Extremely correlated Fermi liquids

or

How I learned to stop worrying and love the infinite U limit

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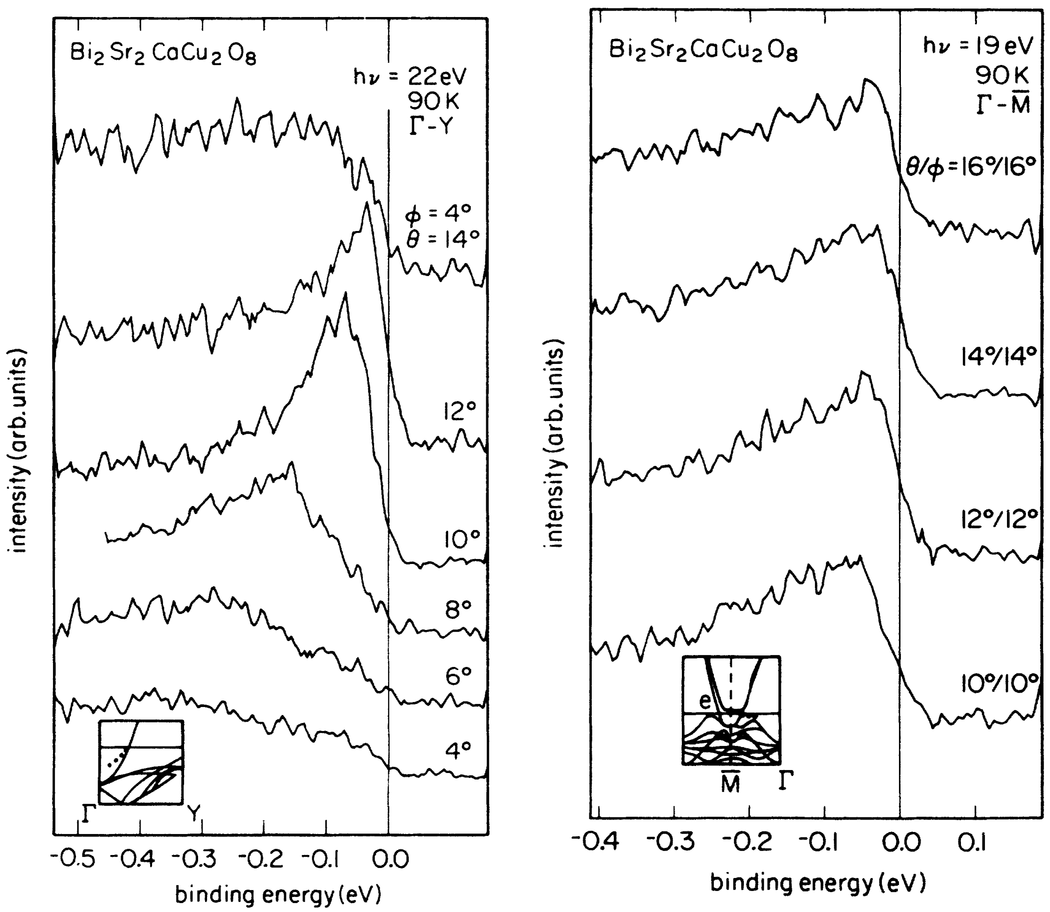
Angle resolved photo emission
ARPES (1990)
Surprising.

$$A(k,\omega) = \sum_{\alpha,\nu} e^{-\beta\varepsilon_\alpha} |\langle \nu | C(k) | \alpha \rangle|^2 \; \delta(\omega + \varepsilon_\nu - \varepsilon_\mu)$$

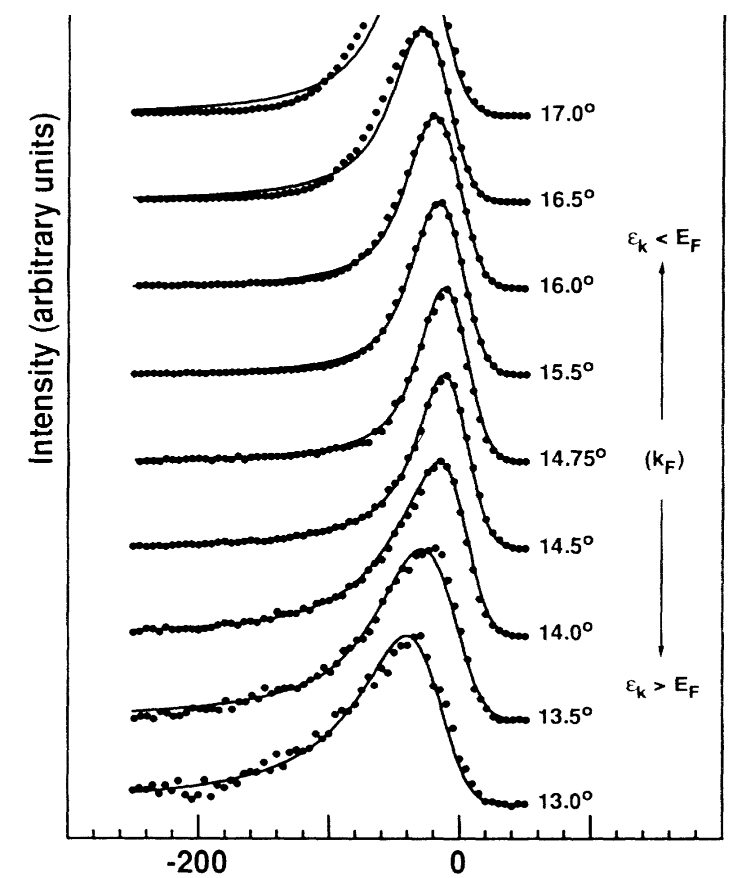
$$A_{FL}(k,\omega) \sim \frac{\Gamma/\pi}{\Gamma^2 + (\omega - E_k)^2}$$
$$\Gamma_{FL} \sim (\omega^2 + \pi^2 T^2)$$

E_k = Quasi hole energy



High-resolution angle-resolved photoemission study of the Fermi surface and the normal-state electronic structure of $Bi_2Sr_2CaCu_2O_8$

C. G. Olson, R. Liu, and D. W. Lynch



Fermi-Liquid Line Shapes Measured by Angle-Resolved Photoemission Spectroscopy on 1-*T*-$TiTe_2$

R. Claessen, R. O. Anderson, and J. W. Allen
Randall Laboratory, University of Michigan, Ann Arbor, Michigan 48109-1120

C. G. Olson and C. Janowitz

What does extreme correlations mean?

$$H = -\sum_{i,j} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

Hubbard model (t,U)

(1) Weak Correlations $U \ll t$

Semiconductors

(2) Intermediate Correlations $U \leq t$

DFT (Band theory), Wide band free electron like metals

(3) Strong Correlations $U \geq t$

Transition metal magnetism, Dense Kondo Heavy Fermi systems,
Iron arsenide superconductors etc

(4) Extreme Correlations $U \gg t$

High Tc systems, cobaltates, possibly some Heavy Fermi systems.

t J model

$$H = P_{d=0} \; (-\sum t_{ij} \; c^{\dagger}_{i} c_{j}) \; P_{d=0} + \frac{1}{2} \sum J_{ij} \vec{S}_i . \vec{S}_j$$

P W Anderson 1987; T M Rice, F C Zhang, 1989

In the work presented here:

- Systematic theory for the t J model using Schwinger Dyson approach.
- Expansion in density via a parameter "λ".
- Lowest non trivial order $O(\lambda^2)$ equations:
  - Simplified ECFL solution (analytical expressions)
  - Numerical solution (preliminary results, preprint soon with Daniel Hansen)
  - Large U Hubbard problem with Edward Perepelitsky and Ehsan Khatami, Marcos Rigol.

- Comparison with normal state cuprate ARPES line shapes (Laser and Synchrotron) at optimal doping using simplified ECFL solution.
- Gey-Hong Gweon + Genda Gu + Shastry.
- Predictions for asymmetry in line shapes near Fermi energy.

Why is the t J model such a difficult theoretical Problem?

- Non canonical field theory- Cannot consult existing text books!
  - Absence of Wicks theorem and Feynman series
  - Absence of any obvious small parameter.
- Gutzwiller projection is a ``singular perturbation", hence a major stumbling block for the dynamics.
- Use an adaptation of Schwinger's method.
  - Bypass Wicks theorem.
  - Uses extra time dependent potentials and magnetic fields to generate exact equations of motion (EOM).
- Freedom intrinsic to the Schwinger Dyson method + insights from spectral sum rules helps us to make progress.
- Describe a new **framework** for calculation with twin self energies and vertices.
- Initial results are promising.

PHYSICAL REVIEW LETTERS

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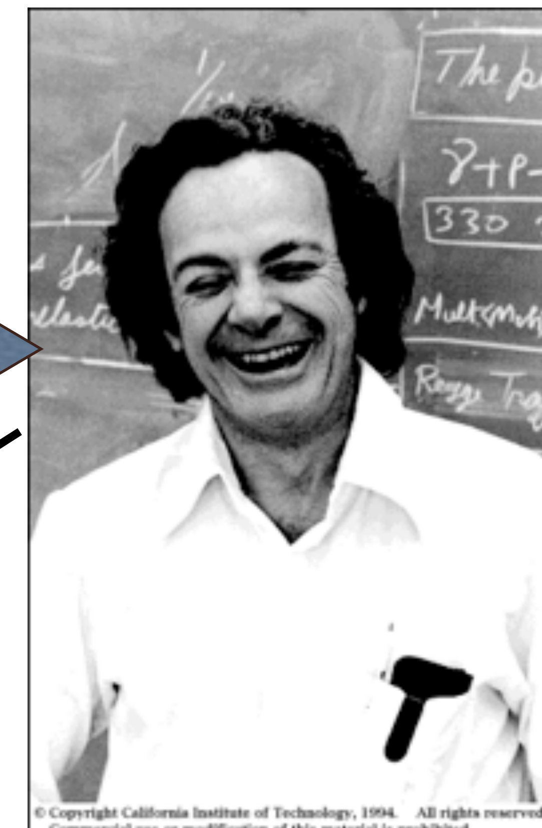
Extremely Correlated Fermi Liquids

B. Sriram Shastry

Seek inspiration from these great framework creators

- Dyson
- Feynman
- Schwinger
- Wick



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Calculation in brief

$$\hat{C}_\sigma = P_{d=0}\ C_\sigma\ P_{d=0}$$

$$\boxed{\mathcal{G}_{\sigma_i\sigma_f}(i\ \tau_i,\ f\ \tau_f) = -\frac{1}{Z}\ Tr\ e^{-\beta H}T_\tau e^{-A}\ \hat{C}_{i\sigma_i}(\tau_i)\hat{C}^\dagger_{f\sigma_f}(\tau_f)}$$

Added time dependent potentials, finally set to zero.

$$A = \sum_i \int_{\tau'} \mathcal{V}_i^{\sigma\sigma'}(\tau')\ \hat{C}^\dagger_{i\sigma}(\tau')\hat{C}_{i\sigma'}(\tau')$$

Schwinger Dyson exact EOM for Greens function

$$\boxed{(\partial_{\tau_i} - \boldsymbol{\mu})\mathcal{G}[i,f] \ = \ -\delta[i,f](\mathbb{1} - \gamma[i]) - \mathcal{V}_i \cdot \mathcal{G}[i,f] - X[i,\mathbf{j}] \cdot \mathcal{G}[\mathbf{j},f] - Y[i,\mathbf{j}] \cdot \mathcal{G}[\mathbf{j},f],}$$

Local Greens function

$$\boxed{\gamma(i) = \mathcal{G}^{(k)}[i^-, i], \qquad \mathcal{G}^{(k)}_{\sigma_1\sigma_2} = \sigma_1\sigma_2\ \mathcal{G}_{\bar{\sigma}_2\bar{\sigma}_1}}$$

Turning off sources, γ becomes n/2(density=n)

$$D = \xi^* \frac{\delta}{\delta\mathcal{V}^*} \quad (^* \text{ represents spin indices})$$

$$\boxed{\begin{aligned} X[i,j] &= -t[i,j]\ (D[i^+] + D[j^+]) + \frac{1}{2}J[i,k]\ (D[i^+] + D[k^+])\delta[i,j] \\ Y[i,j] &= -t[i,j]\ (\mathbb{1} - \gamma[i] - \gamma[j]) + \frac{1}{2}J[i,k]\ (\mathbb{1} - \gamma[i] - \gamma[k])\delta[i,j] \end{aligned}}$$

Symbolic notation makes things simpler

Y represents the hopping matrix element broken into a static and dynamic parts.

$$Y \to (-t + \frac{J}{2}) + Y_1 \quad \left\{ \begin{aligned} X &= [-t + \frac{1}{2}J]\ D \\ Y_1 &= -[-t + \frac{1}{2}J]\ \gamma \\ \hat{G}_0^{-1}(\boldsymbol{\mu}) &\equiv (\boldsymbol{\mu} - \partial_\tau - \mathcal{V})\mathbb{1} - [-t + \frac{1}{2}J] \end{aligned} \right.$$

Fermi gas (non interacting) Greens function

Symbolic EOM for t J model

$$\boxed{\mathcal{G} = (\hat{G}_0^{-1}(\boldsymbol{\mu}) - \lambda\ Y_1 - \lambda\ X)^{-1}.\ (\mathbb{1} - \lambda\ \gamma).}$$

Parameter λ introduced here

Set λ=1 at the end.
At λ=0 it reduces a Fermi gas.
Provides continuity between Fermi gas and tJ model.

$$\boxed{G = (\hat{G}_0^{-1} - UG - U\frac{\delta}{\delta v})^{-1}\ .\ \mathbf{1}}$$

Similarly the symbolic EOM for Hubbard model (Canonical theory)

Parameter λ in the atomic limit

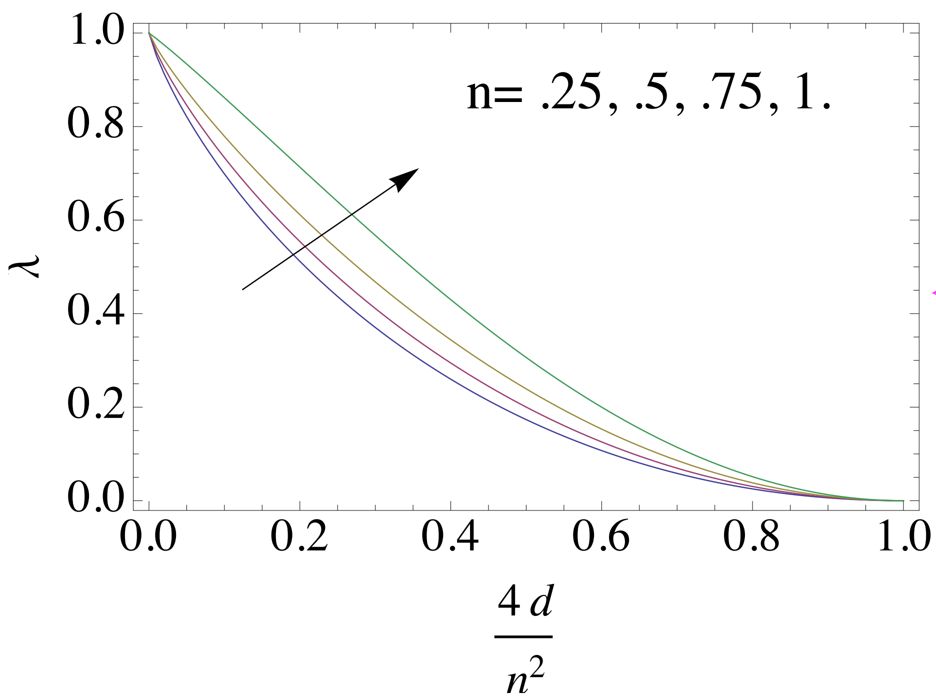
- Atomic limit gives explicit meaning of this parameter.
    - Tuning λ from 0 to 1 eliminates states, and can be mapped exactly to varying the double occupancy.
    - An expansion in powers of λ give virial (i.e. low density) expansion-

We can solve the G exactly and hence compute the chemical potential

$$\boxed{\boldsymbol{\mu} = k_B T \ \log\left(\frac{n}{2-(1+\lambda)n}\right)}$$

Use Maxwell's relation to compute entropy as a function of λ and n (N_s = # sites)

$$\boxed{\frac{S(n,\lambda)}{k_B N_s} = \frac{1}{1+\lambda}\{\log 4 - y\log n - (2-y)\ \log(2-y)\}} \quad y = (1+\lambda)n$$



Parameter λ versus density of double occupancy at various densities "n".

Comparing to standard expression for entropy as a function of d and n, we map λ to the normalized double occupancy density

$$d \sim d_0(1-\lambda)$$

$$d_0 = \frac{n^2}{4}$$ *Uncorrelated density of doubles*

$$\boxed{\mu = \mu_{\mathbf{0}} + k_B T \sum_{m=0}^{\infty}\left[\frac{n}{2-n}\right]^{m+1} \frac{\lambda^m}{m+1}}$$

From this expression conclude that an expansion in λ is effectively an expansion in density "n" as well.

The ECFL Theory in brief

Start from exact EOM

$$\mathcal{G} = (\hat{G}_0^{-1}(\boldsymbol{\mu}) - \lambda\, Y_1 - \lambda\, X)^{-1}.\, (\mathbb{1} - \lambda\, \gamma)$$

$$X = [-t + \frac{1}{2} J]\; D$$ *Recall definition of X*

$$\mathcal{G} = \mathbf{g}.\mu$$

Important decomposition into ``auxiliary Fermi liquid'' g and "caparison factor" (adaptive spectral weight) μ (not to be confused with chemical potential in bold **μ** *).*

$$D.(\mathbf{g}.\mu) = (\mathbf{g}.\Lambda)\ .\mathbf{g}.\ \mu + \mathbf{g}.\ \mathcal{U}$$ *Chain Rule for Derivative*

$$\Lambda \equiv \frac{\delta}{\delta \mathcal{V}}.\, (-\mathbf{g}^{-1}), \qquad \mathcal{U} \equiv \frac{\delta}{\delta \mathcal{V}}.\ \mu$$ *Vertex functions defined*

$$L \equiv [t - \frac{1}{2} J]\ \xi^*.\ \mathbf{g}\ \frac{\delta}{\delta \mathcal{V}^*}$$ *Linear operator L defined*

$$X.\mathcal{G} = \Phi.\mathcal{G} + \Psi$$

Thus arrive at two "self energies"

$$\because \Phi = L.\mathbf{g}^{-1}, \qquad \Psi = -L.\mu$$

EOM transformed exactly into

$$(\hat{G}_0^{-1}(\boldsymbol{\mu}) - \lambda\, Y_1 - \lambda\, \Phi).\ \mathbf{g}.\ \mu = (\mathbb{1} - \lambda\, \gamma) + \lambda\, \Psi$$

EOM bifurcates exactly defining the auxiliary FL and the rest

$$(\hat{G}_0^{-1} - \lambda\, Y_1 - \lambda\, \Phi).\ \mathbf{g} = \mathbf{1}$$ *Auxiliary Fermi liquid*

$$(\mathbf{1} + L)\ .\ \mu = (\mathbf{1} - \lambda\, \gamma)$$ *Adaptive spectral wt*

- *We can set up Schwinger Dyson equations by taking successive functional derivatives.*
- *Generates the analog of the skeleton graph expansion in powers of λ.*
- *We will take terms up to O(λ^2) and study this "second order theory".*

Comment: With some caveats, it might be useful to think of a mapping

$$\lambda \sim \frac{U}{U + z|t|}$$

Hence low order theory in λ is expected to be a VERY GOOD start. (since unlike U, the range of λ is [0,1].)

Theory to O(λ^2): Relevant equations and constraints

Technical Slide

Basic Defs

$$p \equiv (\vec{p}, i\omega_p)$$

$$E(k,p) = \left(\varepsilon_k + \varepsilon_p + \frac{1}{2} \left\{ \hat{J}[0] + \hat{J}[k-p] \right\} \right)$$

$$\mathcal{G}(p) = \mathbf{g}(p)\ \mu(p)$$

Adaptive spectral wt

$$\hat{\mu}(p) = 1 - \frac{n}{2} + \lambda \Psi(p)$$

Auxiliary FL Greens fn

$$\mathbf{g}^{-1}(\vec{k}, i\omega_n) = i\omega_n + \mu - \varepsilon_k^{eff} - \lambda\ \overline{\Phi}(\vec{k}, i\omega_n)$$

Auxiliary FL Self energy

$$\overline{\Phi}[k] = \quad -2\lambda \sum_p E(k,p)(E[p,k] + E[p+q-k,p])\ \mathbf{g}[p]\ \mathbf{g}[q]\ \mathbf{g}[q+p-k]$$

Effective band dispersion

$$\varepsilon_k^{eff} = c(n,\lambda) \times \varepsilon_k - \frac{1}{2}\lambda \sum_q J_{q-k}\ \mathbf{g}(q)$$

NNbr case dispersion vanishes at n~n ~.6 to .8. Exact value uncertain*

Second "Self energy"

$$\Psi(p) = -2\lambda \sum_p E(k,p)\mathbf{g}[p]\ \mathbf{g}[q]\ \mathbf{g}[q+p-k]$$

Exact Schwinger Dyson equations for the two self energies in terms of the two vertex functions.

$$\Phi[k] \ = \ \sum_p E(k,p)\ \mathbf{g}[p]\ \Lambda^{(a)}(p,k)\ e^{i\omega_p 0^+}$$

$$\Psi[k] \ = \ \sum_p E(k,p)\ \mathbf{g}[p]\ \mathcal{U}^{(a)}(p,k)\ e^{i\omega_p 0^+}$$

$$\sum_p \mathcal{G}[p] = \frac{n}{2}$$

Constraint for chemical potential.

- **Comments**
  - The effective band dispersion can vanish. One crude estimate places it at n~.8 (or x~.22). Expect almost non degenerate Fermi behavior near that filling- although higher order terms must prevail.
  - Similarity between expressions for the two self energies.
- **Two schemes reported next**:
  - Numerical solution of these eqns (somewhat high T). Also a few variant schemes, converging to unique scheme only recently.
  - Simplified analytical (engineering) solution at all T, where momentum dependence of Φ(p) and Ψ(p) is ignored.

Simplified ECFL solution (analytical expressions)

$$\mathcal{G}(p) = \frac{1 - \frac{n}{2} + \Psi(p)}{i\omega_n - \xi_p - \Phi(p)}$$

$$g(p) = \frac{1}{i\omega_n - \xi_p - \Phi(p)}$$ *Auxiliary FL*

$$\xi_p \sim (1 - \frac{n}{2})\ \varepsilon_k - \mu$$ *Energy variable*

Recap

$$\Phi(p) = \sum_{k,q} (\varepsilon)^2\ g(p-q)\ g(k)\ g(k+q)$$

$$\Psi(p) = \sum_{k,q} (\varepsilon)\ g(p-q) g(k) g(k+q)$$

$$\Psi(i\omega_n) \sim -\frac{n^2}{4\Delta_0}\quad \Phi(i\omega_n)$$ *Approximation on ignoring k dependence*

$$\mathcal{G}(\vec{p}, i\omega_n) = \frac{n^2}{4\Delta_0} + \frac{1 - \frac{n}{2} + \frac{n^2}{4\Delta_0}(\xi_p - i\omega_n)}{i\omega_n - \xi_p - \Phi(p)}$$

$$\sum_p g(p) = \frac{n}{2} = \sum_p \mathcal{G}(p)$$

Mean inelasticity scale Δ_0 computed from sum rule

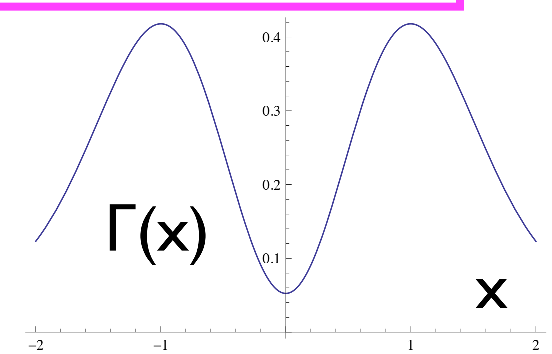
$$\Delta_0 = \int_{-\infty}^{\infty} dx\ f(x)\ \langle \rho_{\mathbf{g}}(\xi, x)\{\xi - x\}\rangle_\xi$$

Simplest Fermi liquid approximation (Analytically convenient).

$$\Gamma(x,T) = \eta + C_\Phi\{x^2 + \pi^2 T^2\}\ e^{-C_\Phi(x^2+\pi^2T^2)/\omega_c}$$

$$\Phi(i\omega_n) \sim \int \frac{dy}{\pi} \frac{\Gamma(x)}{i\omega_n - x}$$

$$\epsilon(\xi, x) \equiv (x - \xi - C_\Phi\ h(x))$$



Aux Fermi liquid fully fixed by this appx.

$$\rho_{\mathbf{g}}(\xi, x) = \frac{1}{\pi} \frac{\Gamma(x)}{\Gamma^2(x) + \epsilon^2(\xi, x)}$$

$$\rho_{\mathcal{G}}(\xi, x) = \frac{\Gamma(x)}{\pi} \frac{\left(\{1 - \frac{n}{2}\} + \left(\frac{n^2}{4}\right)\left\{\frac{\xi - x}{\Delta_0}\right\}\right)_+}{\Gamma^2(x) + \epsilon^2(\xi, x)}.$$

Parameters determining Auxiliary FL:

Extrinsic:

1) η (Elastic Impurity scattering-)
Importantly distinguishes Laser and Synchrotron ARPES

Intrinsic:

2) C_Φ (strength of FL inelasticity)

3) ω_c (High frequency cut off of FL)

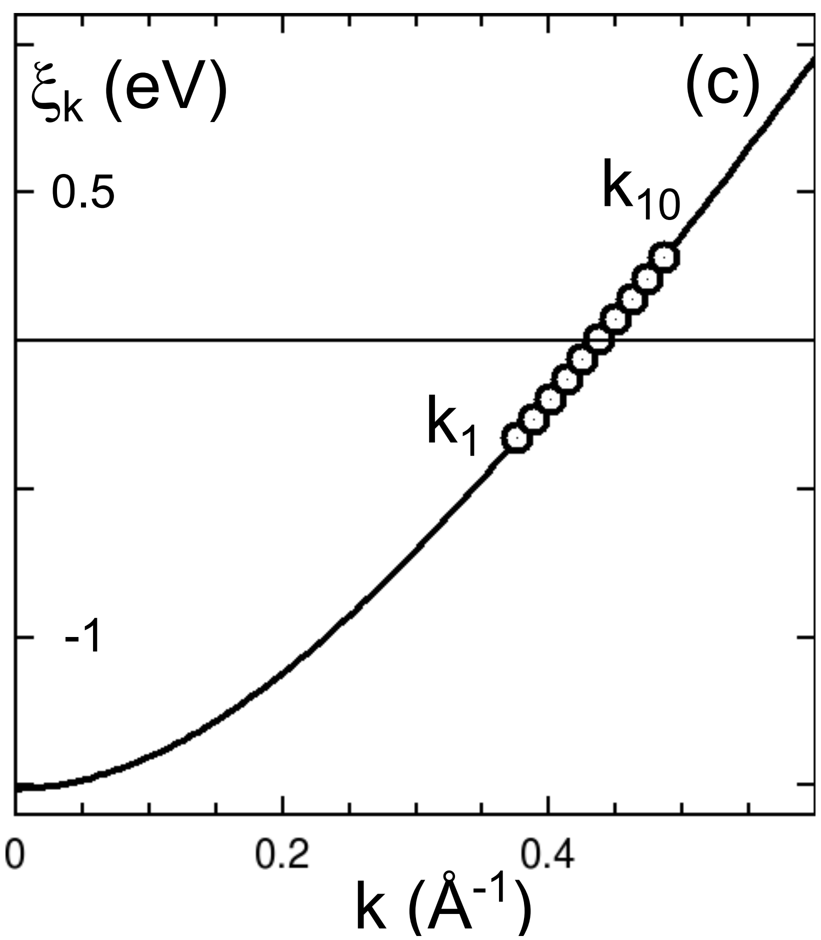
Simplified ECFL solution confronts data:

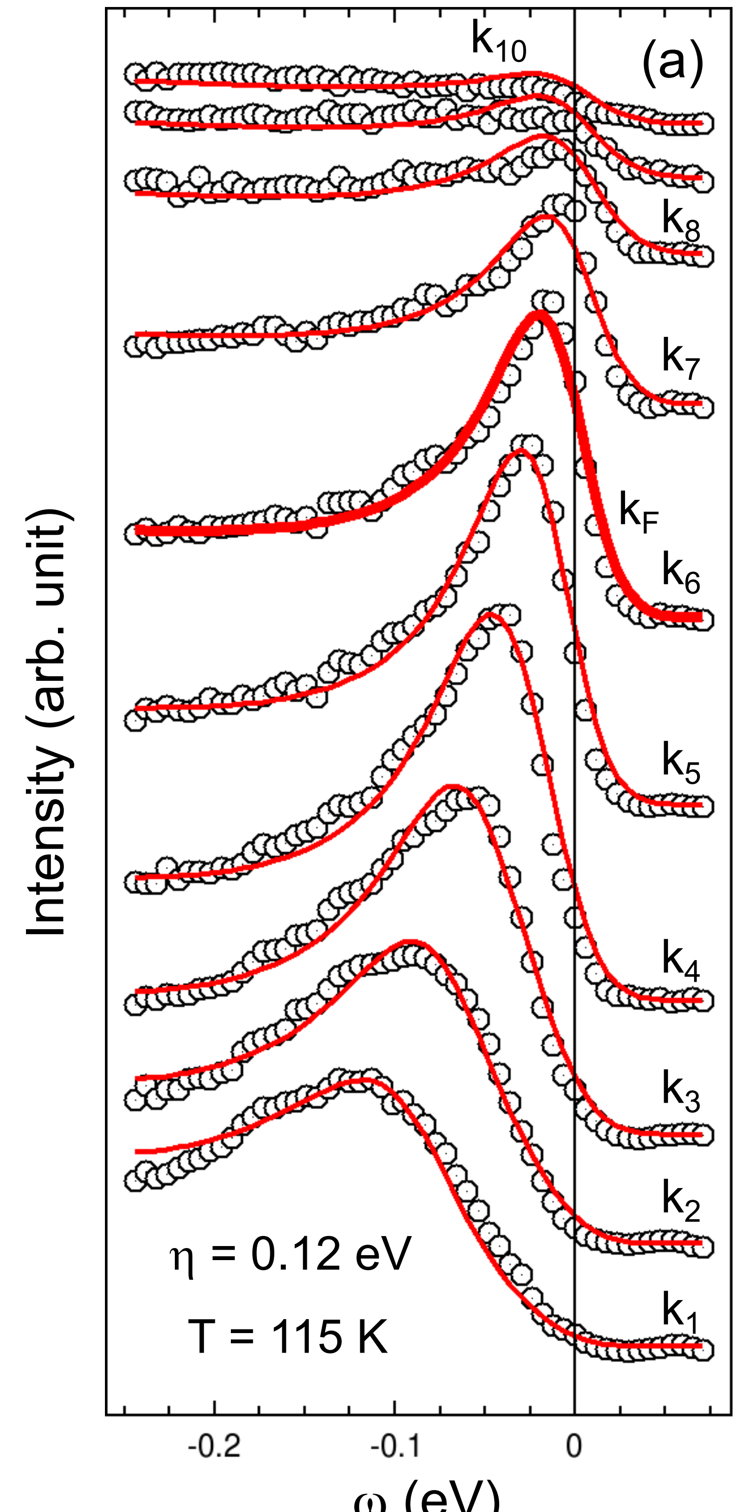
PRL **107,** 056404 (2011) PHYSICAL REVIEW LETTERS week ending 29 JULY 2011

Extremely Correlated Fermi-Liquid Description of Normal-State ARPES in Cuprates

G.-H. Gweon,[1,*] B. S. Shastry,[1,†] and G. D. Gu[2]

Energy dispersion and the 10 chosen values of k to compare theory and experiment.

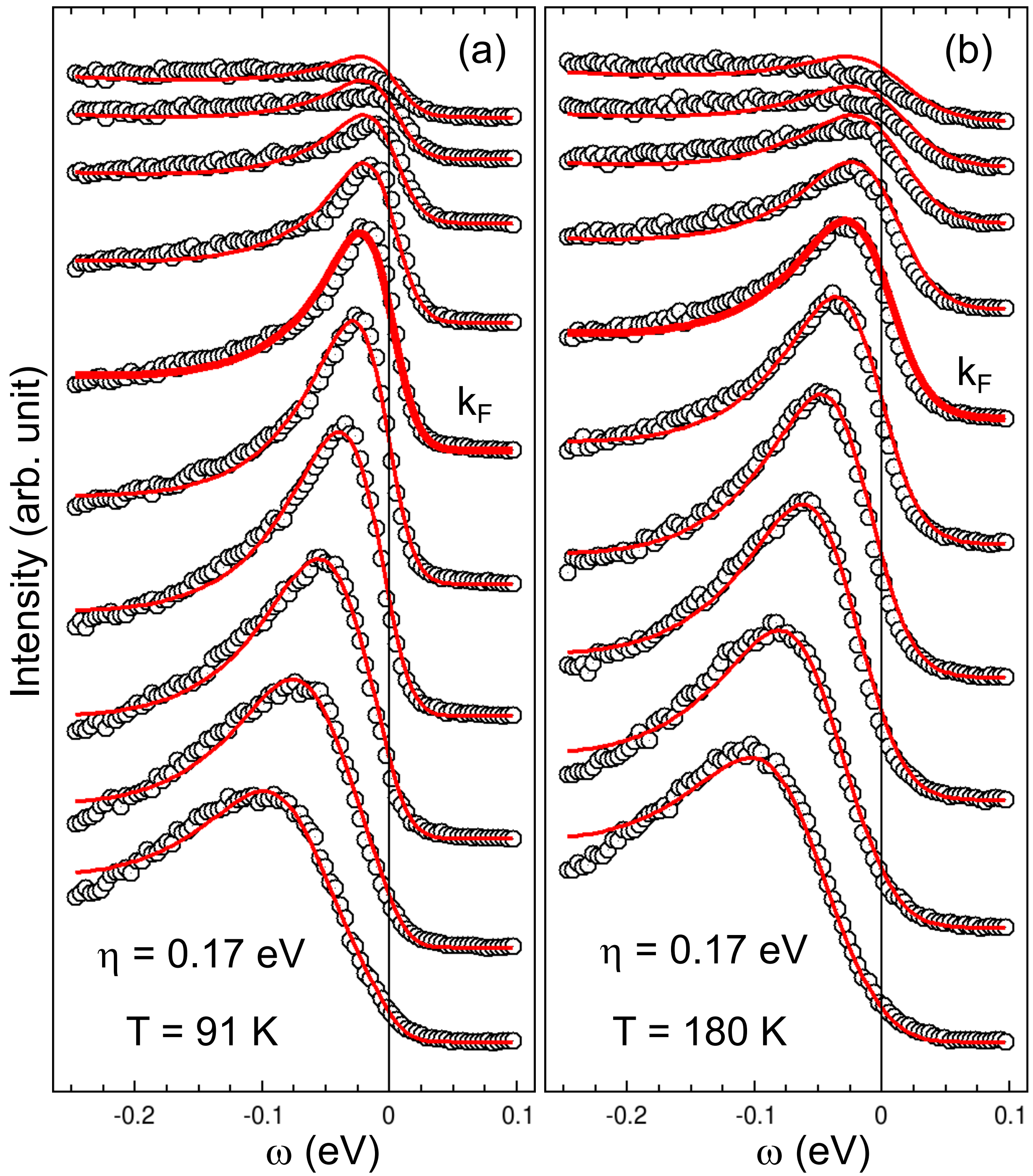




Synchrotron ARPES data from J Campuzzano's group compared to our theory. BISSCO at optimal doping T= 115K along <11> direction. Note that η =.12 eV (rather large)

Highly non Lorentzian therefore seem non Fermi liquid like.
First surprising data from High Tc was ARPES Olson et al.
ARPES probes states that are within .1 to .2 eV of Fermi energy with a resolution of say 20 meV therefore the most precise low energy probe and started the stampede!!

Expected symmetric peaks but spectra encountered in High Tc seemed "bizarre"
A prime mystery in this field.



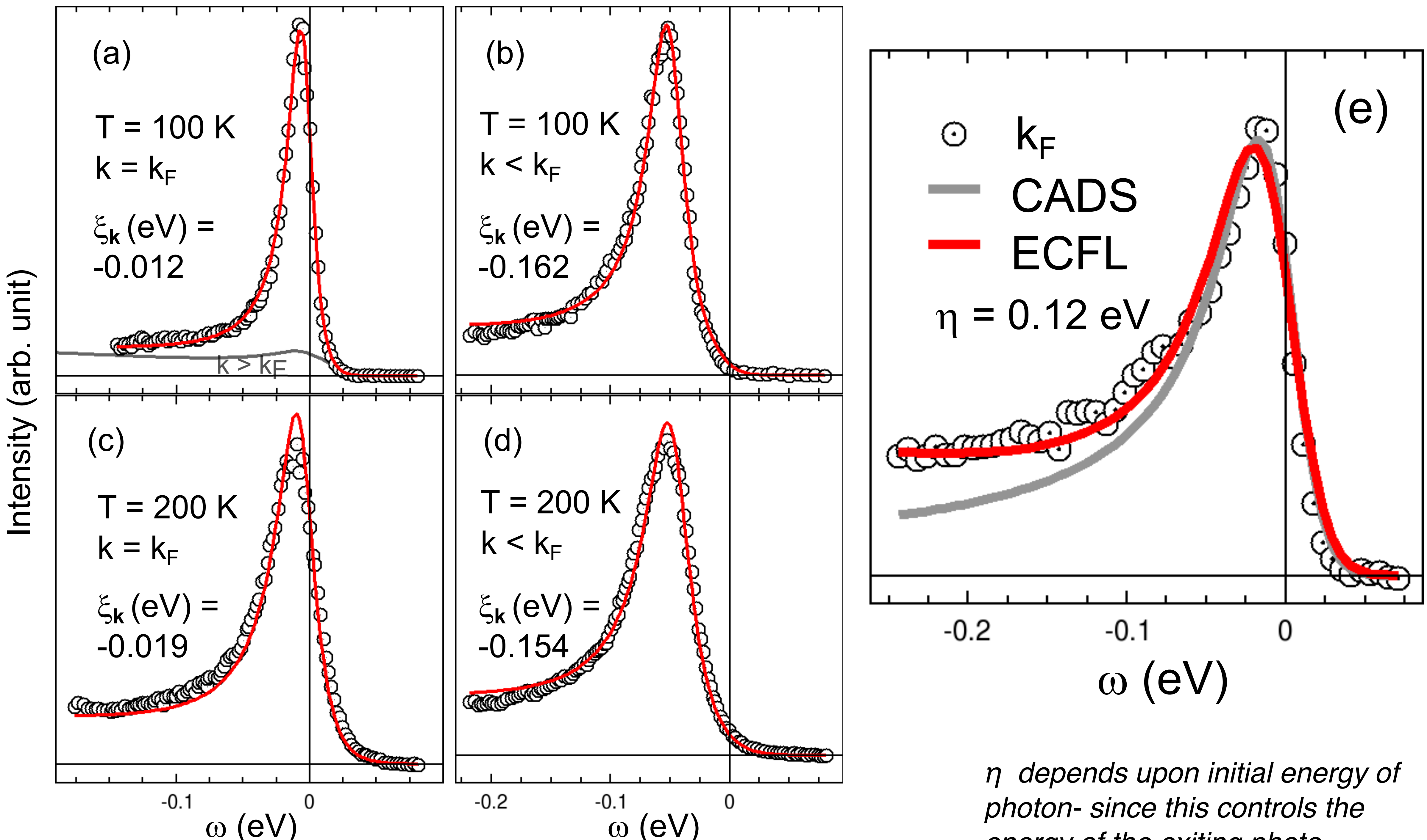
(Bi2212)

Gey-Hong Gweon's recent data UCSC
Similarly Campuzzano's data from 5 yrs ago.

Laser ARPES BISCO 2212

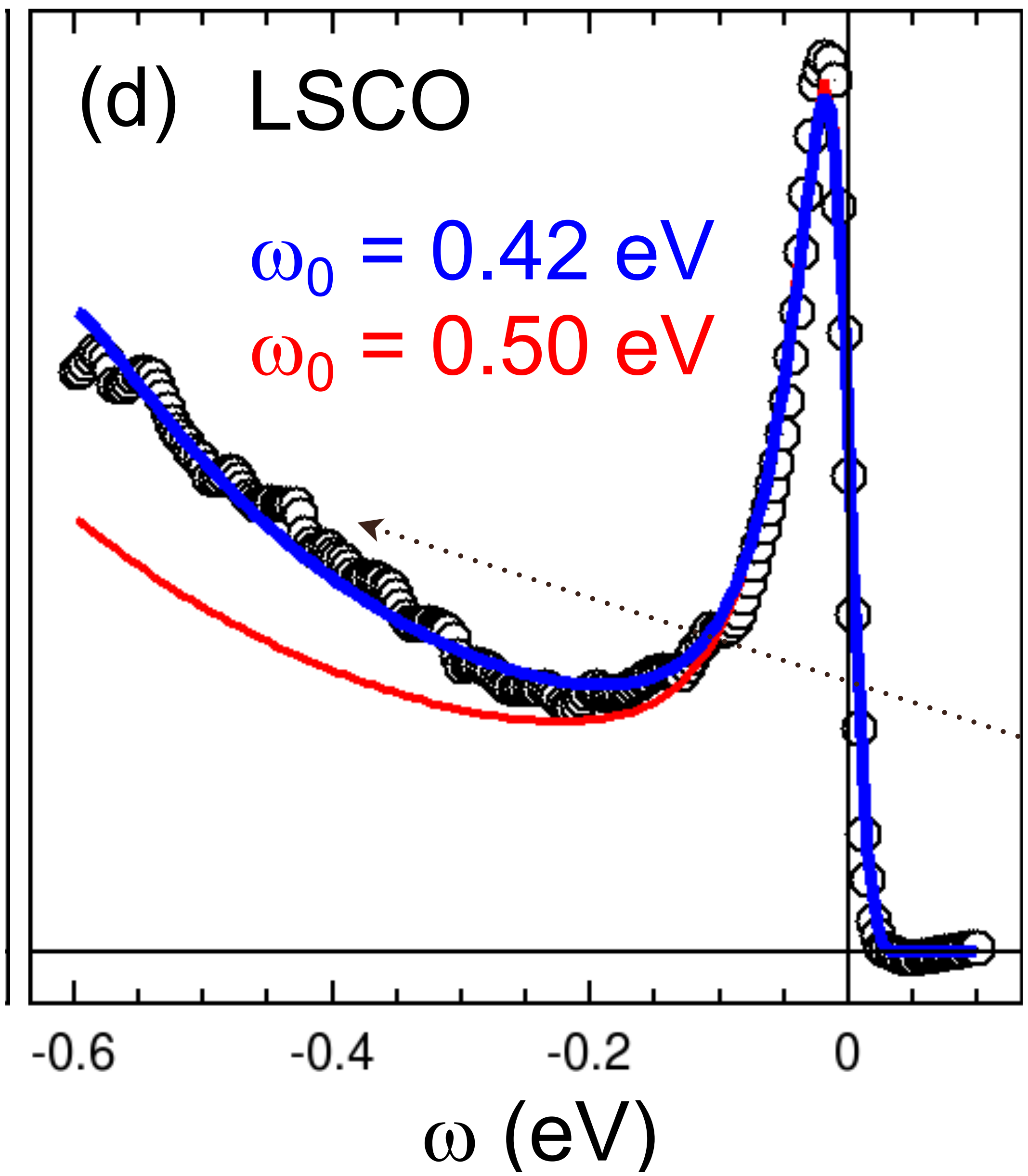
η=.032 eV

Synchrotron ARPES BISCO 2212



Same physical parameters only η different

η depends upon initial energy of photon- since this controls the energy of the exiting photo electron. Lower energy exiting electrons have shorter MFP due to electron gas relaxation processes.

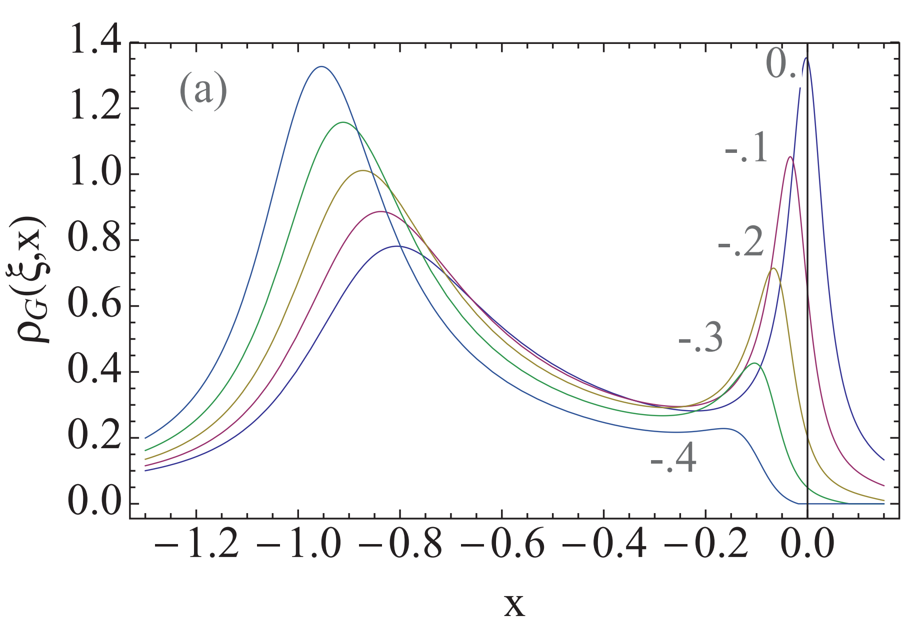


$$\rho_{\mathcal{G}}(\vec{k},\omega) \leftrightarrow A(\vec{k},\omega)$$

Fujimori, ZX Shen data on LSCO

$$A(\vec{k},\omega) = A_{FL}(\vec{k},\omega)\left(1 - \frac{n}{2} + \frac{n^2}{4}\cdot\frac{\xi_{\vec{k}}-\omega}{\Delta_0}\right)_+$$

Smoking gun
Linear rise of intensity
for occupied states.



On a larger energy scale
there are often broad peaks beyond which
the intensity falls.

Some predictions

Yes, really!

Dynamical Particle Hole Asymmetry in Cuprate Superconductors

B Sriram Shastry arXiv:1110.1032, November 2011

Dynamical P-H transformation $(\hat{k} \equiv \vec{k} - \vec{k}_F)$

$$(\vec{\hat{k}}, \omega) \to -(\vec{\hat{k}}, \omega).$$

P-H symmetry is an "Emergent symmetry" at low enough energies: Fixed point symmetry in the asymptotic regime: "Schmalian- Batista"

$$\mathcal{S}_{\mathcal{G}}(\vec{k}, \omega) \equiv f(\omega) f(-\omega) \rho_{\mathcal{G}}(\vec{k}, \omega) = \frac{1}{|M(\vec{k})|} f(-\omega) I(\vec{k}, \omega).$$

This is the Fermi symmetrized spectral function that focuses attention near chemical potential. Here I(k,w) is ARPES intensity and M is dipole matrix element

Construct symmetric and antisymmetric combinations under the above DPH transformation

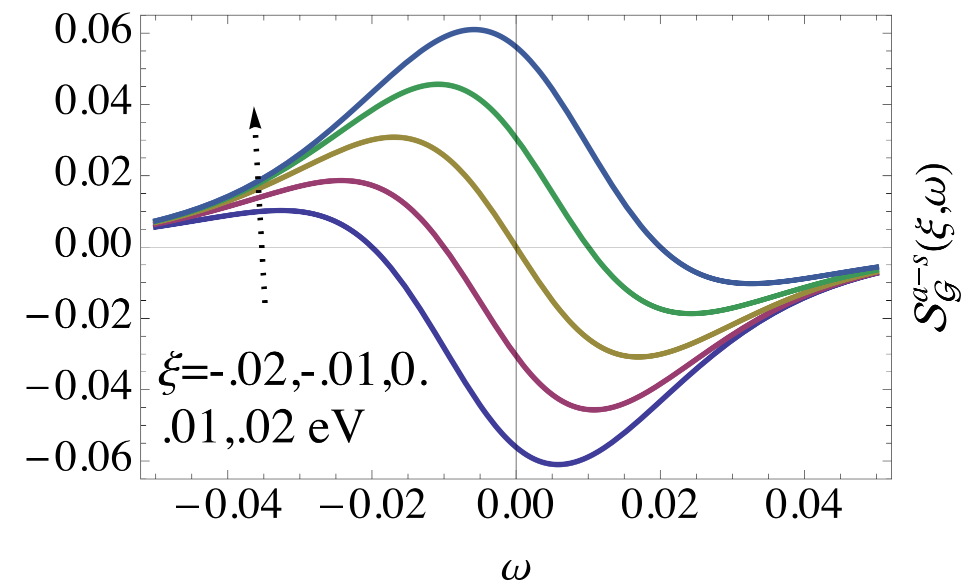
$$\frac{1}{2}\left[\mathcal{S}_{\mathcal{G}}(\vec{k}_F + \vec{\hat{k}}, \omega) \mp \mathcal{S}_{\mathcal{G}}(\vec{k}_F - \vec{\hat{k}}, -\omega)\right]$$

From these form the (dimensionless) asymmetry ratio R

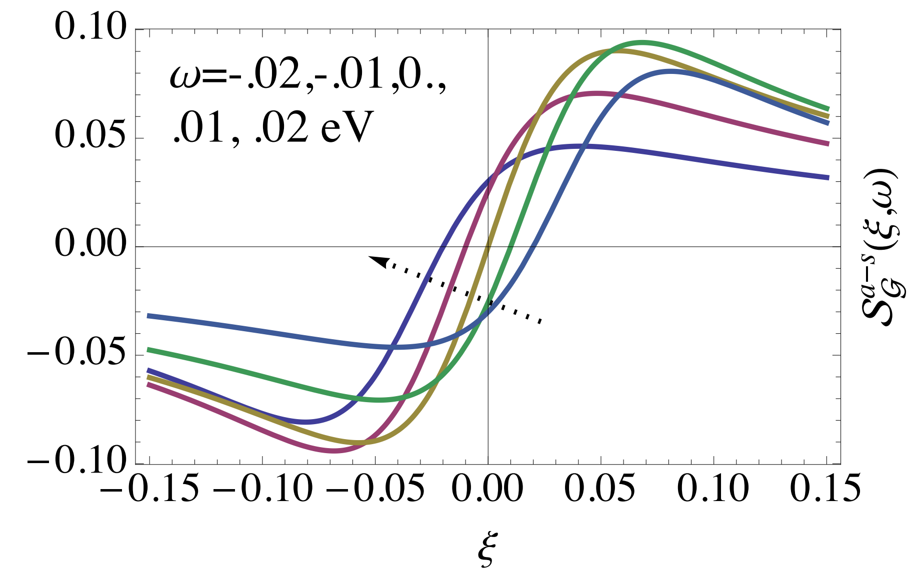
$$\mathcal{R}_{\mathcal{G}}(\vec{k}_F|\vec{\hat{k}}, \omega) = \mathcal{S}^{a-s}_{\mathcal{G}}(\vec{k}_F|\vec{\hat{k}}, \omega) / \mathcal{S}^{s}_{\mathcal{G}}(\vec{k}_F|\vec{\hat{k}}, \omega)$$

Important ratio Can experimentally distinguish between two classes of theories.

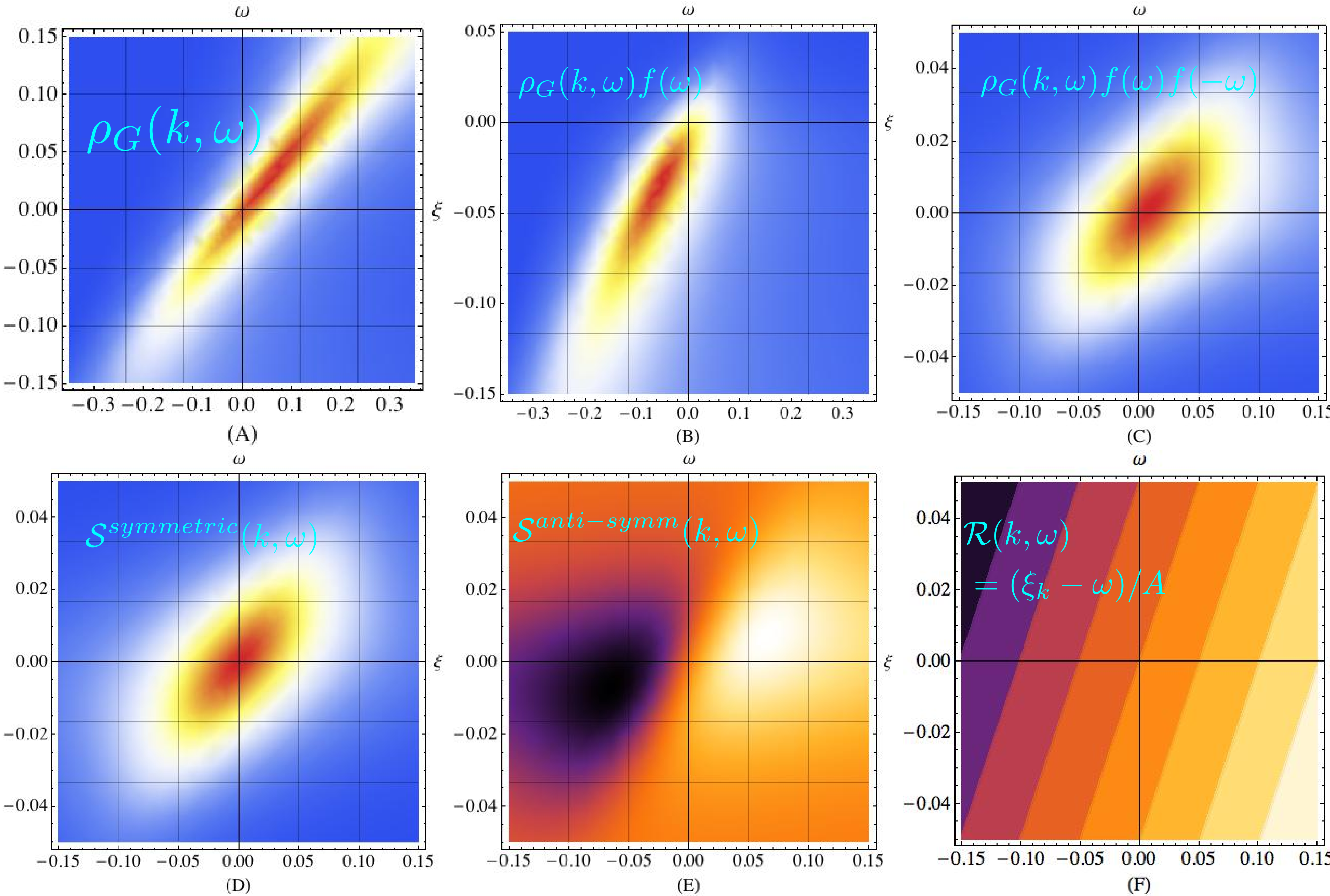
Simplified ECFL theory



Scale of ω is eV. Enormous asymmetry is expected



Scale of ξ is eV.



Requires momentum resolution Δk = .001 Angstrom (perhaps just beyond current reach.)

Asymmetry related comments:

- Experimentally feasible if momentum resolution is attained (not too far from current resolution-).
- Fermi liquids do not have such large asymmetries on a similarly small energy scale. P-H symmetry is emergent at most accessible energy scales in *intermediate coupling Fermi liquids*.
- DMFT: Professor Antoine Georges mentions that remarkably similar asymmetries emerge from the theory by pushing large U. We expect that DMFT and ECFL will be ultimately connected since these are alternate descriptions of the same very strong correlations.
- Asymmetry is a measure of corrections to scaling at the FL fixed point, large asymmetry implies large corrections- has serious implications for Hall constant and Seebeck coefficients- being pursued. Numerical estimates give R~10% (25 meV scale) compared to <1% for weak/ intermediate coupling Fermi liquids" (Hodges, Smith, Wilkins 1972)
- ECFL and Anderson Casey have similar features. A-C line shapes share the feature of non trivial asymmetry of O(1) on fairly small energy scale (~25 meV). However they have too strong a statement about criticality at all densities.
- Asymmetry can be used to discriminate between classes of theories.

$$\boxed{\mathcal{R}_{SECFL} = \frac{\hat{k}.\vec{v}_F - \omega}{\varepsilon_0} \qquad \mathcal{R}_{CA} = \frac{\hat{k}.\vec{v}_F - \omega}{a\ k_B T}}$$

Requires momentum resolution Δk = .001 Angstrom (perhaps just beyond current reach.)

In Summary:

- Presented a Schwinger based systematic low density or λ expansion of t-J model.
- Numerics: (work in progress)
  - Tentatively: expansion indicates an Extremely Correlated Fermi liquid phase colliding with a Quantum Critical Point at T=0 at density n*.
  - Shrinking energy scale follows from bare bandwidth as density increases.
  - Realistic bands (with non zero t') needs to be done.
- Simplified analytical solution:
  - Novel and relevant **non Lorentzian analytical expressions** for line shapes. Satisfy important sum-rules and give a **global perspective** of the spectral functions.
  - Excellent agreement with line shape data at optimal doping.
- Testable predictions for line shape asymmetries
- Superconductivity itself?