DYNAMICAL MEAN-FIELD THEORY AND STRONGLY CORRELATED SUPERCONDUCTORS: CAN REPULSION FAVOUR SUPERCONDUCTIVITY?

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OUTLINE

- Some minutes on Dynamical Mean-Field Theory:
  - ✓what is it?
  - ✓Why and how do we use it?
  - ✓Mott transitions
- Strongly Correlated Superconductors: the (un)popular case of fullerenes
- Mott meets BCS: phonon-driven superconductivity enhanced by correlations
- Is this a general phenomenon? What do I mean?

M. C., M. Fabrizio, C. Castellani, and E. Tosatti, Rev. Mod. Phys. 81, 943 (2009)

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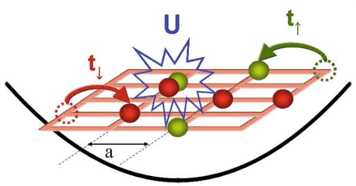
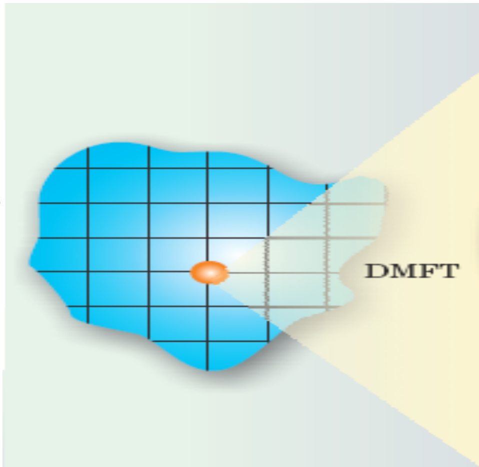
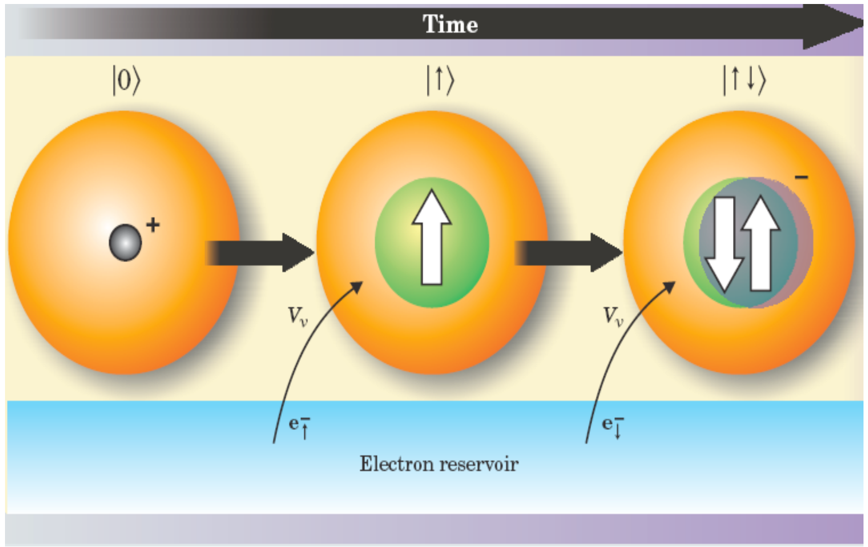
SUPERBAD

DYNAMICAL MEAN-FIELD THEORY

Lattice method: Originally for effective low-energy models (Hubbard)
Suited for correlated electrons with narrow bands (3d, 4f, 5f)







- Mean-Field idea: every site is equivalent
- We sit on a lattice site and focus on its dynamics
- Local changes are equivalent to exchange with a "bath"

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STATIC vs DYNAMICAL MEAN-FIELD THEORY

Lattice Model

$$H = -\sum_{<ij>} J S_i S_j - h \sum_i S_i$$

$$H = -t \sum_{<ij>} c^+_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}$$

Local Model

$$H_{eff} = -h_{eff} S_0$$

$$S_{eff} = \int d\tau d\tau' c^+_{0\sigma}(\tau) G_0^{-1}(\tau - \tau') c_{0\sigma}(\tau') + U \int d\tau n_{i\uparrow}(\tau) n_{i\downarrow}(\tau)$$

Weiss field

$$h_{eff} = h + zJm$$

$$G_0(i\omega_n)^{-1} = i\omega_n + \mu + G(i\omega_n)^{-1} - R\left[G(i\omega_n)\right]$$

$$m = Tr e^{-\beta H_{eff}} S_0$$

$$G(\tau) = - < T c_0(\tau) c^+_0(0) >_{S_{eff}}$$

$$m = tgh\left[\beta(h + Jmz)\right]$$

Curie-Weiss

The Weiss Field is Dynamical

Self-consistency is more "involved"

DMFT AND "IMPURITY MODELS"

Dynamical Mean-Field → No local time-independent Hamiltonian

We can introduce auxiliary fermions describing the **bath**

$$H = Un_{0\uparrow}n_{0\downarrow} - \mu n_0 + \sum_{k\sigma} V_k (c^+_{k\sigma} c_{0\sigma} + c^+_{0\sigma} c_{k\sigma}) + \sum_{k\sigma} \varepsilon_k c^+_{k\sigma} c_{k\sigma}$$

Equivalent to previous slide if $G_0(i\omega_n)^{-1} = i\omega_n + \mu - \sum_k \frac{V_k^2}{i\omega_n - \varepsilon_k}$

Well-known model for magnetic impurities in metals (Kondo physics)

We have to solve this model and **compute the Green's function**

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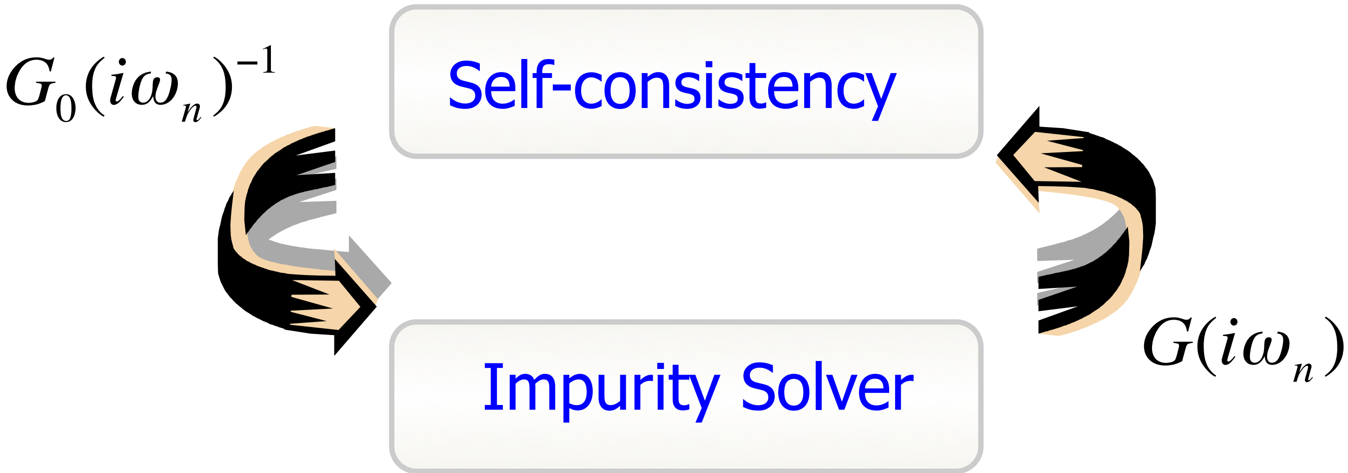
THE IMPURITY SOLVERS, OR "THE COMPUTATIONAL PART"

We need to solve the "impurity model" and compute at least The frequency-dependent Green's function

Numerical methods are much cheaper (or "more") than for the lattice model

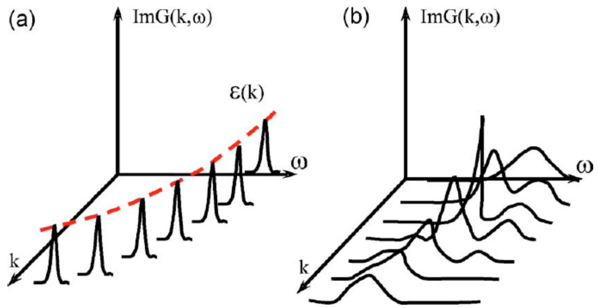
- Exact Diagonalization
- QMC (Continuous-Time Diagrammatic)
- Numerical RG
- Density-Matrix RG
- Iterated Perturbation Theory

ITERATIVE SOLUTION OF AIM



Once converged: compute static and dynamic observables

- Spectral function, optical conductivity,
  non-equilibrium properties



- Superconductivity with s-wave symmetry
- Antiferromagnetism, charge-ordering, ferromagnetism, phase separation

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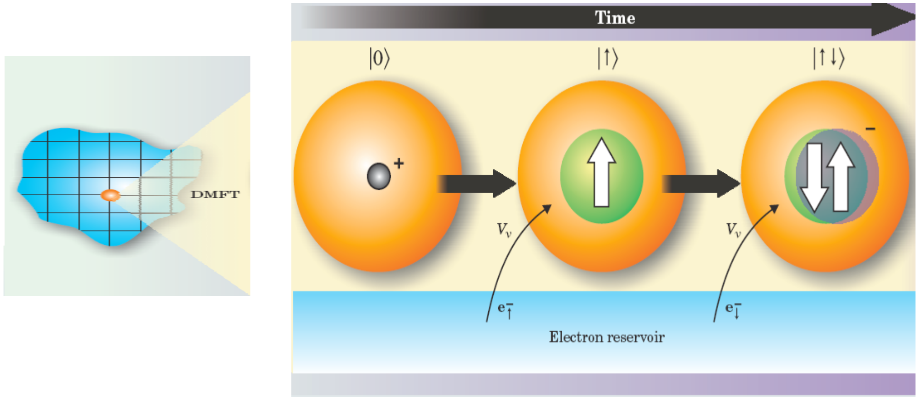
DMFT: pros (hopefully more) and cons



- Does not assume any hierarchy between energy scales (weak or strong coupling…), and treats many scales on equal footing
- Dynamical information (spectroscopy) "for free" (ARPES, optics, …)
- Zero and finite temperature
- Can be merged with DFT

GOOD

- Non-local quantum fluctuations at mean-field level
- Can not treat non-local order parameters (d-wave SC)
- Still needs some non-obvious numerics

BAD

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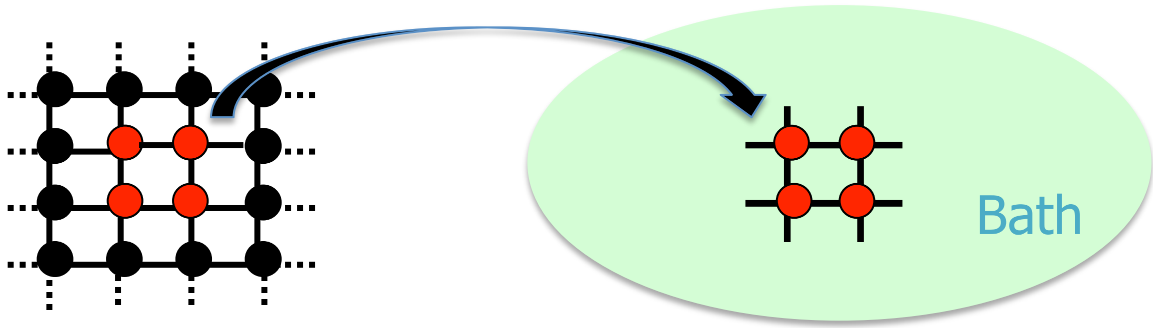
CLUSTER-DMFT

"Straightfoward" generalization: instead of a single site, a cluster is selected



- Not uniquely defined: different recipes (DCA, CDMFT,…)
- Numerics becomes "harder"

Need at least a 2x2 plaquette to treat d-wave SC and the cuprates, even if…

OPTICAL CONDUCTIVITY

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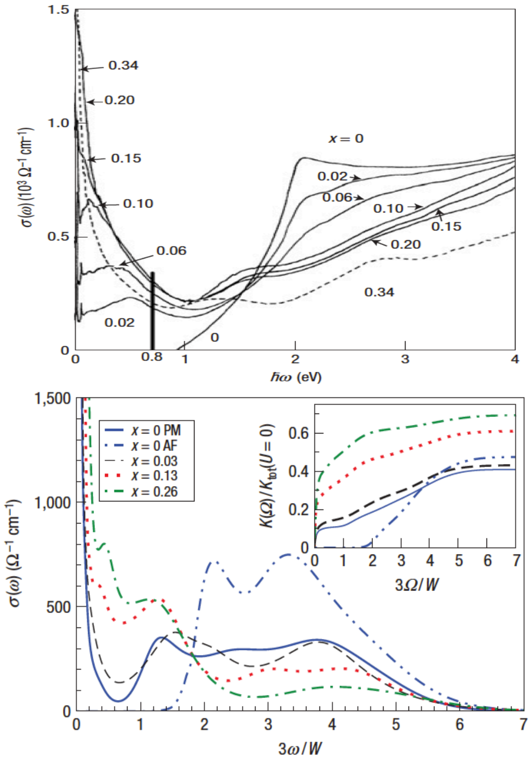
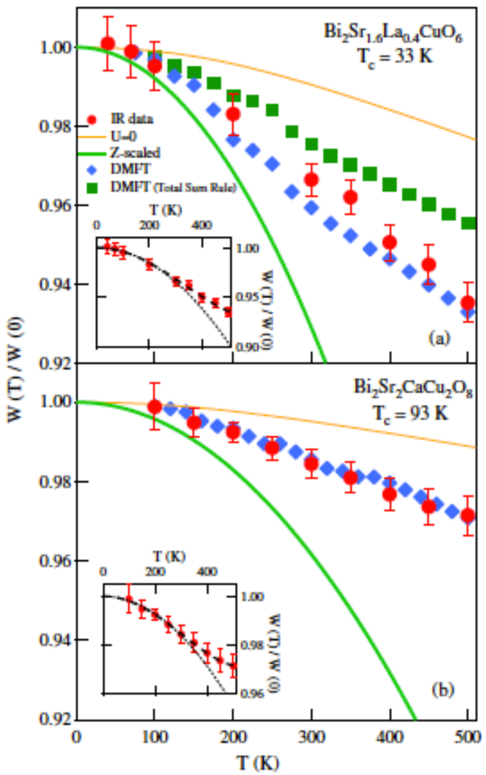
Analysis of spectral weight: already with single-site DMFT
We reproduce the temperature evolution of the integral of $\sigma(\omega)$

The optical conductivity of cuprates corresponds to a moderate U



A. Comanac, L. de' Medici, M.C. and A.J. Millis, Nat. Phys. 4, 287 (2008)



$$W(T) = \int_0^{\Omega} \sigma(\omega, T)\, d\omega$$

D. Nicoletti et al., Phys. Rev. Lett. 105, 077002 (2010)

SUPERBAD

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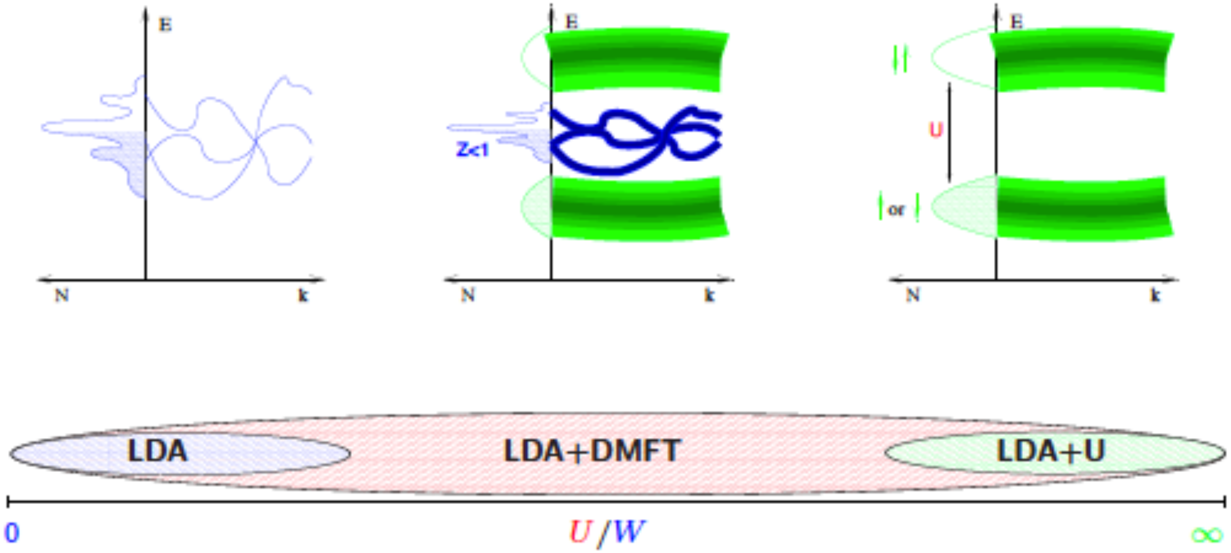
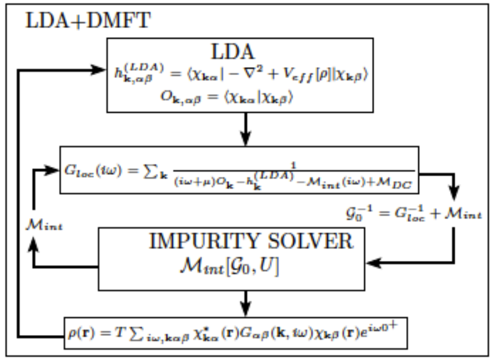
"LDA+DMFT"

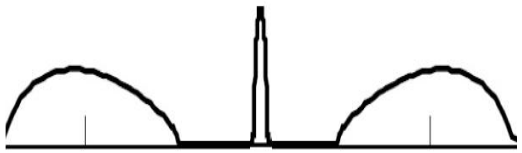




WIDE BANDS

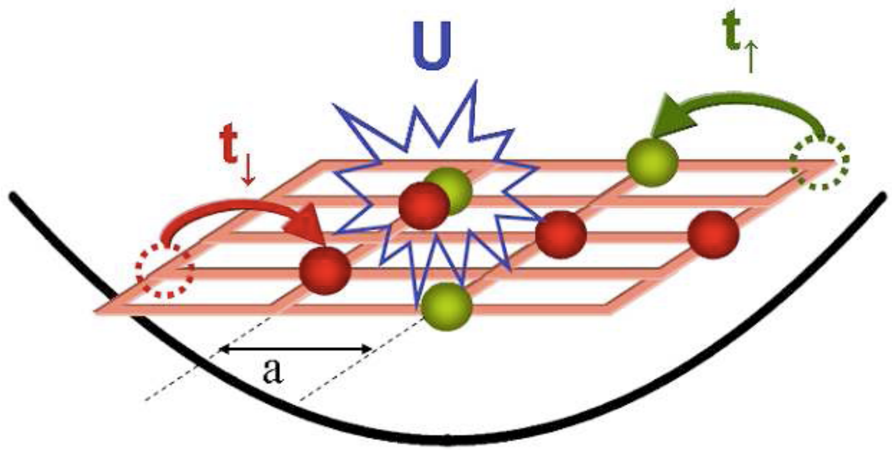
STRONGLY CORRELATED METALS
(bands + atomic features)

MOTT INSULATORS



THE MOTT-HUBBARD TRANSITION

The "smoking gun" of electronic correlations:
Insulating behaviour in partially filled bands



- Main qualitative effect of correlations
- Nonperturbative
- Non-trivial (interplay with magnetism and else)
- Present in the cuprates!

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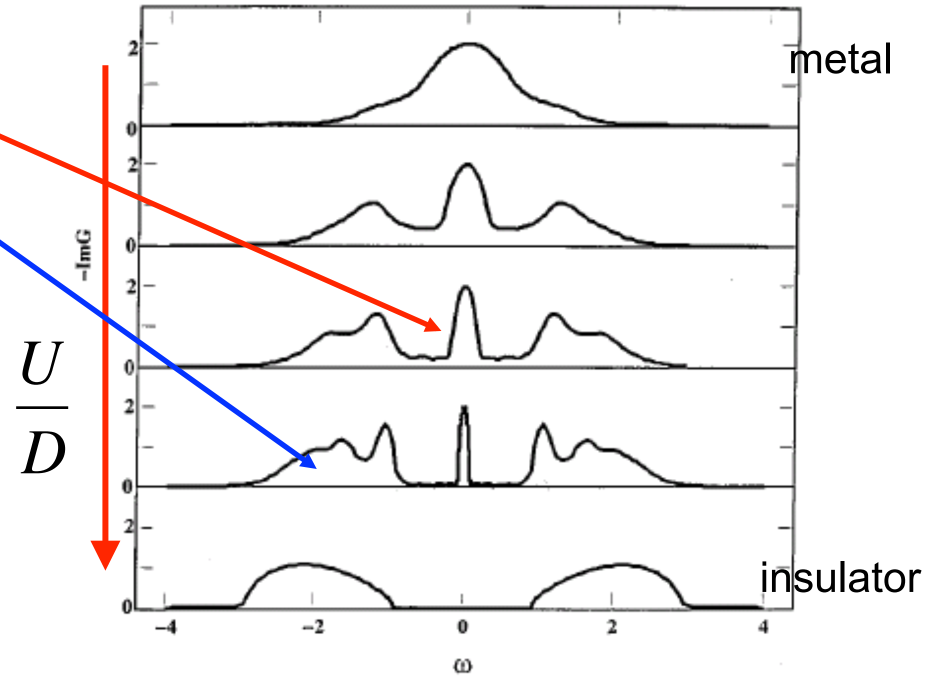
THE MOTT TRANSITION IN DMFT

Spectral function of the Hubbard model as a function of U/D

$$\rho(\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G(\omega)$$

Metallic Quasiparticle peak
and
"Insulating" Hubbard bands
coexist



The QP band shrinks

$$W \rightarrow ZW$$

$$Z = \left(1 - \frac{\partial \Sigma(i\omega_n)}{\partial i\omega_n}\right)^{-1}$$

Mott Transition when

$$Z = \frac{1}{m^*} \rightarrow 0$$

THE MOTT TRANSITION IN DMFT

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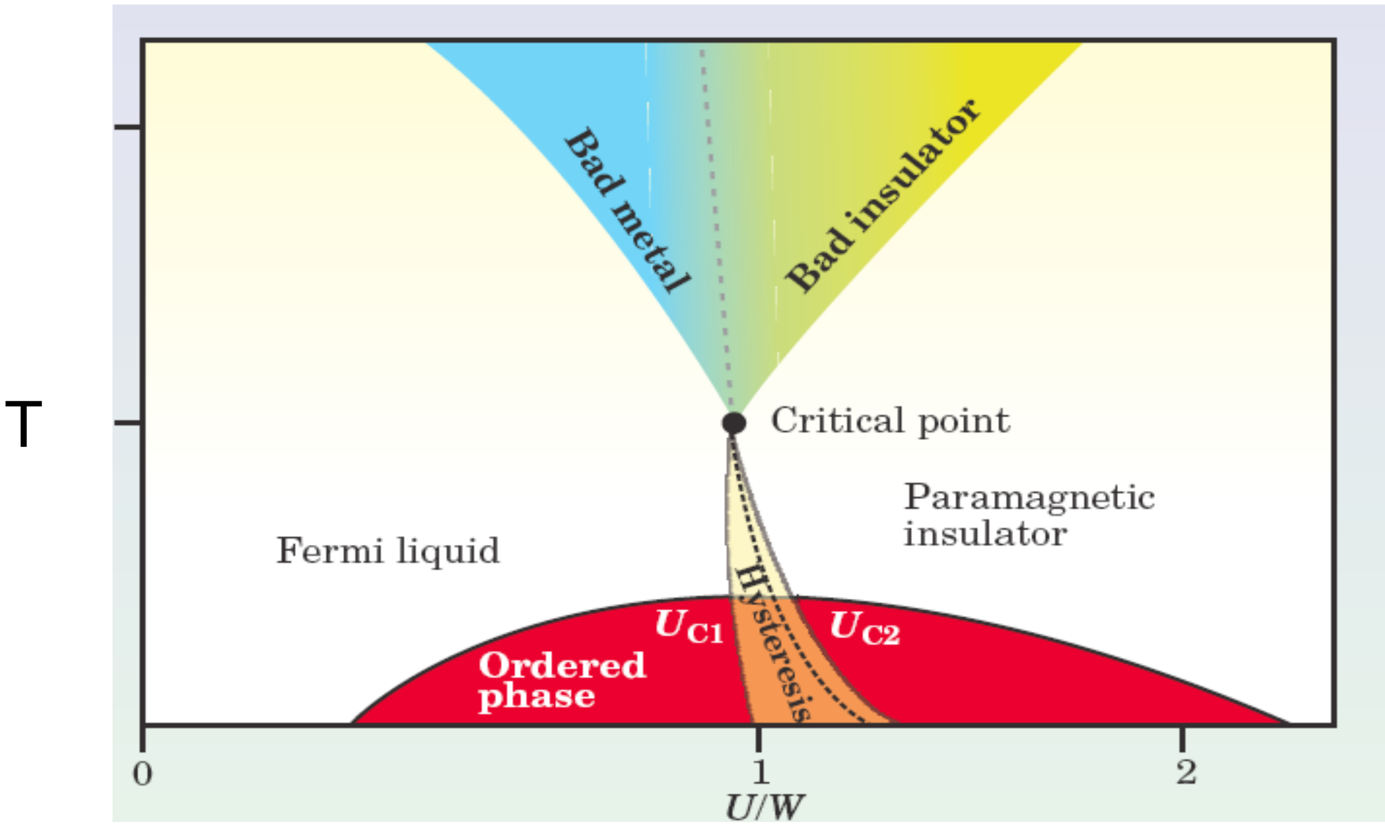

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FRAMEWORK (AND ADVERTISEMENT)

SUPERCONDUCTIVITY after the cuprate earthquake

Conventional

- low T_c
- Phonon-mediated
- **Normal metal above Tc**

Non-Conventional

- high T_c
- “Electronic Mechanism”
- **A strange metallic state**

Are these two distinct fields?

- Cuprates: most likely electronic (though phonons strike back)
- Fullerides: phononic and “high Tc” ~40K
- Heavy Fermions: electronic and low Tc
- Iron based?

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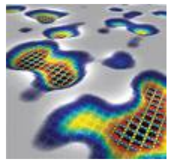
ERC Starting Grant SUPERBAD – IDEAS Program
Post-doc Position(s) available



HOW CAN CORRELATIONS (REPULSION) FAVOUR SUPERCONDUCTIVITY (ATTRACTION)?

$$T_c = \omega_0 e^{-\frac{1}{\lambda - \mu^*}}$$

$\lambda = \rho V$ → Attractive Potential (V); → Density of States (ρ)

Electron-electron Correlations ⇒ Quasiparticles with Reduced bandwidth

$W \longrightarrow ZW$

$Z << 1$

$$\rho \propto \frac{1}{W}$$

⇒ $\rho \longrightarrow \rho/\mathbf{Z}$

Repulsion enhances T_c!

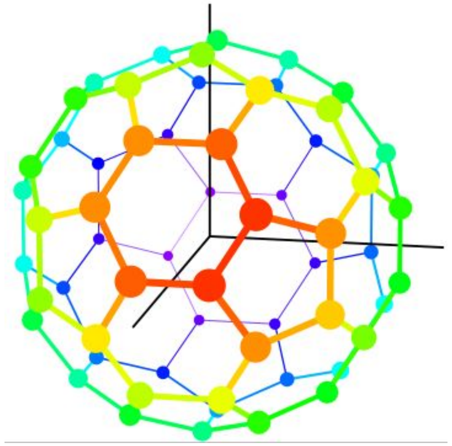
"Typically" V is also renormalized

$V \longrightarrow V\mathbf{Z}^2$ ⇒ $\lambda \longrightarrow \lambda \mathbf{Z} << \lambda$

$T_c \downarrow$

Correlation can enhance Tc if the attraction is not renormalized

THE ALKALI-METAL DOPED FULLERIDES: WHERE DO THEY BELONG?



- Solid C_{60} forms a molecular crystal
- Band insulator with a threefold degenerate (t_{1u}, like p) LUMO

- A_nC_{60}: alkali-metal atoms donate their s electrons to C_{60} bands
- n=3 Superconductors (Tc ~ 35K)

A = K, Rb

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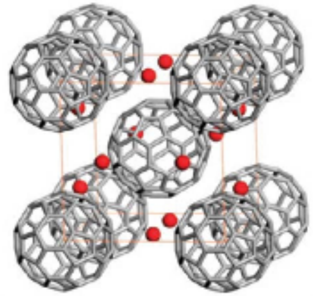
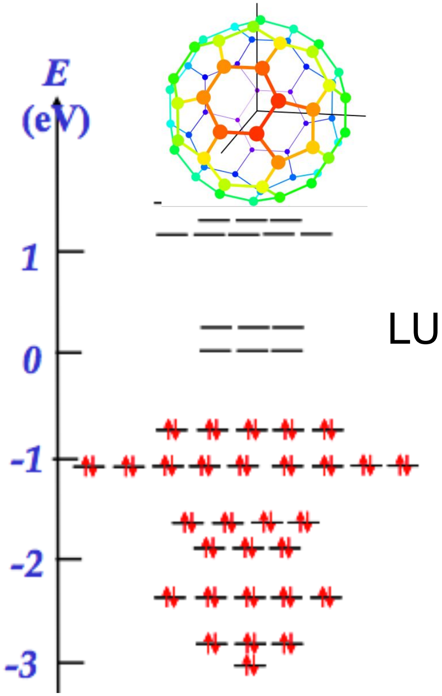
THE ALKALI-METAL DOPED FULLERIDES: WHERE DO THEY BELONG?

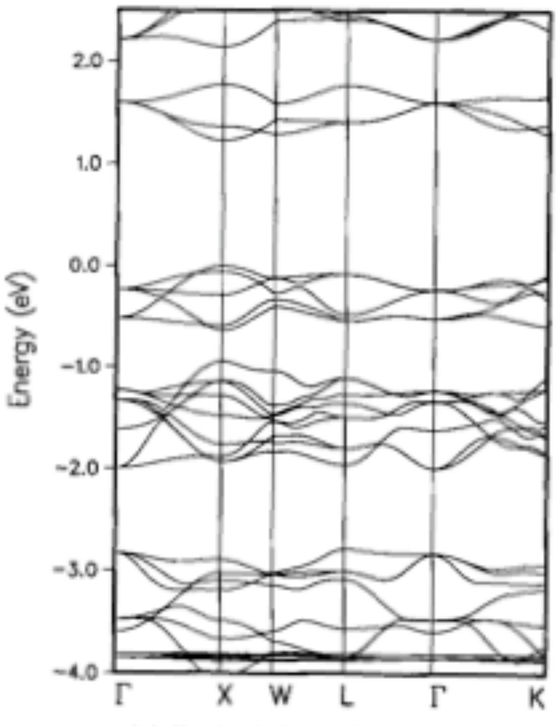


C_{60} molecule MOs



LUMO t_{1u}

Solid C_{60} bands



3 degenerate LUMO bands

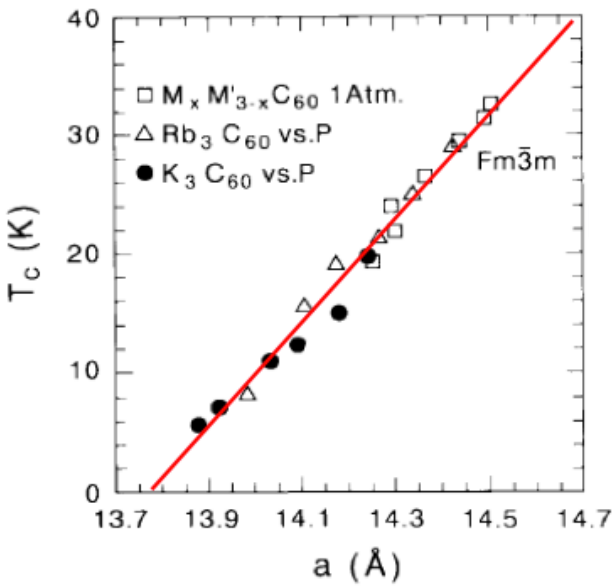
Molecular Crystal: the bands are formed by molecular orbitals

THE FIRST ANSWER: ELECTRON-PHONON

“old” (90s) compounds (K_3C_{60}, Rb_3C_{60})

- Carbon Isotope effect on T_c
- Regular Specific heat jump at T_c
- Increase of T_c and DOS with lattice spacing

Ordinary “BCS” Superconductors with “moderate” effective mass enhancement

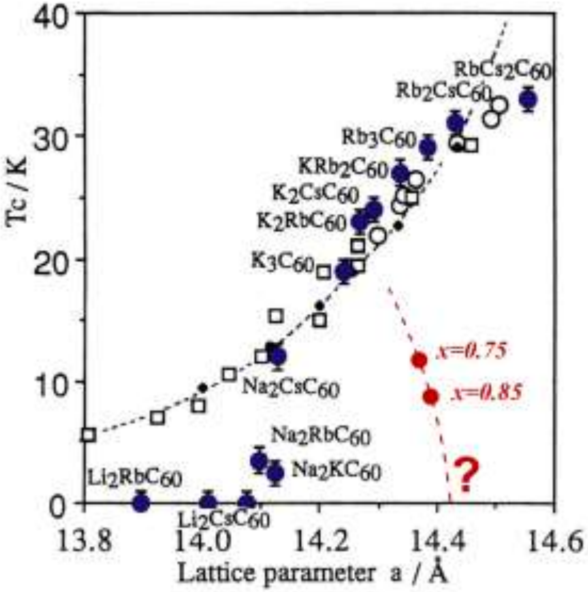


$$T_C \cong 1.14\omega_D e^{-\frac{1}{VN(E_F)}}$$

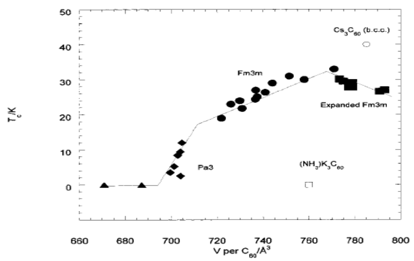
O. Gunnarsson, Rev. Mod. Phys. 69, 575 (1997)

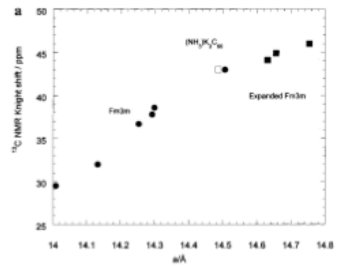
THE STORY BECOMES MORE “INTERESTING”

00s: Expanded (large interball distance) compounds:
T_c decreases with lattice parameter



$(NH_3)_xNaK_2C_{60}$





$Cs_{3-x}Rb_xC_{60}$

While DOS increases

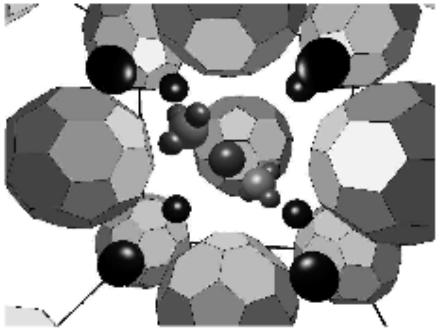
M. Riccò et al.
Phys. Rev. B, 68, 035102 (2003)

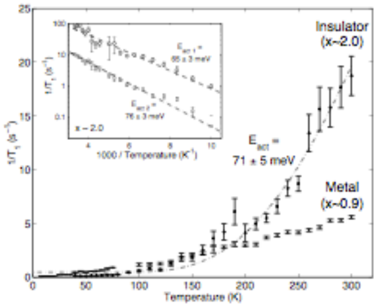
Dahlke, Denning, Henry, Rosseinsky,
J. Am. Chem. Soc. 122, 12352 (2000)

THE STORY BECOMES MORE "INTERESTING"

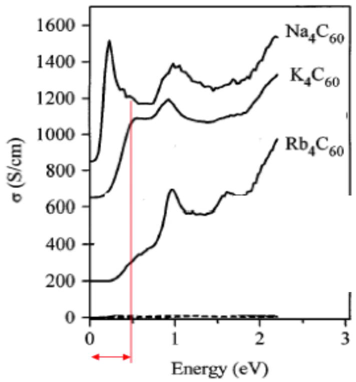
Evidence of Mott Insulating States

A non magnetic
Spin-gapped insulator





$(NH_3)_xNaK_2C_{60}$



K_4C_{60}

M. Riccò et al.
Phys. Rev. B, 68, 035102 (2003)

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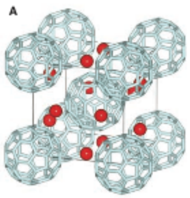
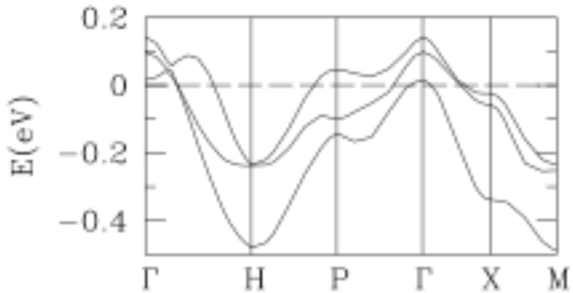
THEORY: A SIMPLIFIED MODEL FOR A_nC_{60}



One C60 per lattice site
Alkali only donate their s electrons

$$-t \sum_{<ija>} c^{+}_{ia\sigma} c_{ja\sigma}$$

hopping Term → 3 bands
W ~ 0.5-0.6 eV



$$+\frac{U}{2}\sum_{i}(n_i - 1)^2$$

Coulomb Repulsion U ~ 1/1.5 eV

It should be a correlated system!

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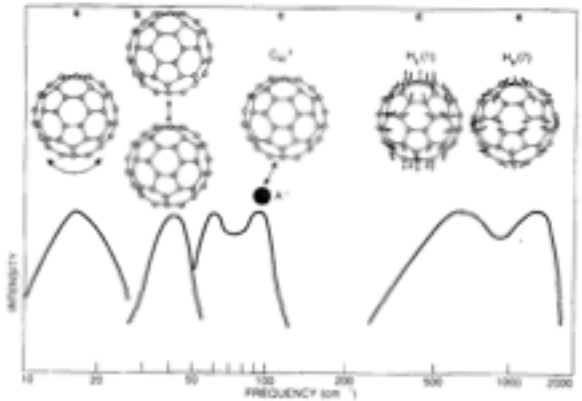
A SIMPLIFIED MODEL FOR A_nC_{60} (2)

$$-J_H(2S_i^2 + \frac{1}{2}L_i^2) - \frac{5}{6}J_H(n_i - 3)^2$$

Hund's rule
(F_2 Slater integral)

Electron-phonon interaction
t_{1u} coupled to H_{1g} phonons



In the antiadiabatic limit
identical with opposite sign

$$J = -J_H + J_{el-ph}$$ $$J_{el-ph} \approx 0.1eV$$ $$J_H \approx 0.07eV$$

J > 0 favors minimum S e L (inverted Hund's rule)

SIMPLE LIMITS

- Rather large U/W
- Smaller attraction than what pure e-ph calculation gives (competes with Hund): we use J=0.02eV
- Standard e-ph superconductivity now seems impossible!

$U << W$

Metal + Attraction J + Repulsion U

S-wave SC $\Delta = \sum_{ia} c^{+}_{ia\uparrow} c^{+}_{ia\downarrow}$

A = U - 10/3 J

Scattering amplitude in Cooper channel

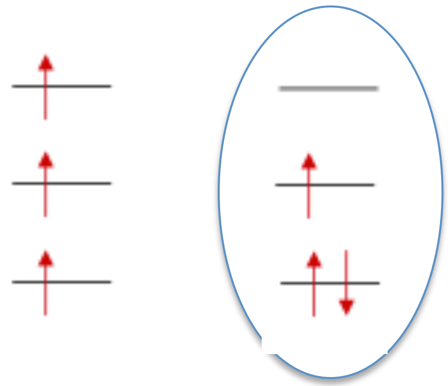
U > J No superconducting instability

SIMPLE LIMITS

$U >> W$ ⇒ The filling is integer
Mott Transition

Three electrons stuck on each site (buckyball)

The J term is still free to act



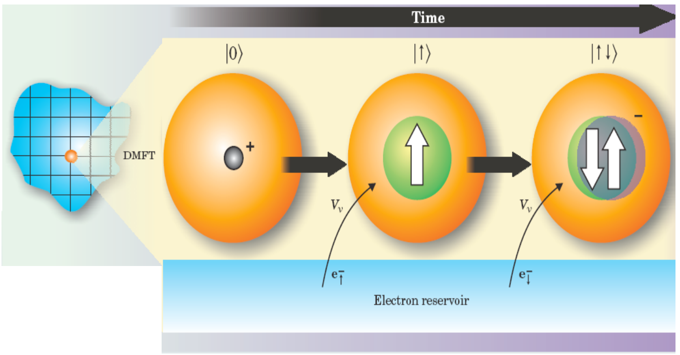
Mott Jahn-Teller Insulator $J > 0$ ⇒ S=1/2
L=1
low spin

GUESS HOW DO WE SOLVE THE MODEL?

Several competing Energy scales

Local (on-ball) Interaction Terms

DYNAMICAL MEAN-FIELD THEORY



A. Georges, G. Kotliar, W. Krauth, M.J. Rozenberg. Rev. Mod. Phys. 68, 13 (1996)

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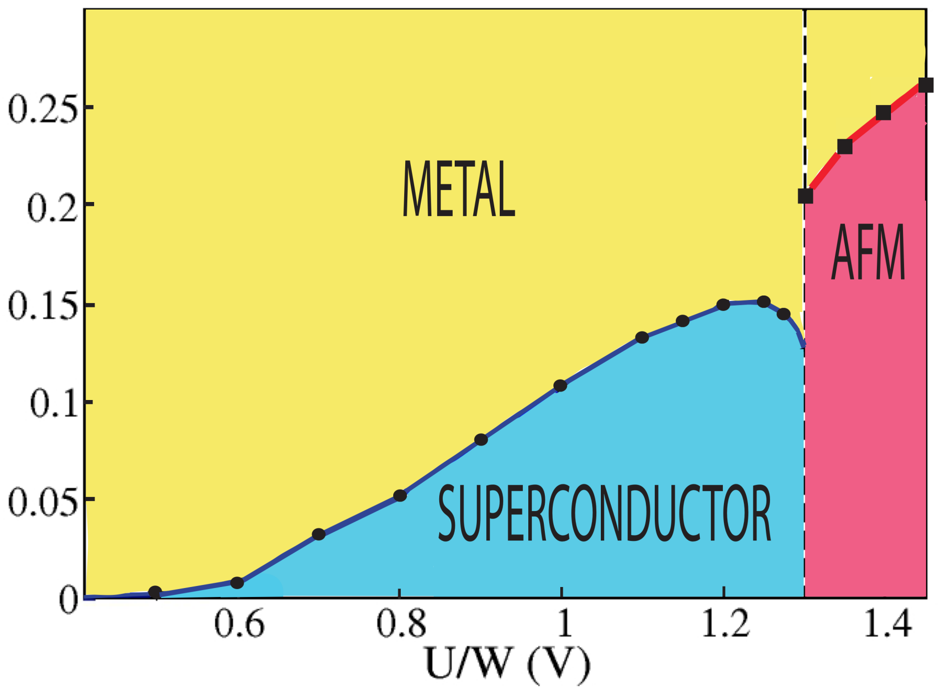
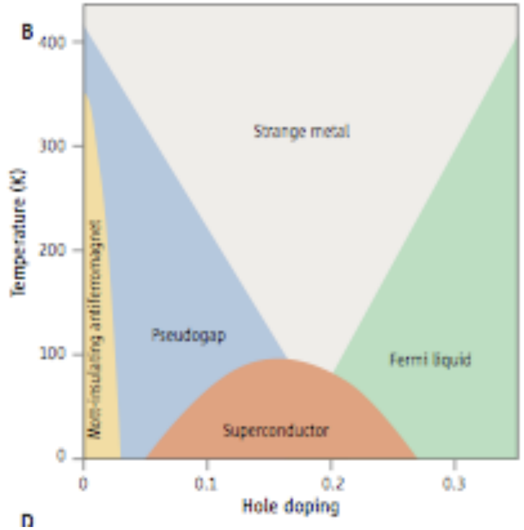
PHASE DIAGRAM



Cuprates

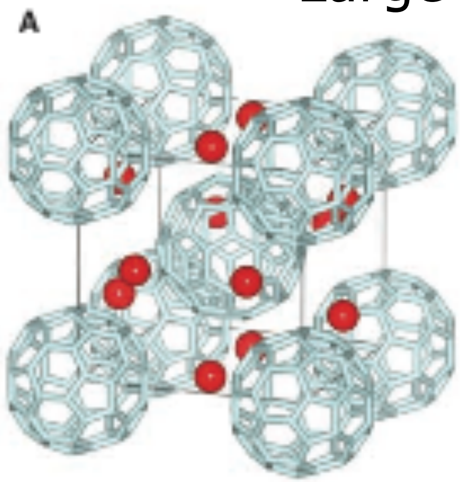


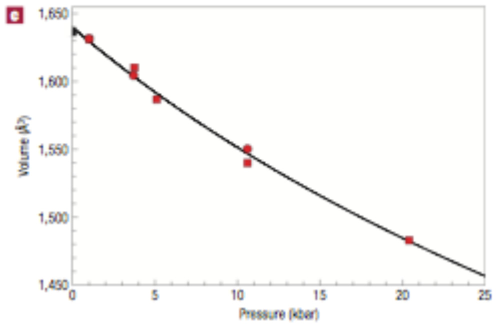
A bell-shaped T_c + first order transition to AFM
AF insulator has S=1/2 (Mott-Jahn-Teller)

M. C., M. Fabrizio, C. Castellani, and E. Tosatti, Rev. Mod. Phys. 81, 943 (2009)
[submitted in 2008. This will be important]

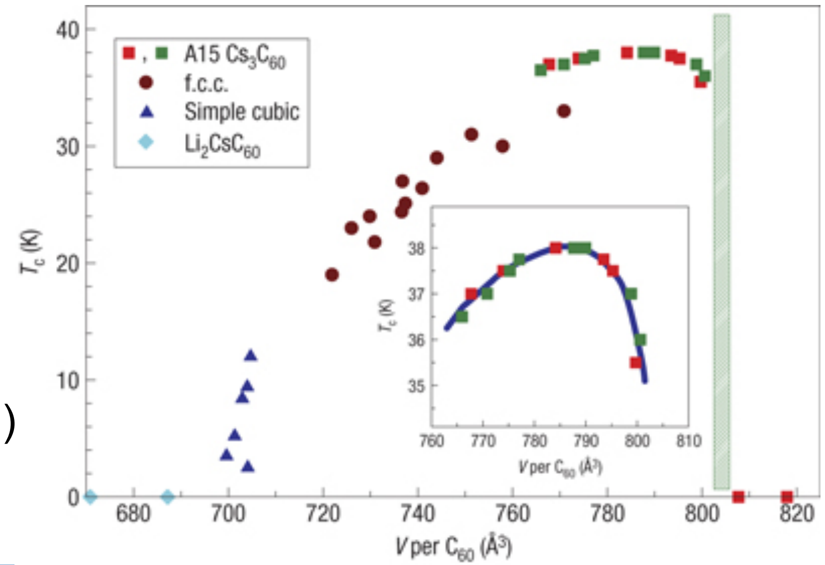
A NEW ENTRY (late 00s): A15 Cs_3C_{60}

Large lattice spacing





T_c = 38K



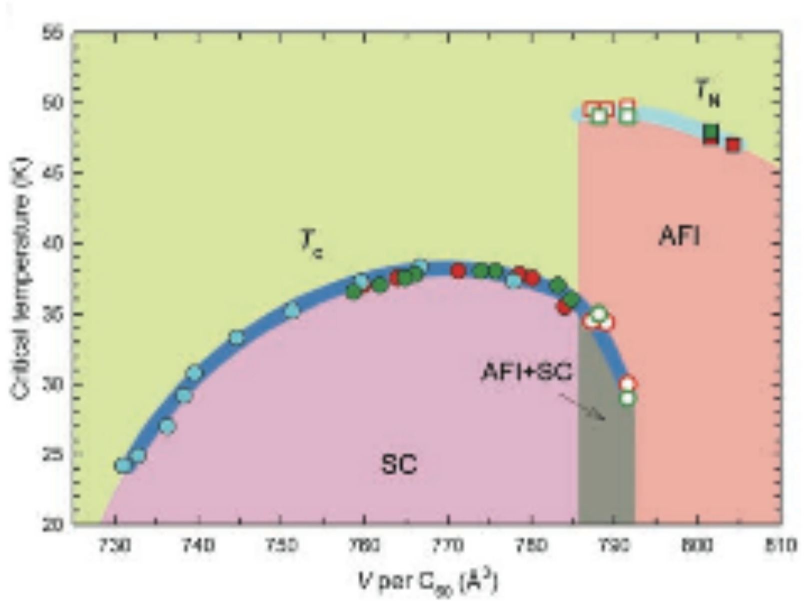
- Non superconducting at ambient pressure
- Superconducting bell from 4 to 7 Kbar

A. Y. Ganin et al. Nature Materials 7, 367 (2008)

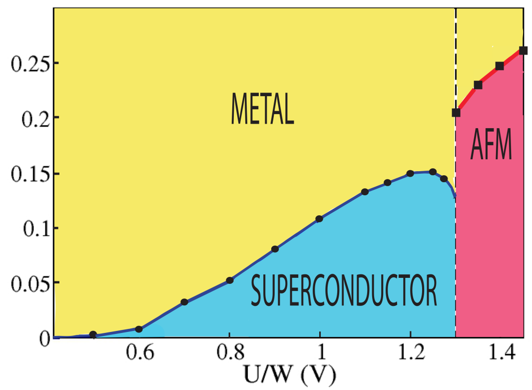
A NEW ENTRY: A15 Cs_3C_{60}

Pressure-driven transition between superconductor and antiferromagnetic insulator

- The Insulating state is a S=1/2 (low spin) AFM



Y. Takabayashi et al., Science 323, 1585 (2009)



The theoretical prediction is confirmed!

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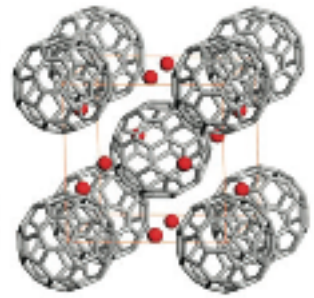
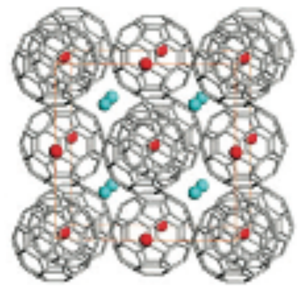
A NEW ENTRY: A15 Cs_3C_{60}

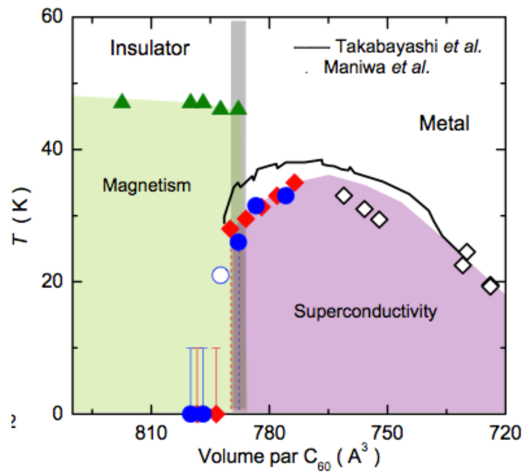
Comparison between A15 (bcc) and fcc Cs3C60

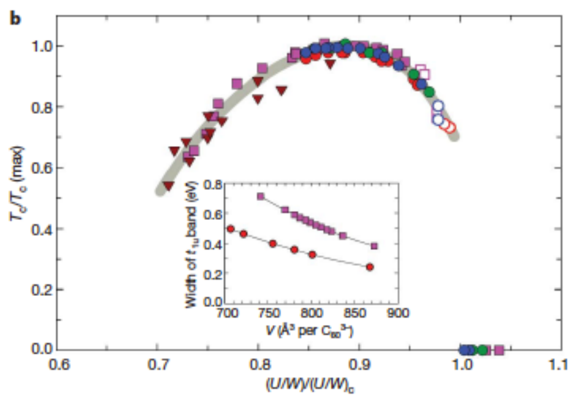
- Frustration reduces T_N by an order of magnitude
- T_c and the dome are essentially identical





The SC dome appears close to Mott





A. Y. Ganin et al. Nature 466, 221 (2010)

Y. Ihara et al. Phys. Rev. Lett. 104 256402 (2010)

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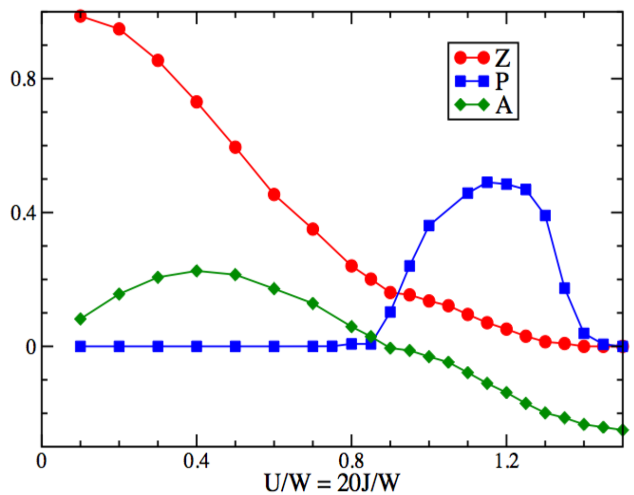
STRONGLY CORRELATED SUPERCONDUCTOR

W ⟶ ZW   Z << 1

A = ZU -10/3 J



U ⟶ ZU

Coulomb Repulsion

J ⟶ J

Electron-phonon

Strongly Correlated Superconductivity: “heavy” quasiparticles
Experiencing the bare attraction and reduced repulsion

Enhanced Superconductivity

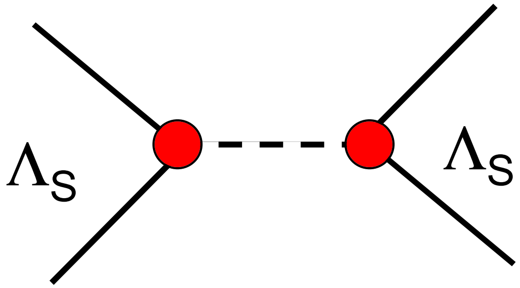
M.C., M. Fabrizio, C. Castellani, and E. Tosatti, Science 296, 2364 (2002)

WHY IS J UNRENORMALIZED?

Physical Argument

J is related to Spin and Orbital Degrees of Freedom
Still active when charge fluctuations are frozen by correlations
Even in the Mott state the singlet energy gain is J

Technical Argument

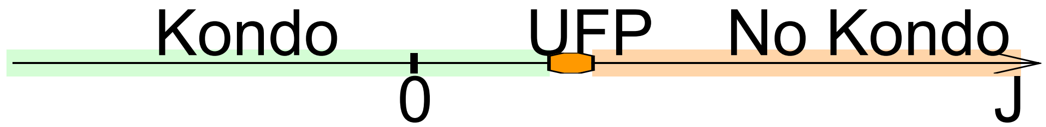


$$J_{QP} = z^2 \Lambda_S^2 J \cong z^2 \chi^2 J \cong J$$

$$\Lambda_S \propto \chi_{loc} \propto \frac{1}{Z}$$

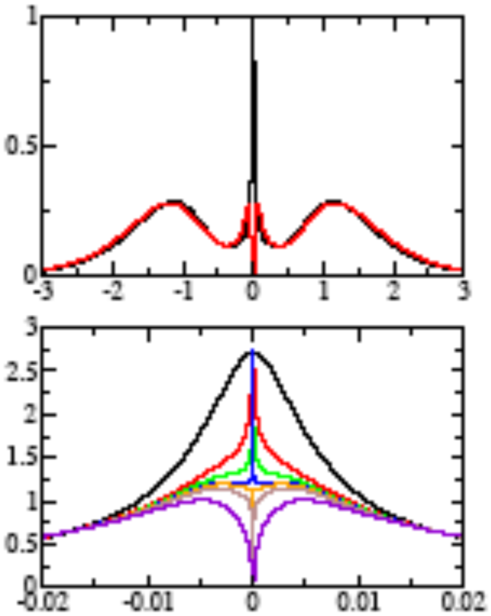
"General Mechanism": realized for any pairing that survives in the Mott state like Superexchange in cuprates

LESSONS FROM THE IMPURITY MODEL



Competition between ordinary Kondo screening leading to a Fermi liquid and J which forms local singlets (for two electrons)

$$\rho_{\pm}(\omega) = \frac{\rho_0}{2}\left(\frac{T_+^2}{\omega^2 + T_+^2} \pm \frac{T_-^2}{\omega^2 + T_-^2}\right)$$



- In the screened phase we obtain the FL Kondo resonance on top of a broader resonance
- In the unscreened phase the narrow peak becomes a Pseudogap
- At the Fixed Point only the broad resonance survives
- Superconductivity is the leading instability: it “cures” the critical point

L. De Leo and M. Fabrizio, Phys. Rev. B. 69, 245114 (2004)

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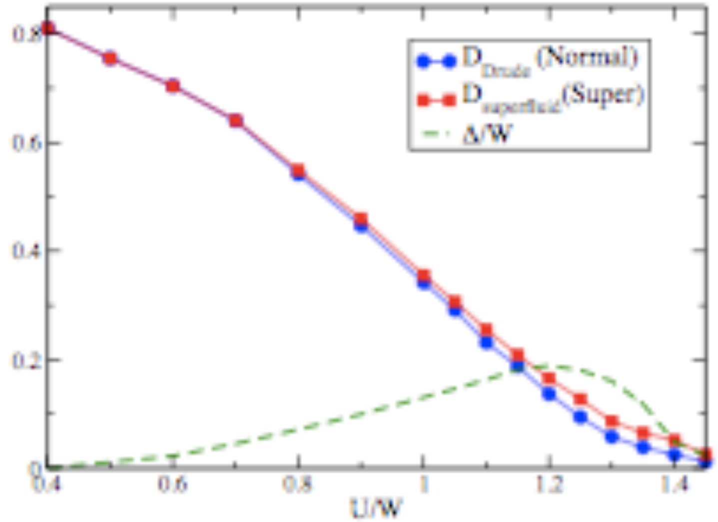
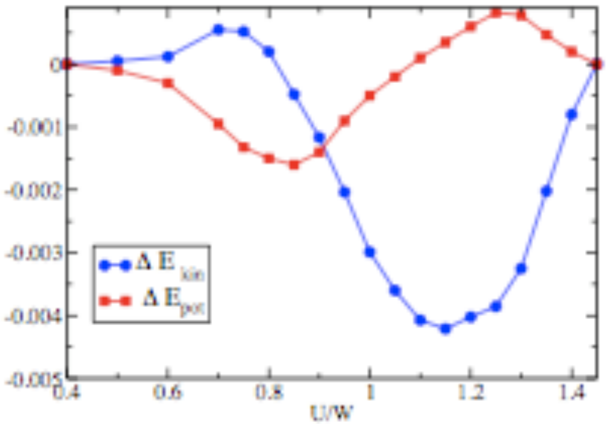
ENERGETIC BALANCE

SUPERCONDUCTIVITY "HEALS"
THE ANOMALOUS METAL CLOSE
TO THE CRITICAL POINT
(normal self-energy becomes regular)

Superfluid contribution
to optical conductivity
larger than the Drude
Weight of the metal





Close to Mott
a kinetic energy gain
stabilizes the SC

(as it happens in u.d. cuprates)

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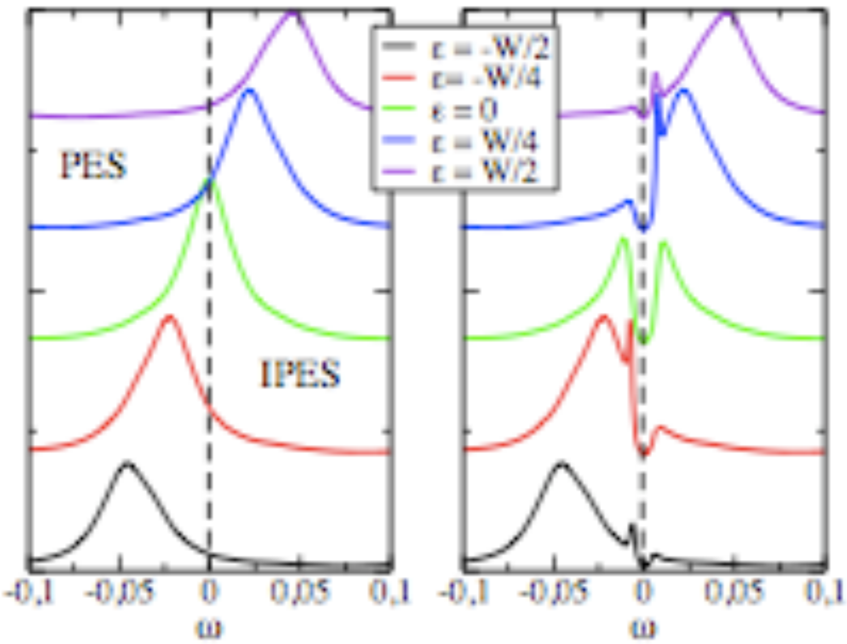
PHOTOEMISSION SPECTRA

Unexpanded Expanded

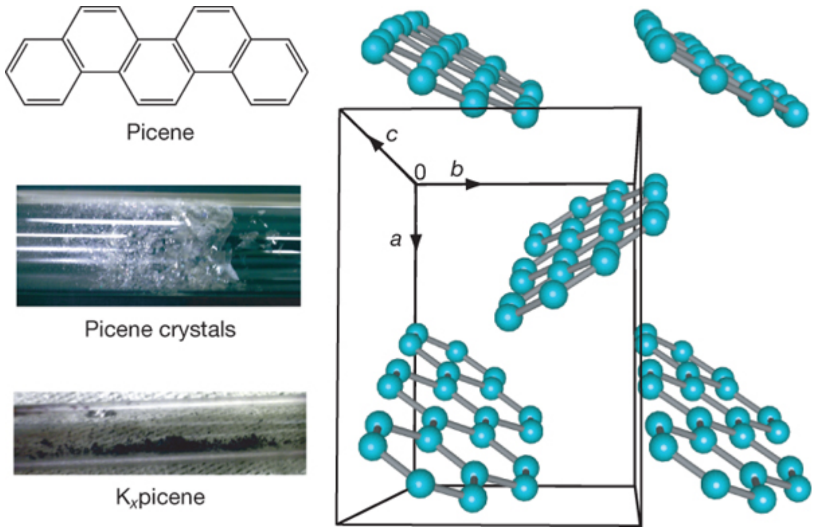


$$\rho(\varepsilon,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G(\varepsilon,\omega)$$

- No pseudogap in the "overdoped" side (small lattice spacing, K_3C_{60})
- Pseudogap in the "underdoped" side (expanded, Cs_3C_{60})

NEW ORGANIC SUPERCONDUCTORS

$C_{22}H_{14}$



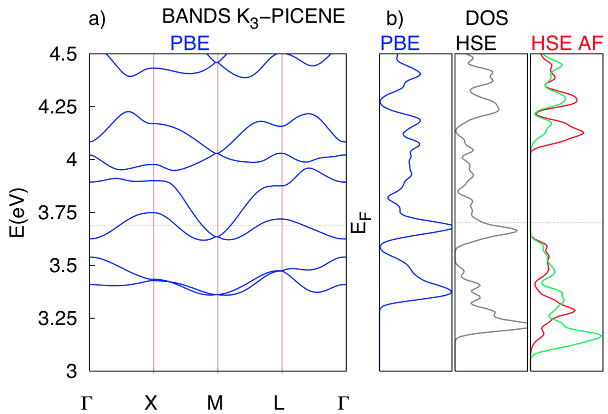
K_x-picene

$2.7 < x < 3.3$ $T_c = 18K$

Mitsuhashi et al. Nature 464, 76 (2010)

Signatures of electron-electron correlations

AFM ordering competing with SC



G. Giovannetti and M.C. Phys. Rev. B 83, 134508(2011)

CONCLUSIONS

- Alkali-doped fullerides display relevant electron correlation effects which dominate the phase diagram and the phonon-driven superconducting phase
- Transition between s-wave superconductor and AFM
- Phonon-driven Superconductivity is favored by strong correlation since it involves spin/orbital degrees of freedom (Strongly Correlated Superconductivity)
- The normal phase is not so normal, and it deviates from Fermi-liquid behavior
- Consequences on energetic balance (optics), specific heat, spin susceptibility, ARPES

M. C., M. Fabrizio, C. Castellani, and E. Tosatti, Rev. Mod. Phys. 81, 943 (2009)