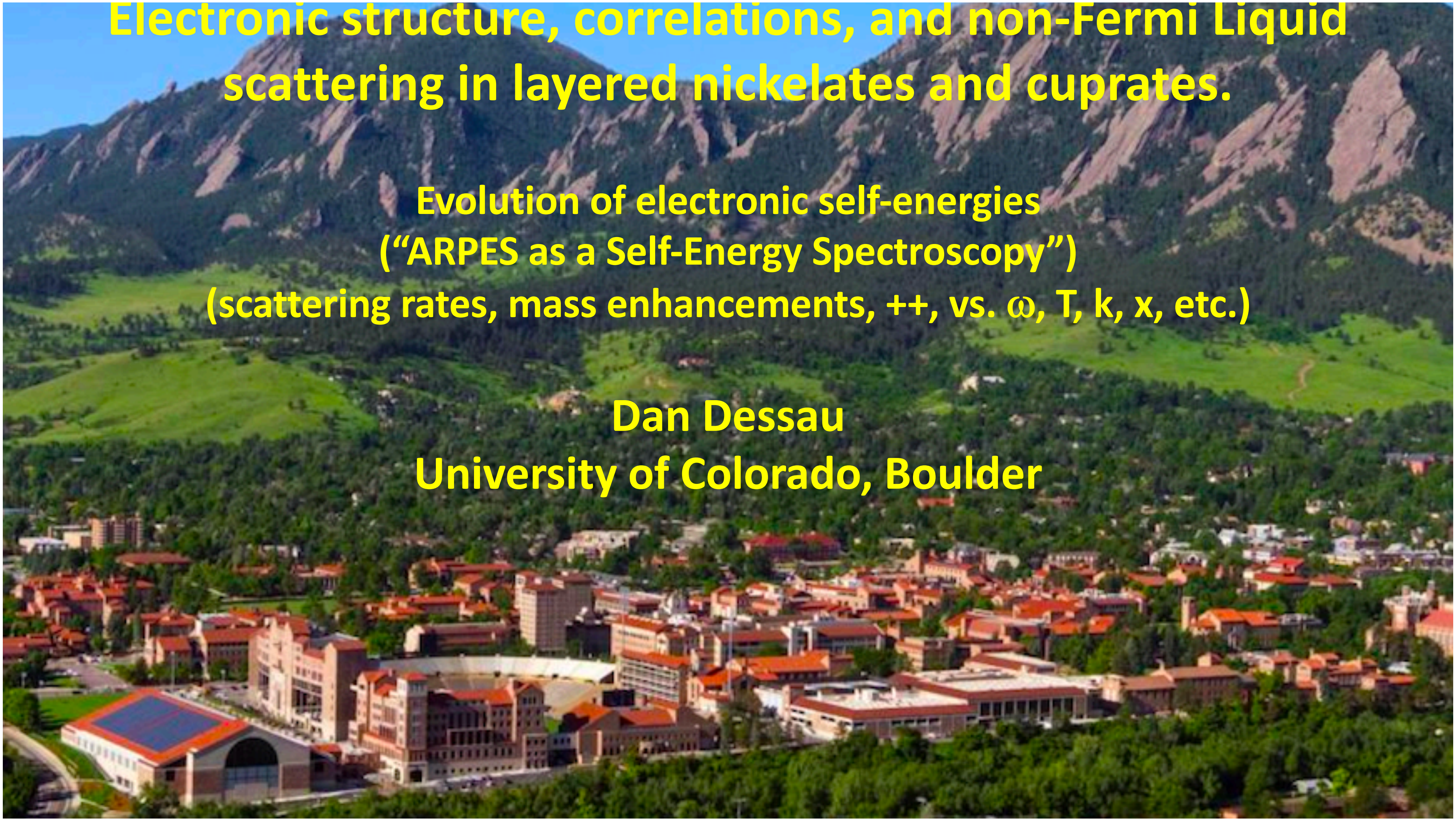

Electronic structure, correlations, and non-Fermi Liquid scattering in layered nickelates and cuprates.

Evolution of electronic self-energies
(“ARPES as a Self-Energy Spectroscopy”)
(scattering rates, mass enhancements, ++, vs. ω, T, k, x, etc.)

Dan Dessau

University of Colorado, Boulder


The original Flatirons
Boulder, CO

Team

Haoxiang Li, T. J. Reber, S. Parham, X. Zhou, K. Gordon, P. Hao, G.B. Arnold (Boulder)

H. Berger (Lausanne)

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J. Zhang, H. Zheng, J. Mitchell (Argonne)

ARPES measurements and analysis.

1) Nodal electron normal state scattering rate in cuprates. Power-law Liquid scattering rates - Beyond linear-in-ω,T. Planckian scattering. Non-quasiparticle. SYK model.

2) Self-energy analysis across entire BZ, including normal and SC state of the cuprates. Beyond 1D MDCs and EDCs. “ARPES as a self-energy spectroscopy.”

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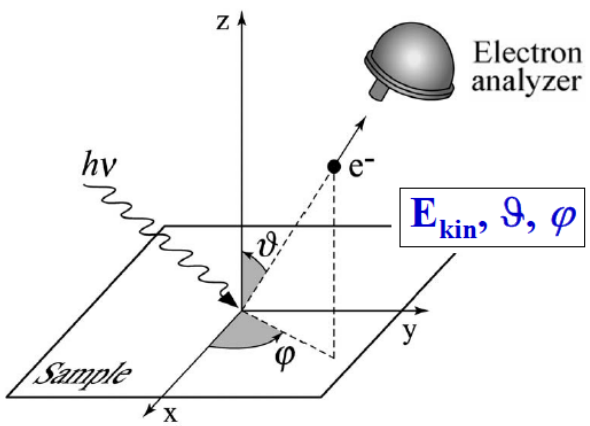
Angle Resolved Photoemission (ARPES) → k-resolved electronic structure



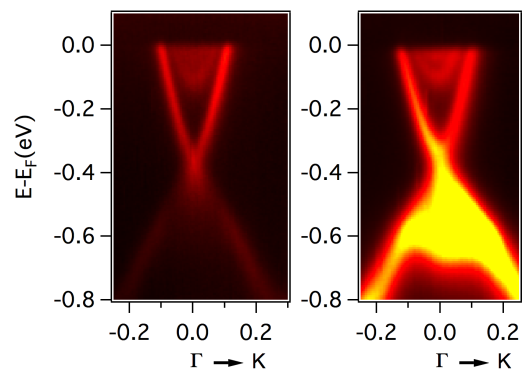
$$E_{kin}=h\nu-\Phi-E_i$$

$$\mathbf{K}=\mathbf{p}/\hbar=\sqrt{2m\boldsymbol{E}_{kin}}/\hbar$$

$$K_x = \frac{1}{\hbar}\sqrt{2mE_{kin}}\sin\vartheta\cos\varphi$$
$$K_y = \frac{1}{\hbar}\sqrt{2mE_{kin}}\sin\vartheta\sin\varphi$$
$$K_z = \frac{1}{\hbar}\sqrt{2mE_{kin}}\cos\vartheta$$

Typically used for peak tracking (band dispersions, Fermi surface mapping).

Example: Massless Dirac-like surface state dispersion in a topological insulator



Bi_2Se_3 surface state dispersion
Y. Cao, D.S.D. et al. Nature Physics 2013

ARPES as a self-energy spectroscopy

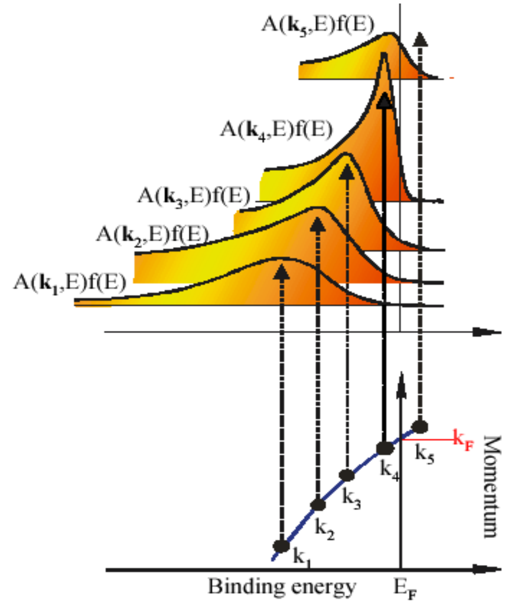
Spectral Function A(k,ω) = -Im G(k,ω)

$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\frac{\Sigma''(\mathbf{k},\omega)}{[\omega-\epsilon_{\mathbf{k}}-\Sigma'(\mathbf{k},\omega)]^2+[\Sigma''(\mathbf{k},\omega)]^2}$$

Bare band energy

Renormalized dispersion
(e.g. kinks, mass renormalization)

Peak widths
(Lifetimes or scattering rates)



Σ=Σ'+iΣ" = electron "self energy".
Contains the details of the electronic interactions.

Major goal: Develop ARPES as a true self-energy spectroscopy. Connect to (and explain) transport, optics, thermodynamics.

Intermediate step: Improve the quantitative accuracy of ARPES measurement and analysis.

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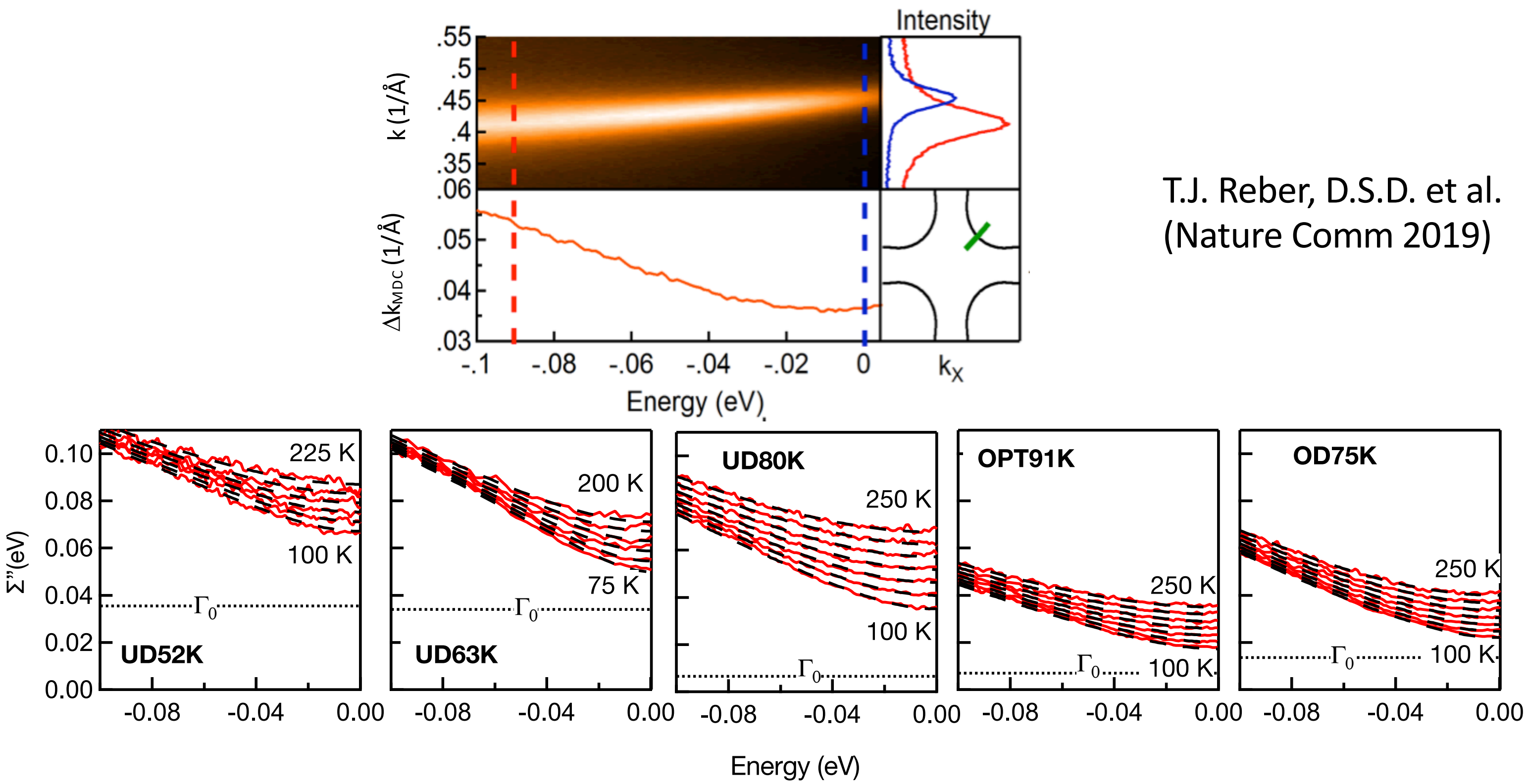
Normal-state nodal ARPES scattering rates (Σ”) as a function of ω,T, doping (Bi2212).

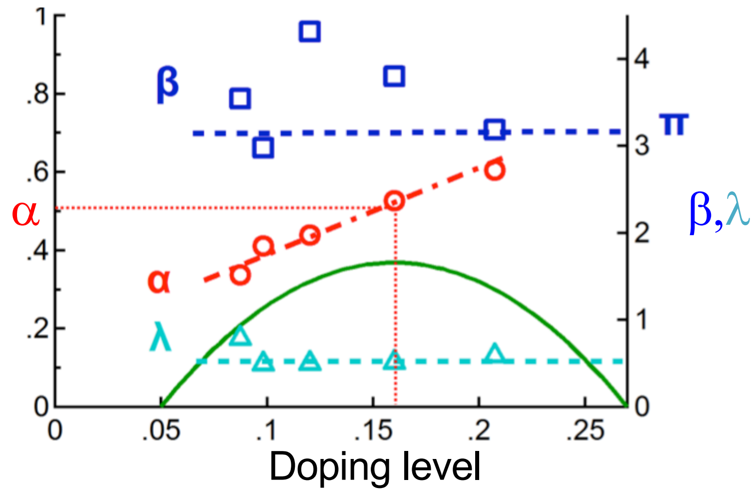


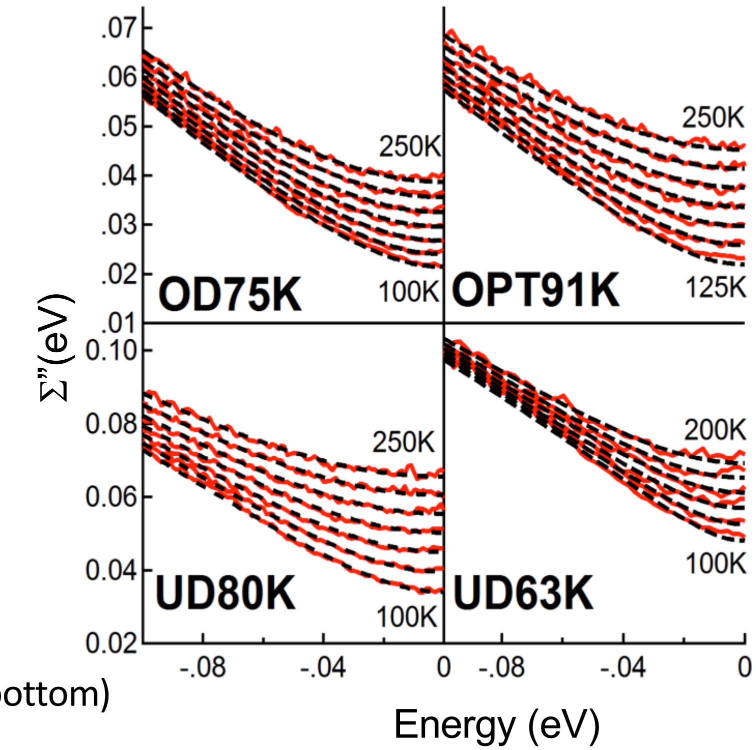
T.J. Reber, D.S.D. et al.
(Nature Comm 2019)

All data looks quadratic at low ω (FL-like), linear at high ω (MFL-like).
All data for one sample (many T and E) fit simultaneously to a more general form of Σ(ω,T).

Ansatz for normal state Σ" - the Power Law Liquid (PLL)
All data on one sample fit simultaneously.

$$\Sigma''_{PLL} = \Gamma_0 + \lambda \frac{[(\hbar\omega)^2 + (\beta k_B T)^2]^{\alpha}}{(\hbar\omega_N)^{2\alpha-1}}$$





ω_N (unit normalization) fixed at 0.5 eV (~ band bottom)

Γ_0=impurities+disorder (discussed later)

$\beta \sim \pi$. Expected from Matsubara and Fermi Liquid (not previously proven).

λ = coupling strength ~ constant=0.5.

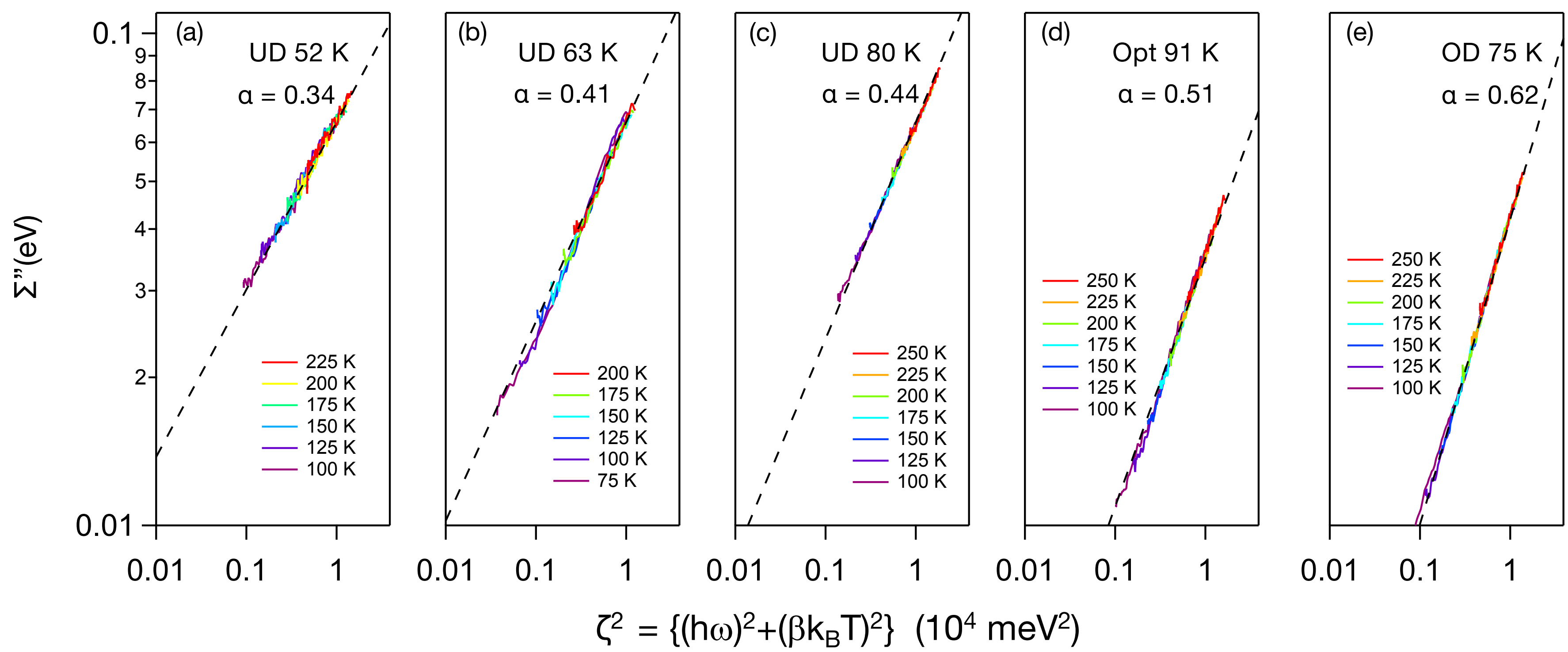
α= 0.5 : ω,T linear (Marginal Fermi Liquid).

α=1 : ω,T quadratic (True Fermi Liquid)

Entire evolution essentially controlled by the one parameter α.

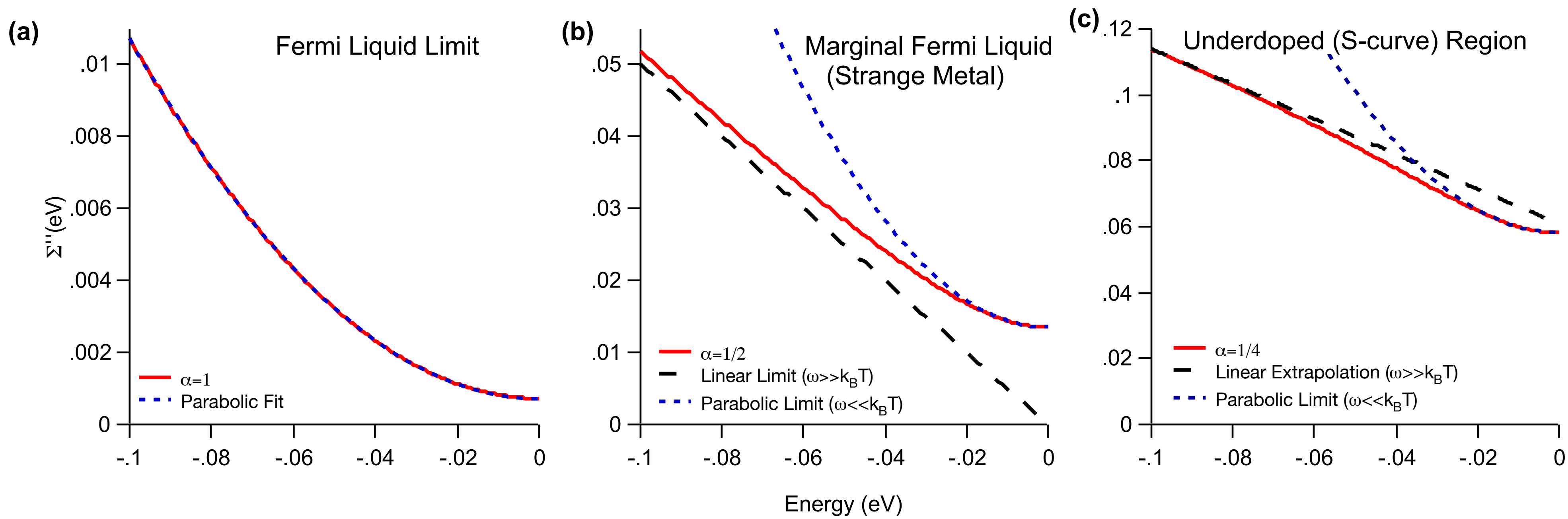
T.J. Reber, D.S.D. et al. (Nature Comm 2019)

Scaling behavior of Σ” as a function of T and ω



Different slopes → different power law exponents α.

Low energy behavior of Σ" as a function of PLL exponent α (T=100K)

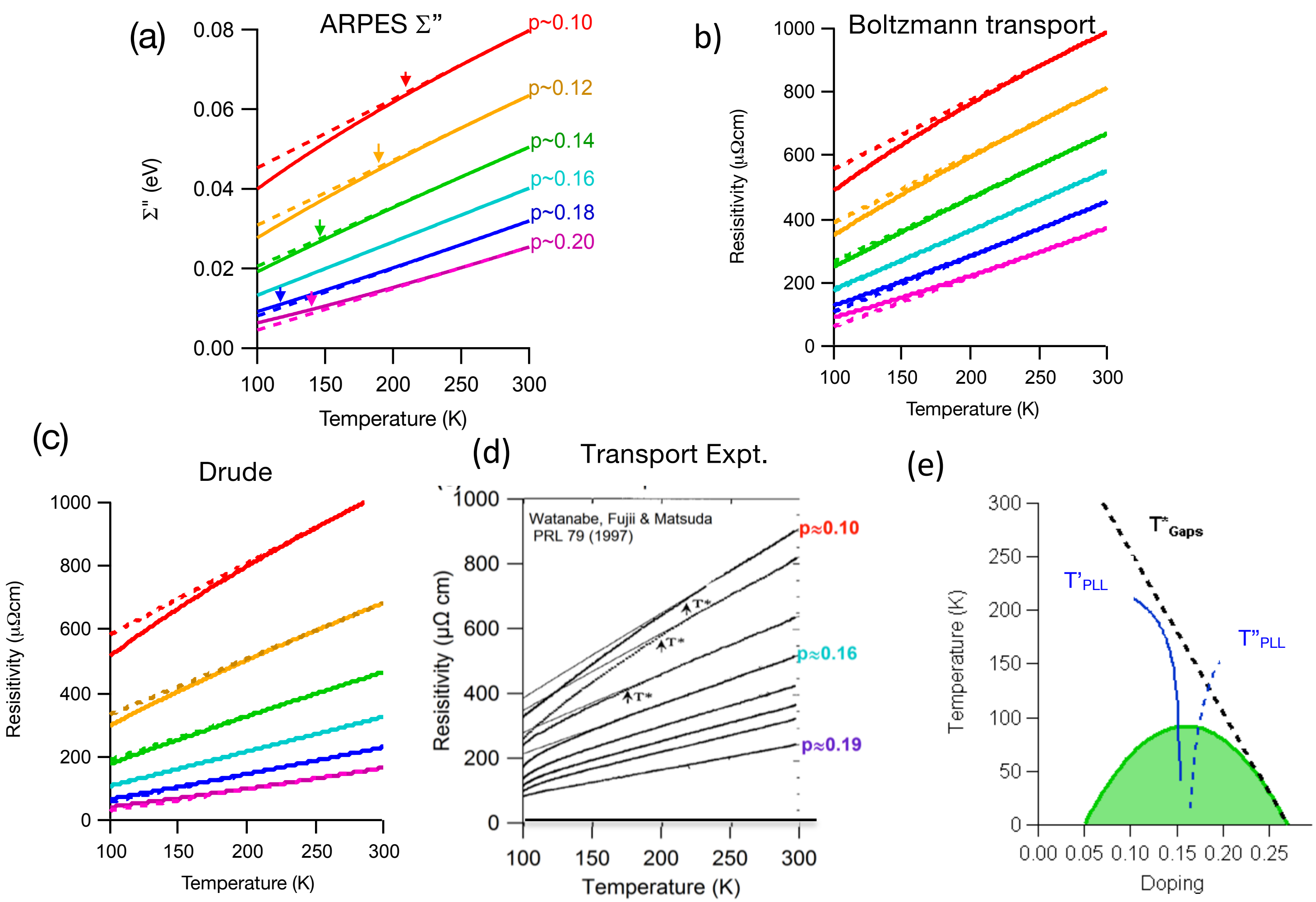


Low energy scattering rate right of middle and right spectra look quadratic.

Fermi Liquid? (No).

Indicative of quasiparticles? (No).

Resistivity vs T from Power Law Liquid Σ”

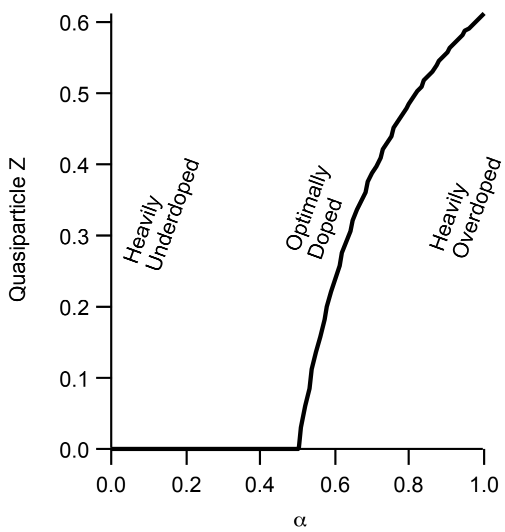


QP Residue and optical conductivity from Power Law Liquid Σ”

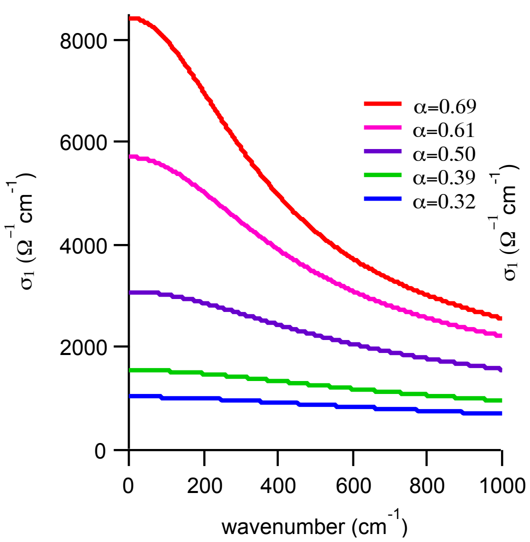
T= 0

T=300K

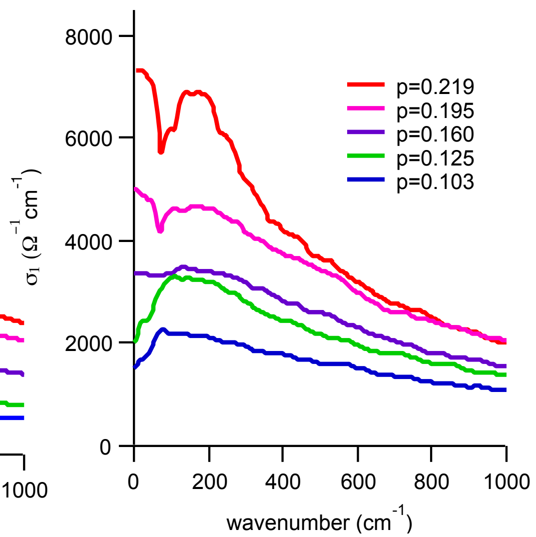
(Analytical calculation)



Calculated from Σ”



From Hwang/Timusk (2004)



“Sharpish” ARPES QP-like peak and optical Drude peak even when T=0 quasiparticle residue is identically zero.

Power Law Liquid as a quantum critical phase (not quantum critical point).

Luttinger liquid physics in 1D. PLL spectra (and ARPES data) don't have the power law spectral weight that the LL physics has.

SYK (Sachdev/Ye/Kitaev) exactly solvable models.

Quantum gravity-based ideas (ADS/CFT)?

Doped Hubbard model?

The superconductivity is born out of these states.

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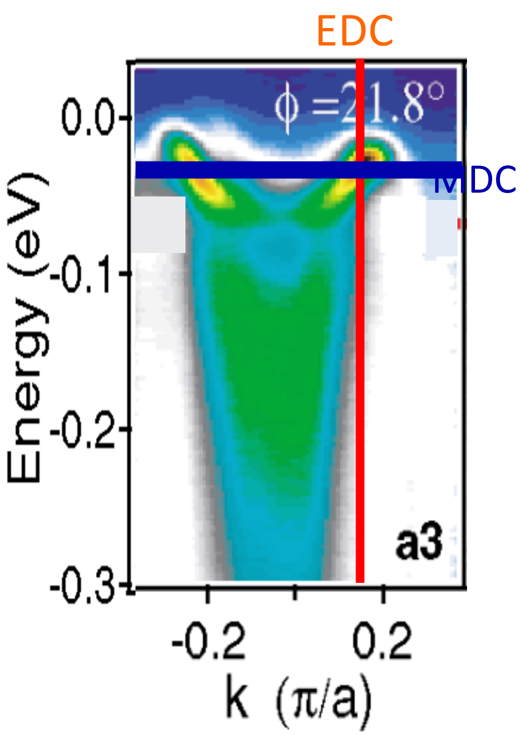
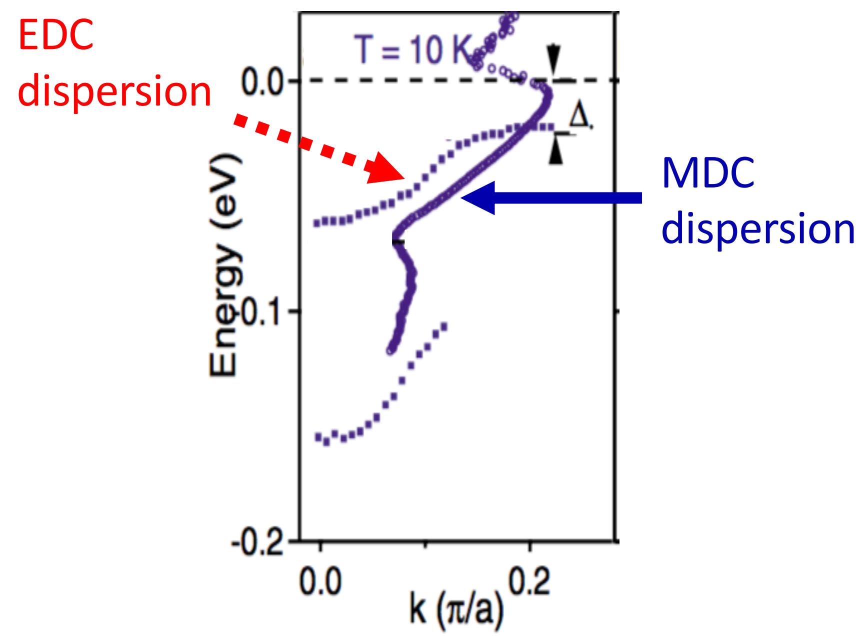
EDCs (Energy Distribution Curves) and MDCs (Momentum Distribution Curves).

Serious trouble for system with large broadening (large self energies) and band curvature.

No problem if spectral peaks are very sharp (self energy small) or if dispersion is linear.





T. Cuk, Z-X. Shen et al. PRL **93**,117003 (2004)

A new step: True 2D fitting (EDCs and MDCs fit simultaneously).

Obtain:

- Bare-band dispersion $\varepsilon(k)$
- Gaps $\Delta(k, T)$
- Fully causal self energy $\Sigma(k,\omega,T)=\Sigma'(k, \omega,T)+i\Sigma''(k, \omega,T)$

All the details of the 1-particle electronic interactions.

Orders of magnitude fewer free parameters.
New level of accuracy → new physics.

Haoxiang Li, D.S.D et al., Nature Comm. **9**, 26 (2018)

Development of a 2D fitting method (EDCs and MDCs together).

Nambu-Gorkov's Green's function

$$G^{-1} = \begin{pmatrix} \omega + \varepsilon_k - \Sigma & \phi \\ \phi & \omega - \varepsilon_k - \Sigma \end{pmatrix}$$

$$G_{11} = \frac{\omega + \varepsilon_k - \Sigma}{(\omega - \Sigma)^2 - \varepsilon_k^2 - \phi^2}$$

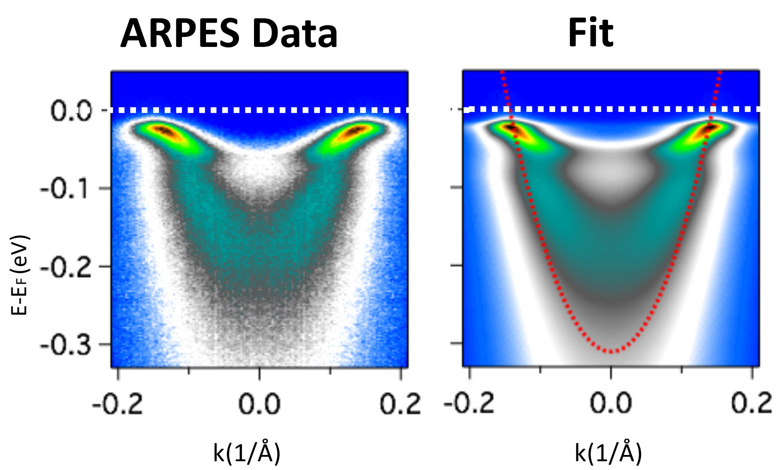
$$A(k,\omega) = -\frac{1}{\pi}\,\mathrm{Im}\,G_{11}$$

$$I(k,\omega) \propto \left(\left|\langle f | A \cdot p | i \rangle\right|^2 \times f(\omega) \times A(k,\omega) \right) \otimes R(k,\omega)$$

Note: $\begin{cases} \phi = \Delta \cdot Z \\ Z = 1 - \dfrac{\Sigma'(\omega)}{\omega} \end{cases}$

Mid-zone cut, lightly underoped Tc=85K Pb-BSCCO sample.

T=50K (UD85K)



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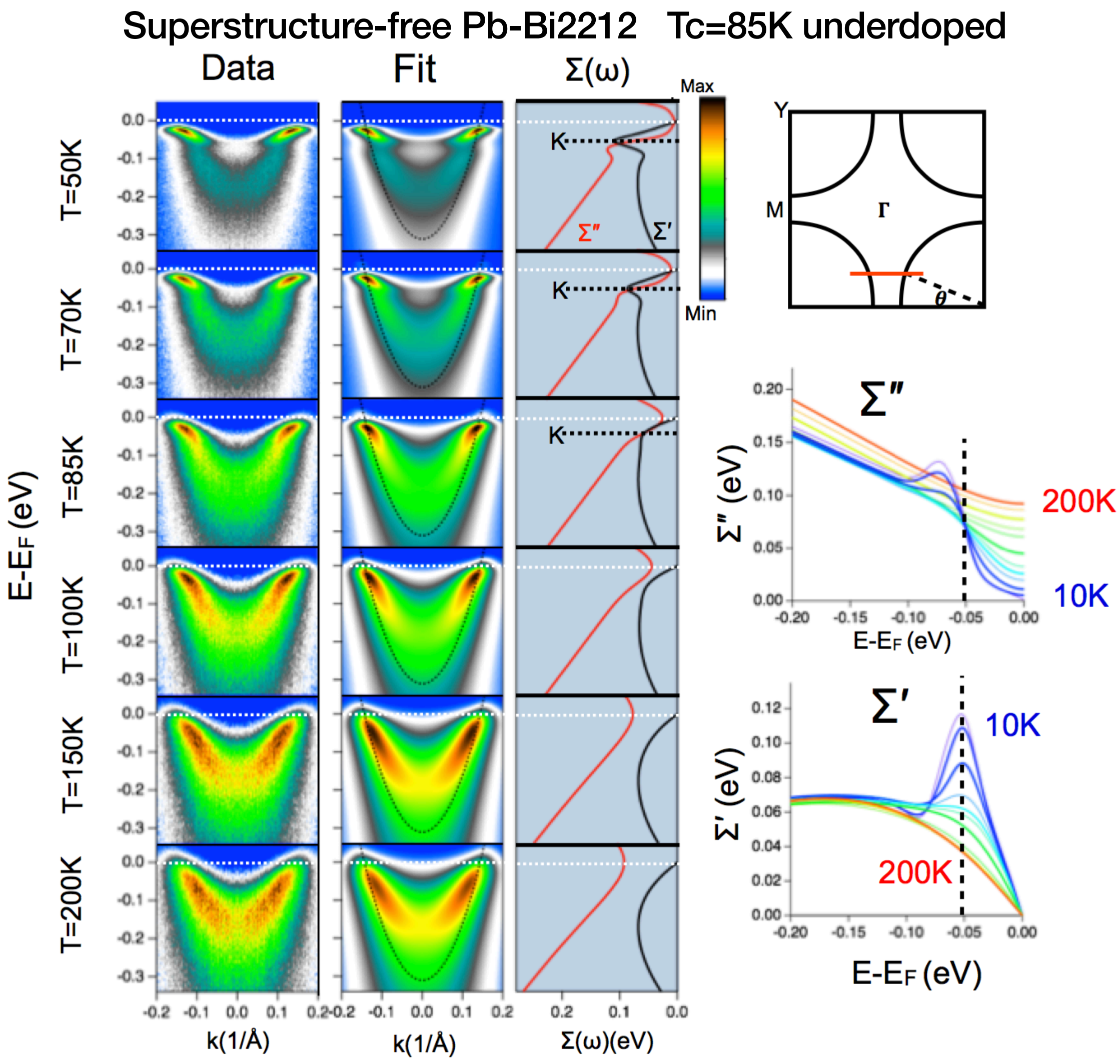


Fully causal treatment within Nambu-Gor'kov:

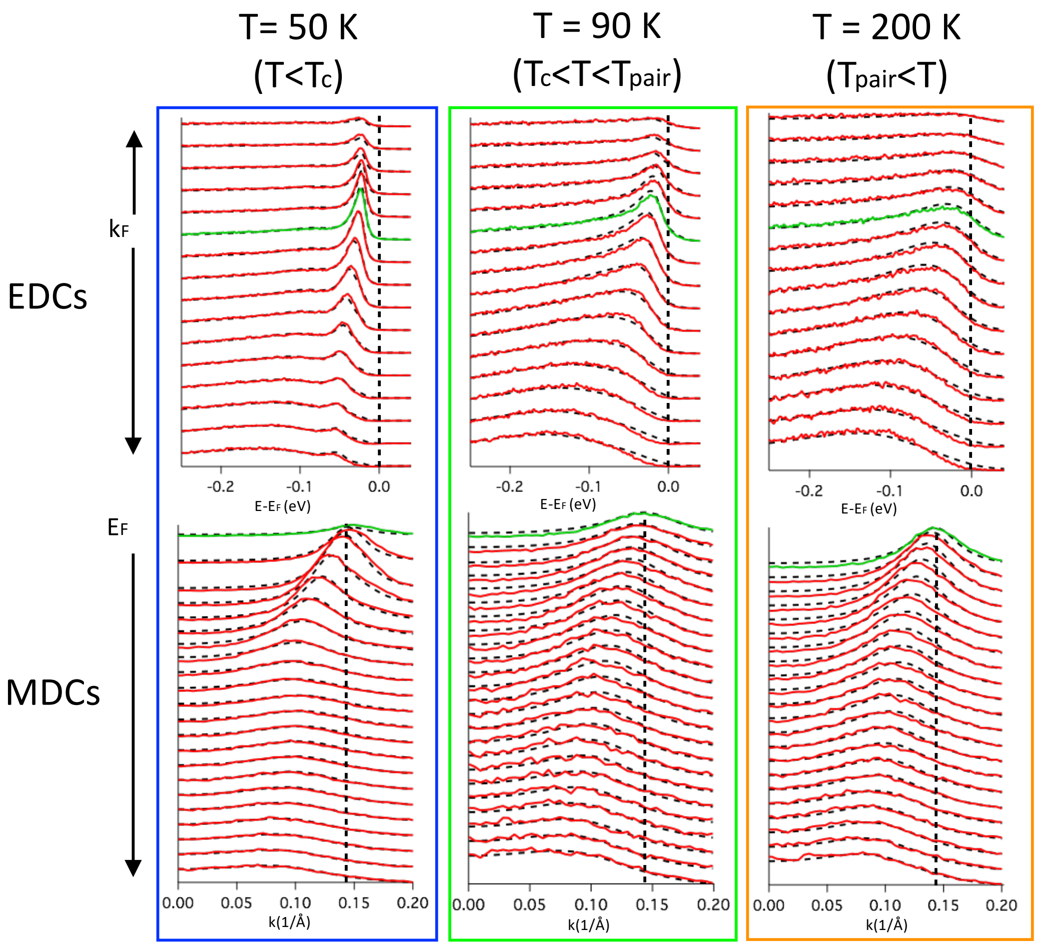
Simultaneous extraction of:

- SC gaps, $\Delta(\boldsymbol{k},T)$
- $\Sigma'(\boldsymbol{k},\omega,T)$ and $\Sigma''(\boldsymbol{k},\omega,T)$
- Renormalization $Z(\boldsymbol{k},w,T)$
- Unrenormalized "bare" bands, $v_F(\boldsymbol{k},T)$, etc.

Orders of mag. fewer free parameters compared to EDC or MDC fitting.

Haoxiang Li, D.S.D et al., Nature Communications **9**, 26 (2018)

2D fit result shown as 1D cuts
(All fits are done simultaneously)

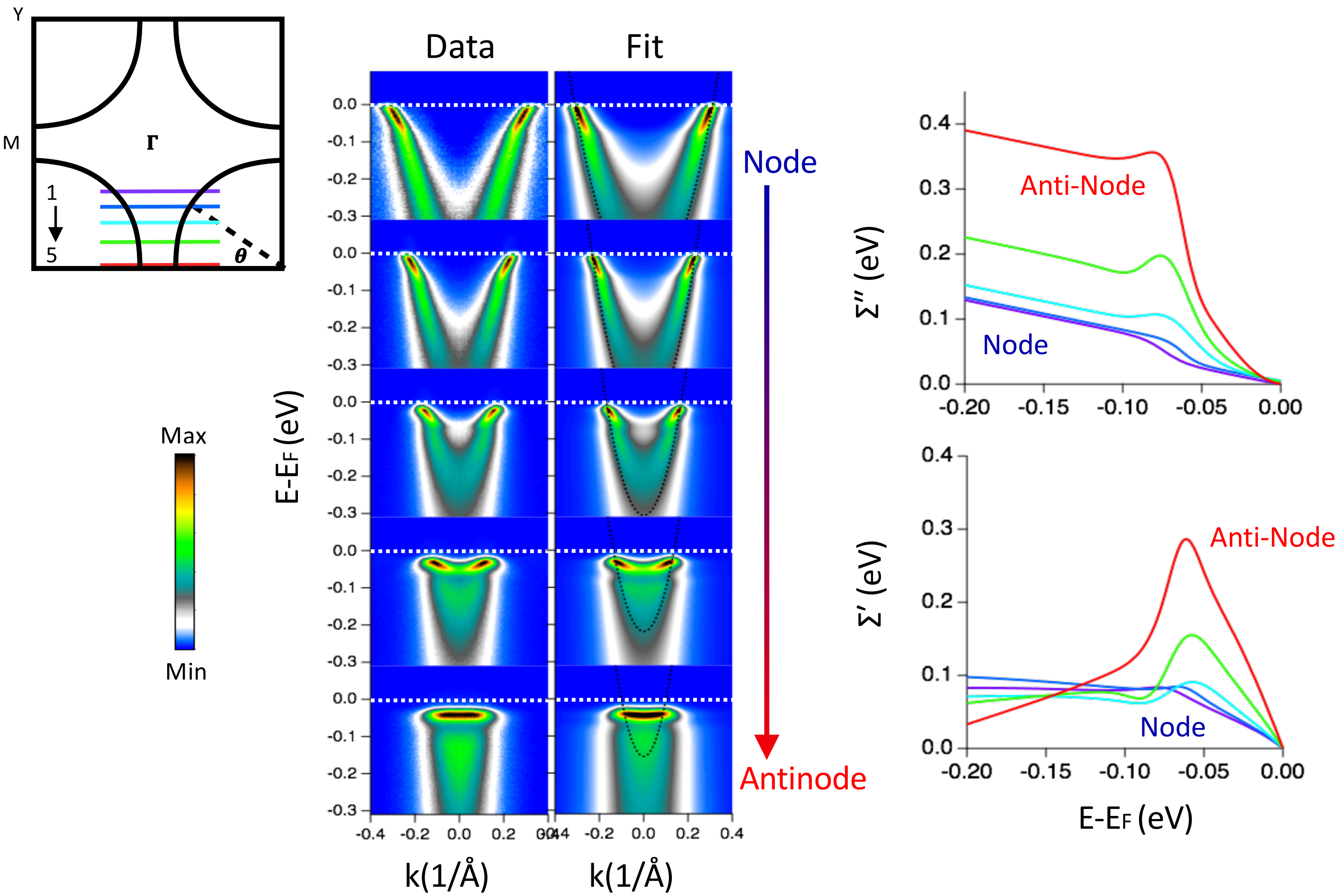


2D fit results are dashed black lines.

Band curvature makes MDCs asymmetric – can not captured in MDC fitting.

Orders of magnitude fewer free parameters than from 1D fits.

Haoxiang Li, D.S.D et al., Nature Communications **9**, 26 (2018)



Pb-$Bi_2Sr_2CaCu_2O_8$

Tc=85K

Lightly UD

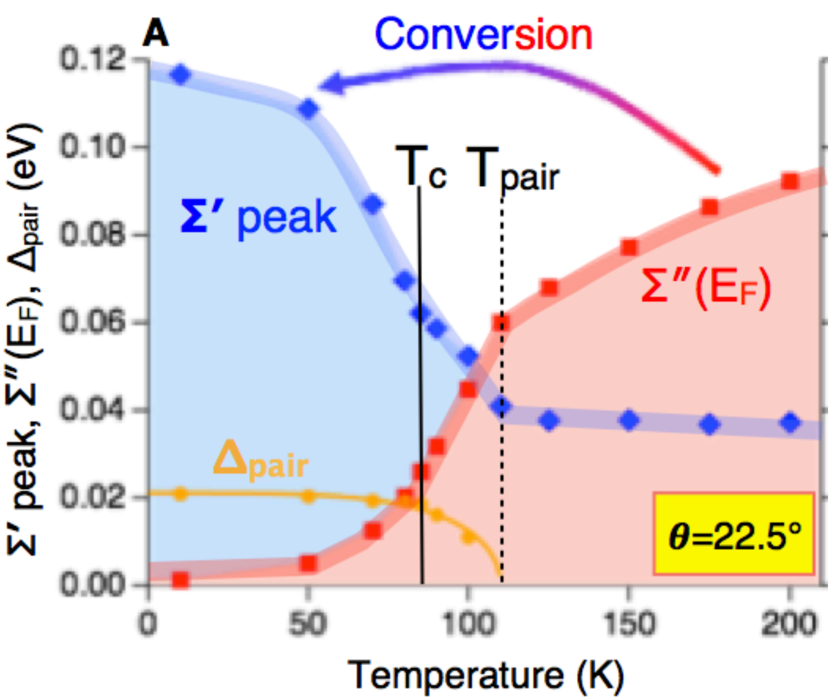
Low T

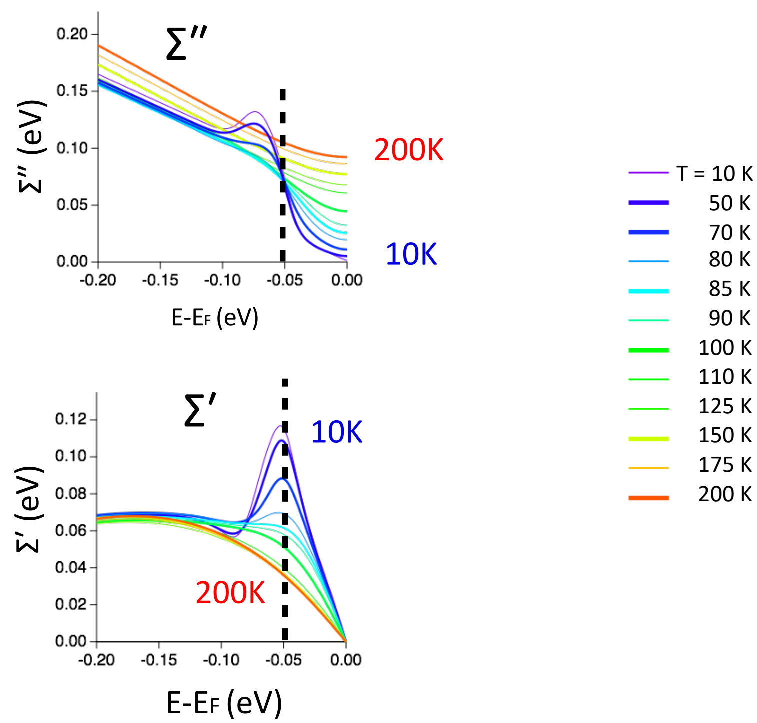
k-dependence

H. Li, D.S.D et al., Nature Communications **9**, 26 (2018)

Coherent organization (conversion) of electronic correlations

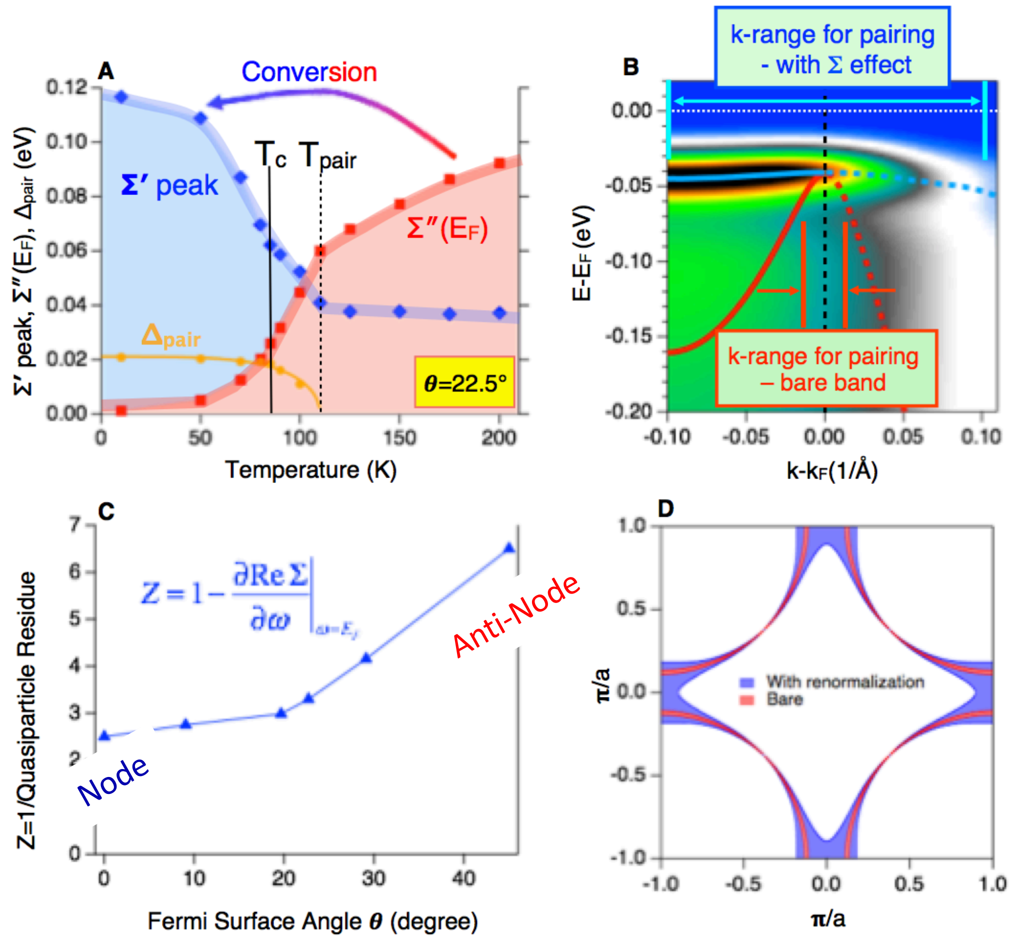
Mid-zone cut shown as an example.





H. Li, D.S.D et al., Nature Communications **9**, 26 (2018)

Increased k-range for pairing due to the correlations



H. Li, D.S.D et al., Nature Communications **9**, 26 (2018)

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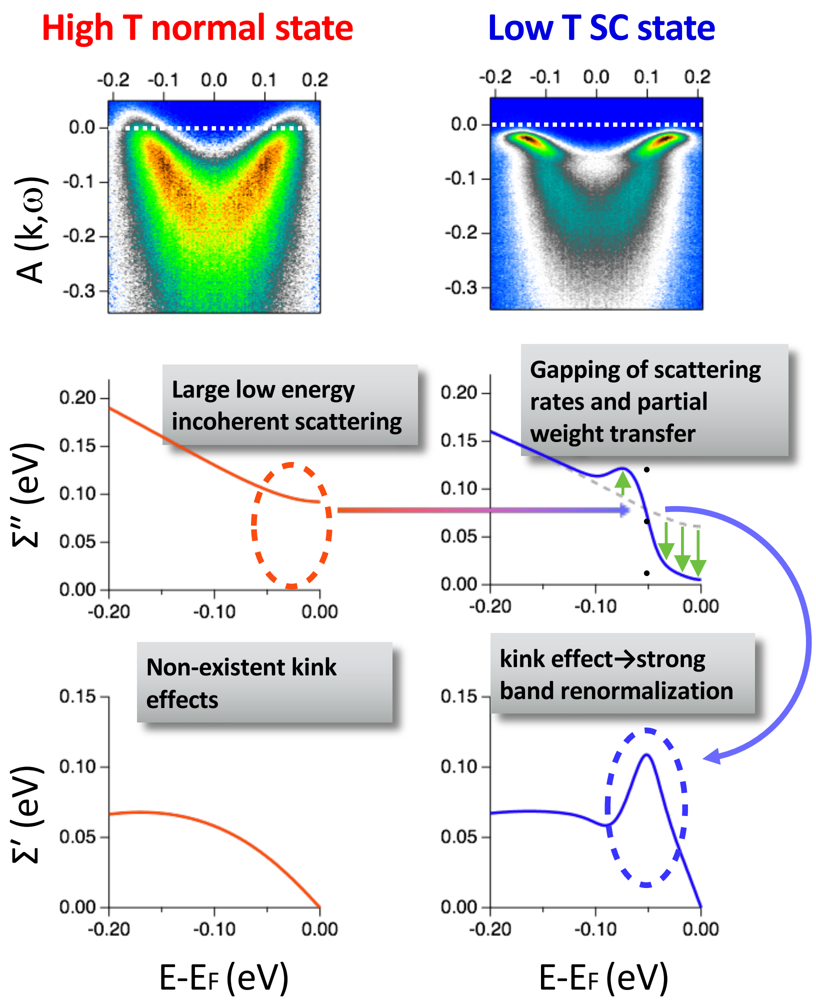

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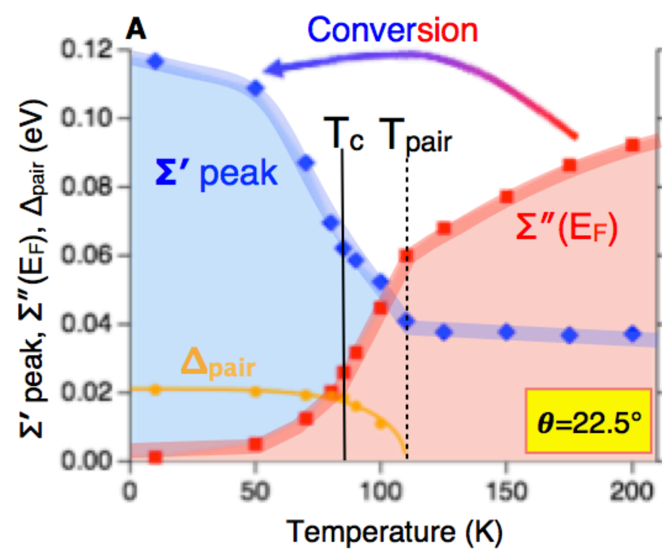
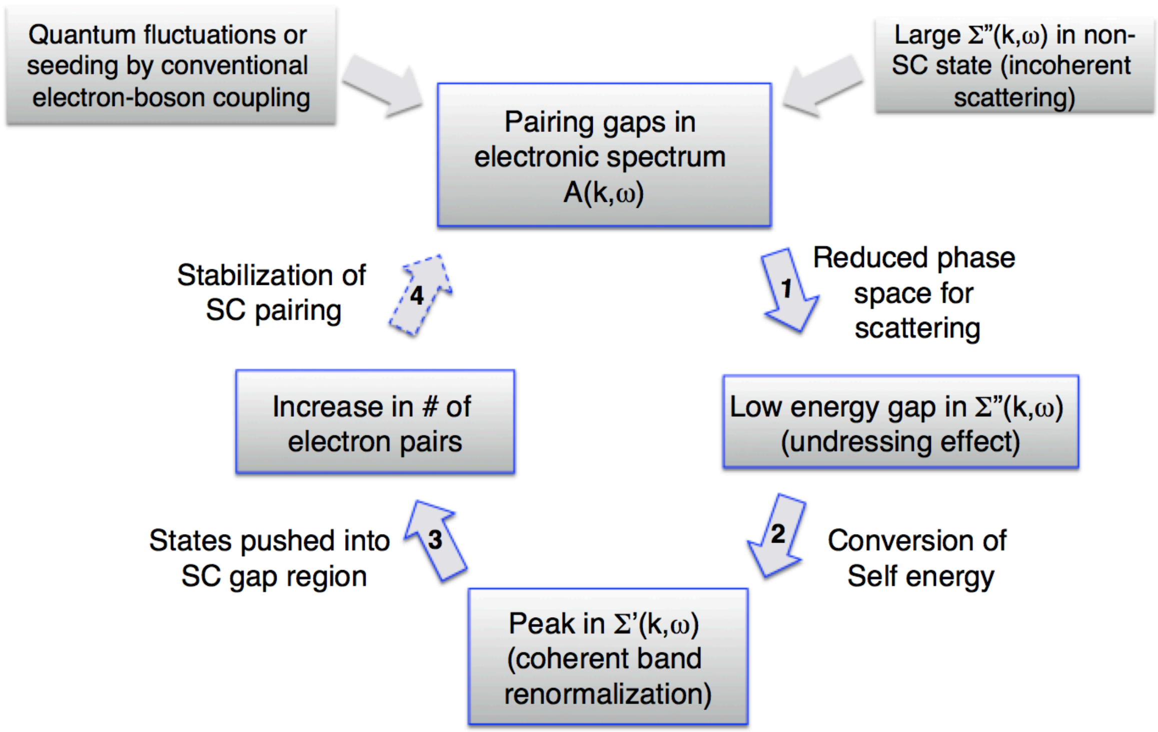


Stronger Σ″ in N-state gives a stronger Σ′ effect in the SC state (strongest at antinode).

H. Li, D.S.D et al., Nature Communications **9**, 26 (2018)

Positive feedback loop due to increasing # of states for pairing.



- Should strengthen any mechanism for pairing (e.g. electron-phonon).
- May support a fully-electronic mechanism, starting from fluctuations.

H. Li, D.S.D et al., Nature Communications **9**, 26 (2018)

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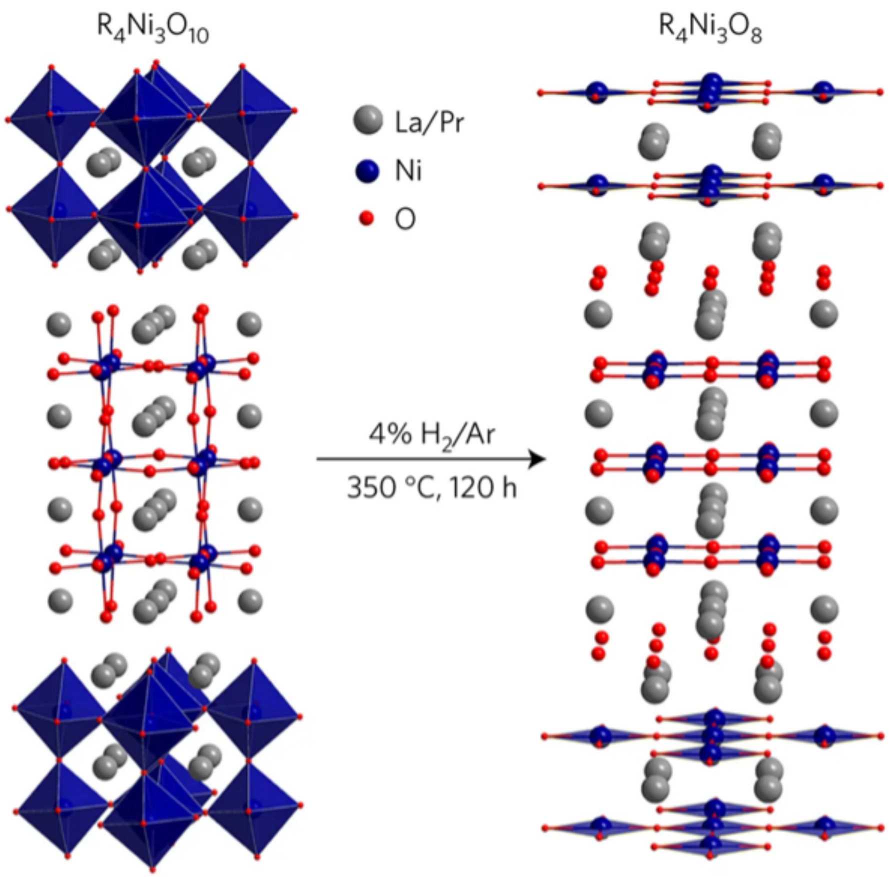
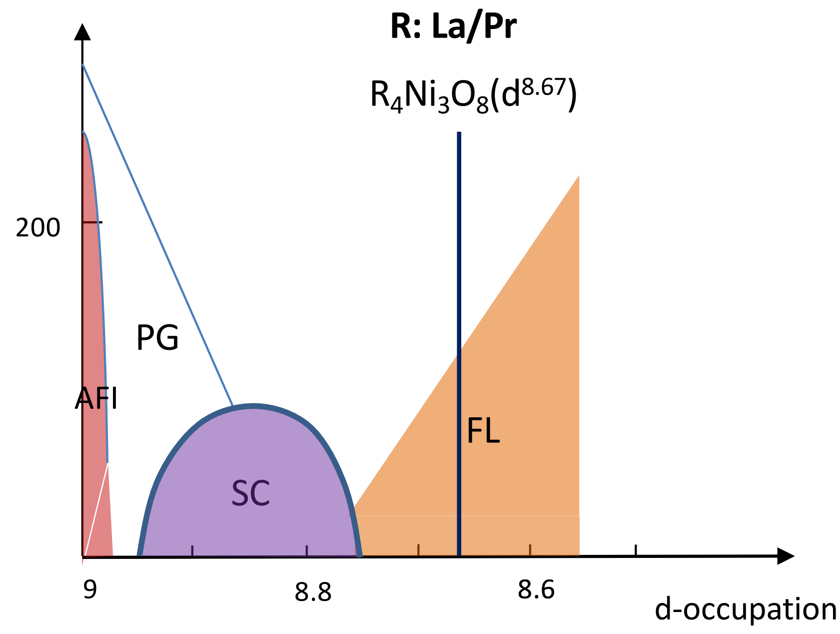
Trilayer nickelates: Quasi-2D trilayer structure and similar d-electron counts to cuprates.





Phase diagram of hole-doped cuprates

[1]J. Zhang, A. S. Botana, etc. Nat. Phys.doi:10.1038/nphys4149

This work is unpublished. For details feel free to contact me at

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