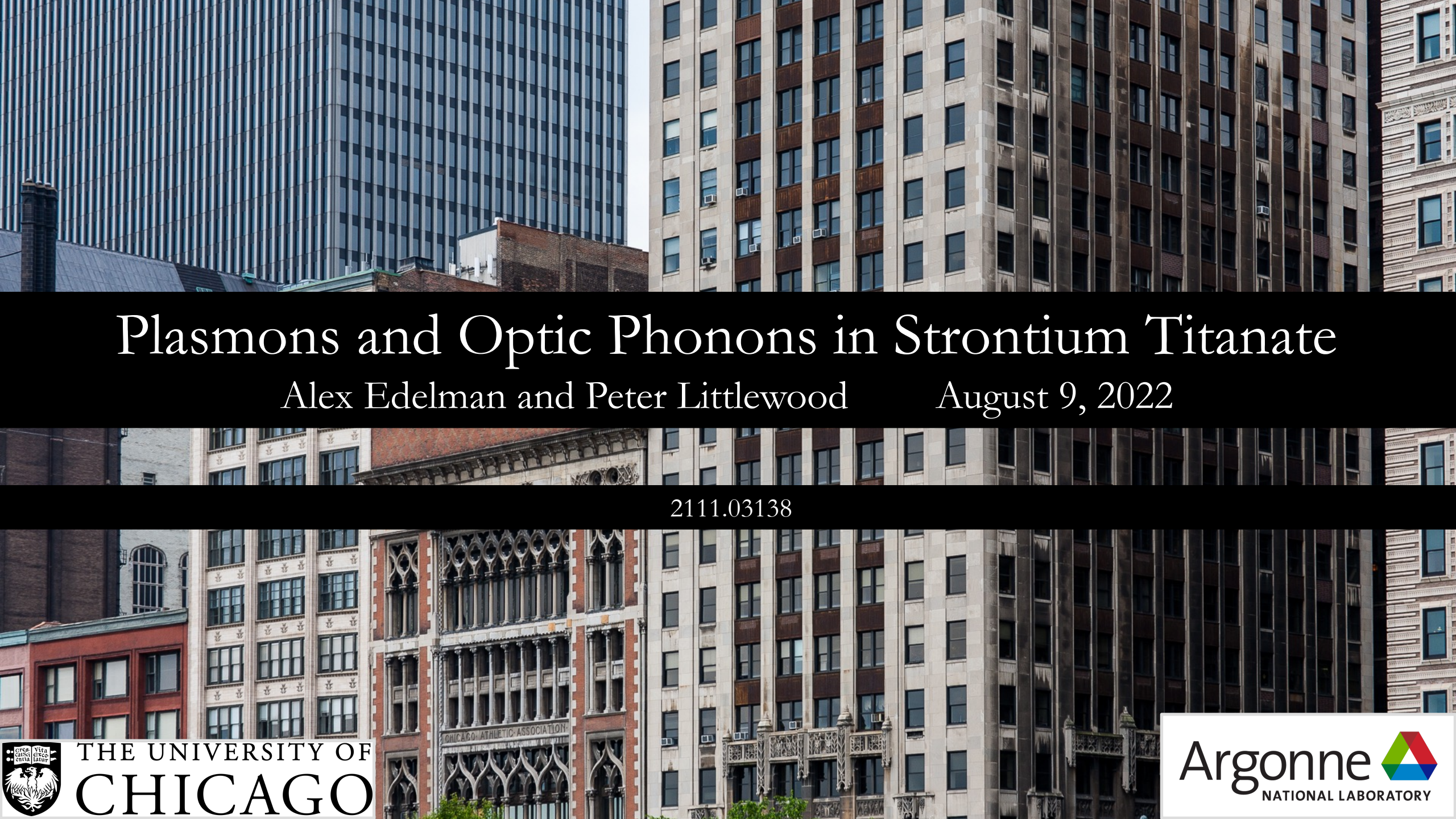


Plasmons and Optic Phonons in Strontium Titanate

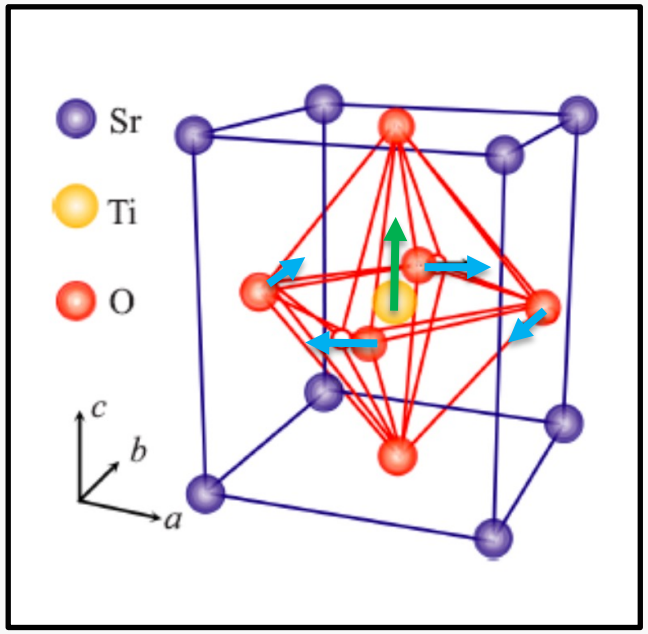
Alex Edelman and Peter Littlewood August 9, 2022

2111.03138

THE UNIVERSITY OF CHICAGO

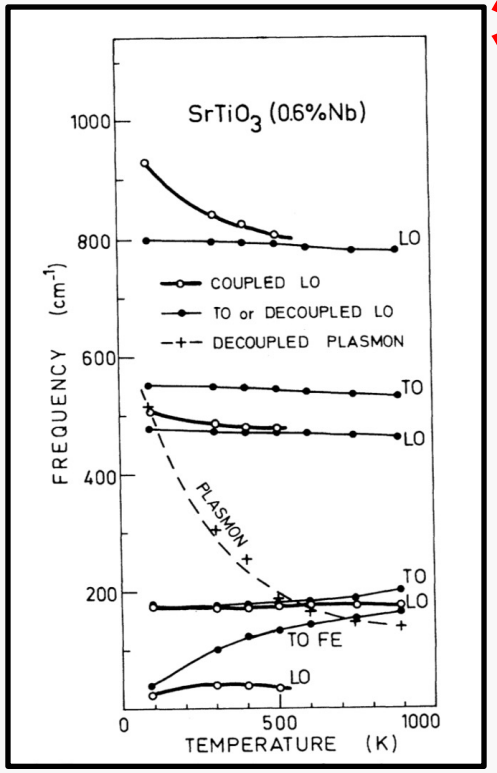
Argonne NATIONAL LABORATORY

A “quantum parelectric”



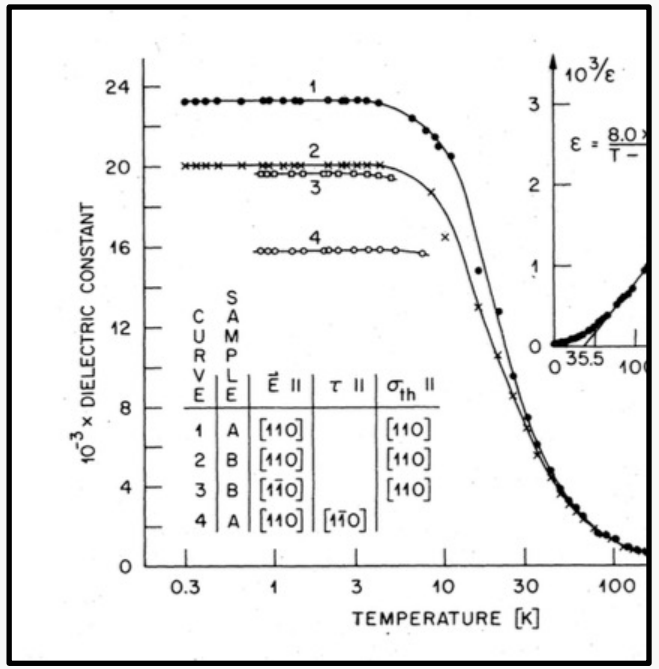
105K: cubic to tetragonal

37K: quantum paraelectric



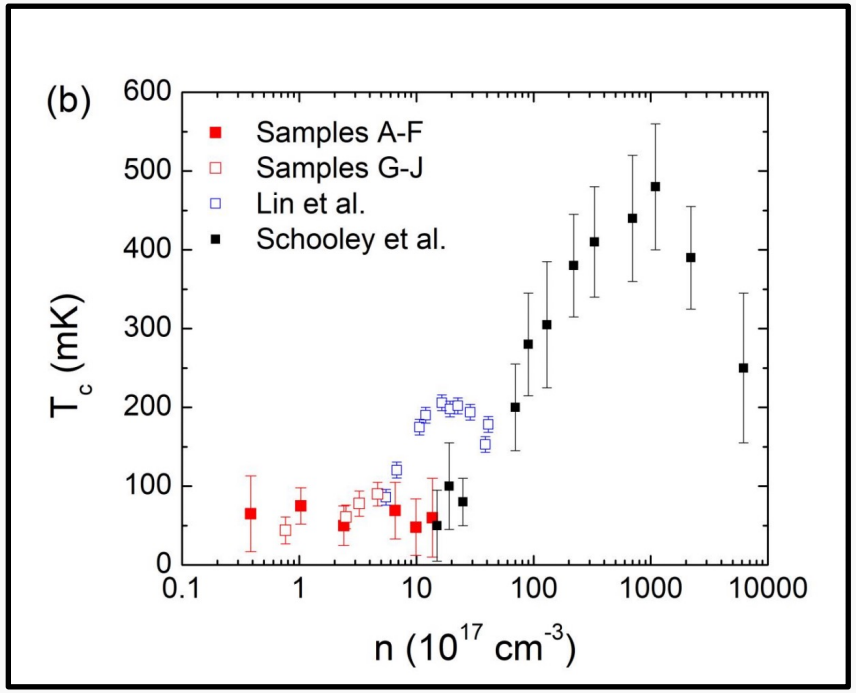
Gervais, PRB (1993)

*

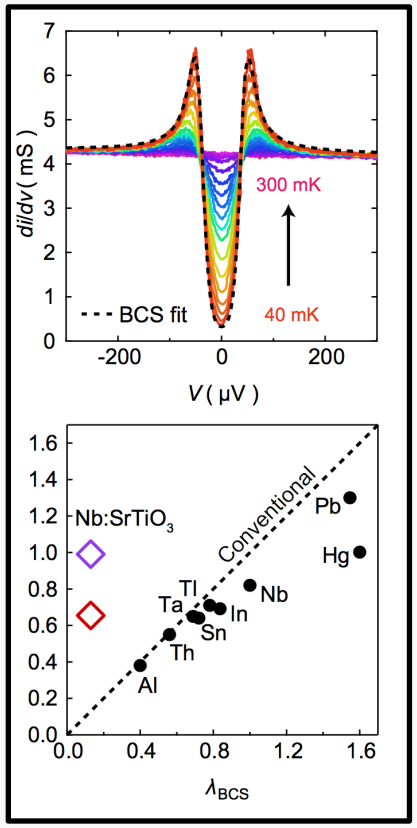


Müller, PRB (1979)

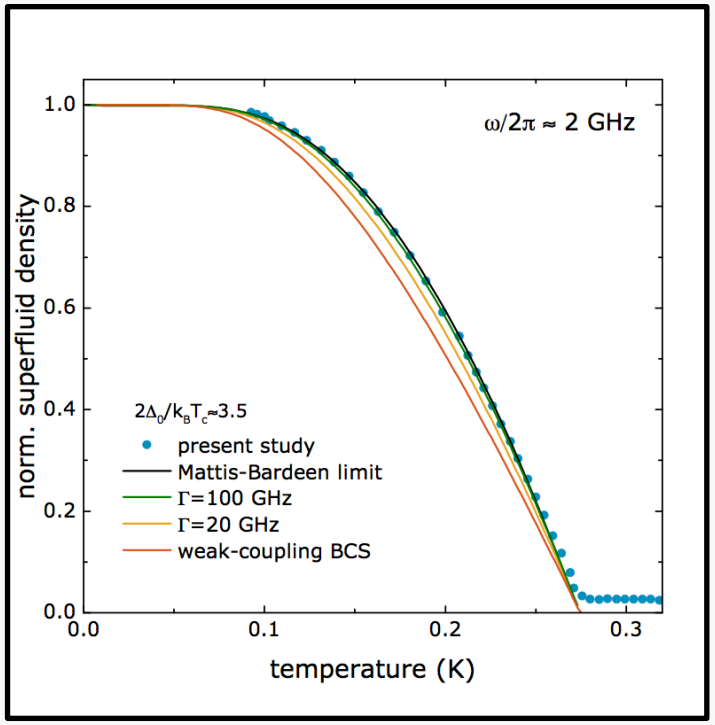
A very low-density but "boring" superconductor



1904.03121



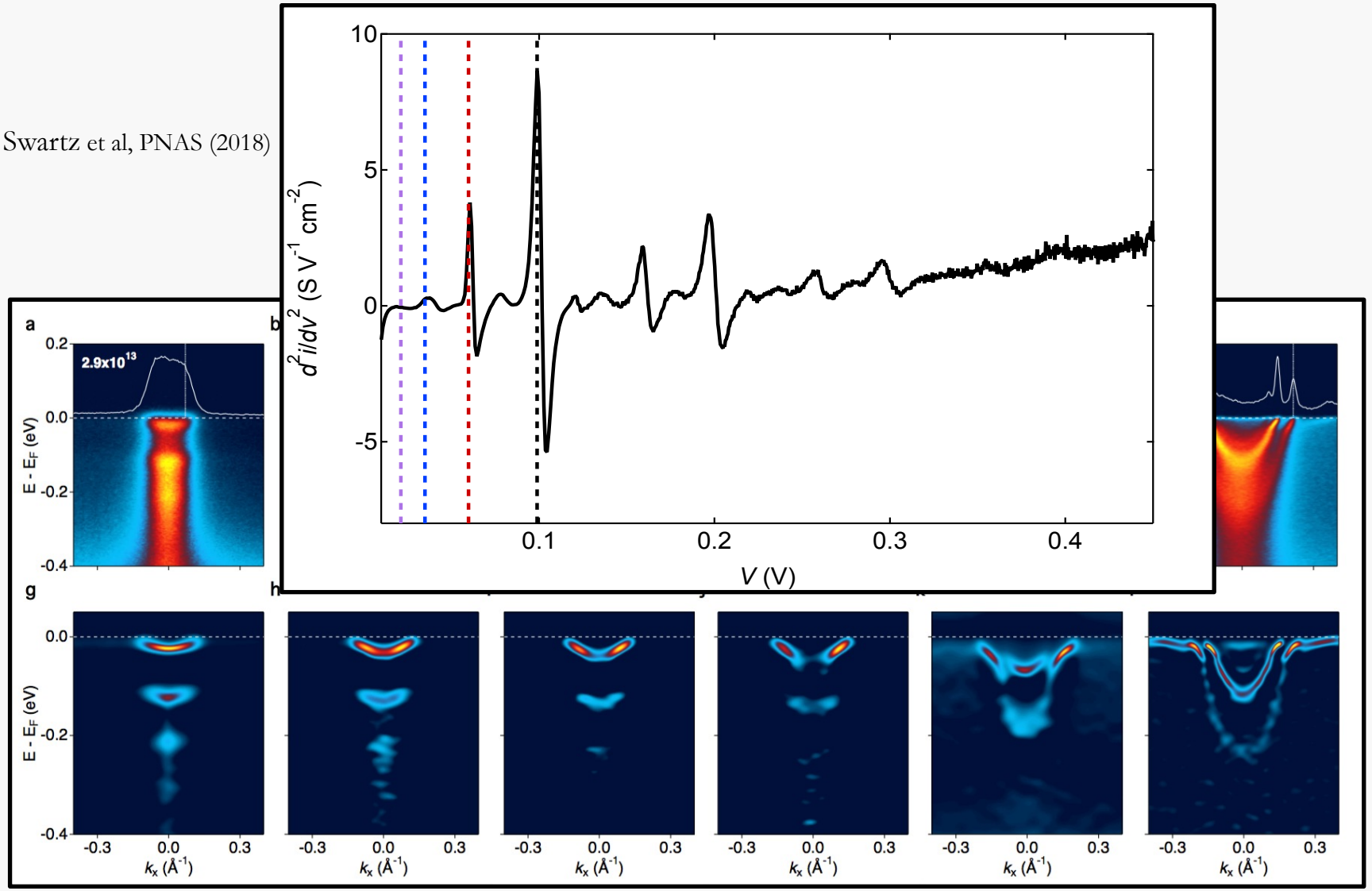
Swartz et al, 1608.05621



Thiemann et al, 1703.0471

Strong electron-phonon coupling

Swartz et al, PNAS (2018)



Wang et al, Nature Materials (2016)

This talk

- A too-brief introduction to STO
- A minimal model
- Domed superconducting phase diagrams are generic
- Normal state properties are puzzling

The Minimal Model

$$H = \sum_{\mathbf{k}\ \sigma} c^\dagger_{\mathbf{k}}(\epsilon_{\mathbf{k}} - \mu)c_{\mathbf{k}} + \Omega \sum_{\mathbf{k}\ \sigma} b^\dagger_{\mathbf{k}} b_{\mathbf{k}} + \sum_{\mathbf{k}\ \sigma} g(\mathbf{k})\rho_{\mathbf{k}}(b_{\mathbf{k}} + b^\dagger_{-\mathbf{k}}) + \sum_{\mathbf{k}} V(\mathbf{k})\rho_{\mathbf{k}}\rho_{-\mathbf{k}}$$

$$g^2(\mathbf{k}) = \frac{\lambda\Omega\gamma}{\mathbf{k}^2}$$

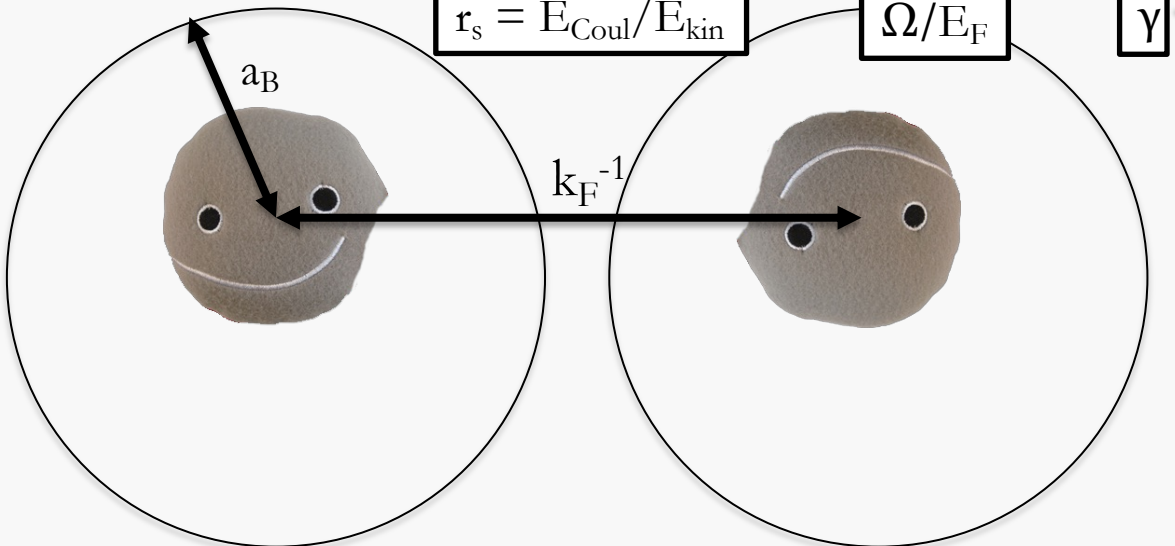
$$V_{\mathrm{Coul}}(\mathbf{k}) = \frac{\lambda}{\mathbf{k}^2}$$

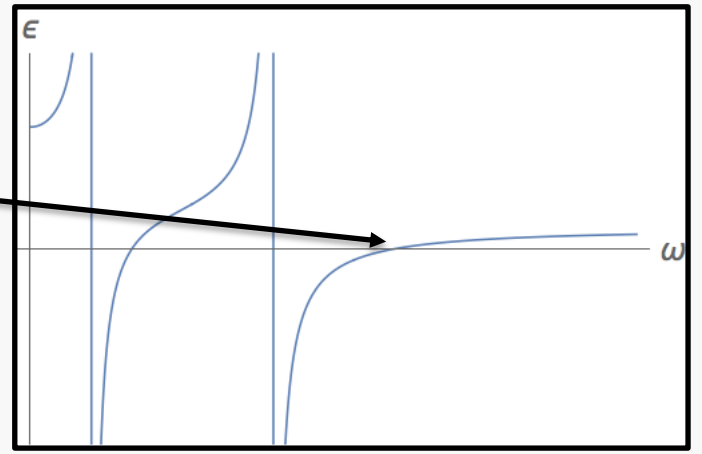
Parameters of the theory:

$r_s = E_{Coul}/E_{kin}$

Ω/E_F

γ

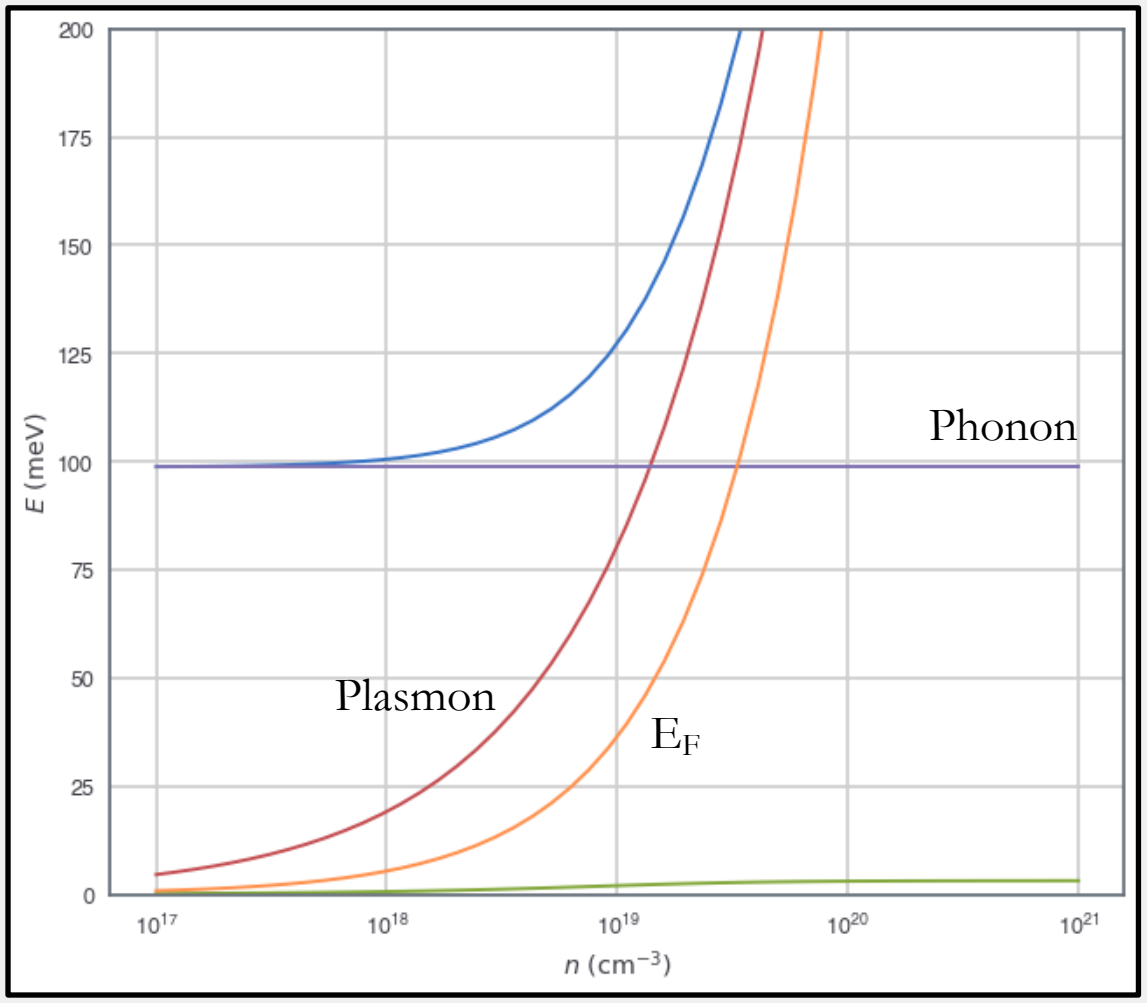


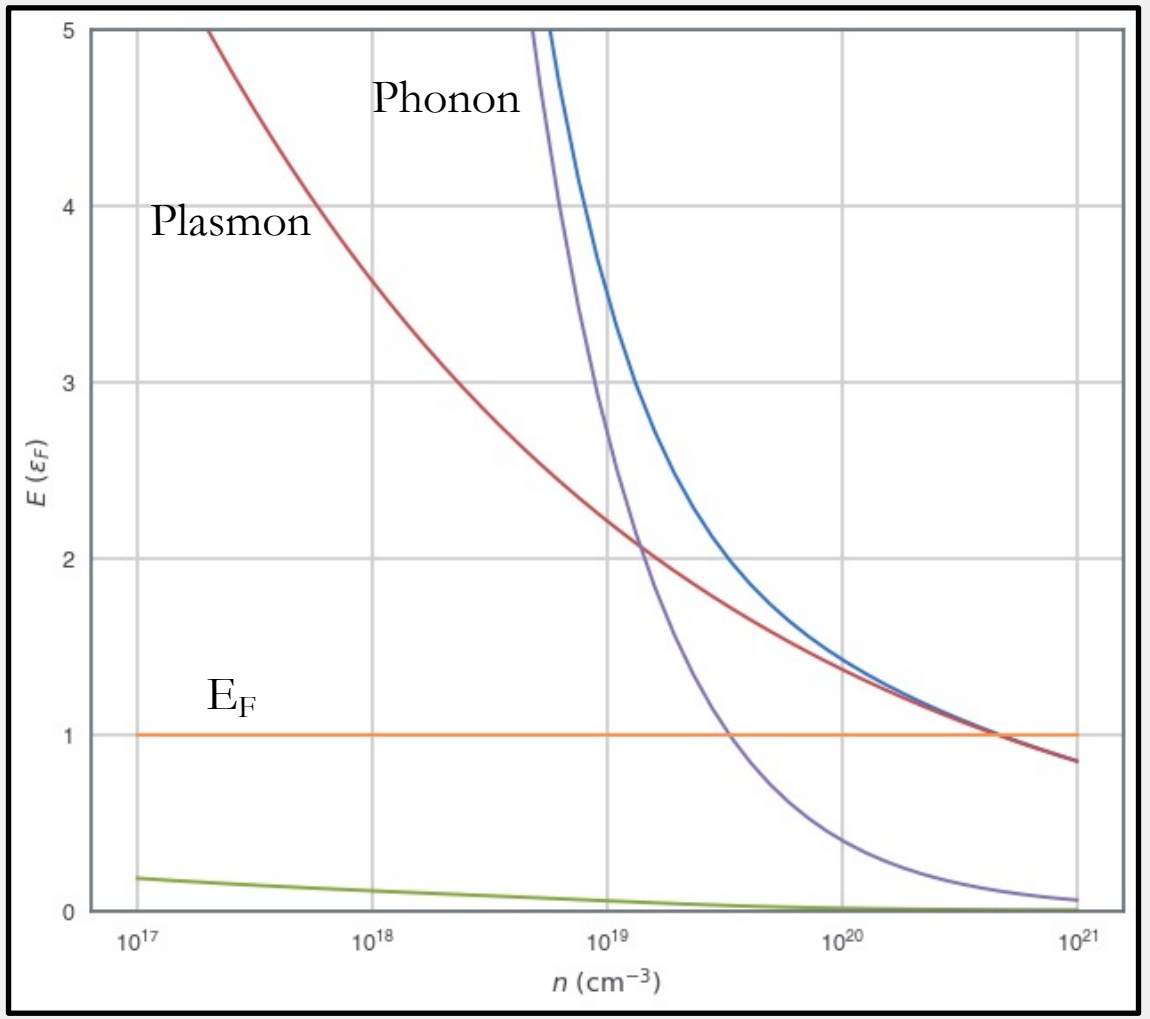


Rock salt:

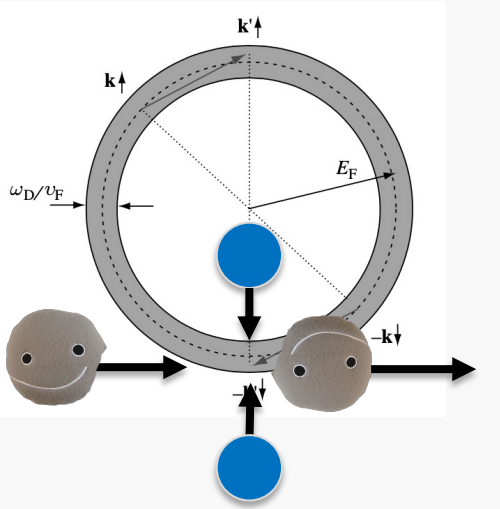
$$\gamma = \frac{1}{2}\left(\frac{1}{\epsilon_\infty} - \frac{1}{\epsilon_0}\right)$$

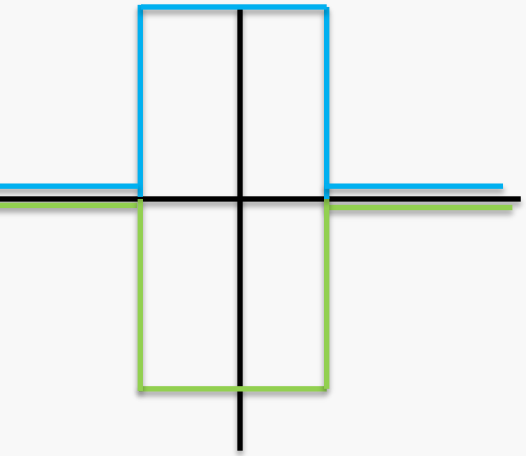
Coupled Modes



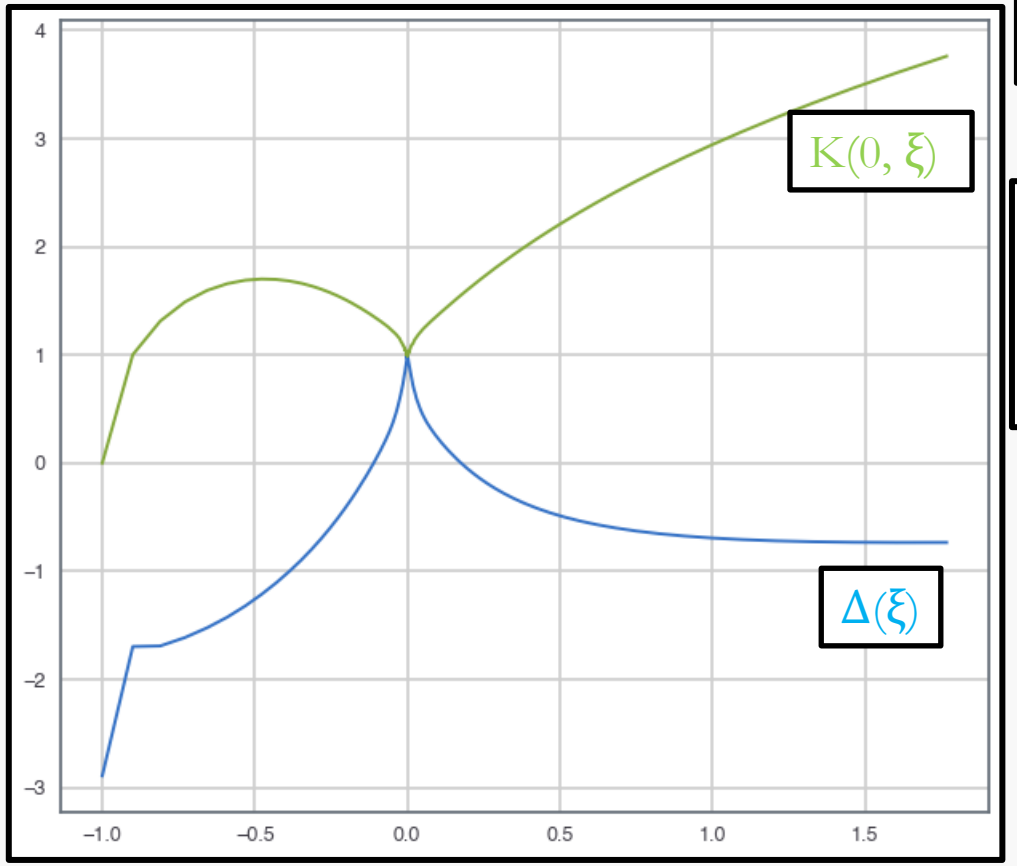


Establishing a Gap



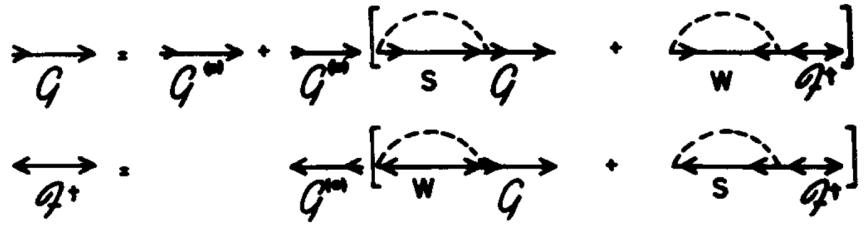


BCS



$$S(\mathbf{p}, ip) = -\int \frac{d^3q}{(2\pi)^3} \frac{1}{\beta} \sum_{iq} V_{\text{eff}}(\mathbf{q}, iq)\mathcal{G}(\mathbf{p}+\mathbf{q}, ip+iq)$$

$$W(\mathbf{p}, ip) = -\int \frac{d^3q}{(2\pi)^3} \frac{1}{\beta} \sum_{iq} V_{\text{eff}}(\mathbf{q}, iq)\mathcal{F}(\mathbf{p}+\mathbf{q}, ip+iq)$$



Spectral representation

$$\frac{\Delta}{Z}(\omega,\epsilon) = -\int d\epsilon'\ N(\epsilon) \int_0^\infty \frac{d\eta}{\pi} \Im F(\eta,\epsilon') \tanh(\beta\eta/2) \times \left(V_0(\epsilon,\epsilon') + \int_0^\infty \frac{d\Omega}{\pi} \Im V(\Omega,\epsilon,\epsilon') \left(\frac{1}{\eta+\Omega+\omega} + \frac{1}{\eta+\Omega-\omega} \right) \right)$$

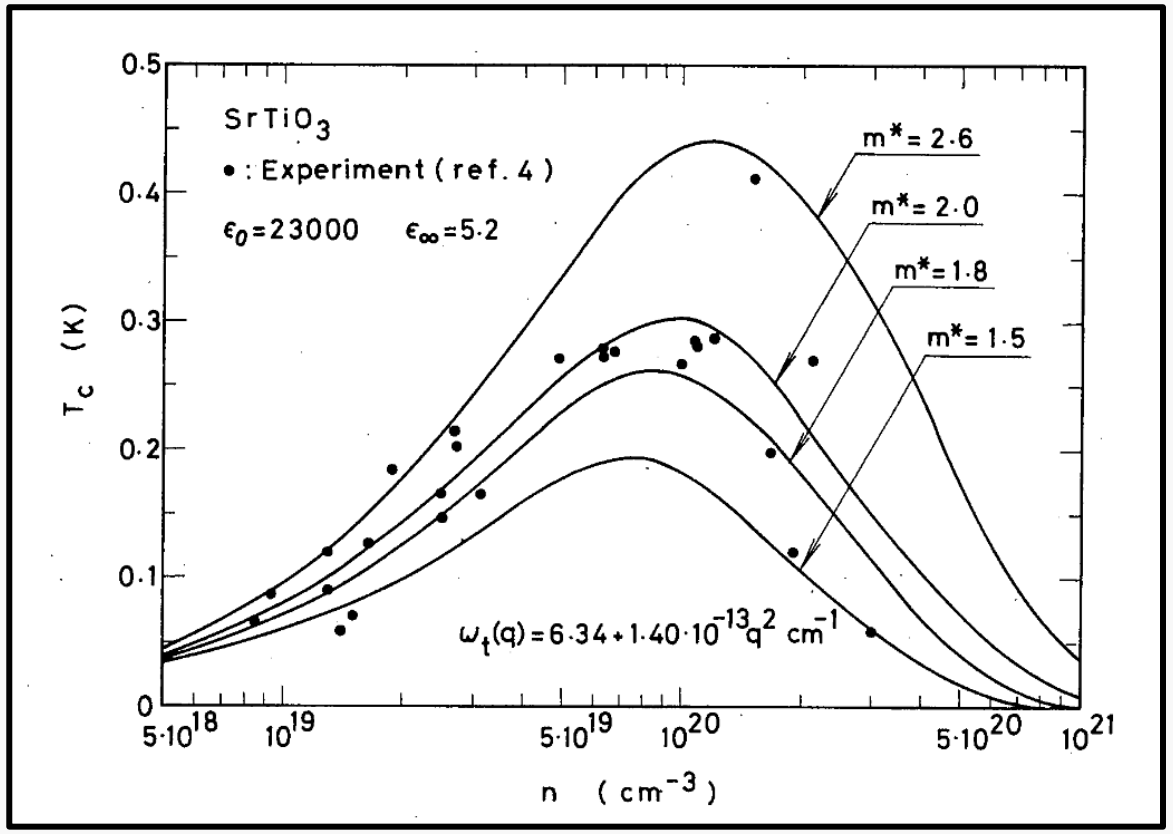
Kirzhnits, Maksimov, Khomskii (1972)

$$V_0(\xi+\mu,\xi'+\mu) + 2\int_0^\infty \frac{d\Omega}{\pi} \frac{\Im V(\Omega,\xi+\mu,\xi'+\mu)}{|\xi'|+|\xi|+\Omega}$$

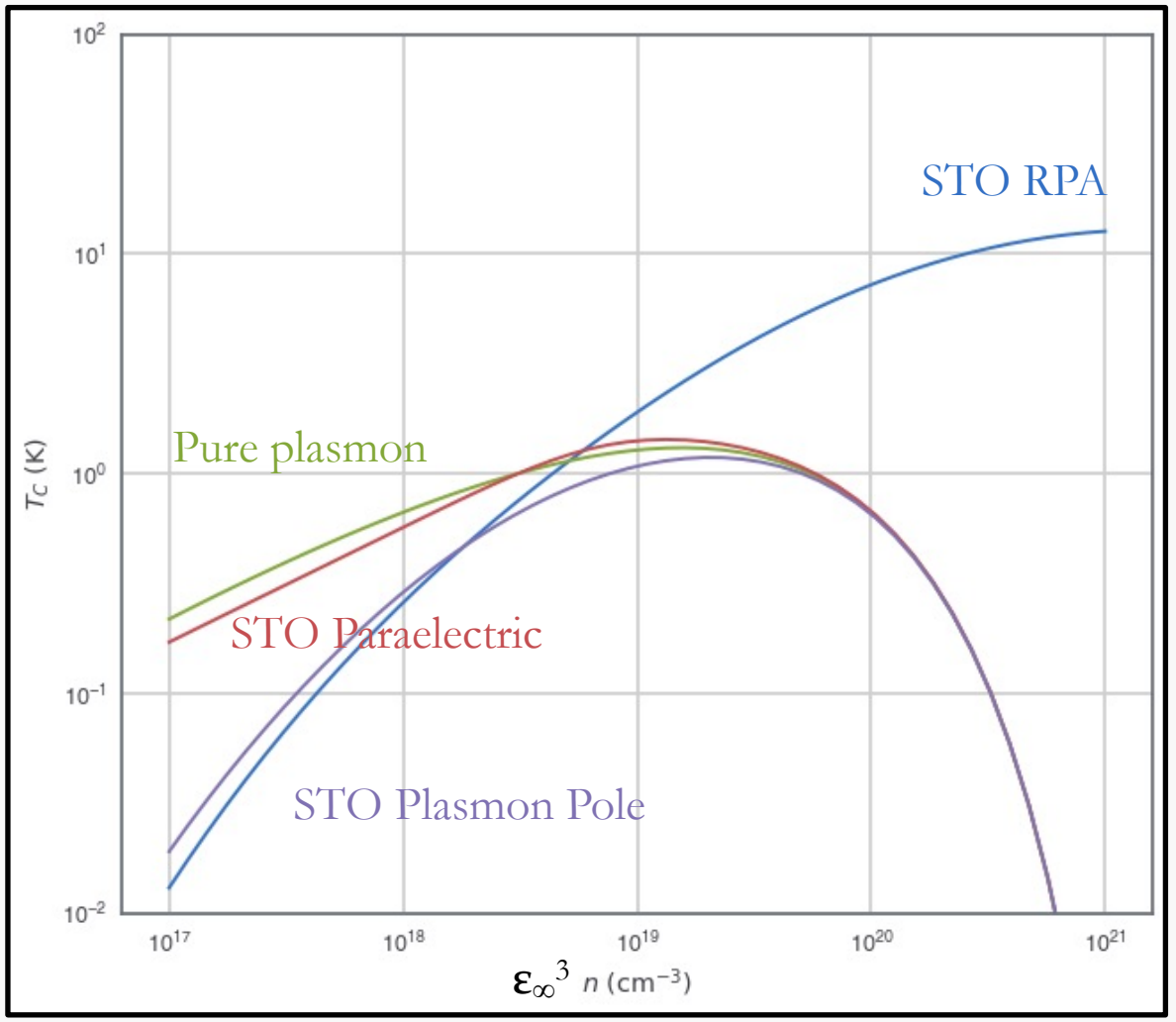
Weak Coupling

- $\omega_D << E_F$
- No cutoffs
- No μ^*

Roughly matches the data but is very generic

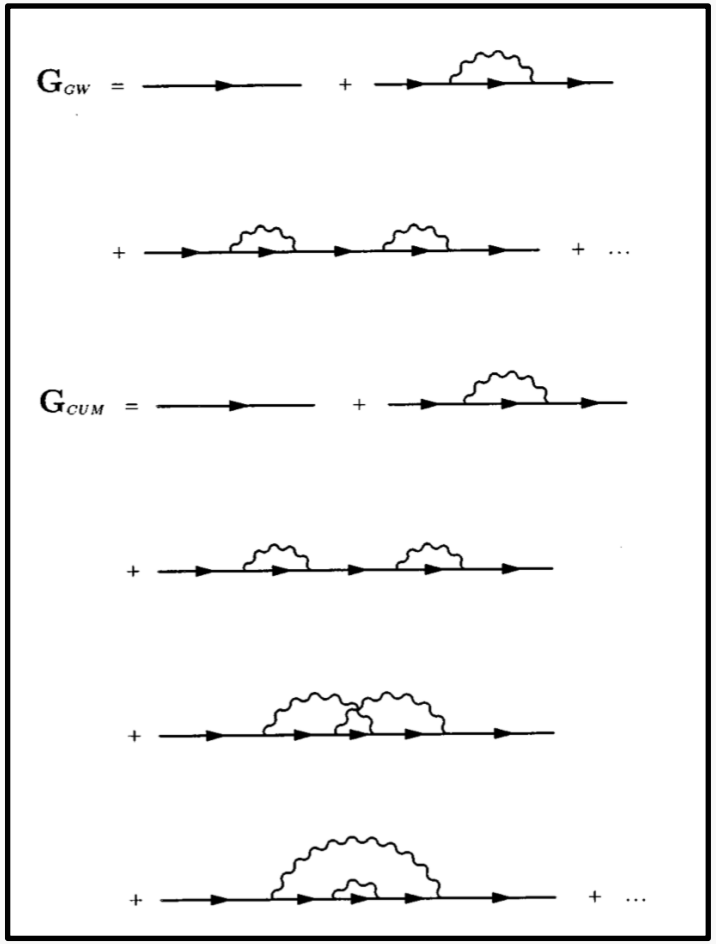


Takada (1980)



Spectral Functions and Cumulants

$$H = \sum_{\mathbf{k}} c^{\dagger}_{\mathbf{k}}(\epsilon_{\mathbf{k}} - \mu)c_{\mathbf{k}} + \Omega \sum_{\mathbf{k}} b^{\dagger}_{\mathbf{k}} b_{\mathbf{k}} + \sum_{\mathbf{k}} g(\mathbf{k})\rho_{\mathbf{k}}(b_{\mathbf{k}} + b^{\dagger}_{-\mathbf{k}}) + \sum_{\mathbf{k}} V(\mathbf{k})\rho_{\mathbf{k}}\rho_{-\mathbf{k}}$$

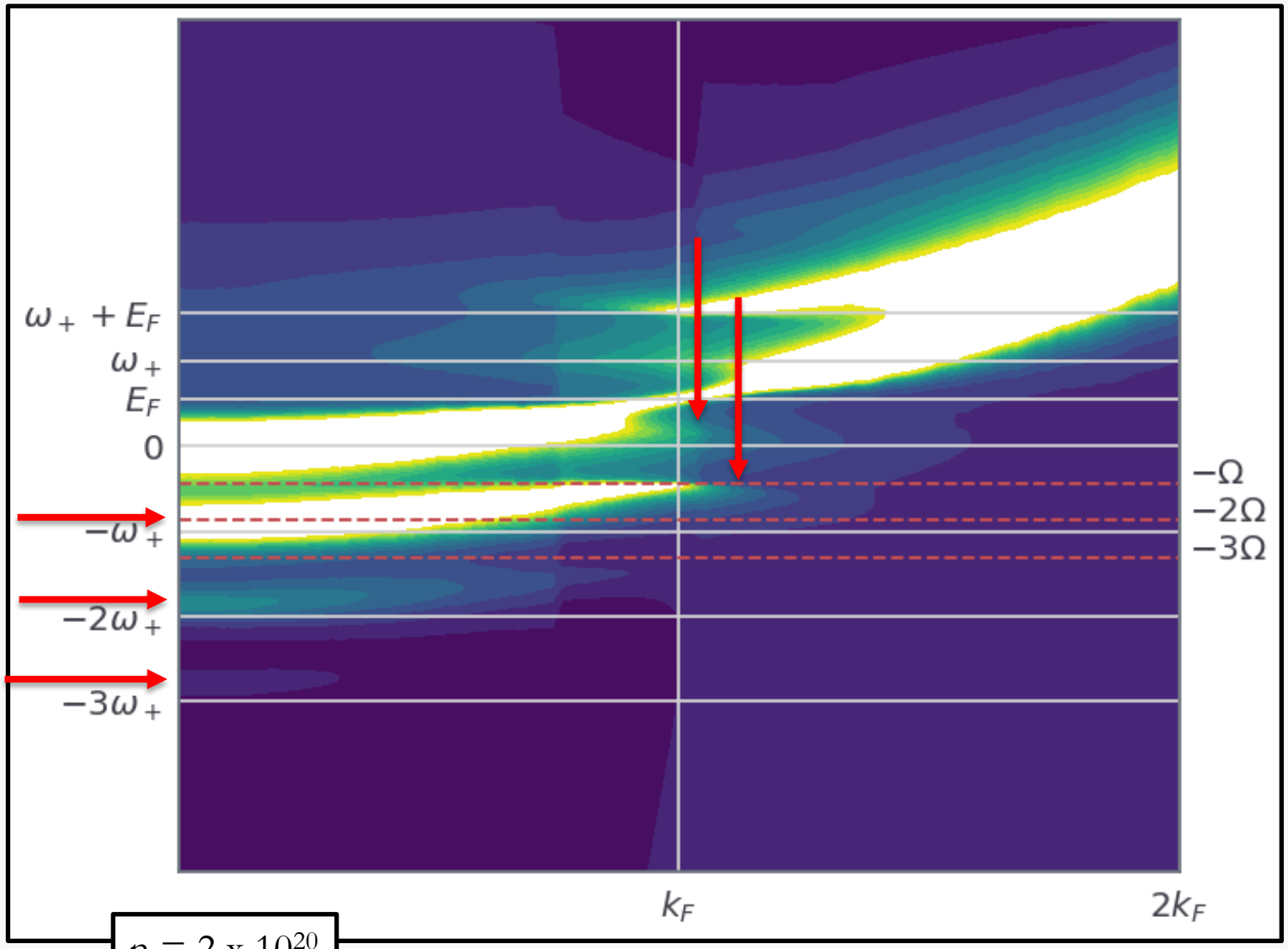


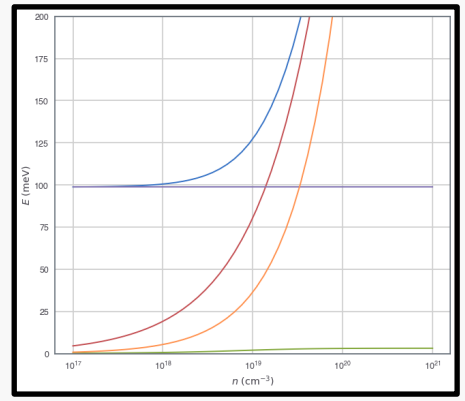
$$V_{\text{eff}}(\omega, \mathbf{k}) = \frac{V_{\text{Coul}} + V_{\text{ph}}}{1 - \Pi_{\text{RPA}}(V_{\text{Coul}} + V_{\text{ph}})}$$

$$G = \underbrace{\qquad\qquad}_{n} = G_0 \exp \qquad\qquad + \ldots$$
$n!$

$$A(\mathbf{k}, \omega) = \frac{2|\text{Im}\Sigma|}{(\omega - \epsilon_{\mathbf{k}} + \mu - \text{Re}\Sigma)^2 + (\text{Im}\Sigma)^2}$$

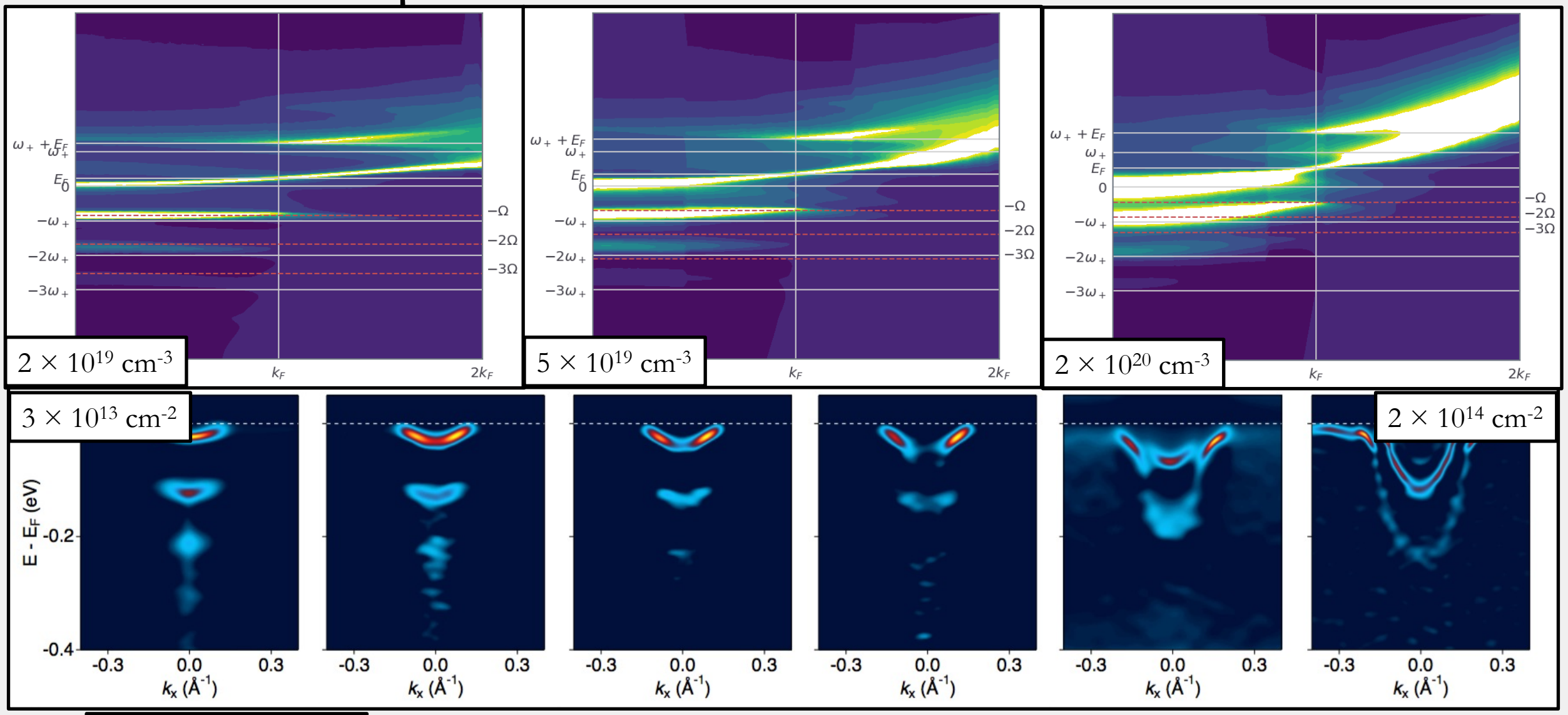
What's in a typical spectral function





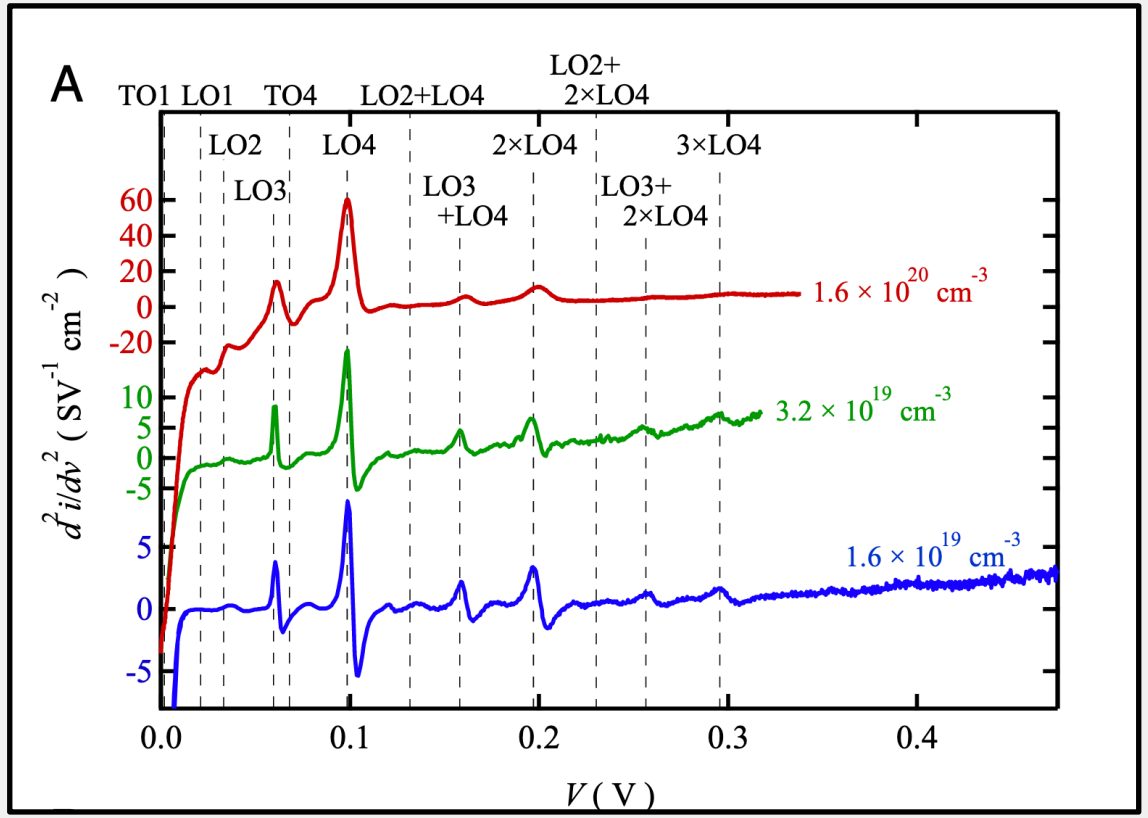
n = 2 x 10^{20}

Spectral Functions vs ARPES

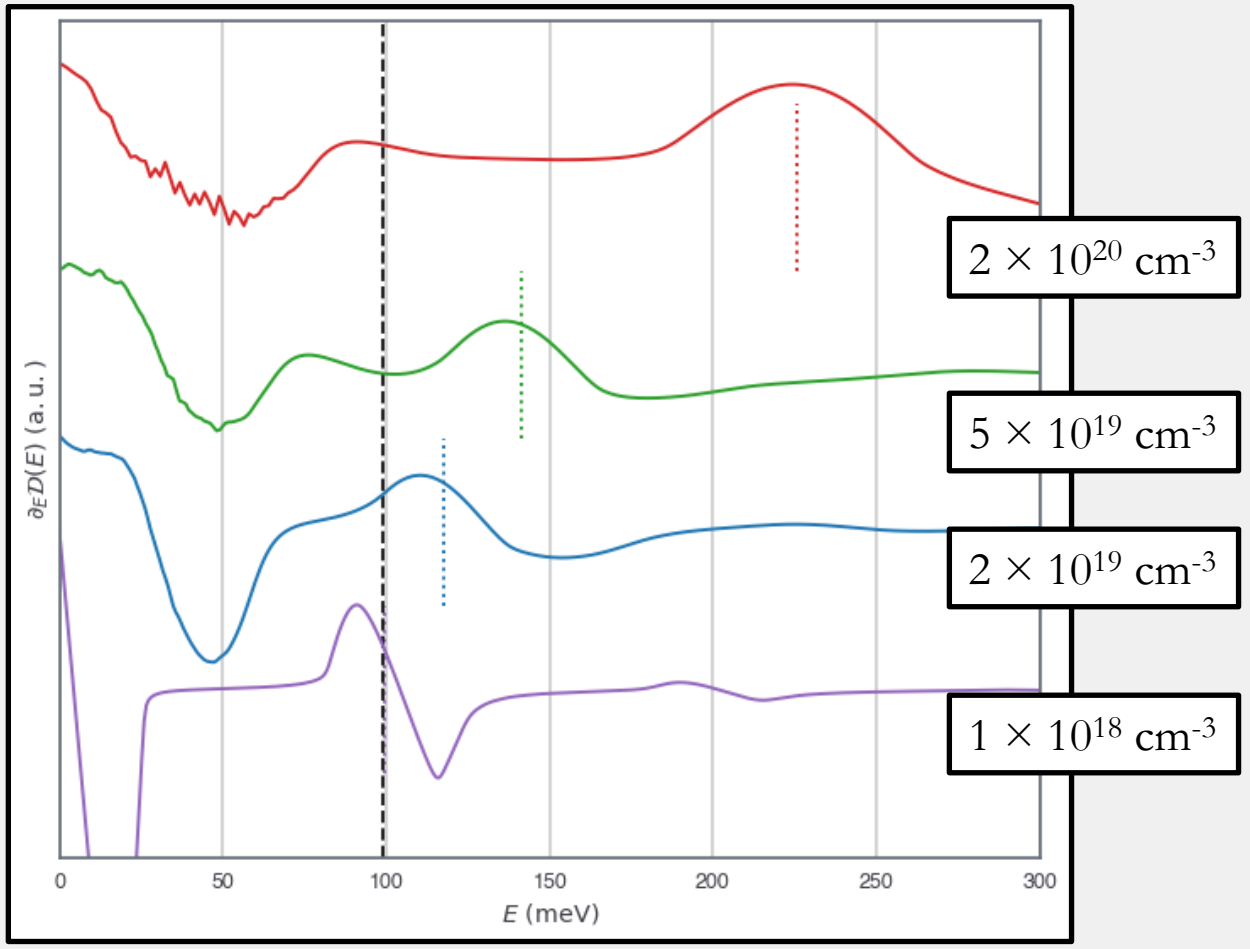


Wang et al, Nat Mat (2016)

∂DoS vs Tunneling

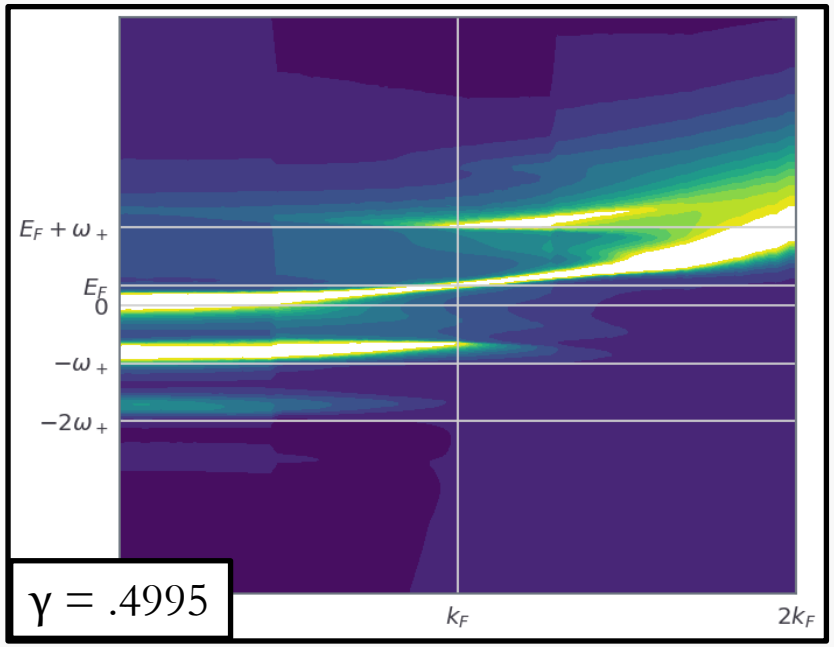


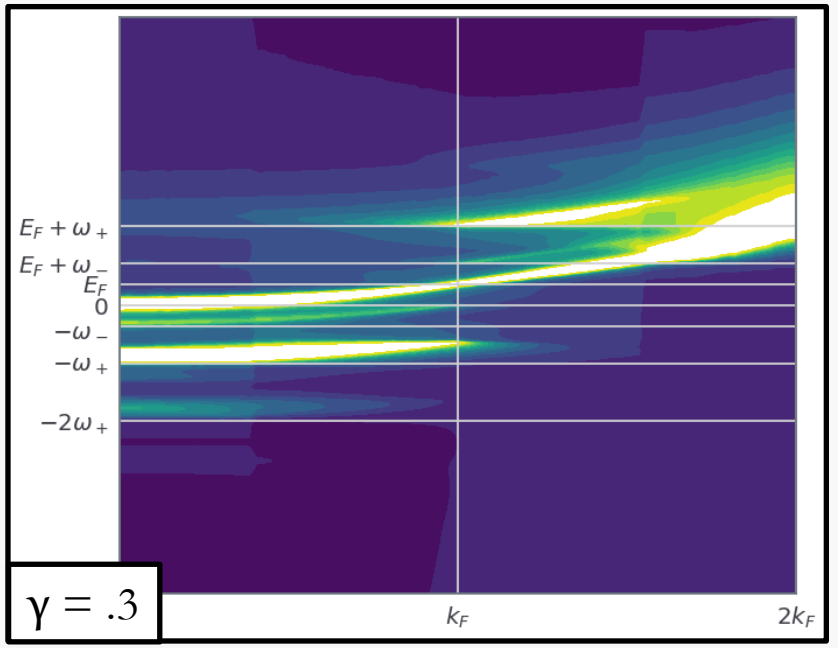
Swartz et al, PNAS (2018)



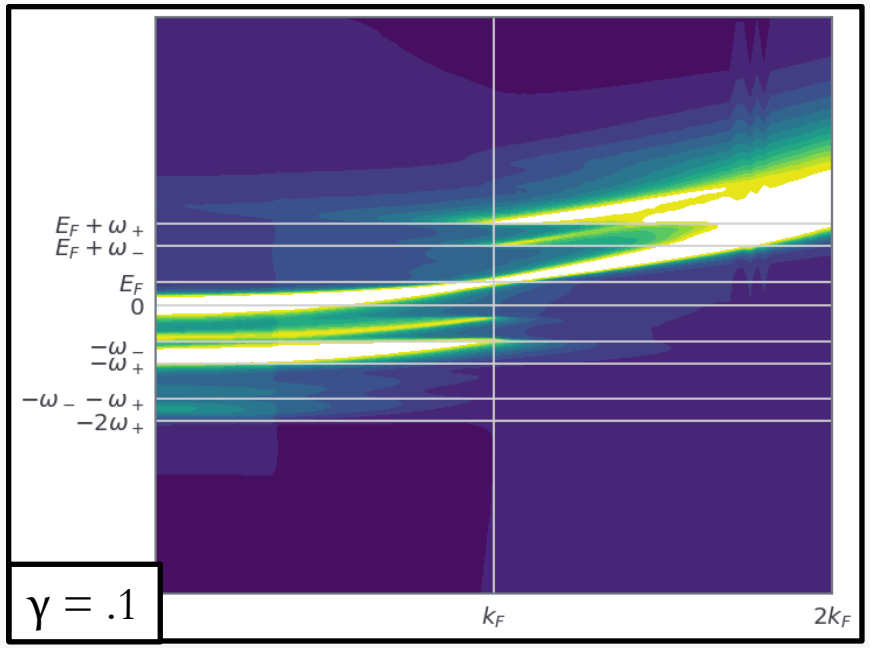
$n = 5 \times 10^{19}$ cm^{-3}

Proximity to the Critical Point



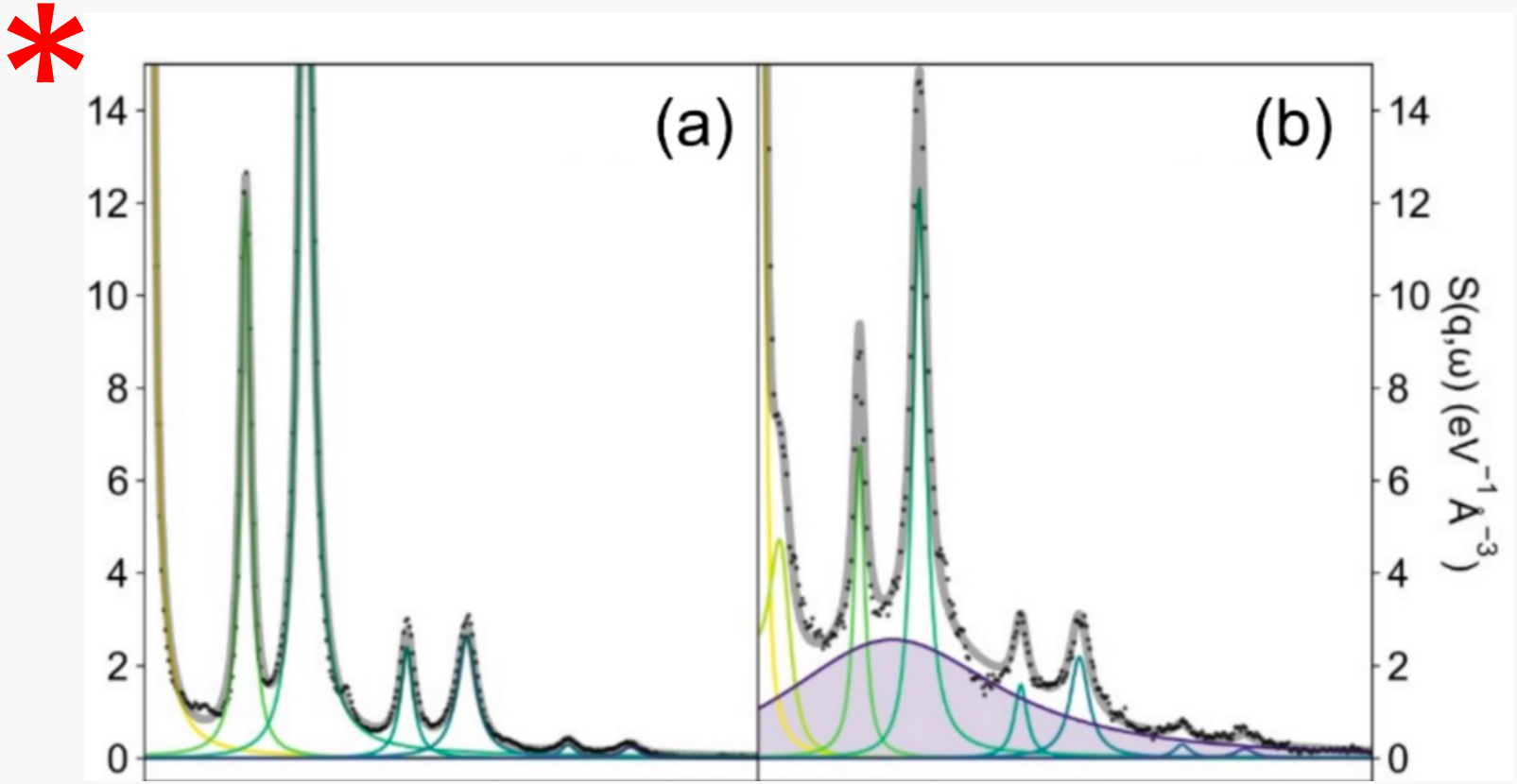


($\varepsilon_0 \sim 14$)



($\varepsilon_0 \sim 7$)

Coming soon



C. Kengle, S. Rubeck, and many others

Parting Thoughts

- We have uncovered a conspicuous discrepancy between the standard superconducting theory of STO and the absence of a plasmon in the normal state
- The dynamical signatures of a system are more indicative of what's happening than a phase diagram