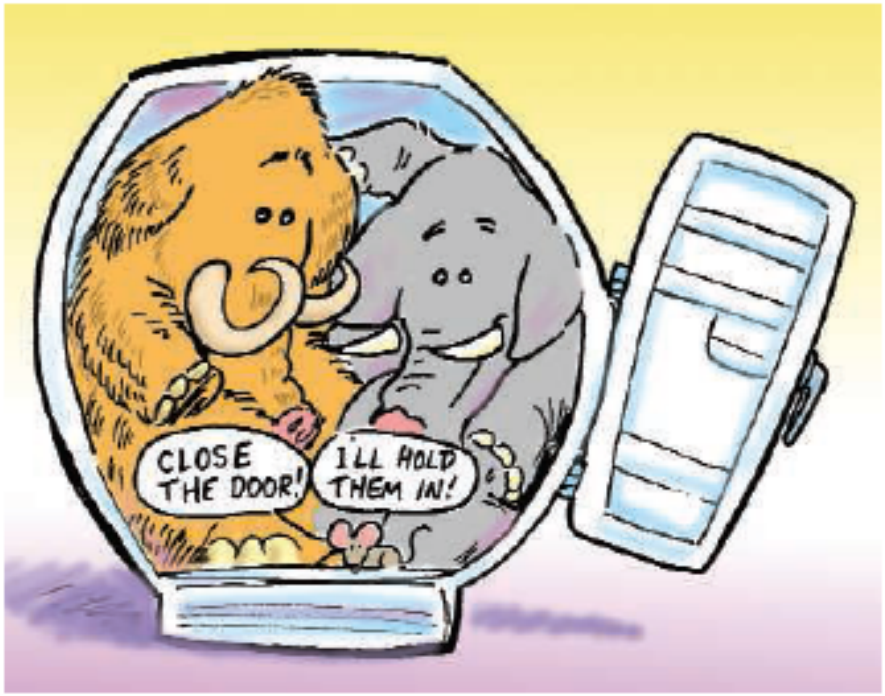
$$\alpha^2(\omega) \equiv \frac{\alpha^2 F(\omega)}{F(\omega)} \sim \text{constant}$$

4 Electron–Phonon Superconductivity

F. Marsiglio University of Alberta, Dept. of Physics, Edmonton, Canada
and
J.P. Carbotte McMaster University, Physics Dept. Hamilton, Canada

So what's wrong?

1) How did $\mu = UN(E_F)$ get reduced to μ^*?

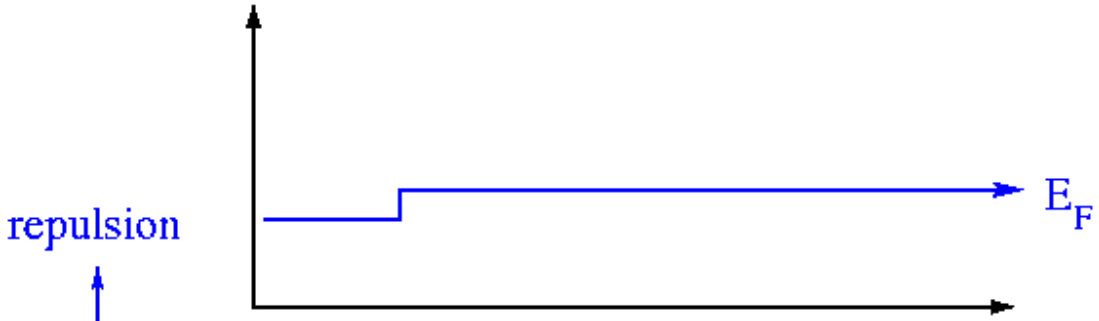


"We have a mammoth and an elephant in our refrigerator—do we care much if there is also a mouse?"

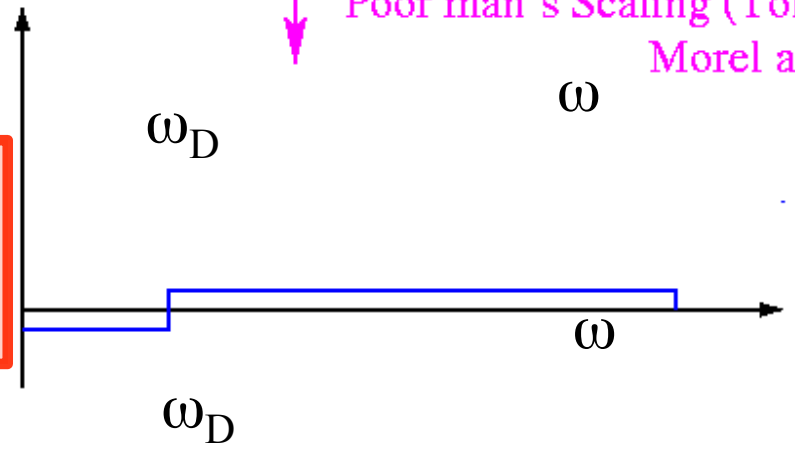
Phil Anderson

Is There Glue in Cuprate Superconductors?
Philip W. Anderson
Science **316**, 1705 (2007);

Eliashberg Theory



Poor man's Scaling (Tolmachev et al., Morel and Anderson)



But…
Never seen in QMC simulations
Many other ways for U to be Reduced

IOP FTC

IOP PUBLISHING

JOURNAL OF PHYSICS: CONDENSED MATTER

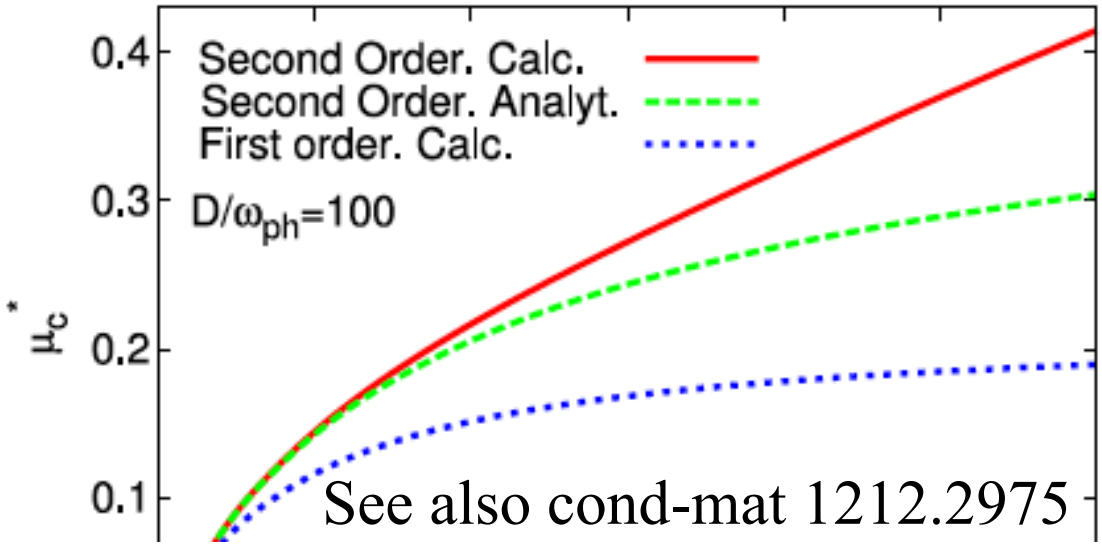
J. Phys.: Condens. Matter **24** (2012) 492202 (5pp)

doi:10.1088/0953-8984/24/49/492202

FAST TRACK COMMUNICATION

The theory of electron–phonon superconductivity: does retardation really lead to a small Coulomb pseudopotential?

Johannes Bau



See also cond-mat 1212.2975

Retardation effects and the Coulomb pseudopotential in the theory of superconductivity

Phys. Rev. B **87, 054507 (2013)**

Johannes Bauer,[1,2] Jong E. Han,[1,3] and Olle Gunnarsson[1]

www.usatoday.com

USA TODAY

Sports

SECTION C

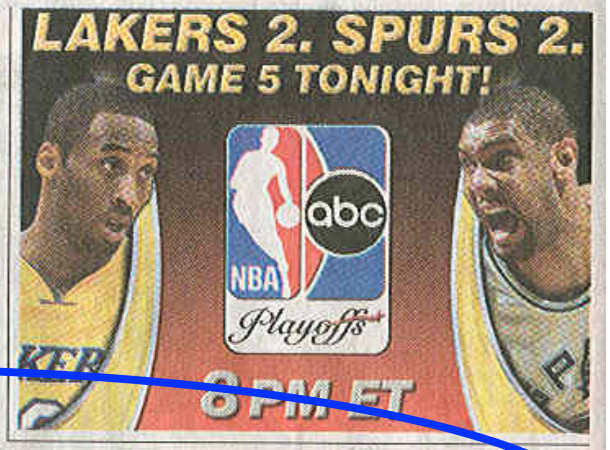
Thursday, May 13, 2004

By Joseph Kaczmarek, AP

Big number: Little Matth Man, led by groom [illegible] the longest of the long shots at 50-1. The draw and odds, 3C

Latest on Preakness

Derby winner Smarty Jones is the favorite, The Cliff's Edge might not run and Imperialism almost didn't come. Preakness news: In focus, 3C



Sportsline

Baseball/American League — Coverage, 3-4C

Kansas City 4, Toronto 3	Cleveland 6, Boston 4
Texas 9, Tampa Bay 8	Oakland 2, Detroit 1
Baltimore at Chicago (ppd.)	Anaheim 11, New York 2
Minnesota 4, Seattle 3	

National League — Coverage, 3, 6C

Pittsburgh at Colorado (ppd.)	St. Louis 5, Atlanta 2
Milwaukee 4, Montreal 3	Florida 5, Houston 2
New York at Arizona	Cincinnati at San Diego
Chicago at Los Angeles	Philadelphia at San Francisco

Basketball/NBA playoffs — Coverage, 10C

Miami 100, Indiana 88	Minnesota at Sacramento

'Boss' buys tickets for military personnel

New York Yankees owner George Steinbrenner purchased 350 tickets for tonight's Game 2 of the NHL's Eastern Conference final between the Philadelphia Flyers and Tampa Bay Lightning for military personnel stationed at MacDill Air Force Base in Tampa. He also donated them to some of the families of servicemen and servicewomen fighting the war in Iraq. Steinbrenner also had donated more than 700 tickets for Game 2 of Tampa Bay's semifinals matchup against the Montreal Canadiens on April 25. Steinbrenner, [illegible]

Reuters

BCS formula up for tweaking

Stoops wants votes made public

By Steve Wieberg
USA TODAY

Architects of the Bowl Championship Series are close to drawing up a simpler and, they say, more fail-safe formula for selecting two teams to play for college football's national title.

The revisions won't be announced until next month. But Big East Conference Commissioner and outgoing BCS coordinator Mike Tranghese said Wednesday that they'll likely streamline a convoluted mathematical formula, essentially giving one-third weight to the Associated Press media poll, one-third to the USA TODAY/ESPN Coaches Poll and a final one-third to a computer rating.

It no longer would include a separate strength-of-schedule rating, an escalating penalty for losses and probably bonuses for "quality" wins. A final determination is awaiting analysis by outside mathematicians.

The modifications, [illegible] should avert a repeat of [illegible] messy split-championship outcome which saw Southern California ranked No. 1 in the voting polls but left out of the BCS' championship game because of lower computer and strength-of-schedule ratings.

"If you can't make it public, then you'd better throw the coaches' poll out," he said. "There needs to be more accountability. If there's not, then that the potential for offending opponents.

Stoops wan

By Steve Wieberg
USA TODAY

Architects of the Bowl Cha
Series are close to drawing up
and, they say, more fail-safe f

What is important, what can we 'throw out' ?

Copper-Oxygen Planes

http://www.cnms.ornl.gov/images/gordon-bell-1.gif

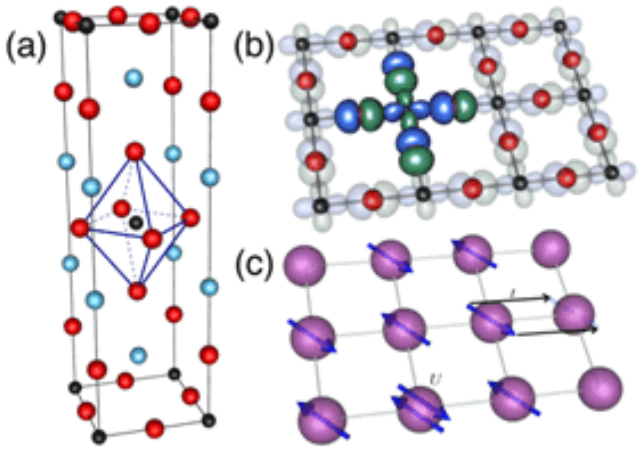
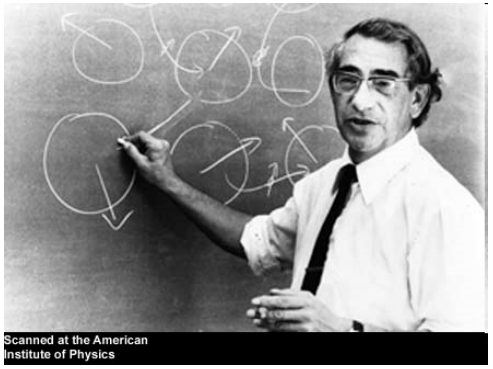


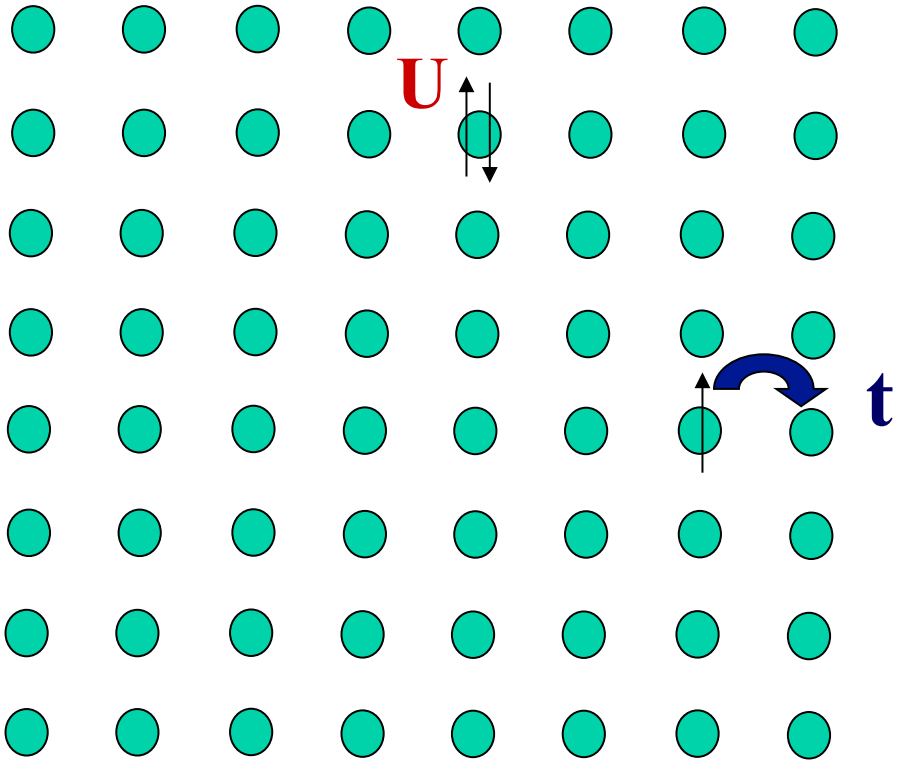
Fig. 1: (a) The crystal structure of La2CuO4, a typical cuprate, where black, red, and blue sphere represent Cu, O, and La, respectively. (b) The CuO2 plane with outlines of the Cu dx2-y2 and O px and py orbitals. Also shown in full color is the Zhang-Rice singlet state that forms from hybridization of the Cu orbitals with the neighboring O orbitals. (c) Pictorial representation of the single band 2D Hubbard model with on-site Coulomb repulsion U and inter-site hopping t.

High T_c Cuprates: a Case Study

The (single band) Hubbard model

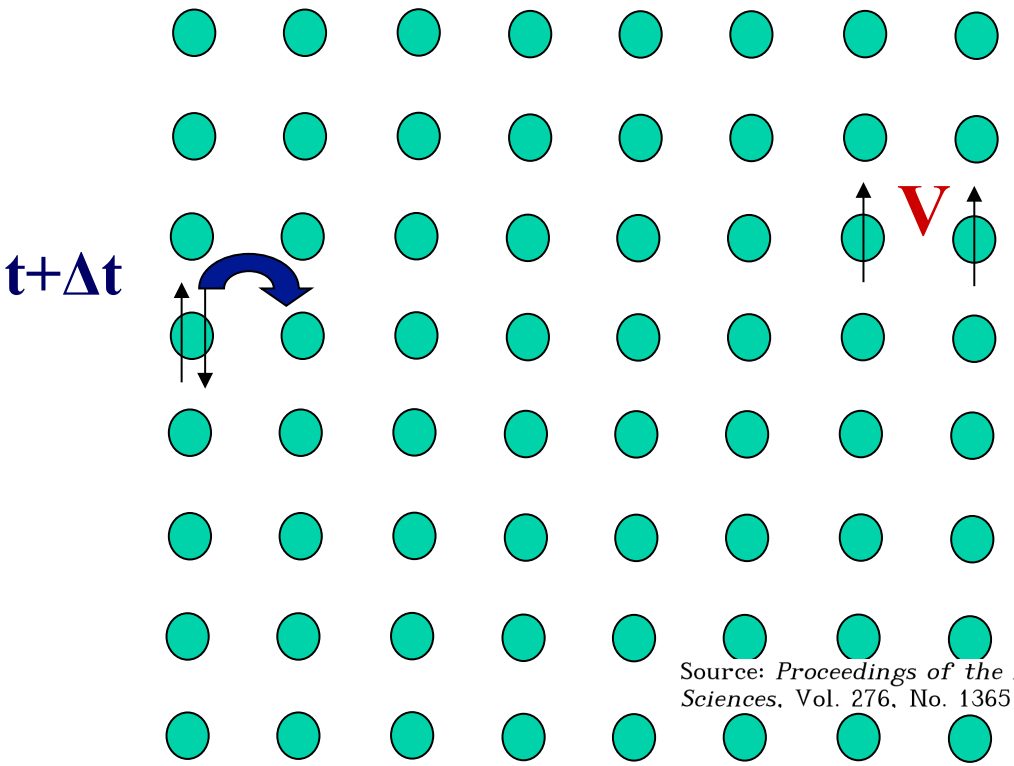


J. Hubbard



$$H = -t \sum_{\langle ij \rangle, \sigma} (\hat{c}^{\dagger}_{i\sigma} \hat{c}_{j\sigma} + \hat{c}^{\dagger}_{j\sigma} \hat{c}_{i\sigma}) + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

Does it have the 'right stuff' (Doug Scalapino)?



Doug Scalapino

Nearest neighbour interactions

$$(ij|\ 1/r\ |ij) \sim \frac{2e^{-\kappa|\mathbf{R}_i-\mathbf{R}_j|}}{|\mathbf{R}_i-\mathbf{R}_j|}\ \mathrm{Ry}\ (6\ \mathrm{eV})$$

Electron correlations in narrow energy bands

By J. Hubbard

Theoretical Physics Division, A.E.R.E., Harwell, Didcot, Berks

(*Communicated by B. H. Flowers, F.R.S.—Received* 23 *April* 1963)

Source: *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, Vol. 276, No. 1365 (Nov. 26, 1963), pp. 238-257

$$(ii|\ 1/r\ |ij) \sim q\,\mathrm{Ry} \sim \tfrac{1}{2}\mathrm{eV},$$
$$(ij|\ 1/r\ |ik) \sim \tfrac{1}{4}q\,\mathrm{Ry} \sim \tfrac{1}{10}\mathrm{eV},$$
$$(ii|\ 1/r\ |jj) \sim (ij|\ 1/r\ |ji) \sim q^2\,\mathrm{Ry} \sim \tfrac{1}{40}\mathrm{eV},$$

Modulated hopping Δt
3-site hopping (t-J model)
Exchange term J

phonons, oxygen (or other) orbitals, longer range hopping, polarons, lunar effects, etc.

Or have we missed a key ingredient all along?

VOLUME 87, NUMBER 20 PHYSICAL REVIEW LETTERS 12 NOVEMBER 2001

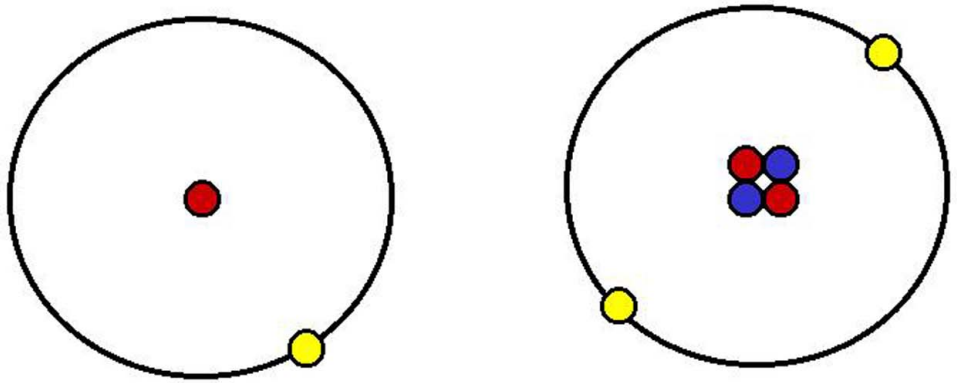
Dynamic Hubbard Model

J. E. Hirsch
Department of Physics, University of California–San Diego, La Jolla, California 92093-0319
(Received 24 July 2001; published 26 October 2001)

…a parable involving the lowly Helium atom…

atoms

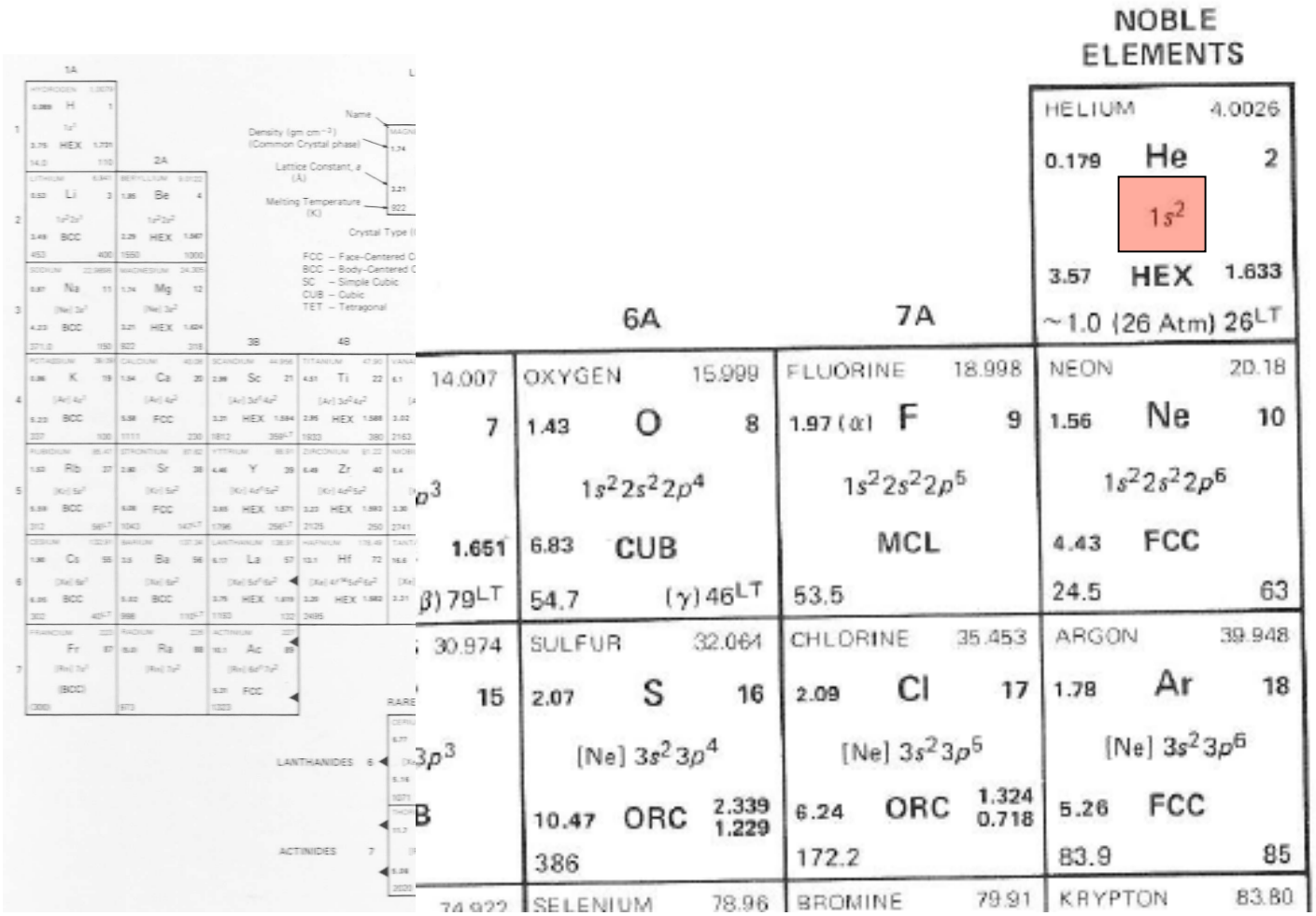
hydrogen **helium**

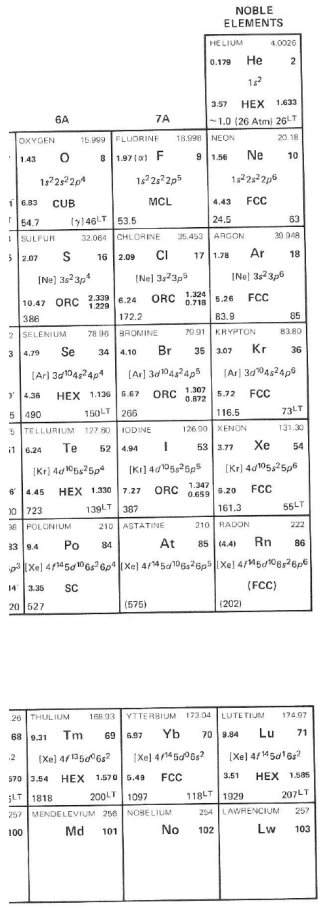


proton (+) **neutron** **electron (-)**

Neutrons and protons are held together in the nucleus by the "strong" force, which has to overcome the electrical repulsion of the two positively charged protons in helium (and in more complex atoms too). Electrons are held around the atom by the electrical attraction between their negative charge and the positive charge of the protons in the nucleus.

Ashcroft and Mermin, inside front cover





But the real 2-electron wave function is given by

$$|\psi\rangle = a_1|1s\ 1s\rangle + a_2|1s\ 2s\rangle + a_3|1s\ 3s\rangle + a_4|2s\ 2s\rangle + a_5|2p\ 2p\rangle + \ldots$$

May 4, 2006

Further Computations of the He Atom Ground State

Charles Schwartz *

Department of Physics, University of California
Berkeley, California 94720

Abstract

Recently reported computations have been extended to give ten more decimals of accuracy in the ground state energy of the Schrodinger equation for the idealized Helium atom. With the F basis - Hylleraas coordinates with negative powers and a logarithm of s - carried to the fiftieth order (N = 24,099 terms) we find the eigenvalue

E = -2.90372 43770 34119 59831 11592 45194 40444 66969 25309 ...

IOP Publishing
Eur. J. Phys. 34 (2013) 111–128

European Journal of Physics
doi:10.1088/0143-0807/34/1/111

The spectral decomposition of the helium atom two-electron configuration in terms of hydrogenic orbitals

Joel Hutchinson[1], Marc Baker[1] and Frank Marsiglio[1,2,3]

Joel

Marc

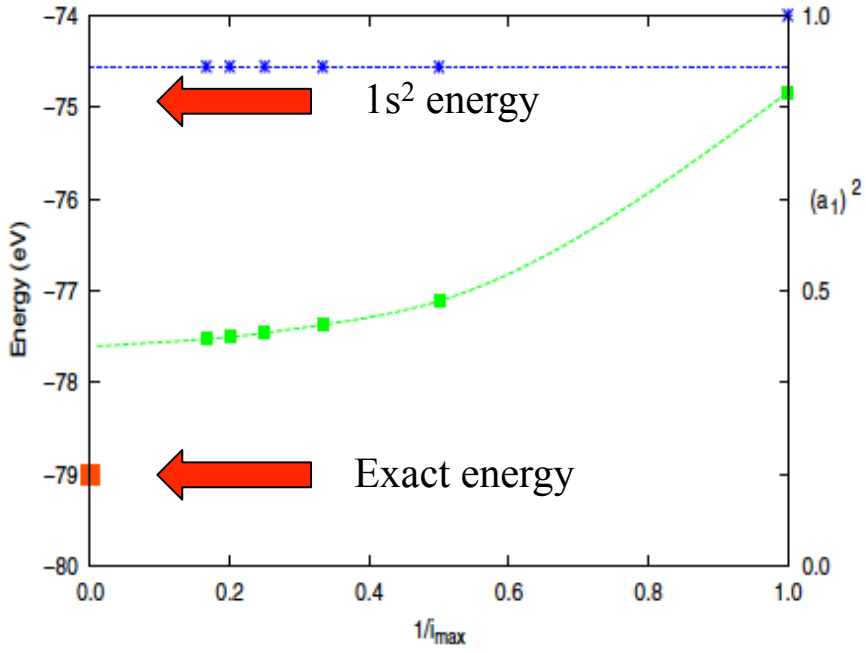


Table 1. Results for some overlaps, a_i.

i	Basis state	a_i	$\lvert a_i\rvert^2$	Total Probability
1	100 100	0.9624	0.9263	0.9263
2	100 200	−0.2148	0.0461	0.9725
3	100 300	−0.0752	0.0057	0.9781
4	100 400	−0.0427	0.0018	0.9799
5	100 500	−0.0289	0.0008	0.9807
6	100 600	−0.0213	0.0005	0.9812
7	100 700	−0.0166	0.0003	0.9815
8	21−1 211	0.0260	0.0007	0.9822
9	210 210	−0.0184	0.0003	0.9825
10	200 200	−0.0146	0.0002	0.9827
11	200 300	−0.0090	0.0001	0.9828
12	100 320	0	0	0.9828

Not 1.000 !

Why is this important?

$$U(Z) = \int d^3r\, d^3r'\, |\varphi_{1s}(r)|^2 \frac{e^2}{|r - r'|} |\varphi_{1s}(r')|^2$$

$$= \frac{5}{4} Z \times 13.606 \text{ eV},$$

$$\varphi_{1s}(r) = \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} e^{-Zr/a_0}$$

Experimental values:

$$U_{\text{eff}}(1) = I - A = 12.86 \text{ eV} = U(1) - 4.15 \text{ eV} \quad (2a)$$

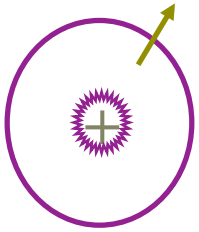
$$U_{\text{eff}}(2) = I_{II} - I_I = 29.92 \text{ eV} = U(2) - 4.10 \text{ eV}. \quad (2b)$$

4 eV ≈ 46 000 K !

J.E. Hirsch, PRL 87, 206402 (2001)

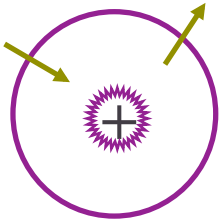
In essentially **all** the lattice models used to understand electron correlations in solids, the "playing field" is static (phonons are a different matter).

In He, when one electron is present, it occupies the 1s orbital:



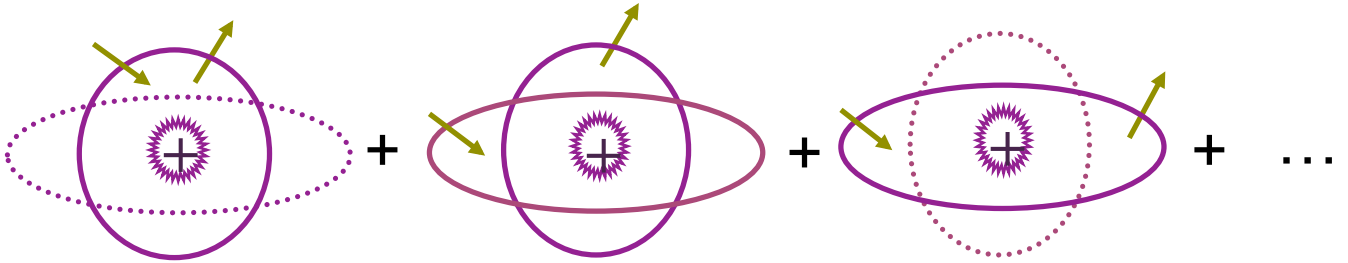
When two electrons are present, in Hubbard-like models they (doubly) occupy the 1s orbital:

- For Hubbard model:



$$\psi(\vec{r}_1,\vec{r}_2) = \Phi_{1s}(\vec{r}_1)\Phi_{1s}(\vec{r}_2)$$

- For real atom

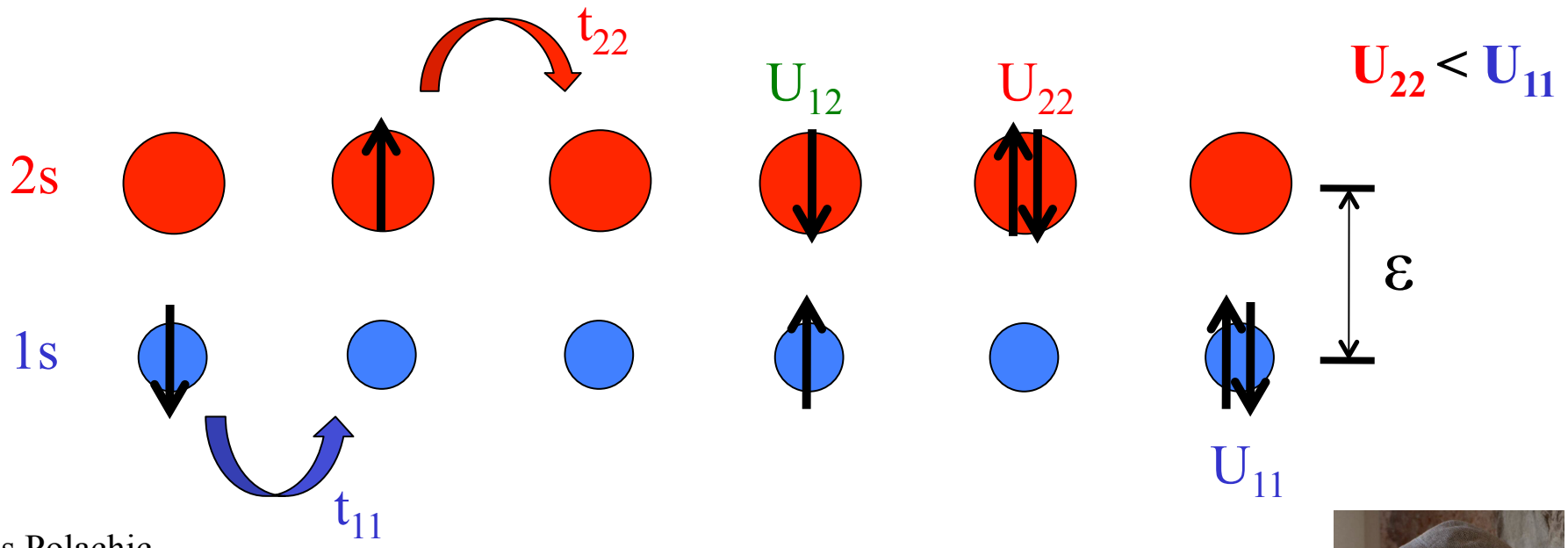


$$\psi(\vec{r}_1,\vec{r}_2) = \sum_{mn} c_{mn}\Phi_m(\vec{r}_1)\Phi_n(\vec{r}_2)$$

This is like what happens in general relativity; the presence of mass alters the underlying space-time structure.

This is like what happens in general relativity; the presence of mass alters the underlying space-time structure.

Here, the presence of a second electron alters the nature of the orbitals that model the conduction band.



Chris Polachic

Lindsay Forestell

Exact Diagonalizations (very small clusters!)

AND

Dynamical Mean Field Theory (DMFT)

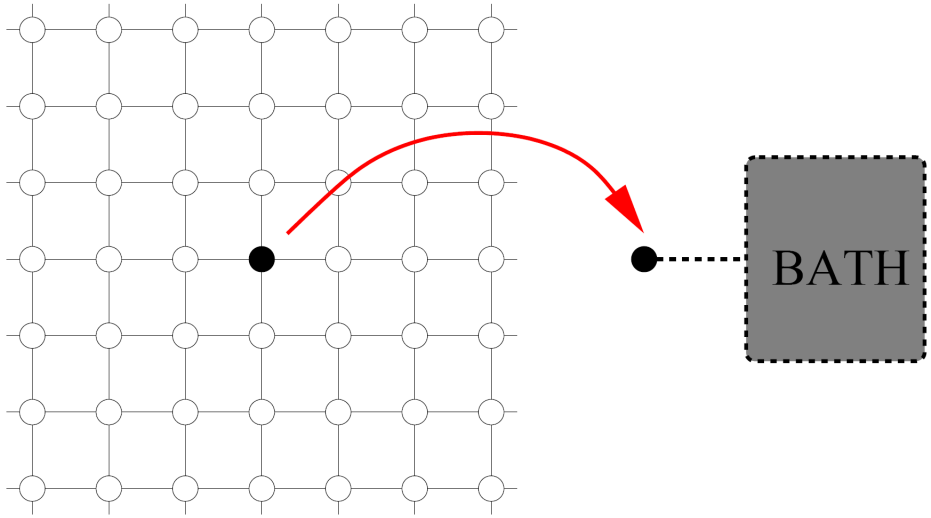
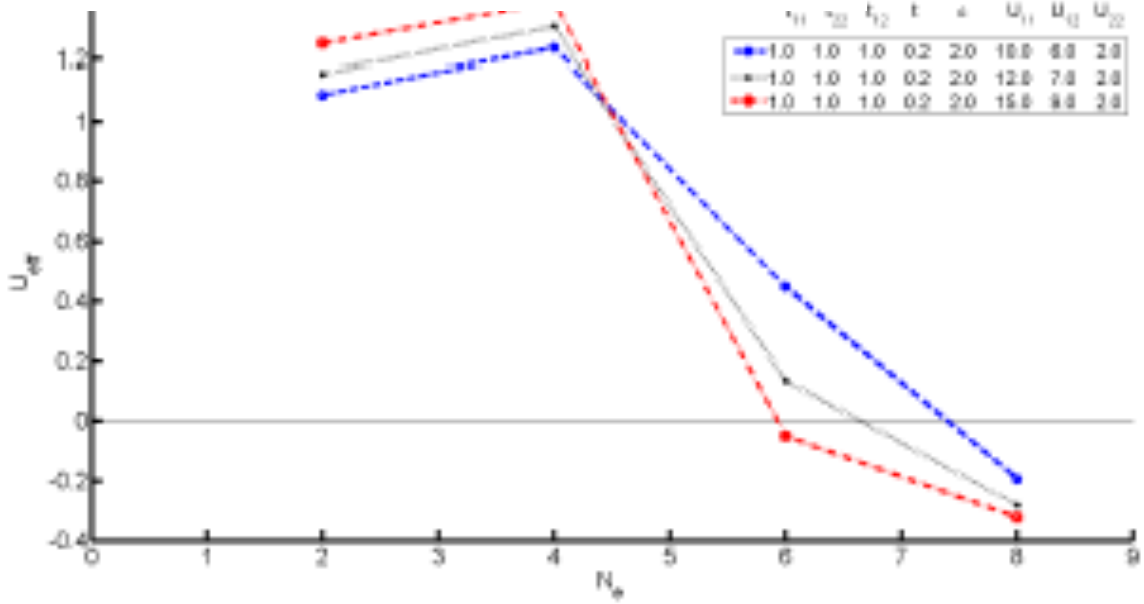
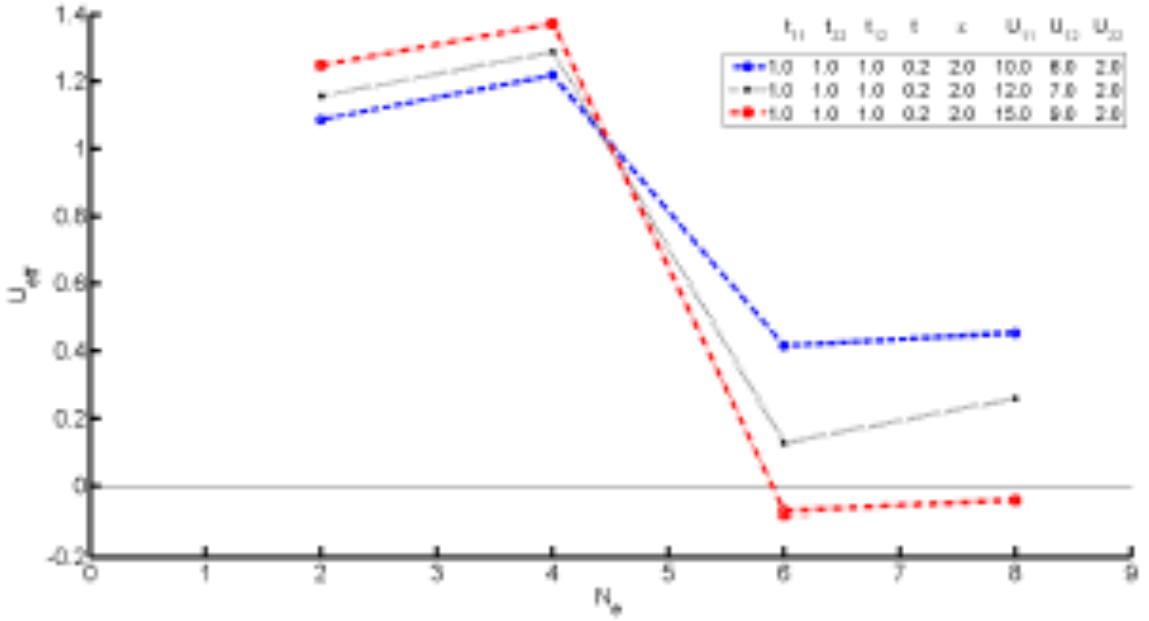


FIGURE 4. Mean-field theory replaces a lattice model by a single site coupled to a self-consistent bath.

Antoine Georges, arXiv:cond-mat/0403123

$$U_{eff} = E_0(N_e) + E_0(N_e - 2) - 2E_0(N_e - 1)$$





Lindsay Forestell

This is like what happens in general relativity; the presence of mass alters the underlying space-time structure.

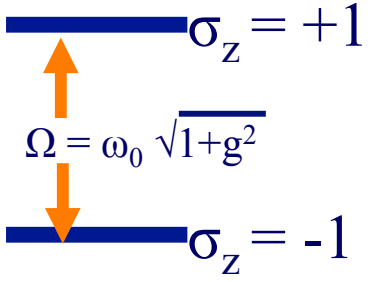
Here, the presence of a second electron alters the nature of the orbitals that model the conduction band.

A simple way to model this:

hopping term

$$H_{DHB} = -\sum_{<i,j>\sigma} t_{ij}\left(c^{+}_{i\sigma}c_{j\sigma} + c^{+}_{j\sigma}c_{i\sigma}\right) - \mu\sum_{i\sigma} n_{i\sigma} +$$

$$\sum_{i}\left(\omega_o\sigma_i^x + g\omega_o\sigma_i^z\right) + \sum_{i}\left(U - 2g\omega_o\sigma_i^z\right)n_{i\uparrow}n_{i\downarrow}$$



$t_e = t$ (electron in an empty lattice)

Th
a

$t_h = tS^2$ (electron in an almost full lattice)

where S = Franck-Condon factor.

Dynamic Hubbard Model

J.E. Hirsch, PRB 65, 184502 (2002)

$$H_{\mathrm{DHM}} = \sum_{<i,j>\sigma} t_{ij}(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}) - \mu\sum_{i,\sigma} n_{i\sigma}$$

$$+\sum_{i}(\omega_0\sigma^x_i + g\omega_0\sigma^z_i) + \sum_{i}(U - 2g\omega_0\sigma^z_i)n_{i\uparrow}n_{i\downarrow}$$

Parameter	
t	electron hopping
U	`bare' electron-electron repulsion
g	electron-pseudospin coupling strength
ω_0	energy (time) scale associated with pseudospin

How do we check this out? (i) effective model
(ii) exact diagonalizations
(iii) Dynamical Mean Field Theory

PHYSICAL REVIEW B 82, 155122 (2010)

Two-site dynamical mean field theory for the dynamic Hubbard model

G. H. Bach
Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2G7

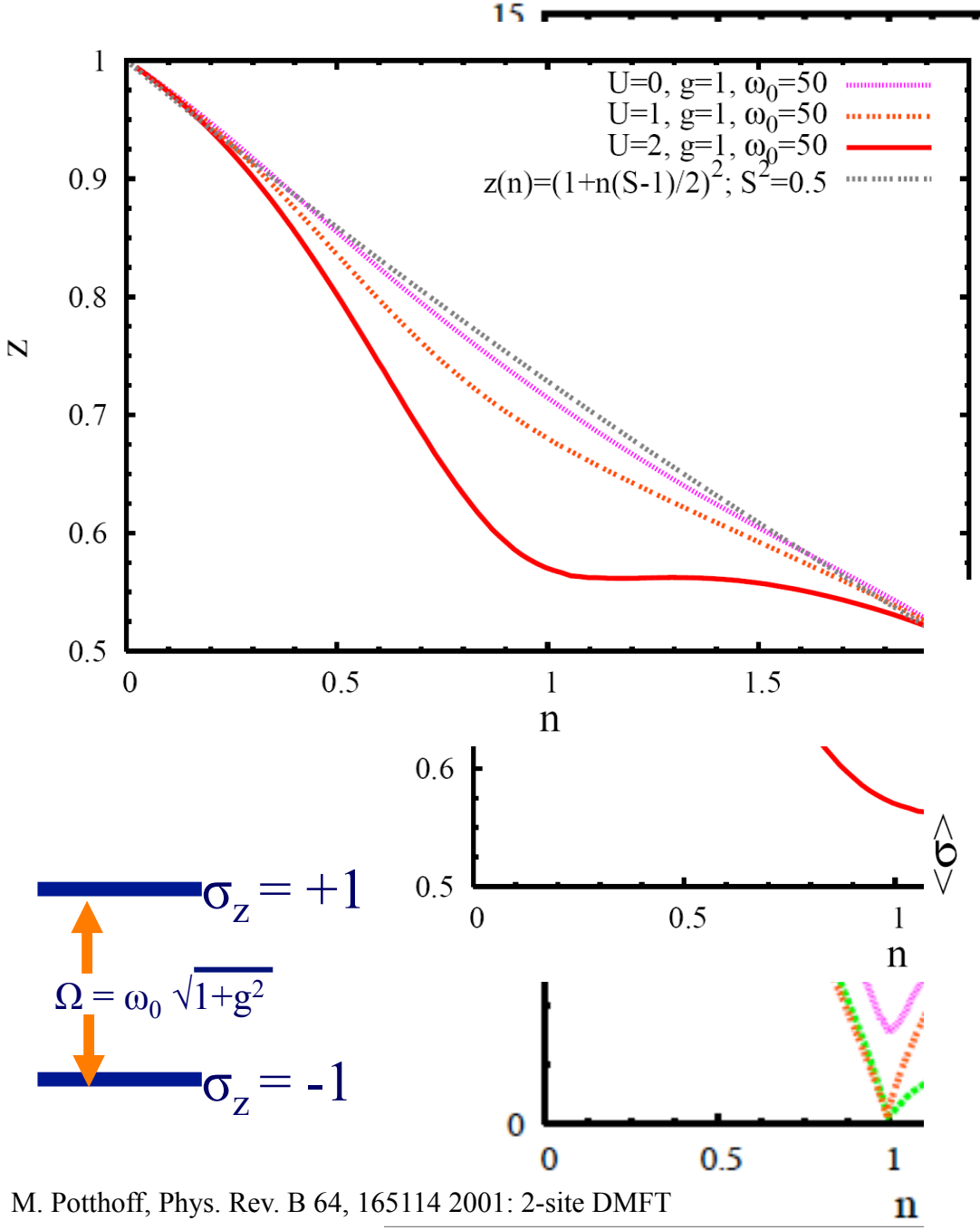
J. E. Hirsch
Department of Physics, University of California–San Diego, La Jolla, California 92093-0319, USA

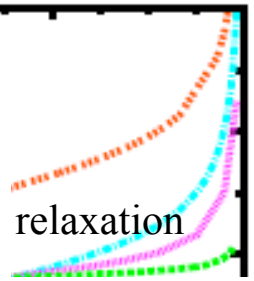
F. Marsiglio
Department of Physics, University of Alberta, Edmonton, Alberta, Canada T6G 2G7
(Received 4 August 2010; published 15 October 2010)

Giang Bach

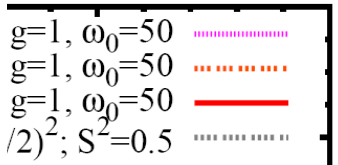
Mott physics vs. orbital relaxation

G.H. Bach et al., PRB 82, 155122 (2010)

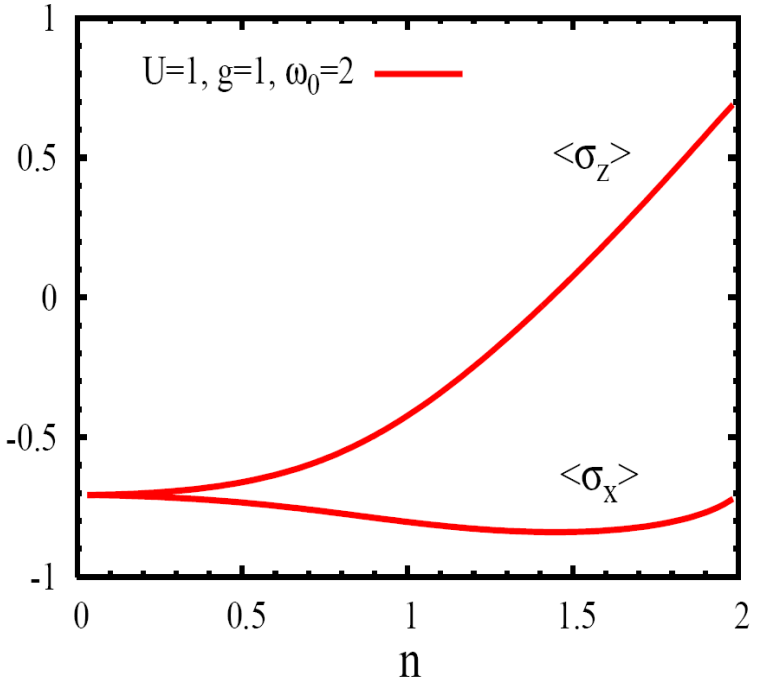




$z = V^2$



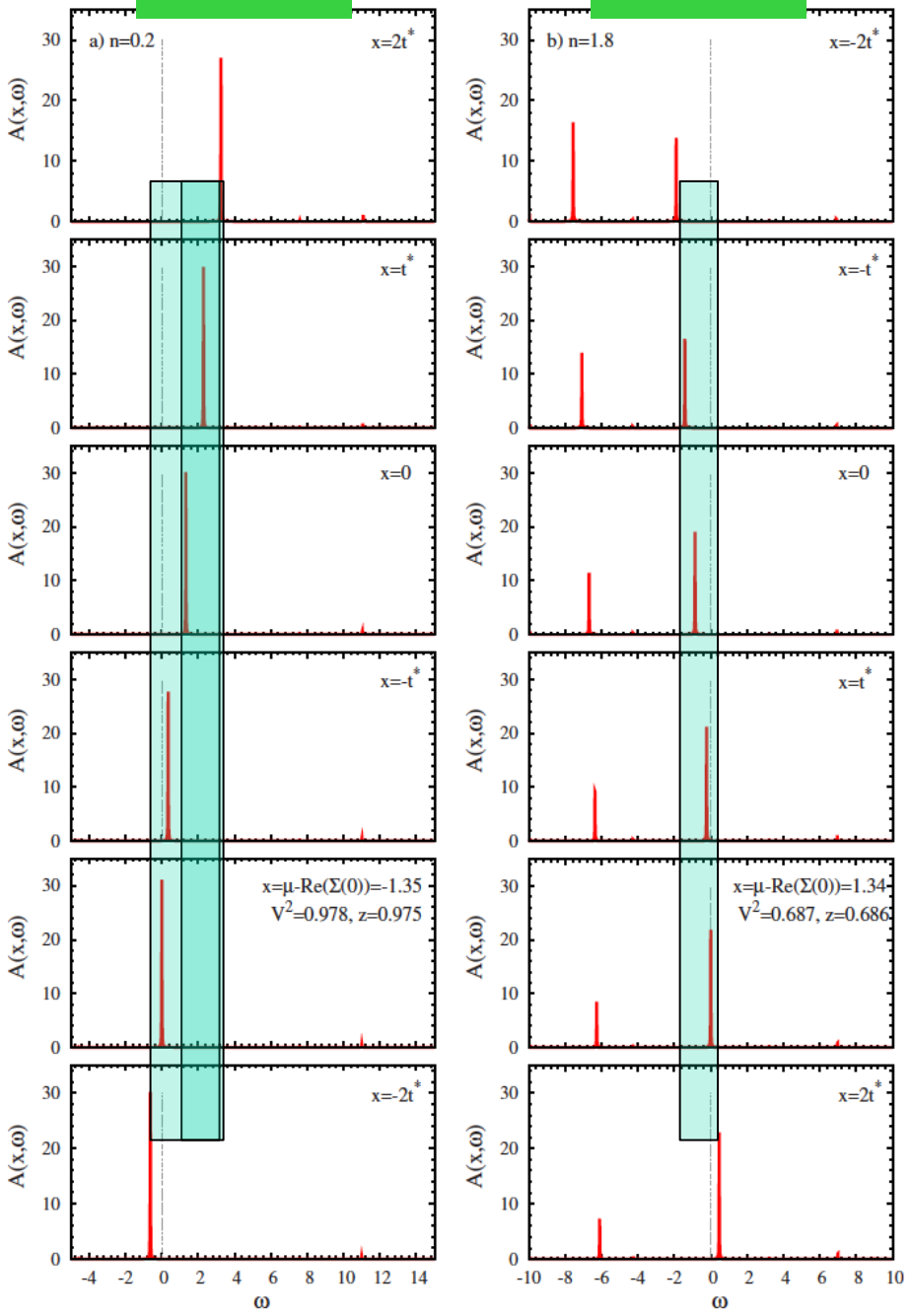
Pseudspin expectation values



M. Potthoff, Phys. Rev. B 64, 165114 2001: 2-site DMFT

n = 0.2

n = 1.8



G.H. Bach et al., PRB 82, 155122 (2010)

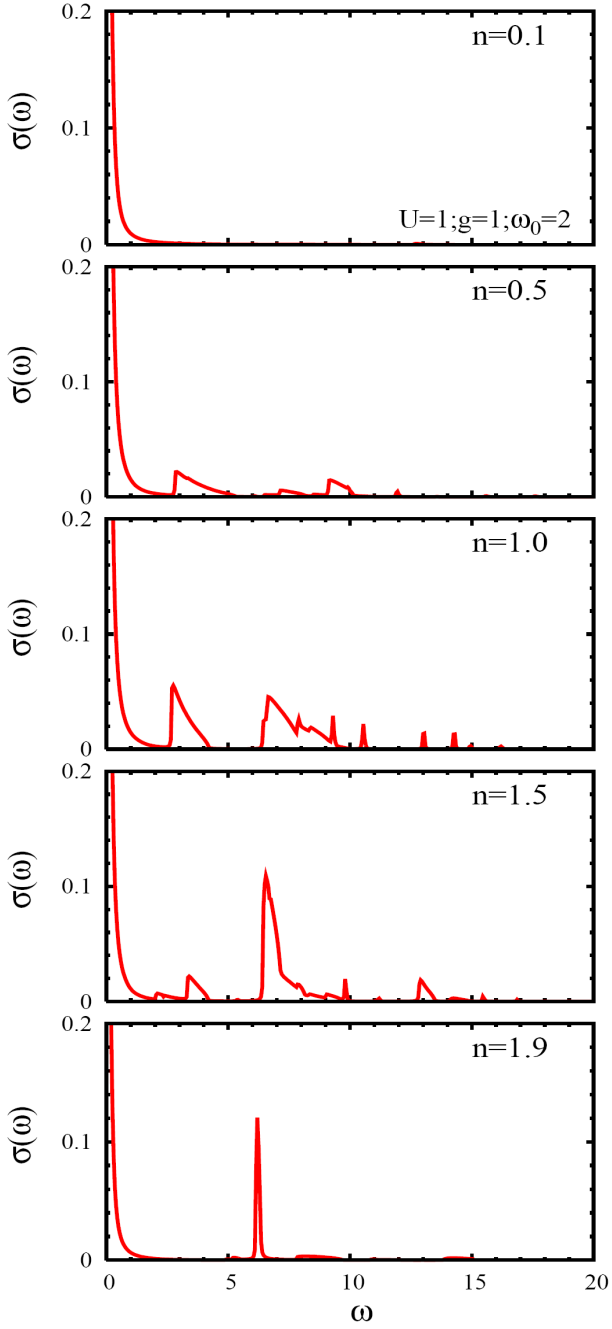
FIG. 12. (Color online) The spectral function for various energies, as shown, for (a) $n=0.2$ and (b) $n=1.8$. Here, we have used $U=1$, $g=1$, and $\omega_0=2$ (see pink curve in Fig. 9). The second last frame in each instance shows the spectral function at an energy corresponding to the Fermi level, and the weight under the peak at $\omega=0$ corresponds to the quasiparticle residue, z.

$U=1,\ g=1,\ \omega_0 = 2$

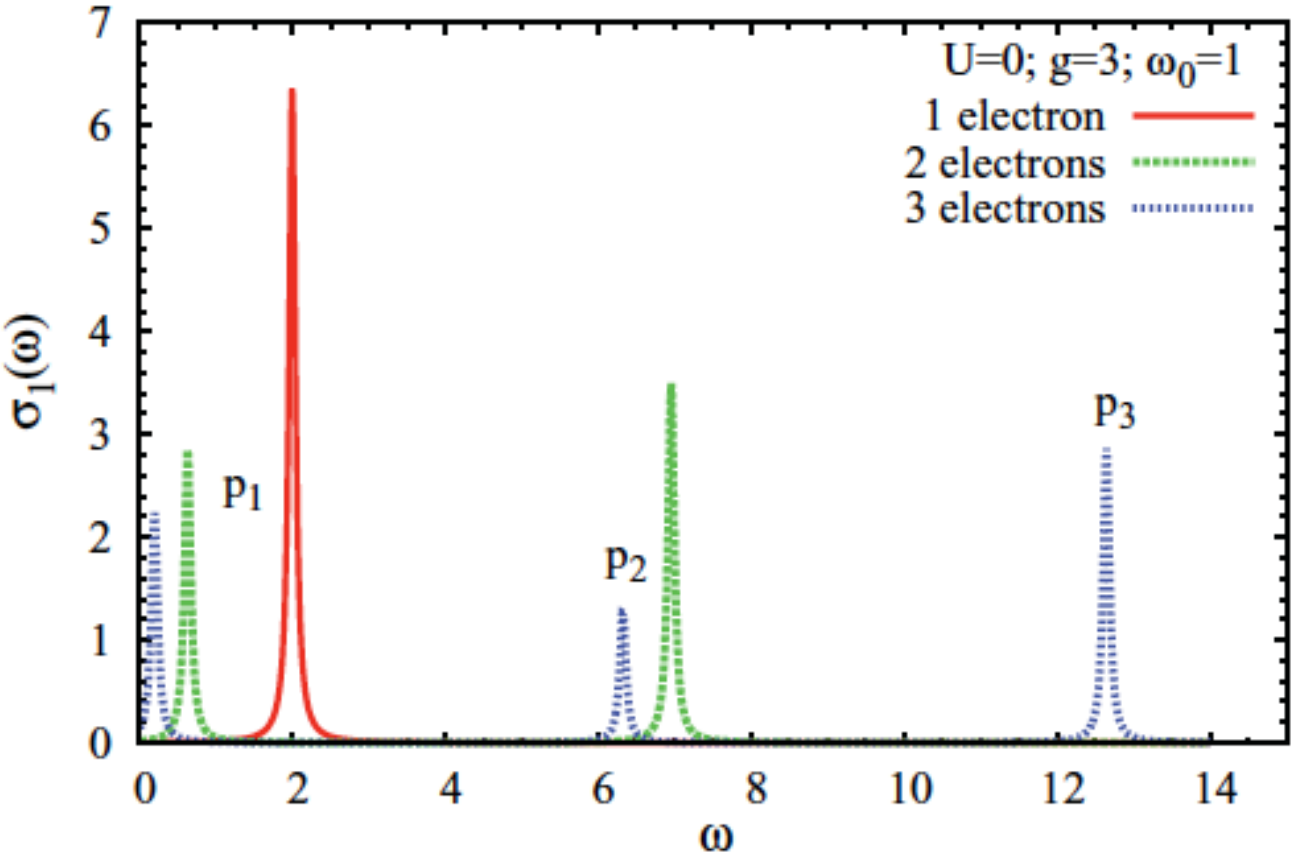
Optical conductivity

G.H. Bach et al., PRB 82, 155122 (2010)

See also G.H. Bach and F.M. PRB 85, 155134 (2012)



$$\sigma_1^{(3)}(\omega) = \frac{\pi e^2 t}{2\hbar^2}\left[S^2\delta\left(\omega - \frac{2tS^2}{\hbar}\right) + 4S^2\bar{S}^2\frac{t}{\Omega_0}\delta\left(\omega - \frac{\Omega_0}{\hbar}\right) + \bar{S}^4\frac{t}{\Omega_0}\delta\left(\omega - \frac{2\Omega_0}{\hbar}\right)\right]. \quad (29)$$



$$\sigma_1^{(1)}(\omega) = \frac{\pi e^2 t}{2\hbar^2}\delta(\omega - 2t/\hbar),$$

Dimer calculations

G.H. Bach and F.M. PRB 85, 155134 (2012)

How do we measure this ?

Optical Sum Rule (Kubo)

$$\int_0^\infty d\nu\ \sigma_1(\nu) = \frac{\pi e^2}{\hbar^2}\frac{1}{N}\sum_k (\frac{\partial^2 \epsilon_k}{\partial k^2}) n_k$$

for all bands (or quadratic dispersion): $= \frac{\pi e^2 n}{2m} = \omega_P^2/8$

for tight-binding band (with nearest neighbour hopping): $\frac{\partial^2 \epsilon_k}{\partial k^2} = -a^2 \epsilon_k$

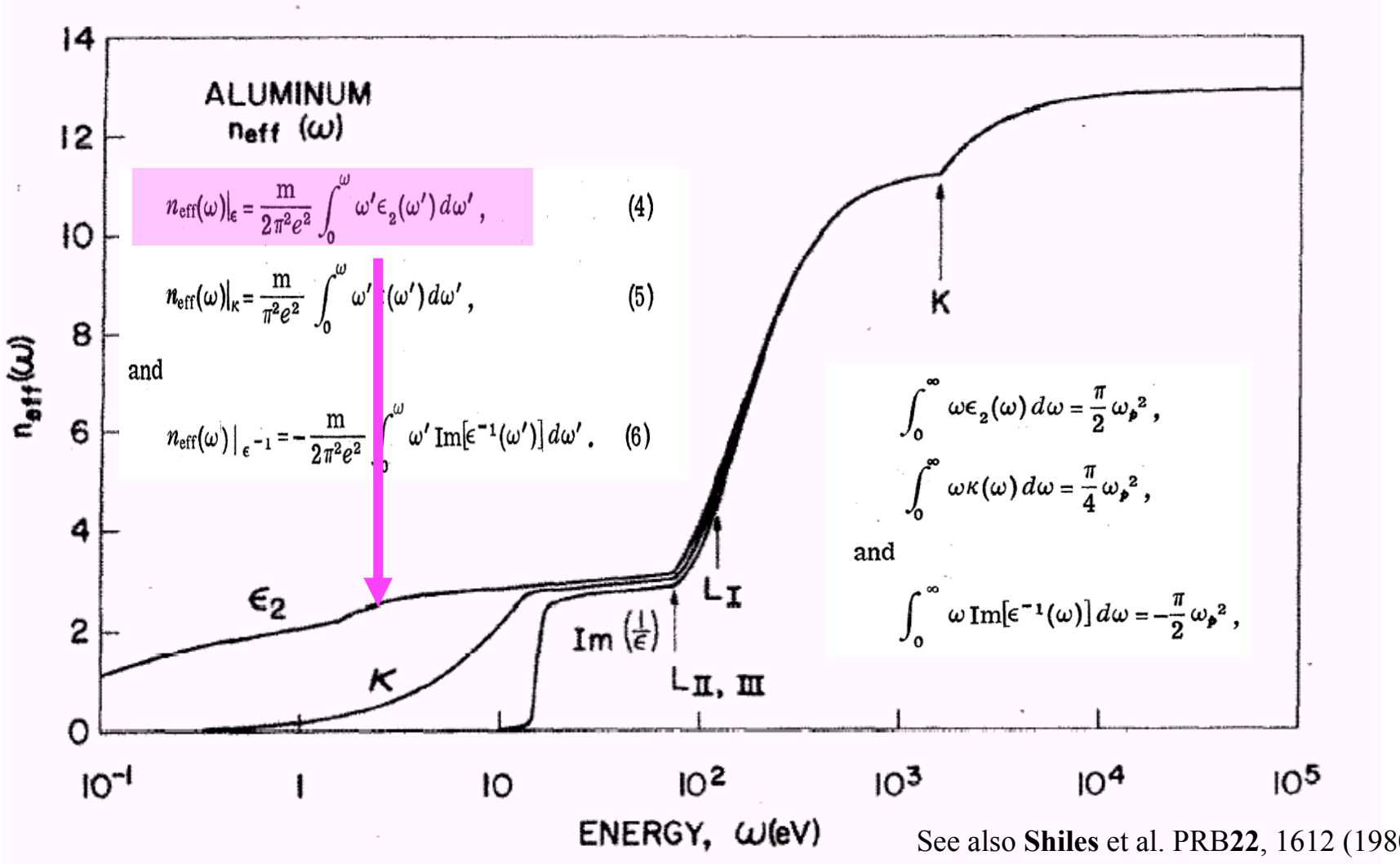
$$\int_0^\infty d\nu\ \sigma_1(\nu) = \frac{\pi e^2 a^2}{2\hbar^2} < -E_k >$$

PHYSICAL REVIEW B VOLUME 17, NUMBER 12 15 JUNE 1978

Finite-energy f-sum rules for valence electrons

D. Y. Smith
Argonne National Laboratory, Argonne, Illinois 60439

E. Shiles
Argonne National Laboratory, Argonne, Illinois 60439
and Virginia Commonwealth University, Richmond, Virginia 23284



See also **Shiles** et al. PRB**22**, 1612 (1980)

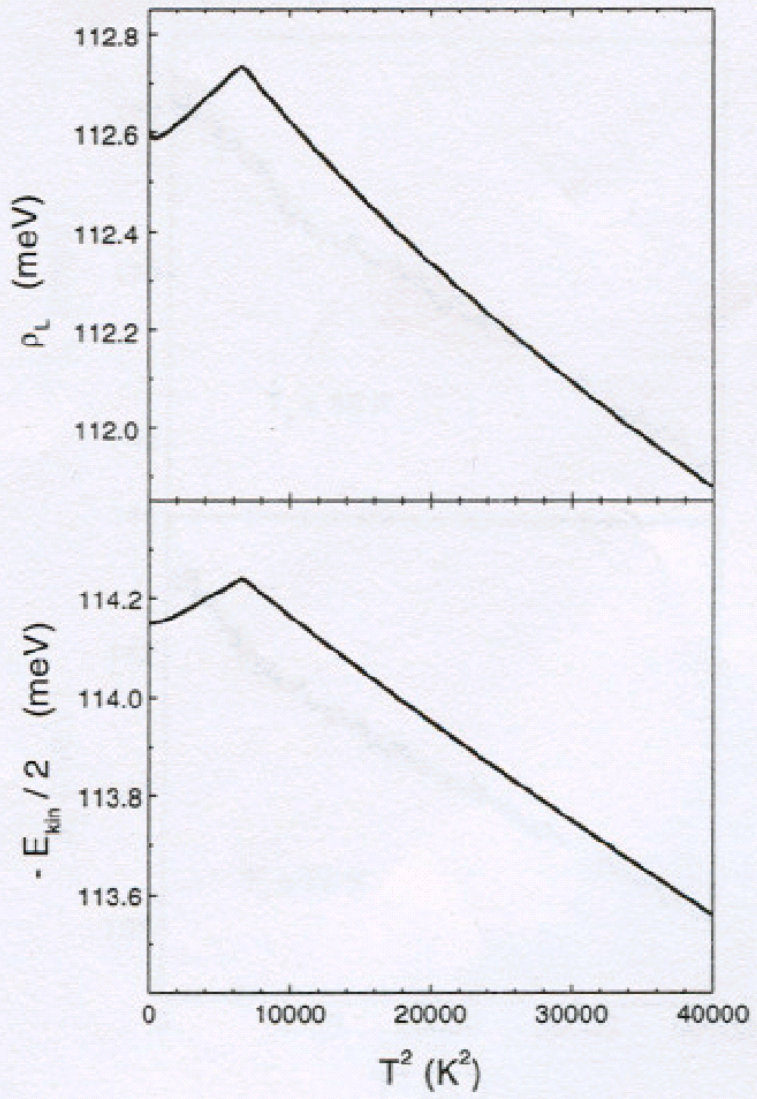


FIG. 6: BCS prediction of the spectral weight function.

van der Marel et al. cond-mat/0302169

why is there temperature dependence in the normal state ?

Answer:
1) n_k ---> f_k (Fermi-Dirac)
2) interactions

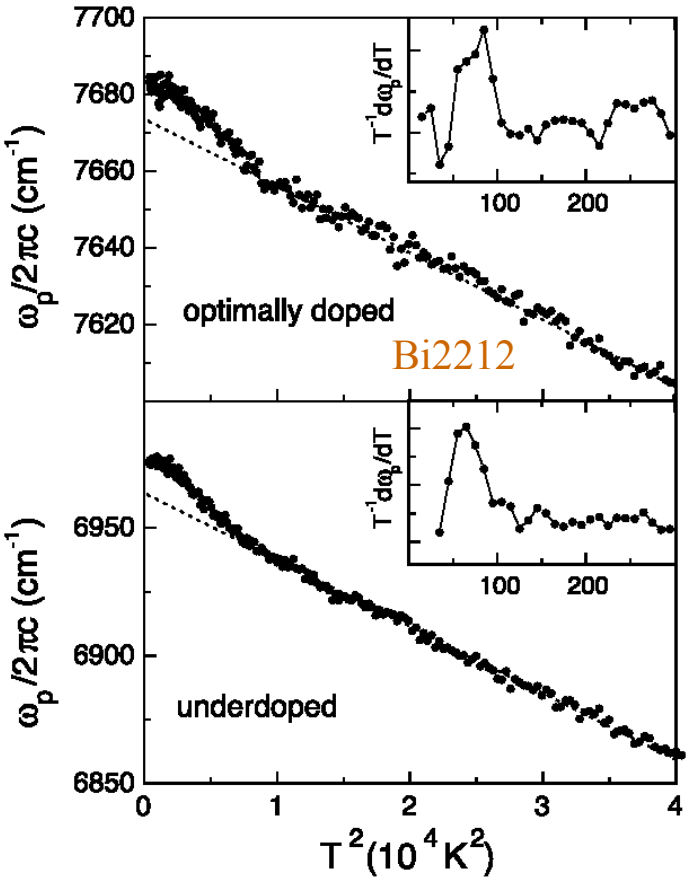
$$E_{kin} = 2 \Sigma \varepsilon_k n_k$$

Note: Absolute value of kinetic energy **decreases** in the superconducting state.
This is **conventional** behaviour

Superconductivity-Induced Transfer of In-Plane Spectral Weight in $Bi_2Sr_2CaCu_2O_{8+\delta}$

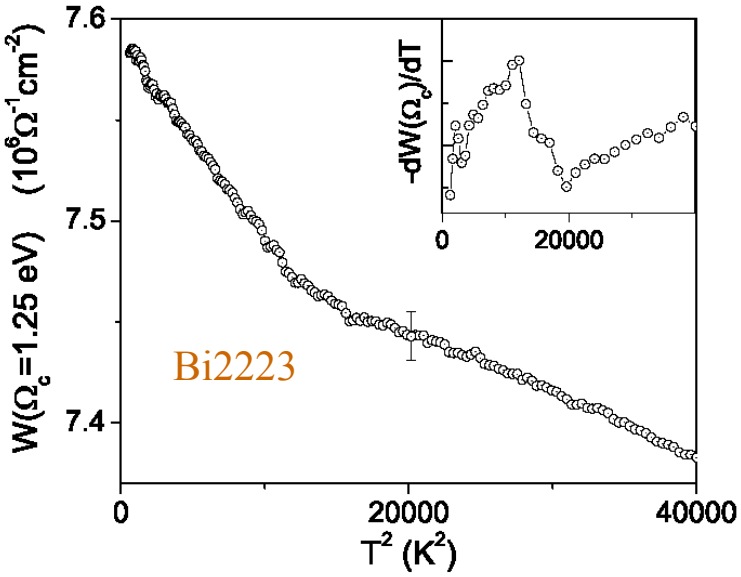
H. J. A. Molegraaf,[1] C. Presura,[1] D. van der Marel,[1]*
P. H. Kes,[2] M. Li[2]

Science 22 March 2002 295: 2239-2241



In-plane optical spectral weight transfer in optimally doped $Bi_2Sr_2Ca_2Cu_3O_{10}$

F. Carbone, A. B. Kuzmenko, H. J. A. Molegraaf, E. van Heumen, E. Giannini and D. van der Marel
DPMC, University of Geneva, 24, Quai Ernest-Ansermet, Geneva 4, Switzerland



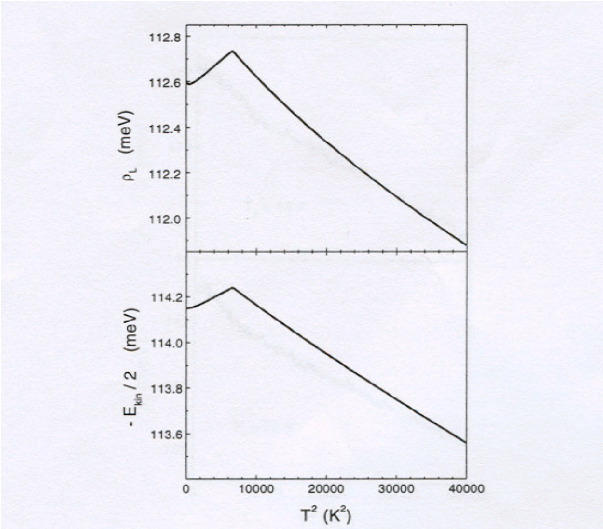
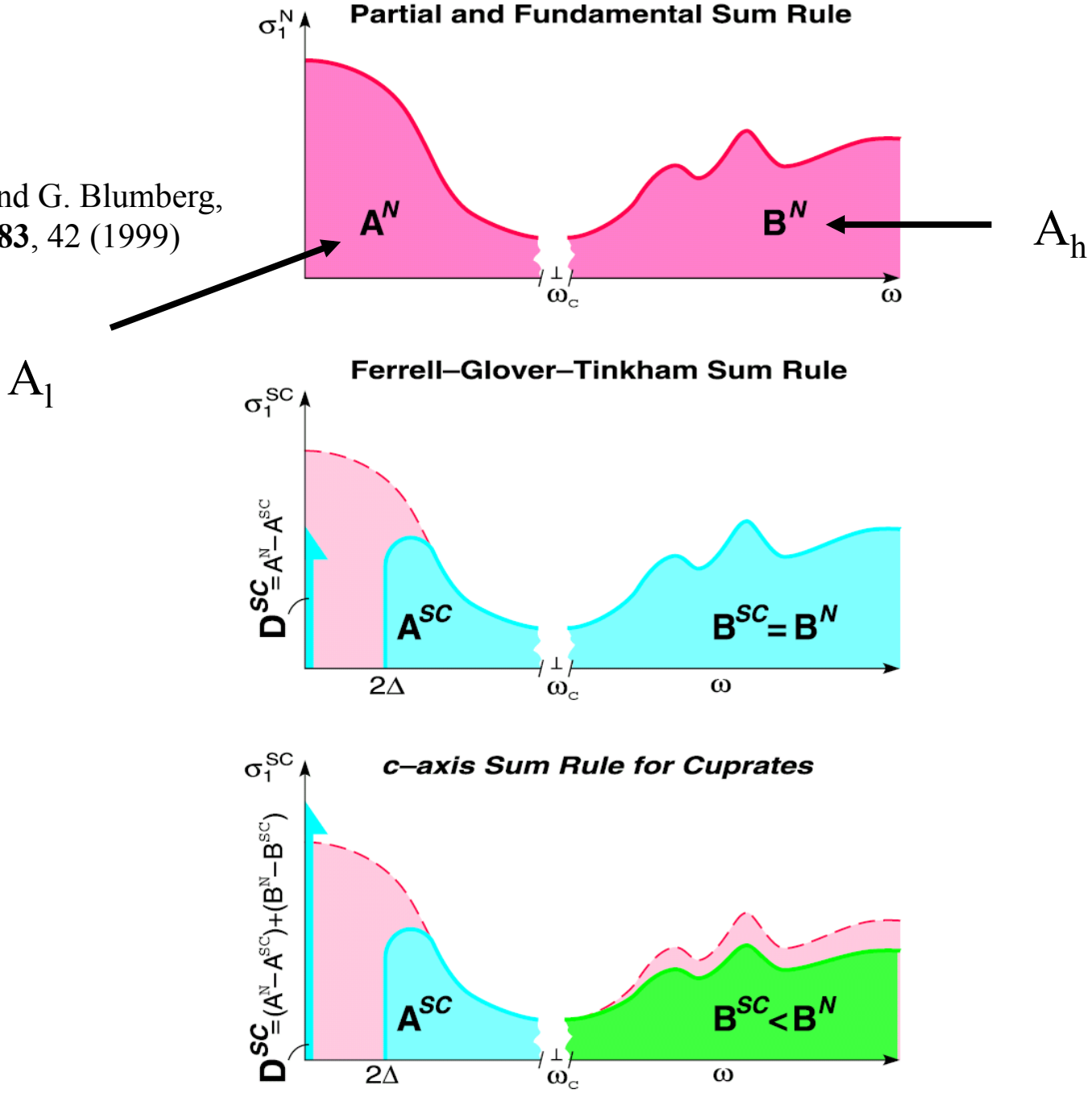


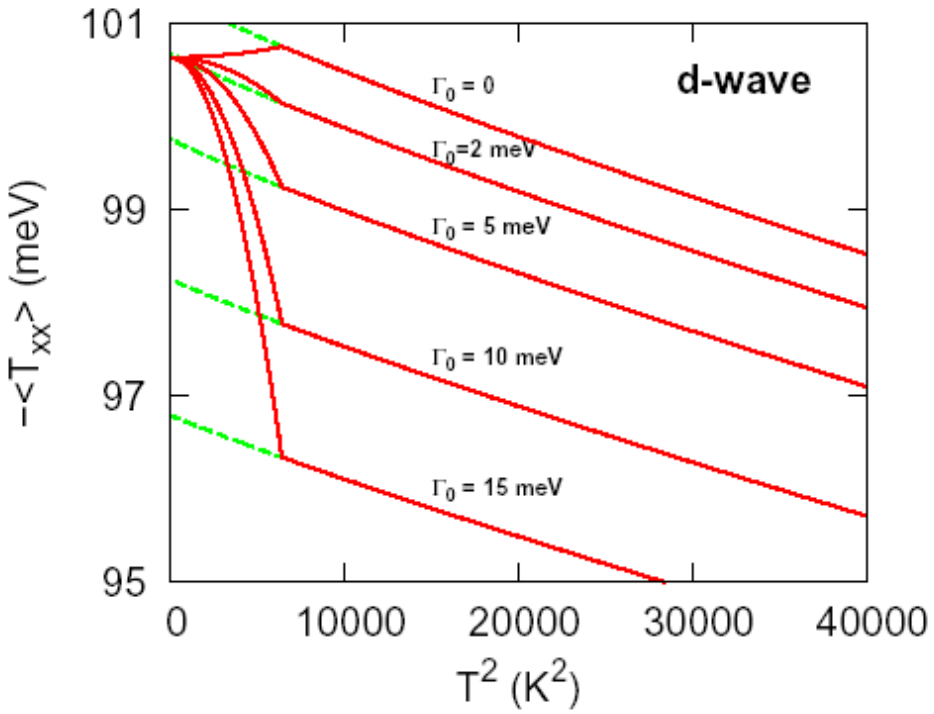
FIG. 6: BCS prediction of the spectral weight function.

M.V. Klein and G. Blumberg,
Science **283**, 42 (1999)

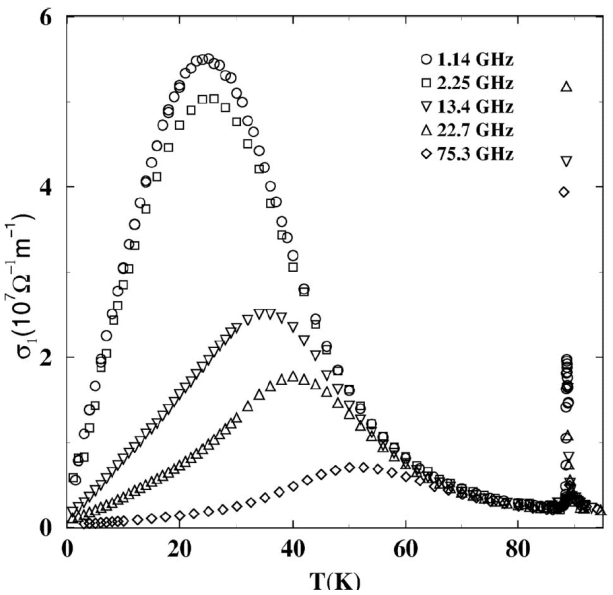


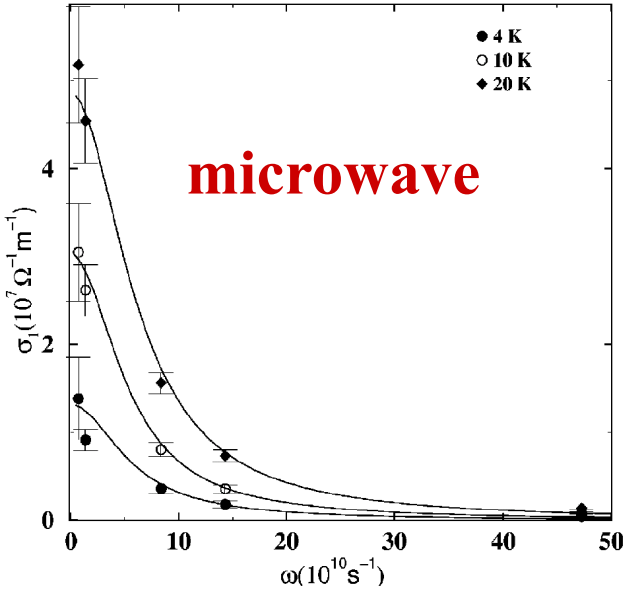
Anomalous sum rule change at Tc

Using a phenomenology of scattering rate collapse:



FM, Phys. Rev. B73, 064507

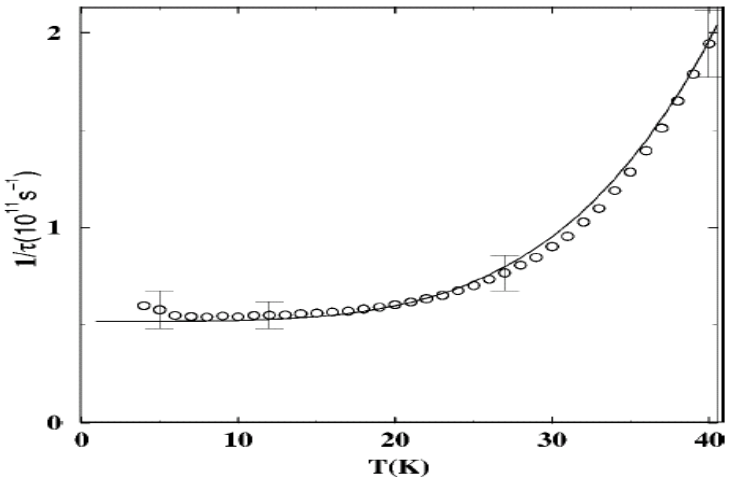




PHYSICAL REVIEW B VOLUME 60, NUMBER 2 1 JULY 1999-II

Microwave spectroscopy of thermally excited quasiparticles in $YBa_2Cu_3O_{6.99}$

A. Hosseini, R. Harris, Saeid Kamal, P. Dosanjh, J. Preston,* Ruixing Liang, W. N. Hardy, and D. A. Bonn



use $1/\tau = 1/\tau_0\,(T/T_c)^4$ below T_c

Also in photoemission, M.R. Norman et al.

Phys. Rev. Lett. 79, 3506–3509 (1997)

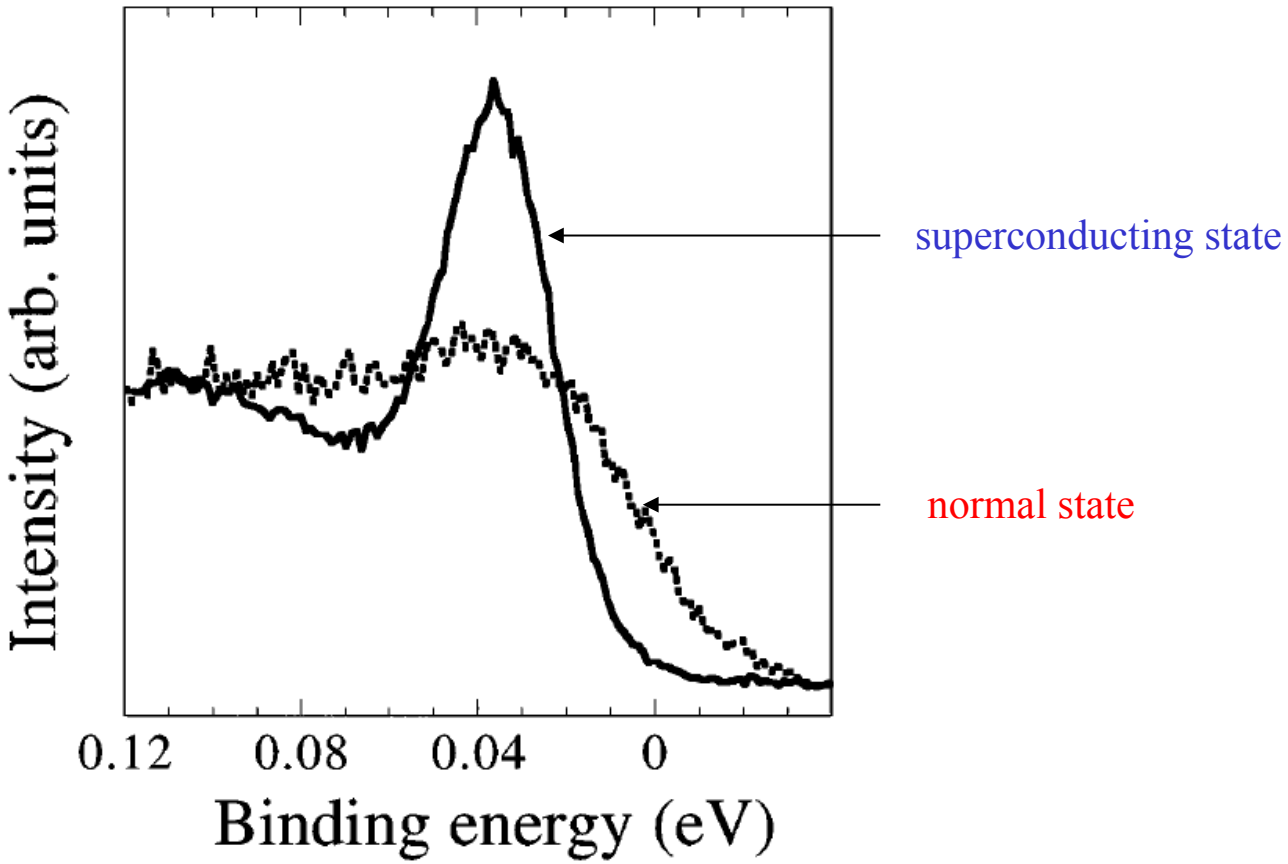


FIG. 1. Comparison of data at $\bar{M}$ in the normal state (105 K, dashed line) and the superconducting state (13 K, solid line) for a slightly overdoped (T_c = 87 K) Bi2212 sample with photon polarization $\Gamma - \bar{M}$.

Summary

I've tried to make the case that the BCS pairing formalism gives an excellent description of the superconducting state

but…

The actual **mechanism** is an active subject of current interest for all superconductors

Key Points

What are the essential ingredients buried in the parameter μ* ?

(i) Maybe the Hubbard and Hubbard-like models don't really capture the essence of electron correlations in metals.

(ii) The Dynamic Hubbard model tries to incorporate orbital relaxation --- the fact that orbitals expand, etc. when doubly occupied. Do these processes play an important role for superconductivity?

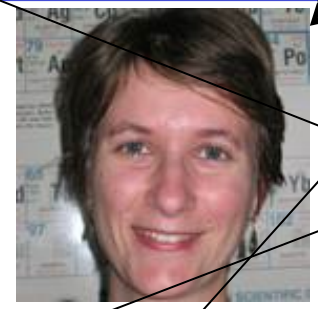
Moreover…

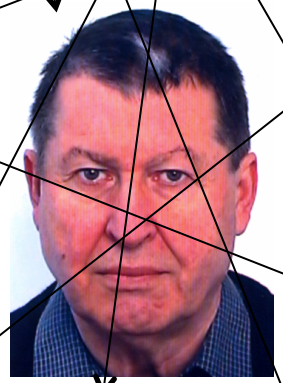
- We find a fundamental electron-hole asymmetry. This asymmetry is apparent in tunneling, and more indirectly through other probes.
- Pairing (requiring further study) results in energy lowering through kinetic energy (not potential energy), as seen in several optical conductivity studies (Basov, van der Marel, Bontemps, Timusk, etc.)

Many thanks to my collaborators: Benfatto, Carbotte, Knigavko,
Schachinger, Timusk, van der Marel,
Forestell, Kuzmenko, Carbone, van Heumen,
Polachic, Chandler, Bach, Hirsch, Baillie, Blois, and Zhou

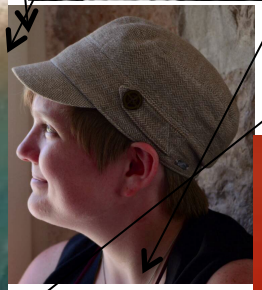
Funding: NSERC, CIAR, ICORE

Many thanks to my collaborators: Benfatto, Carbotte, Knigavko, Schachinger, Timusk, van der Marel, Forestell, Kuzmenko, Carbone, van Heumen, Polachic, Chandler, Bach, Hirsch, Baillie, Blois, and Zhou

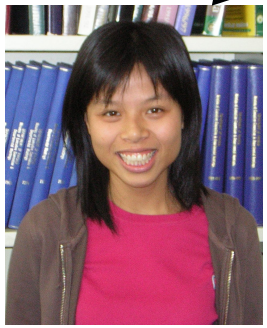



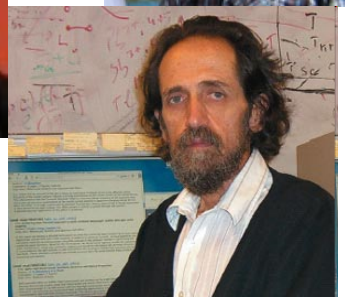
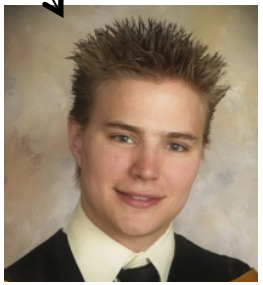








Funding: NSERC, CIAR, ICORE