Peierls vs. Mott: Resolving the VO_2 Controversy

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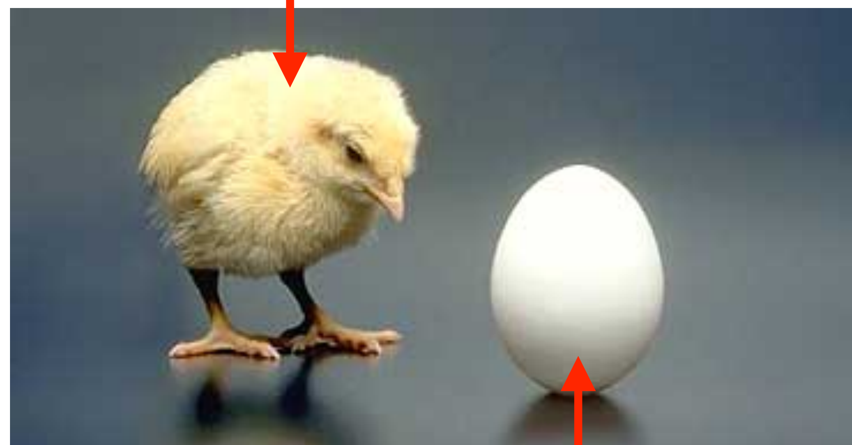
Peierls



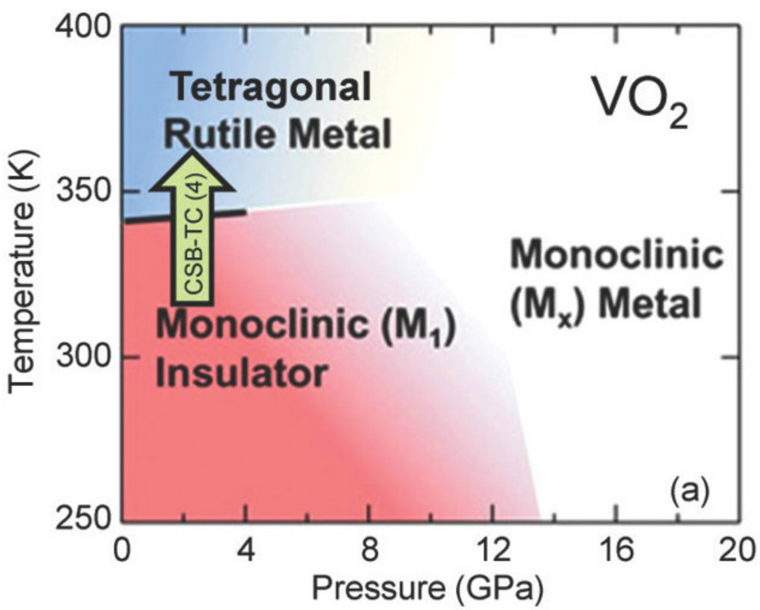
Mott

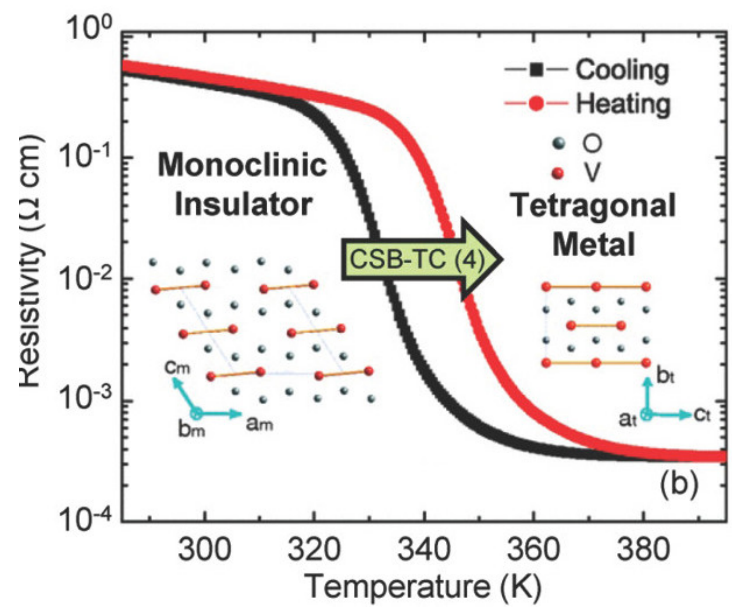
Collaborators:

Oscar Najera (Orsay)
Marcello Civelli (Orsay)
Marcelo Rozenberg (Orsay)
Tsung-Han Lee (FSU, Rutgers)
Serge Florens (Grenoble)

Funding: *NSF grants:*
DMR-1410132
…

Metal-Insulator Transition

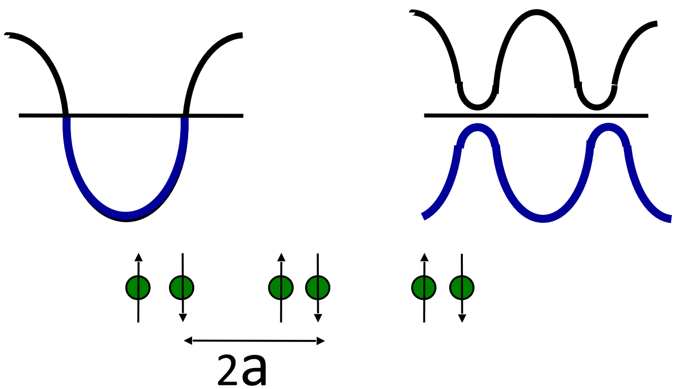


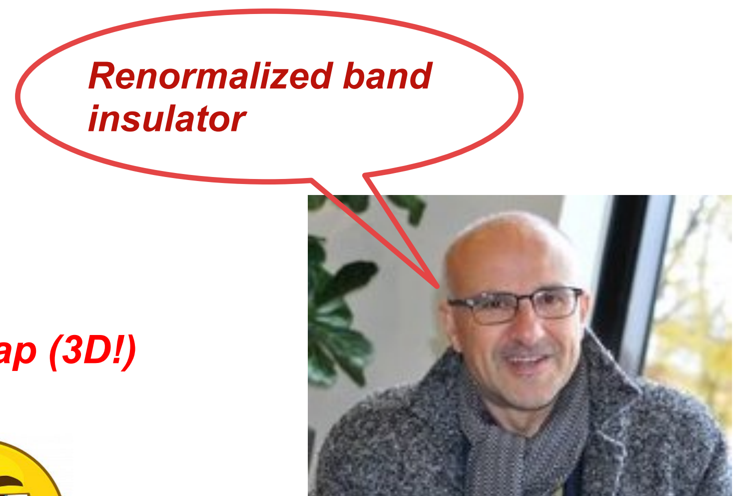


Structural transition - dimerization
Resistivity jump

Peierls?

Peierls opening of a gap (weak coupling effect):





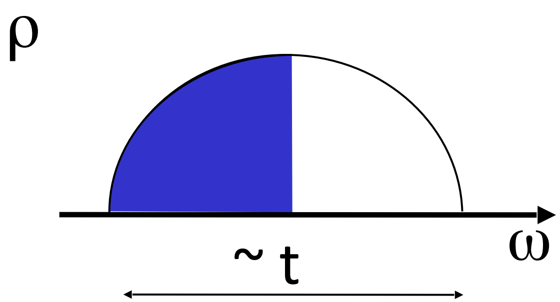
VO_2 DFT Band-structure (DFT): <u>insufficient</u> for gap (3D!)

Correlations: band gap increase?
(S. Biermann + A. Georges, 2005,…)

Mott?

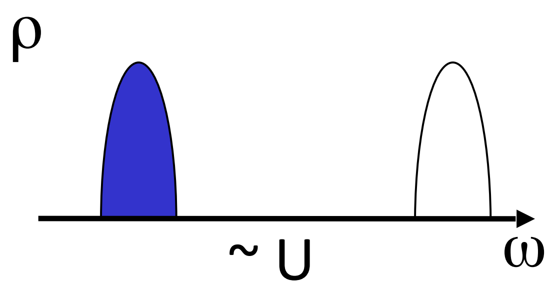
$$H = -\sum_{\langle ij\rangle,\sigma} t_{ij}(c_{i\sigma}^{+}c_{j\sigma} + c_{j\sigma}^{+}c_{i\sigma}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$

U = 0



metal

t = 0



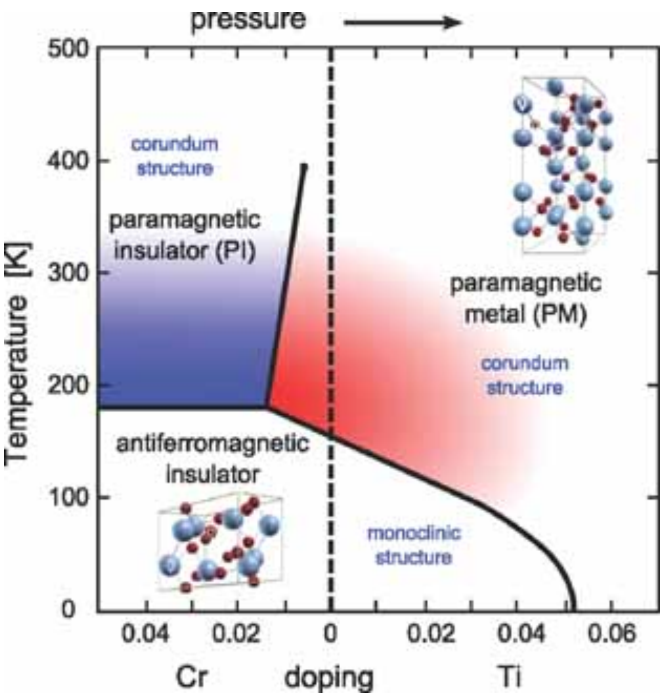
insulator

Thermally driven transition??

Thermally-Driven Mott Transitions?

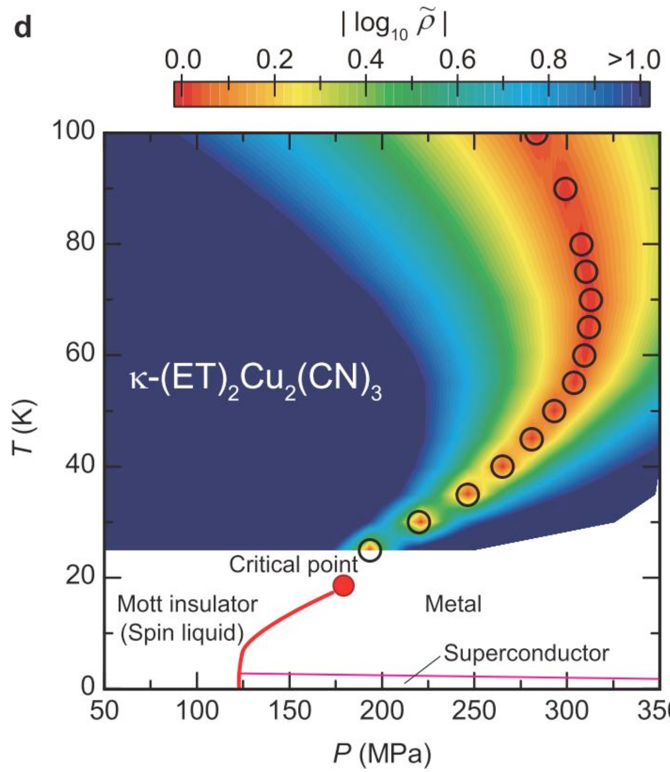
Transition-Metal Oxides: V_2O_3

Mc Whan (1973)



Organic Mott Systems

Kanoda (2005)



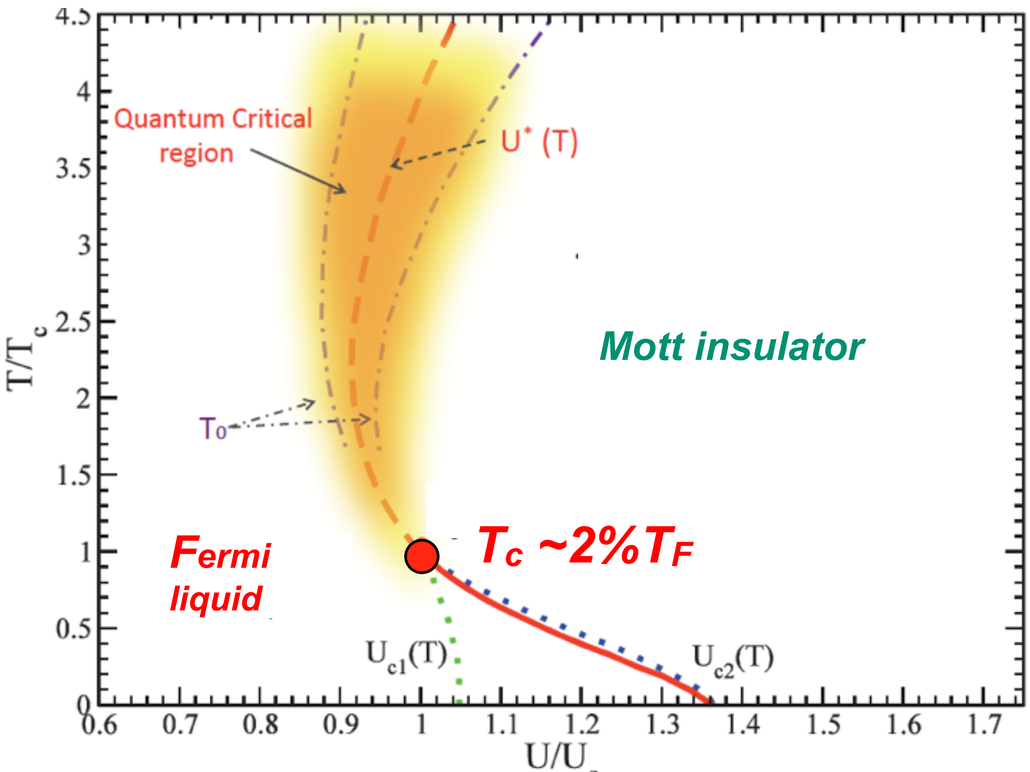
Finite temperature transport: the Mott transition at half-filling

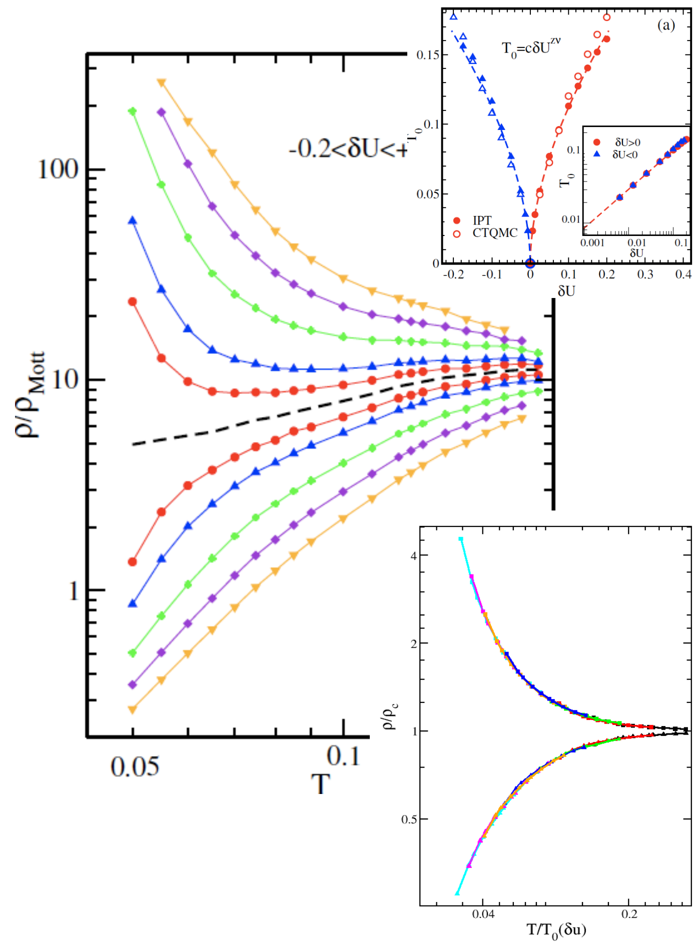
PRL 107, 026401 (2011) PHYSICAL REVIEW LETTERS week ending 8 JULY 2011

Quantum Critical Transport near the Mott Transition

H. Terletska,[1] J. Vučičević,[2] D. Tanasković,[2] and V. Dobrosavljević[1]

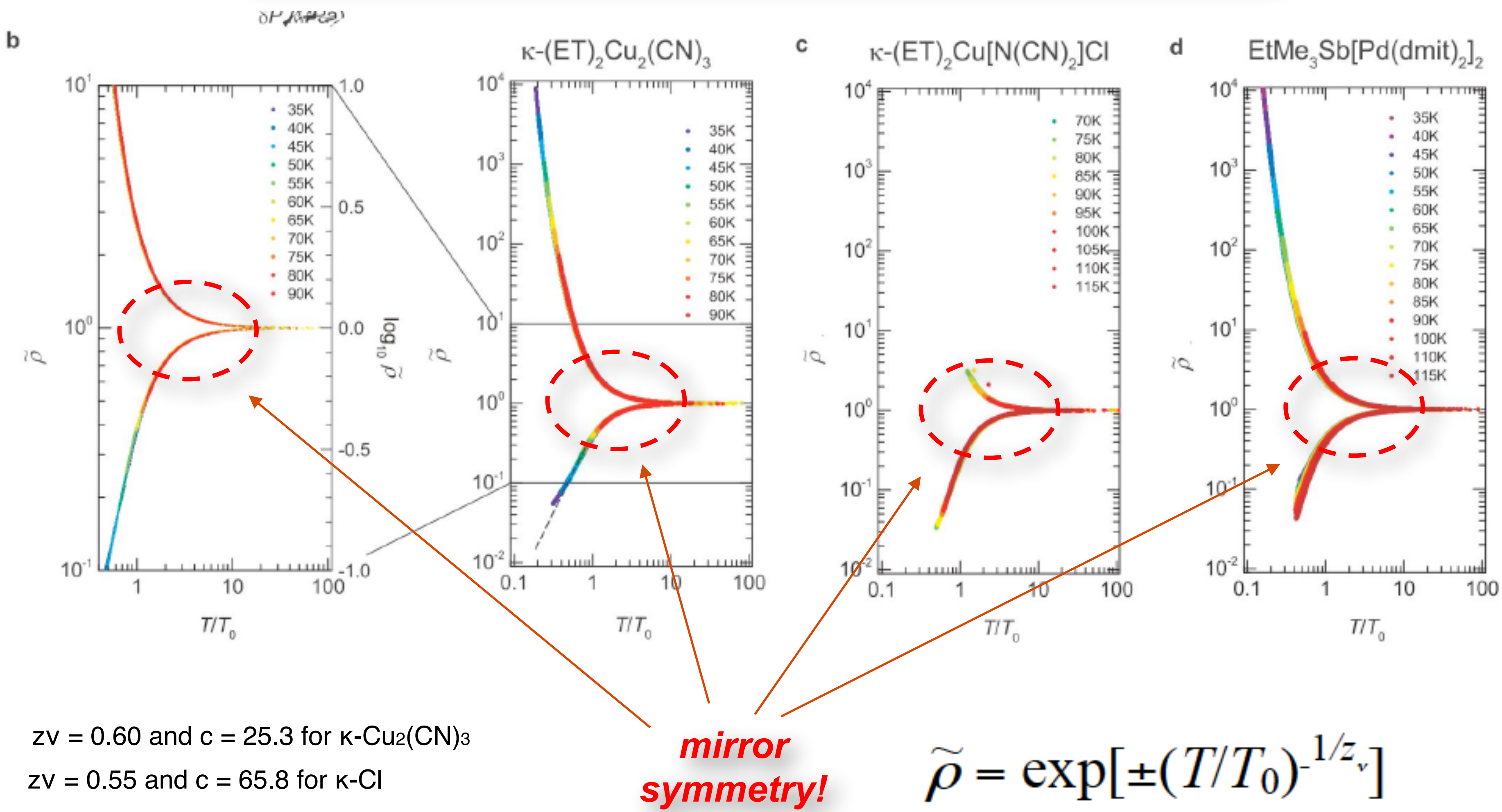
(single-site) DMFT Theory





Mott organics: universal high-T scaling

K. Kanoda et al., Nature Physics (2015)



zν = 0.60 and c = 25.3 for κ-$Cu_2(CN)_3$

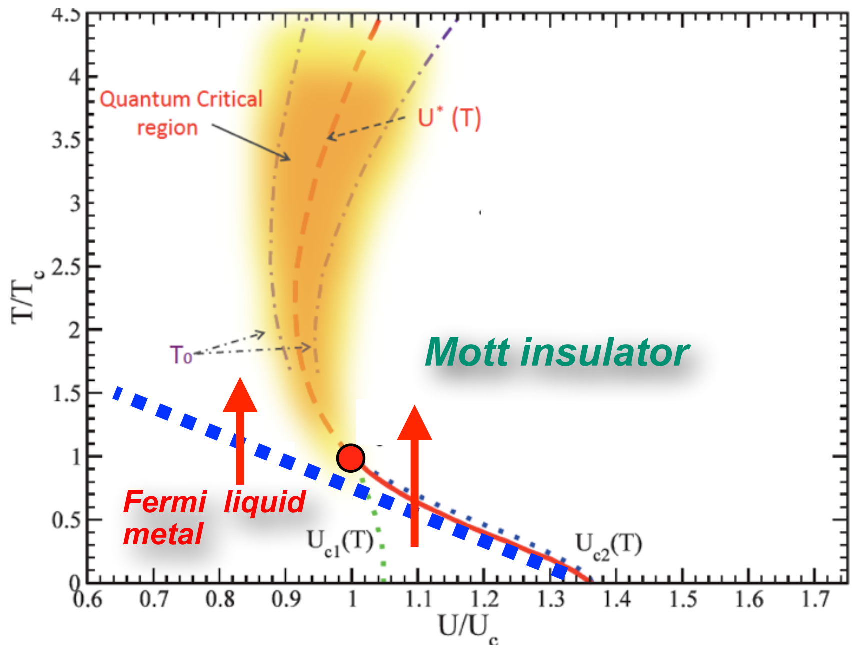
zν = 0.55 and c = 65.8 for κ-Cl

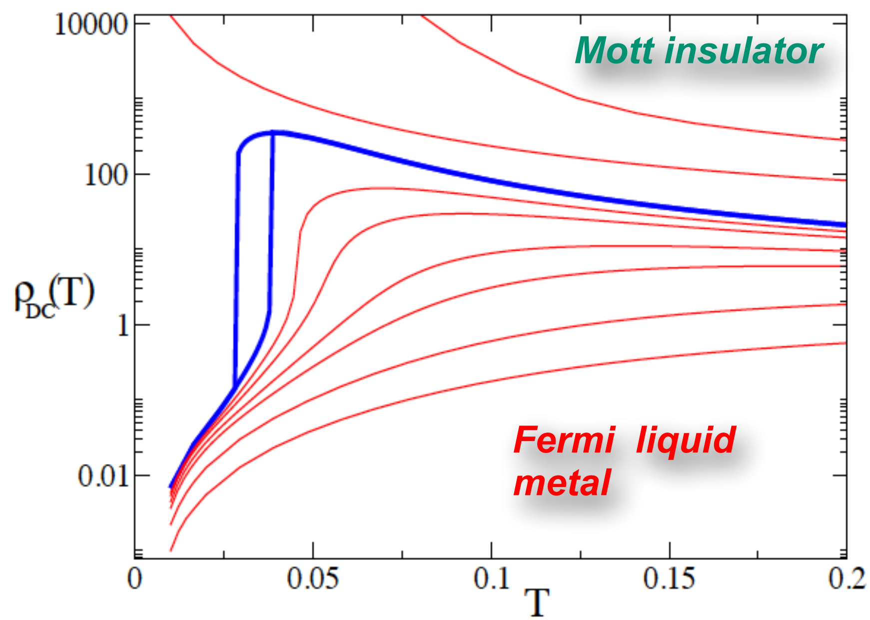
zν = 0.65 and c = 18.9 for $EtMe_3Sb$-dmit

$$\tilde{\rho} = \exp[\pm(T/T_0)^{-1/z_\nu}]$$

"stretched exponential"

Thermally-Driven Mott Transition?



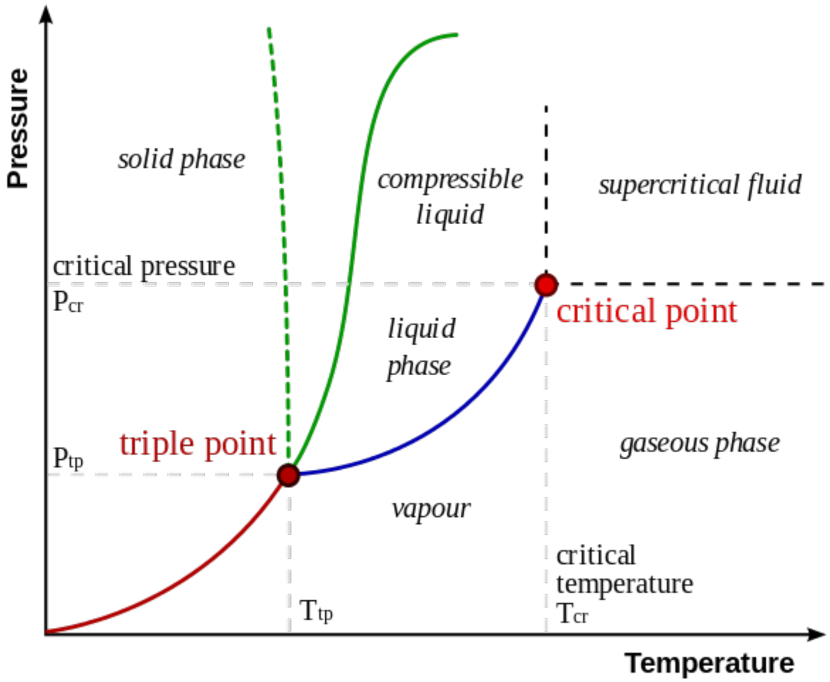


Low-T Insulator to High-T Metal:

WHY?

Entropy: Clausius-Clayperon Equation

(http://en.wikipedia.org/wiki/Clausius–Clapeyron_relation)



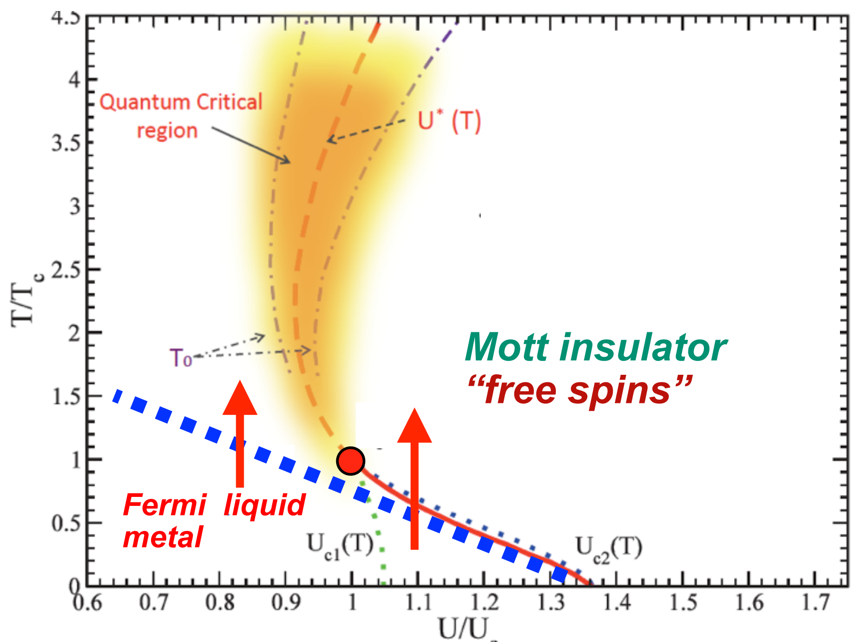
$$\frac{\mathrm{d}P}{\mathrm{d}T} = \frac{L}{T\,\Delta v} = \frac{\Delta s}{\Delta v}$$

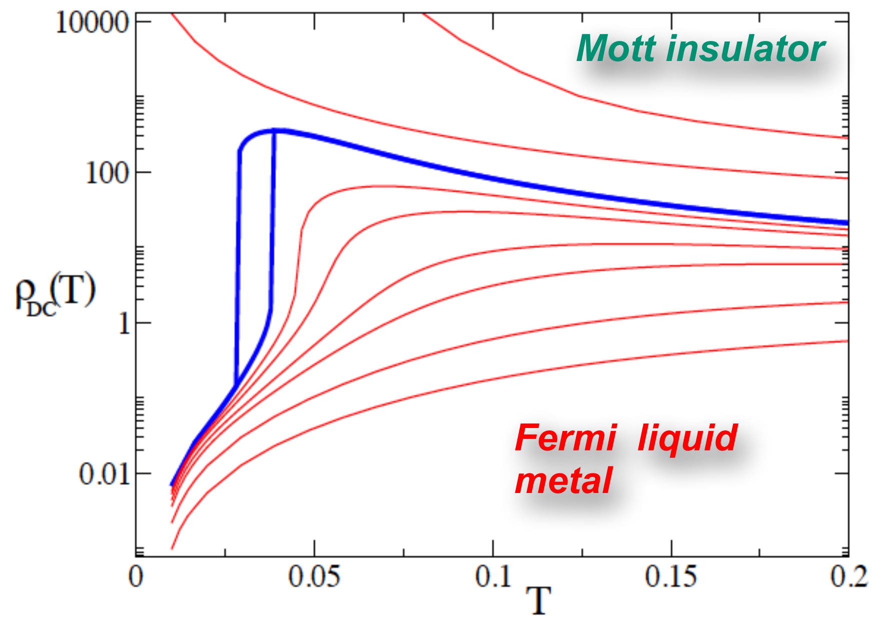
Rudolf Clausius
1822-1888
German
Mathematician / Physicist

Benoit Paul Emile Clapeyron
1799-1864
French
Engineer / Physicist

Gas has more entropy than liquid!

Thermally-Driven Mott Transition?

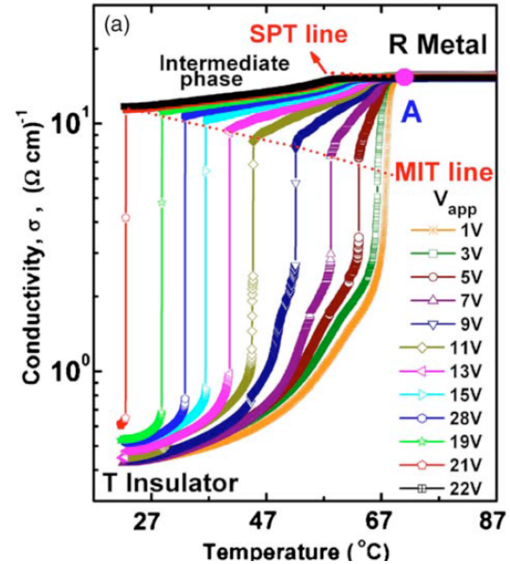




Low-T Insulator to High-T Metal:

Mott insulator has more (spin) entropy than FL

(no inter-site spin correlations)



New experiments: MIT by heating, but without structural change?

Metallic Monoclinic Phase?

(Hyun-Tak Kim, 2007)

PRL **109,** 166406 (2012) PHYSICAL REVIEW LETTERS week ending 19 OCTOBER 2012

Decoupling of Structural and Electronic Phase Transitions in VO_2

Zhensheng Tao, Tzong-Ru T. Han, Subhendra D. Mahanti, Phillip M. Duxbury, Fei Yuan, and Chong-Yu Ruan*

PRL **113,** 216402 (2014) PHYSICAL REVIEW LETTERS week ending 21 NOVEMBER 2014

Direct Observation of Decoupled Structural and Electronic Transitions and an Ambient Pressure Monocliniclike Metallic Phase of VO_2

J. Laverock,[1] S. Kittiwatanakul,[2] A. A. Zakharov,[3] Y. R. Niu,[3] B. Chen,[1] S. A. Wolf,[2,4] J. W. Lu,[4] and K. E. Smith[1,5]

Can one have a T-driven transition from a low T insulator to a high T metal without a structural (symmetry) change???

("Pure Mott")

?

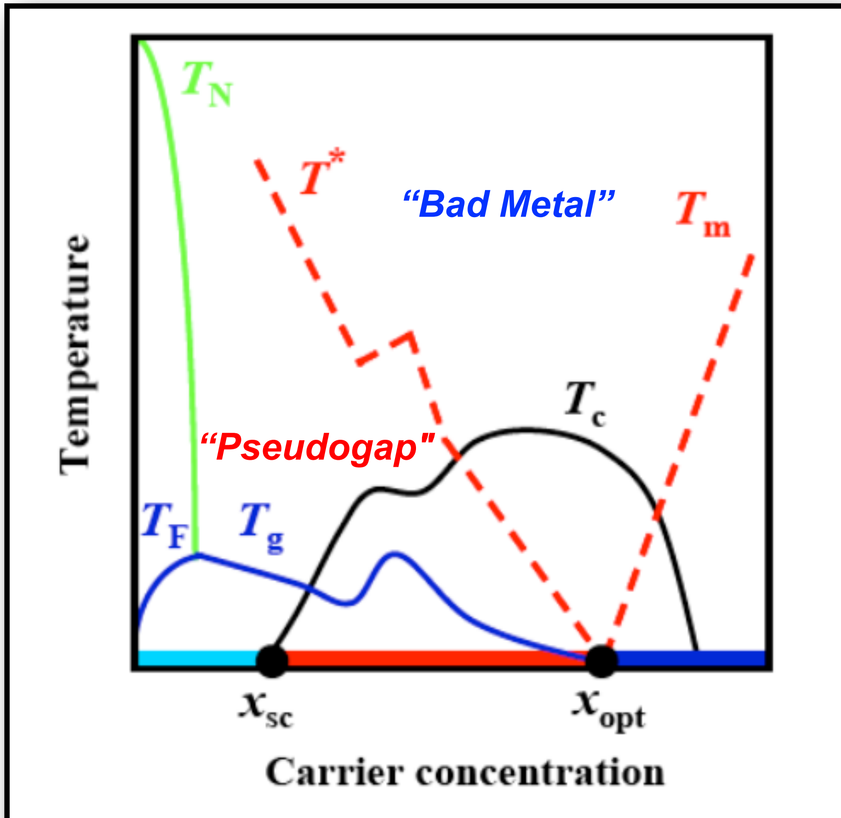
Taming the Mott Insulator: Super-exchange?

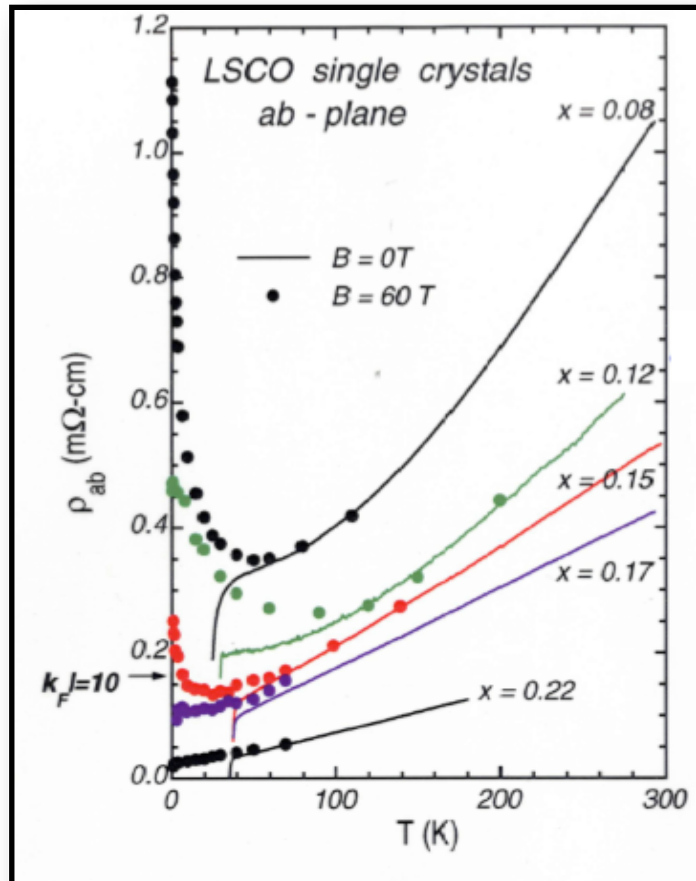
$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$

Generates AFM correlations, order

Not too important in most transition metal oxides due to Hund's rule coupling (FM correlations)

Exception: cuprates - spin gap from J

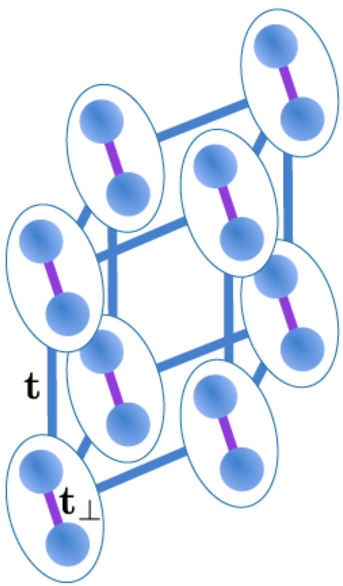


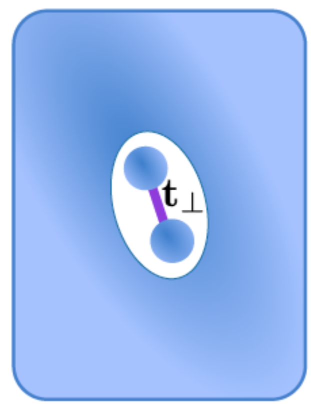


PHYSICAL REVIEW B **95**, 035113 (2017)

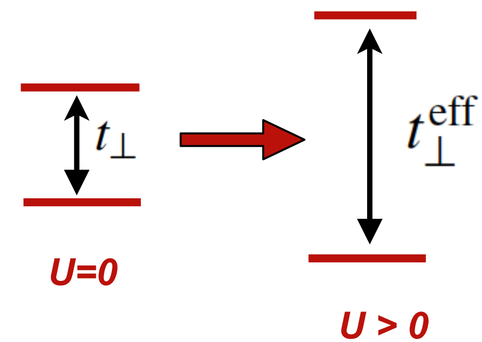
Resolving the VO_2 controversy: Mott mechanism dominates the insulator-to-metal transition

O. Nájera,[1] M. Civelli,[1] V. Dobrosavljević,[2] and M. J. Rozenberg[1]





$$t_\perp^{\text{eff}} = t_\perp + \mathrm{Re}[\Sigma_{12}]$$



Dimer hopping

$$H = \left[-t \sum_{\langle i,j\rangle\alpha\sigma} c^\dagger_{i\alpha\sigma} c_{j\alpha\sigma} + t_\perp \sum_{i\sigma} c^\dagger_{i1\sigma} c_{i2\sigma} + \text{H.c.} \right] + \sum_{i\alpha} U n_{i\alpha\uparrow} n_{i\alpha\downarrow},$$

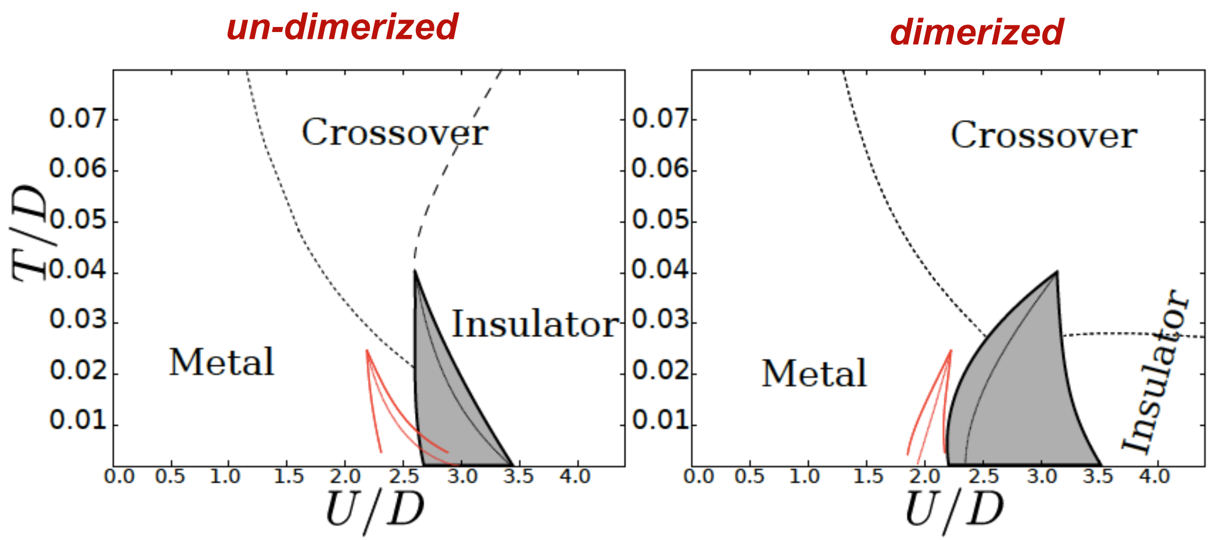
Spin correlations from dimerization:

Cluster DMFT on dimer ("RVB")

(CTQMC, ITP., Exact Diag.)

"Freeze" structure (dimerization), change T

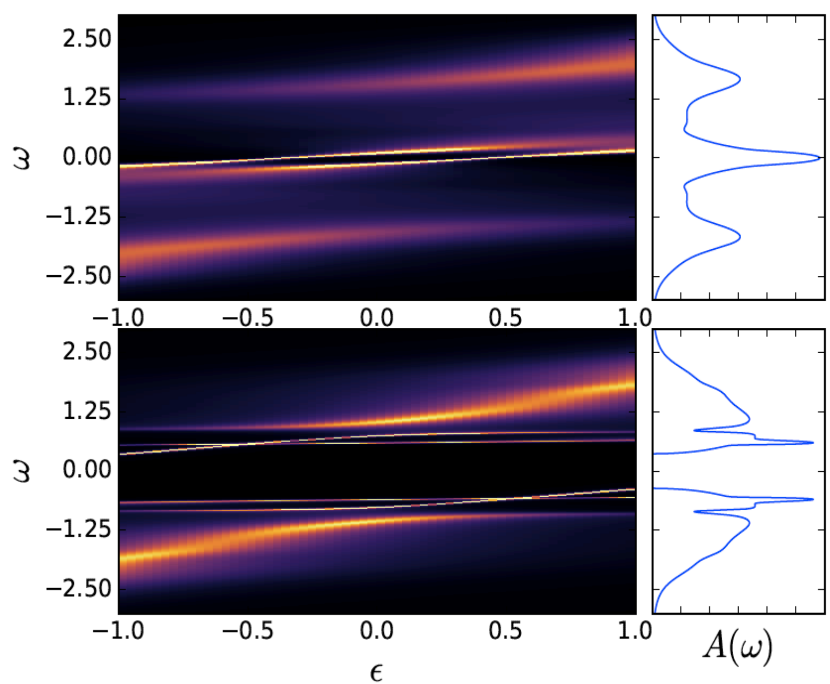
The tale of two singlets: removing entropy



MIT coexistence region: "spin-gap"

low T insulator
high T metal

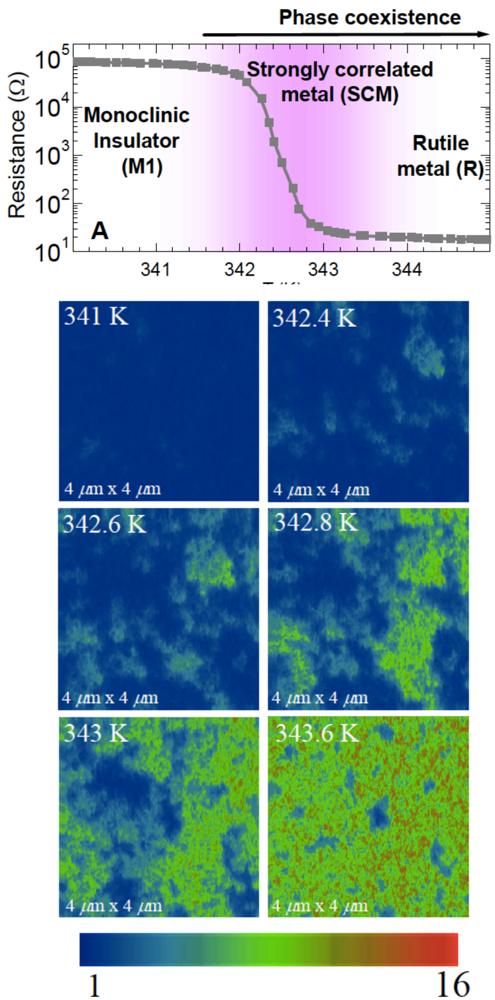
(Clausius-Clayperon)



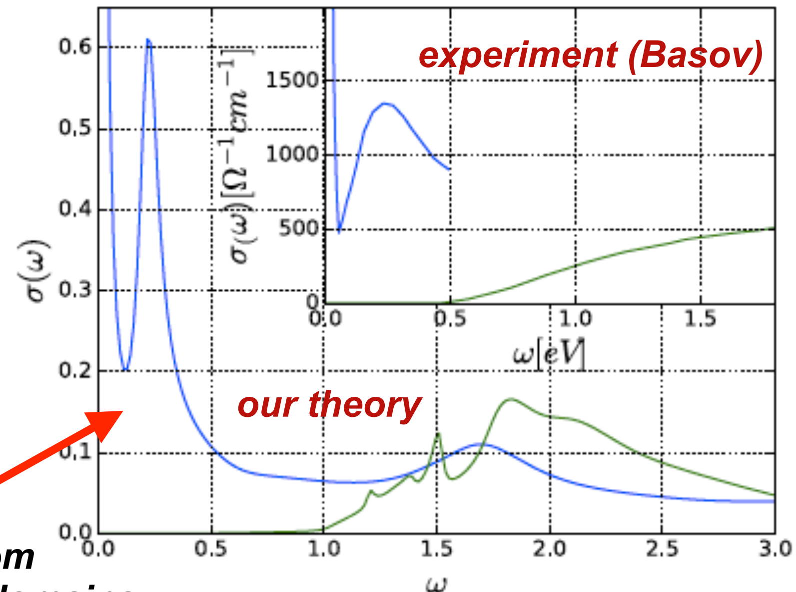
Monoclinic (dimerized) metal:
two overlapping quasiparticle bands

Monoclinic (dimerized) insulator:
gap opens due to singlet formation

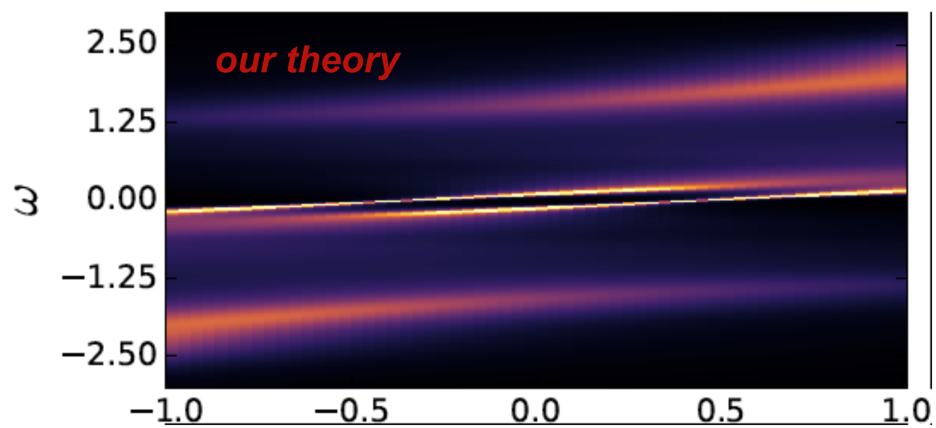
Monoclinic Metallic Phase as seen in optics



Basov, Science (2007)



signal from metallic domains

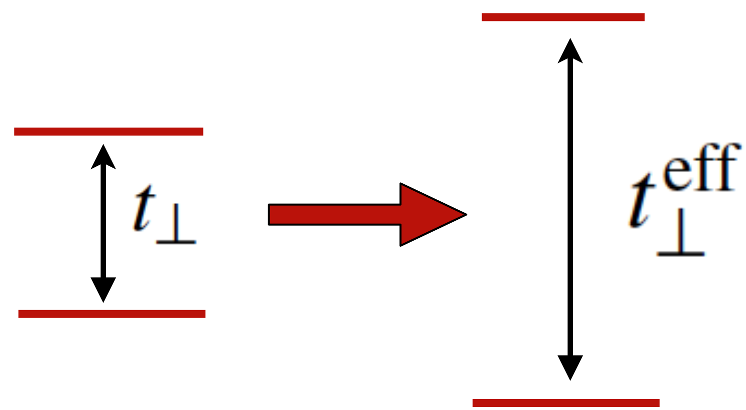


Metallic dimerized domains form before structural transition

What really happens?

inter-site spin correlation

$$t_\perp^{\mathrm{eff}} = t_\perp + \mathrm{Re}[\Sigma_{12}]$$



metal

insulator

Spin correlations large in insulators, weak ("screened") in metals

(note: effect ignored in "plain vanilla" RVB theory)

Where else is this important?

PRL 117, 136601 (2016) PHYSICAL REVIEW LETTERS week ending 23 SEPTEMBER 2016

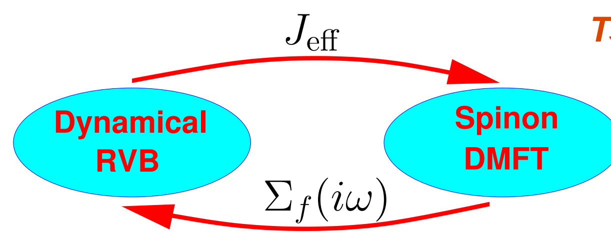
Fate of Spinons at the Mott Point

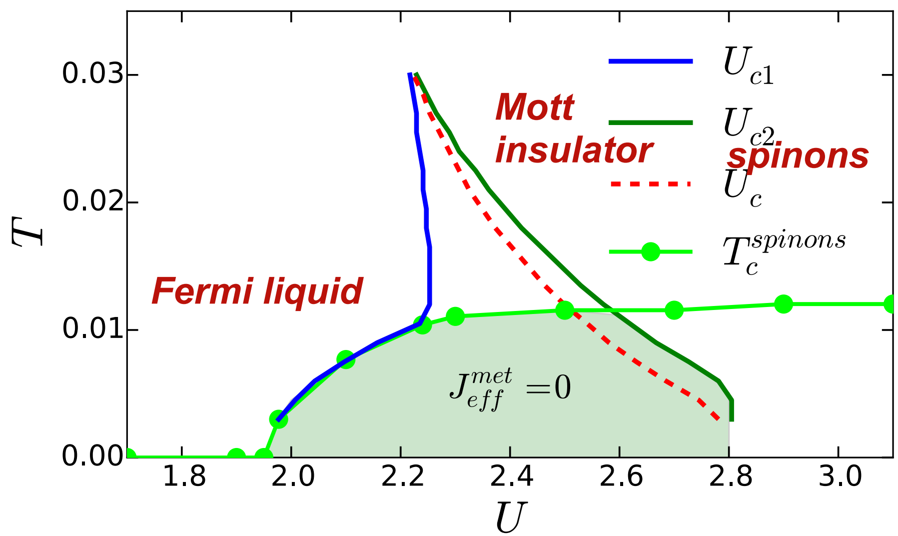
Tsung-Han Lee,[1] Serge Florens,[2] and Vladimir Dobrosavljević[1]

Tsung-Han Lee

Slave-rotor representation:

$$d^{\dagger}_{j,\sigma} = f^{\dagger}_{j,\sigma} e^{i\theta_j}$$





Spinion excitations destroyed by charge fluctuations as soon as the Mott gap closes

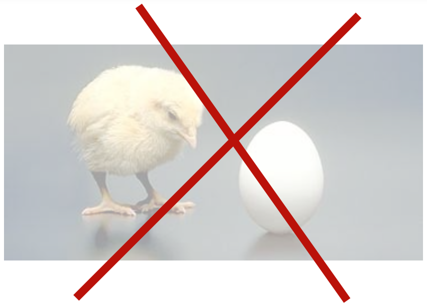
Physical picture of the Mott transition

The Fermi liquid and the (spinon) magnetic fluid are not "miscible"

→ ***Generic first-order transition in kappa-organics and VO_2***

Destruction of spin correlations when charge gap closes

omelette



oil and water

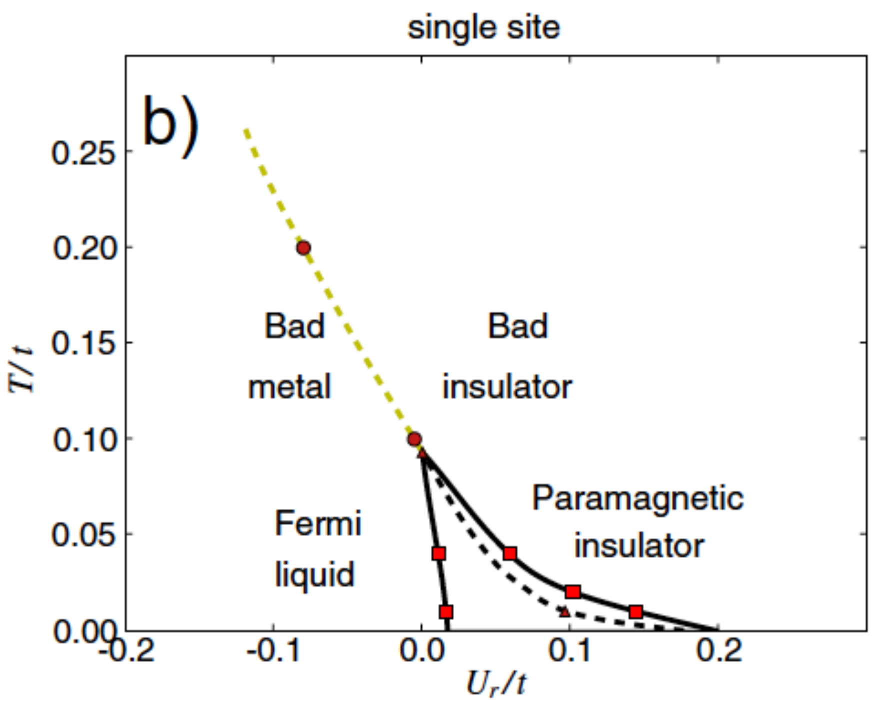
Super-exchange correlations: phase diagram at half-filling

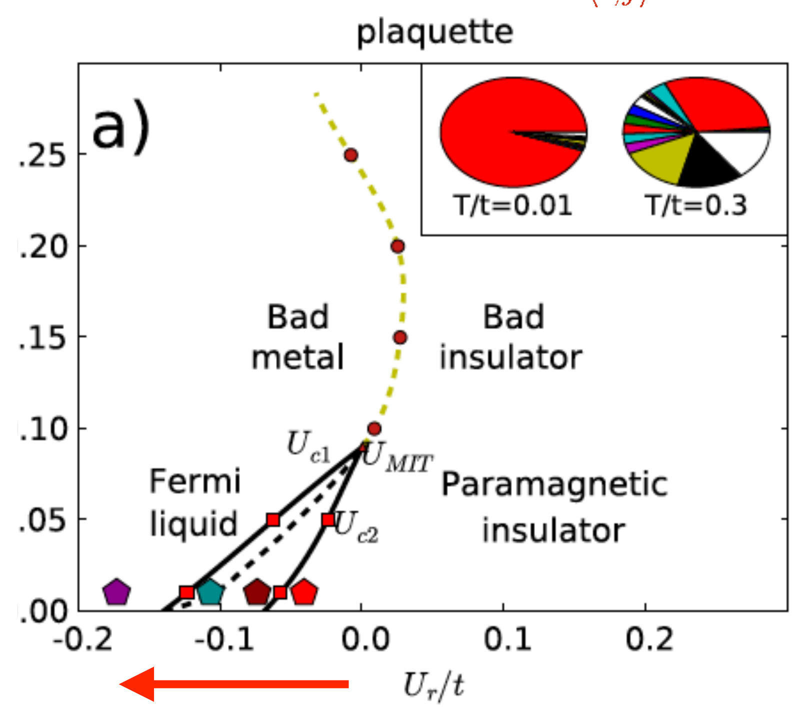
PRL **101,** 186403 (2008) PHYSICAL REVIEW LETTERS week ending 31 OCTOBER 2008

Cluster Dynamical Mean Field Theory of the Mott Transition

H. Park, K. Haule, and G. Kotliar

$$H = J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j$$





High dimensions (d=3)

Low dimensions d=1,2:

M2, MMP(M3) phase of VO_2 ??