第５回HPC-Phys勉強会

ボルツマン機械を用いて解き明かす 高温超伝導の発現機構

Mechanism of Formation of High-Temperature Superconductivity Revealed by Boltzmann Machine Learning

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Acknowledgement:
Prof. Takeshi Kondo (ISSP)

Y. Yamaji, T. Yoshida, A. Fujimori, and M. Imada, arXiv:1903.08060.

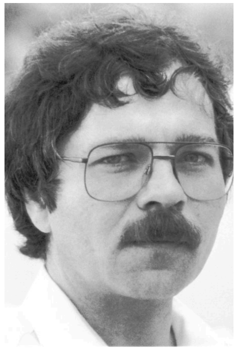
重点課題7

$$A(\vec{k},\omega) = -\frac{1}{\pi}\mathrm{Im}G[\Sigma](\vec{k},\omega)$$

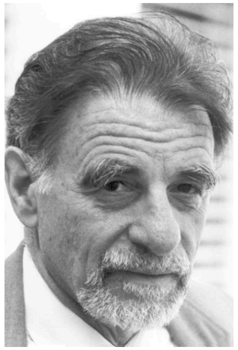
An enigmatic inverse problem:
Origin of high-temperature superconductivity

1986 High-temperature superconductivity
in copper oxides

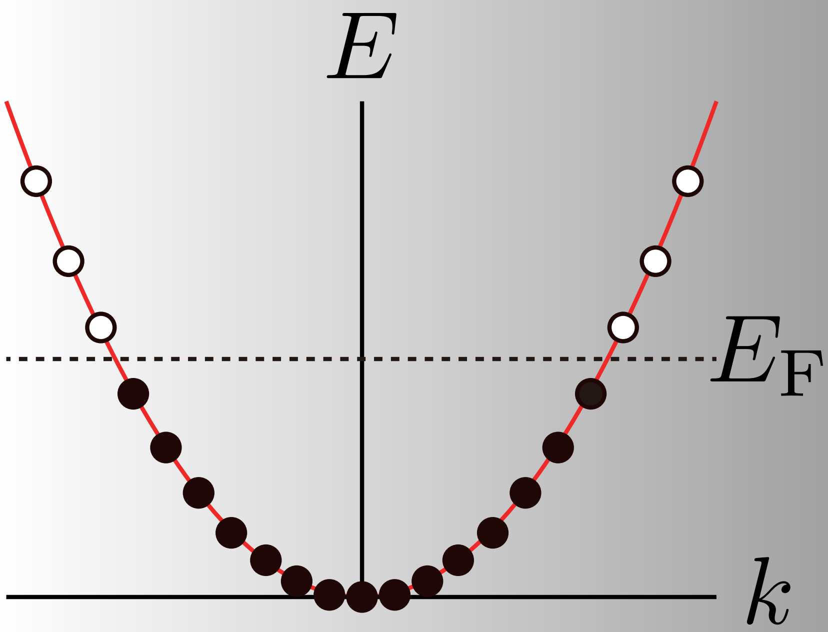
J. G. Bednorz



K. A. Müller

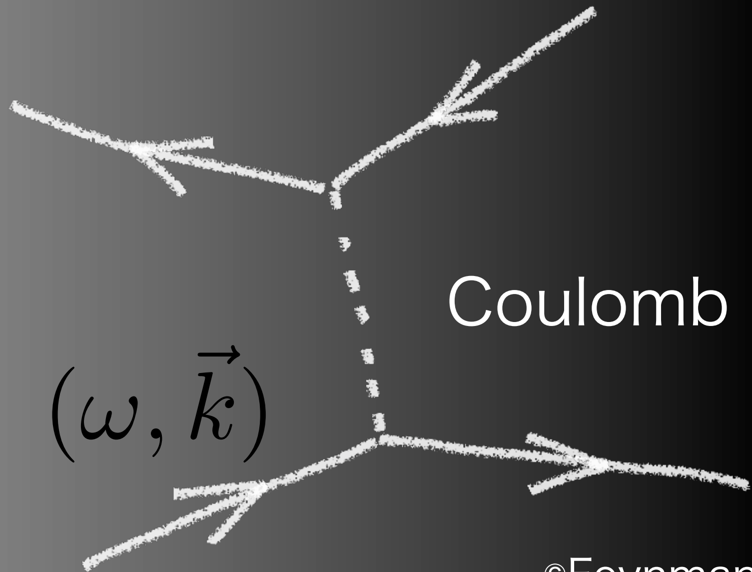


Life of Electrons in Crystalline Solids



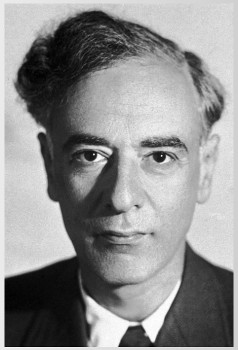
E. Fermi

W. Pauli



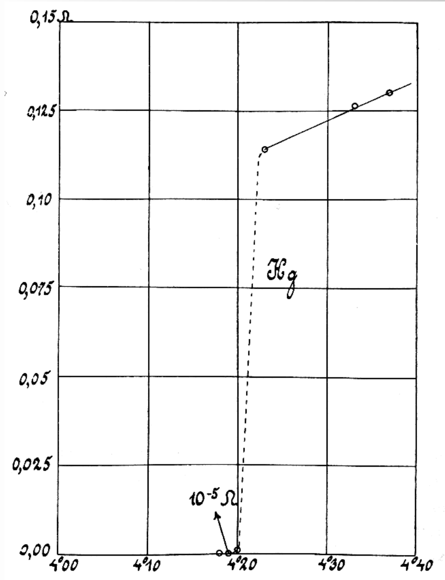
©Feynman

L. D. Landau 1956



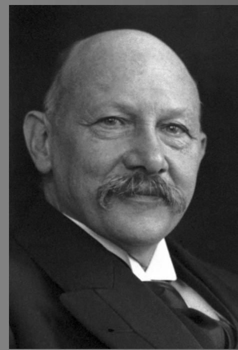
<u>Landau's Fermi liquid theory</u>
strongly interacting electrons and free electrons are adiabatically connected

Life of Electrons in Superconductivity



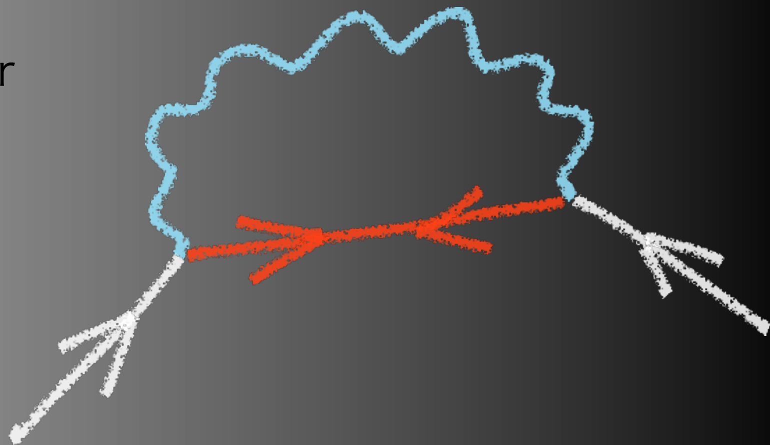
1911 Zero electric resistance of Hg

H. Kamerlingh Onnes



1957 BCS theory

J. Bardeen, L. N. Cooper, J. R. Schrieffer



Propagation of *Free* Electron

$$\left(i\frac{\partial}{\partial t} - \hat{H}_0\left[\vec{x}, \frac{\partial}{\partial \vec{x}}\right]\right) G(\vec{x}-\vec{x}', t-t') = \delta(\vec{x}-\vec{x}')\delta(t-t')$$

For a single electron in vacuum

$$\hat{H}_0\left[\vec{x}, \frac{\partial}{\partial \vec{x}}\right] = -\frac{\nabla^2}{2m} - \mu$$

After Fourier transformation

$$G(\vec{k},\omega) = \frac{1}{\omega + i\delta - \frac{|\vec{k}|^2}{2m} + \mu}$$

Spectral weight

$$A(\vec{k},\omega) = \lim_{\delta\to+0} -\frac{1}{\pi}\mathrm{Im}G(\vec{k},\omega) = \delta\left(\omega - \frac{|\vec{k}|^2}{2m} + \mu\right)$$

Description of Many-Body Electrons

Many-body Schrödinger eq.

$$i\frac{\partial}{\partial t}\Phi(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N) = \hat{H}\Phi(\vec{x}_1, \vec{x}_2, \ldots, \vec{x}_N)$$

$$\hat{H} = \sum_{j=1}^{N}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial \vec{x}_j^2} + V_{\text{ext}}(\vec{x}_j)\right] + \frac{e^2}{4\pi\varepsilon}\sum_{j<\ell}\frac{1}{|\vec{x}_j - \vec{x}_\ell|}$$

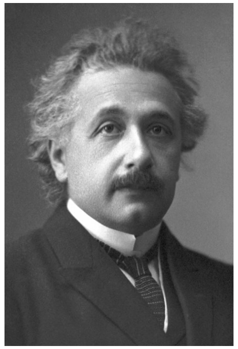
EOM of *single-particle* Green's function

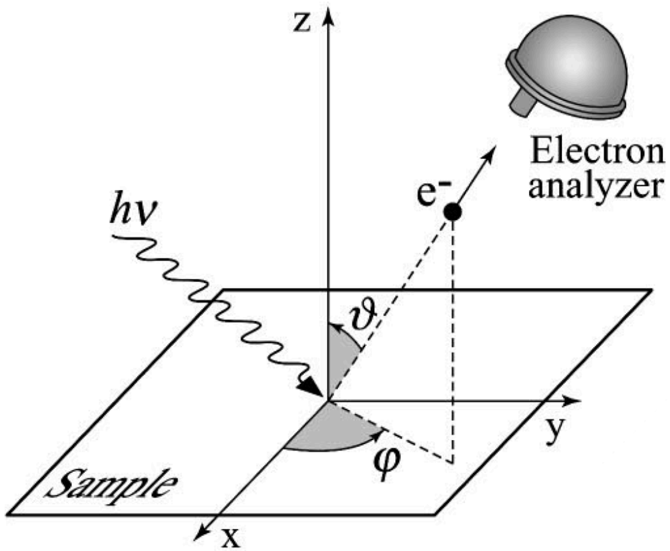
$$\left(i\frac{\partial}{\partial t} - \hat{H}_0\left[\vec{x}, \frac{\partial}{\partial \vec{x}}\right]\right)G(\vec{x}-\vec{x}', t-t')$$

$$-\int d\vec{x}_1 dt_1 \Sigma(\vec{x}-\vec{x}_1, t-t_1)G(\vec{x}_1-\vec{x}', t_1-t')$$

$$= \delta(\vec{x}-\vec{x}')\delta(t-t')$$

$$A(\vec{k},\omega) = -\frac{1}{\pi}\mathrm{Im}G[\Sigma](\vec{k},\omega)$$





Photoemission geometry

Damascelli, Hussain, & Shen,
Rev. Mod. Phys. 75, 473 (2003)

$$(E = \hbar\omega, \vec{p} = \hbar\vec{k})$$

Rigorous Relation between Self-Energy and Spectral Weight

Normal self-energy $\mathrm{Im}\Sigma^{\mathrm{nor}}(\vec{k},\omega)$

∼Scattering rate

Anomalous self-energy $\mathrm{Im}\Sigma^{\mathrm{ano}}(\vec{k},\omega)$

∼Rate of anomalous scattering

∼ω-distribution of attractive force

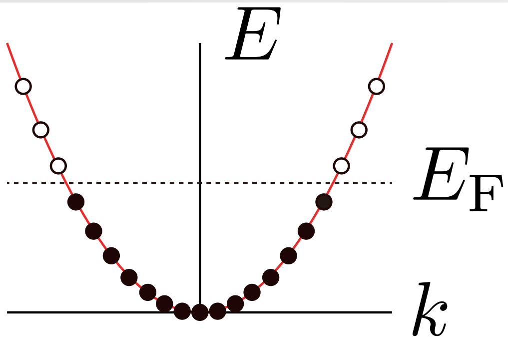
$$\Sigma(\vec{k},\omega)=\Sigma^{\mathrm{nor}}(\vec{k},\omega)+\frac{\Sigma^{\mathrm{ano}}(\vec{k},\omega)^2}{\omega+i\delta+E(-\vec{k})+\Sigma^{\mathrm{nor}}(-\vec{k},-\omega)^*}$$

Spectral weight

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

$$G(\vec{k},\omega)=\frac{1}{\omega+i\delta-E(\vec{k})-\Sigma(\vec{k},\omega)}$$

Self-Energy in BCS Superconductors



$$E_F \sim \mathcal{O}(10^4)\ \mathrm{K}$$

$$\Theta_D \sim \mathcal{O}(10^2)\ \mathrm{K}$$: Scale of phonon

$$T_c \sim \mathcal{O}(1-10)\ \mathrm{K}$$

Eliashberg eqs. for BCS SC

$$k_B T_c / E_F,\ k_B \Theta_D / E_F \ll 1$$

$$\Sigma^{\mathrm{nor/ano}}(\omega) = \int d\omega' K^{\mathrm{nor/ano}}[\Delta](\omega,\omega')\alpha^2(\omega')F(\omega')$$

SC gap function
$$\Delta(\omega) = \frac{\Sigma^{\mathrm{ano}}(\omega)}{1 - \dfrac{\Sigma^{\mathrm{nor}}(\omega) - \Sigma^{\mathrm{nor}}(-\omega)^*}{2\omega}}$$

$\alpha^2(\omega)F(\omega)$: Coupling² x DOS of phonon

A. B. Migdal, Sov. Phys. JETP 7, 996 (1958).
G. Eliashberg, Sov. Phys. JETP 11, 696 (1960).

cf.) P. Morel, P. W. Anderson,
Phys. Rev. **125**, 1263 (1962).

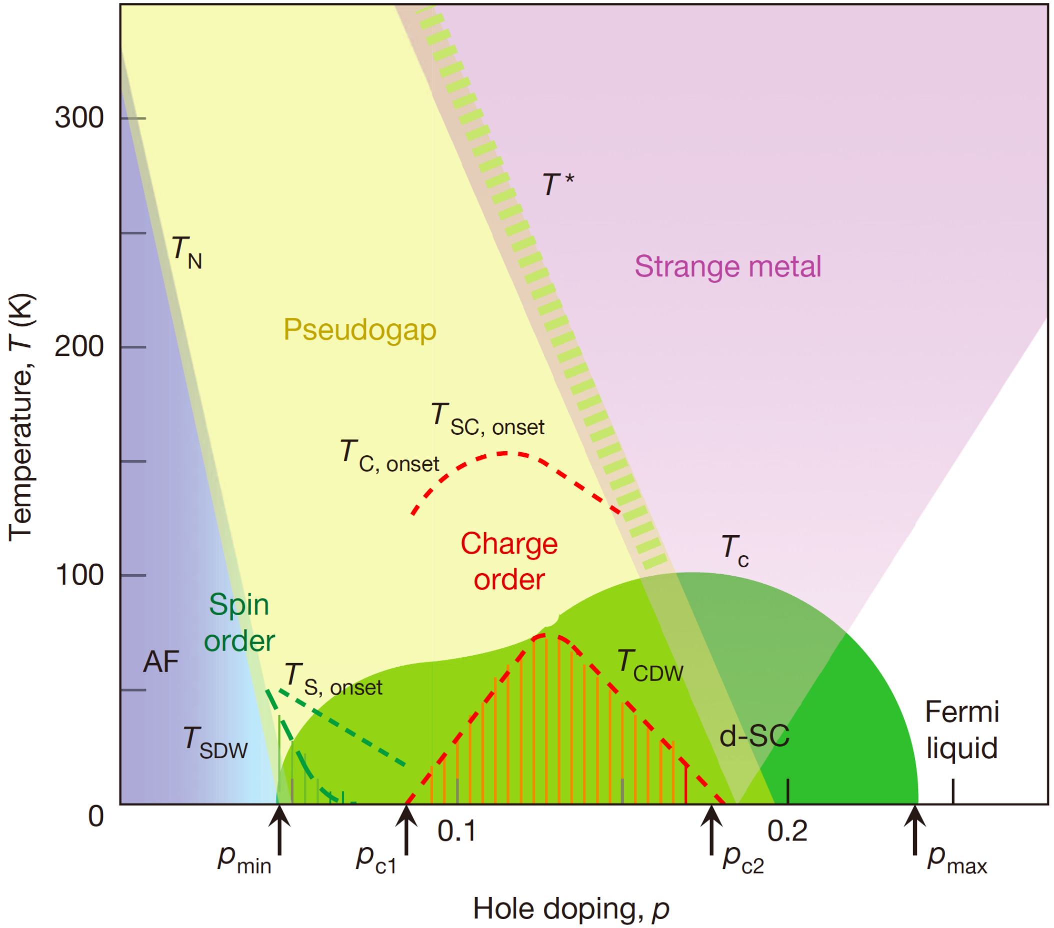
Ratio of DOS
$$\frac{\mathrm{DOS_s}(\omega)}{\mathrm{DOS_n}(\omega)} = \mathrm{Re}\left\{\frac{\omega}{\sqrt{\omega^2 - \Delta(\omega)^2}}\right\}$$

J. R. Schrieffer, D. J. Scalapino, and J. W. Wilkins, Phys. Rev. Lett. 10, 336 (1963).
W. L. McMillan and J. M. Rowell, Phys. Rev. Lett. 14, 108 (1965).

From STS, Σ^{nor} and Σ^{ano} separately obtained

Self-Energy in Cuprate Superconductors

B. Keimer, S. A. Kivelson, M. R. Norman, & S. Uchida, Nature 518, 179 (2015).



$$E_F \sim \mathcal{O}(10^4)\ \mathrm{K}$$

$$E_{\mathrm{pair}} \sim\ 10^3 - 10^4\ \mathrm{K?}$$

$$T_c \sim \mathcal{O}(100)\ \mathrm{K}$$

Competing energy scales, E_F and E_{pair}, prevent us from separating Σ^{nor} and Σ^{ano}

Modeling self-energy:
H. Li, *et al.*,
Nat. Commun. **9**, 26 (2018).

Extension of Eliashberg theory:
J. M. Bok, *et al.*,
Sci. Adv. **2**, e1501329 (2016).

A new approach:

✔Fewer assumptions

✔More flexible representation of Σ

to reveal unexpected physics

beyond biased expectation

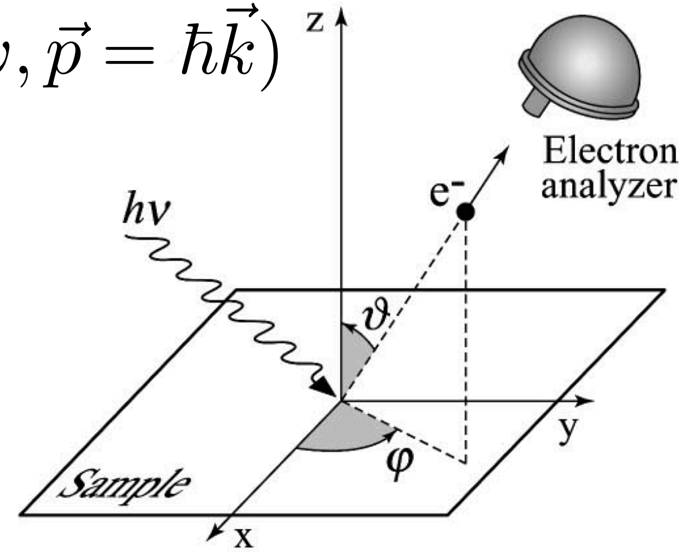
Photoemission Electron Spectroscopy of Crystalline Solids

Intensity of photoelectron

$(E = \hbar\omega, \vec{p} = \hbar\vec{k})$

$$I(\vec{k},\omega) = I_0(\vec{k},\nu,\vec{A}) \times n(\omega, k_{\mathrm{B}}T) A(\vec{k},\omega)$$

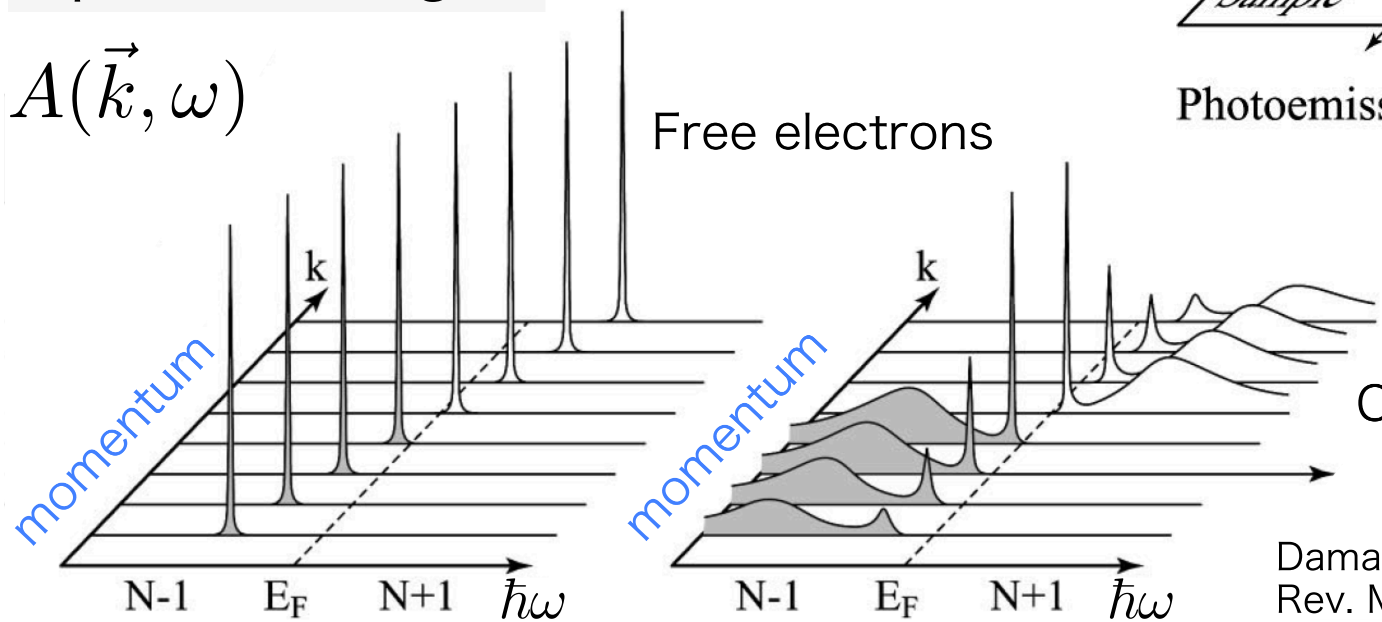
Fermi-Dirac distribution



Photoemission geometry

Spectral weight

$A(\vec{k},\omega)$



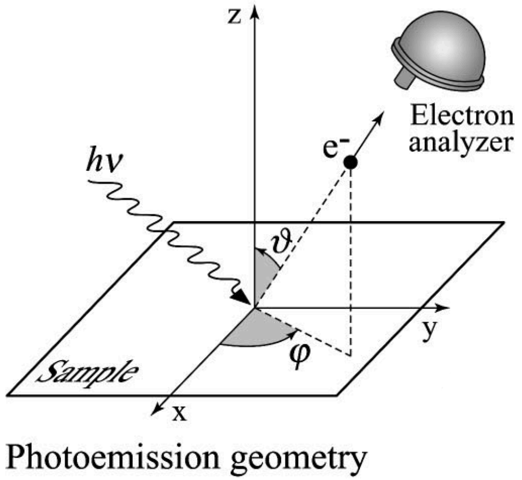
Free electrons

Correlated electrons

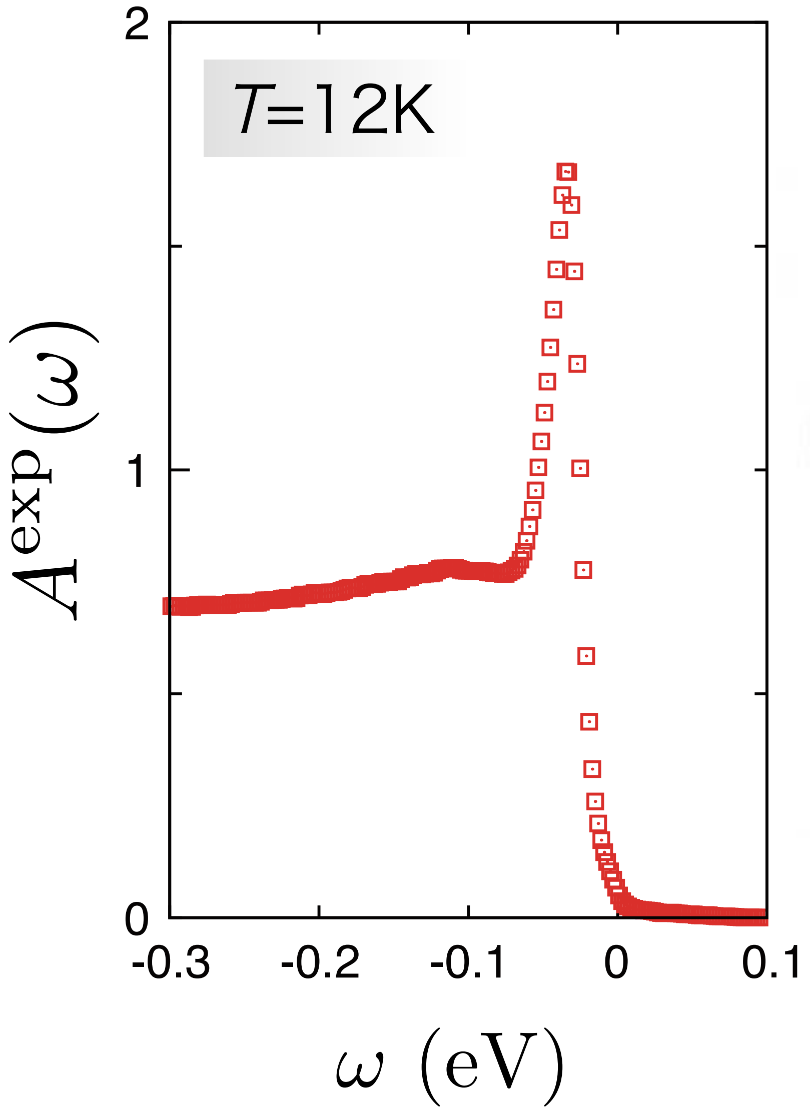
Damascelli, Hussain, & Shen, Rev. Mod. Phys. 75, 473 (2003)

Spectrum of Cuprate Superconductors for $T < T_c$

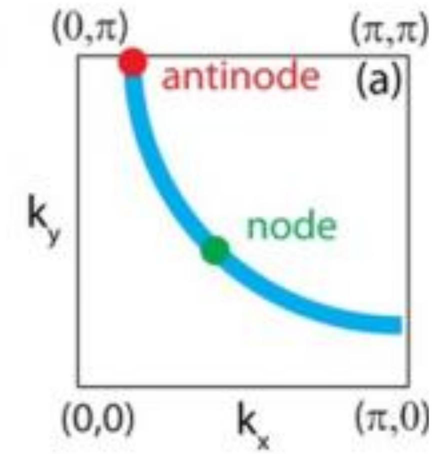
Angle-resolved photoemission



T. Kondo, *et al.*,
Nat. Phys. 7, 21 (2011).
$Bi_2Sr_2CaCu_2O_{8+\delta}$
Optimally doped sample
(T_c=90K)



$$\vec{k} = \vec{k}_{\mathrm{AN}}$$



Underdetermined Non-Linear Inverse Problem

$$A(\vec{k},\omega) = -\frac{1}{\pi}\mathrm{Im}G[\Sigma](\vec{k},\omega)$$

Known: Single-component spectral weight $A(\vec{k},\omega)$

Unknown: Two components of self-energy $\Sigma(\vec{k},\omega)$

$$\Sigma(\vec{k},\omega) = \Sigma^{\mathrm{nor}}(\vec{k},\omega) + \frac{\Sigma^{\mathrm{ano}}(\vec{k},\omega)^2}{\omega + i\delta + E(-\vec{k}) + \Sigma^{\mathrm{nor}}(-\vec{k},-\omega)^*}$$

We need to separately obtain $\Sigma^{\mathrm{nor}}(\omega)$ and $\Sigma^{\mathrm{ano}}(\omega)$ from a single-component spectral function $A(\omega)$

Prior Knowledge to Solve the Underdetermined Problem

Prior knowledge about the self-energy

Rigorous

- Causality $-\mathrm{Im}\Sigma^{\mathrm{nor}}(\omega) > 0$

  -Krammers-Krönig relation

$$\mathrm{Re}\Sigma^{\mathrm{nor/ano}}(\omega) = \frac{1}{\pi}\mathcal{P}\int d\omega' \frac{\mathrm{Im}\Sigma^{\mathrm{nor/ano}}(\omega')}{\omega' - \omega}$$

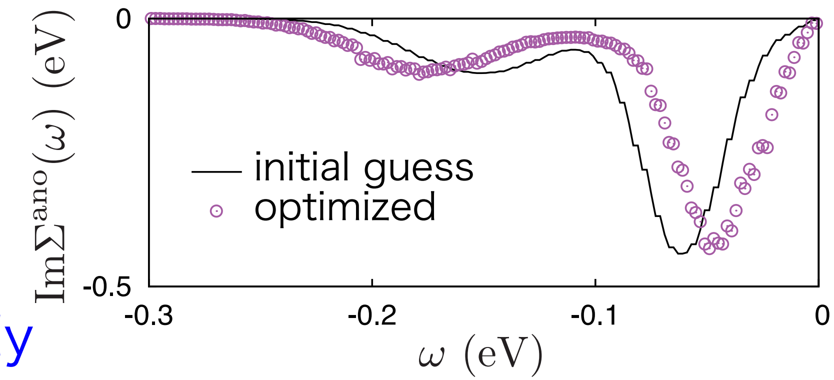
- Structure of self-energy

$$\Sigma(\vec{k},\omega) = \Sigma^{\mathrm{nor}}(\vec{k},\omega) + \frac{\Sigma^{\mathrm{ano}}(\vec{k},\omega)^2}{\omega + i\delta + E(-\vec{k}) + \Sigma^{\mathrm{nor}}(-\vec{k},-\omega)^*}$$

-Im Σ^{ano} is an odd function of ω

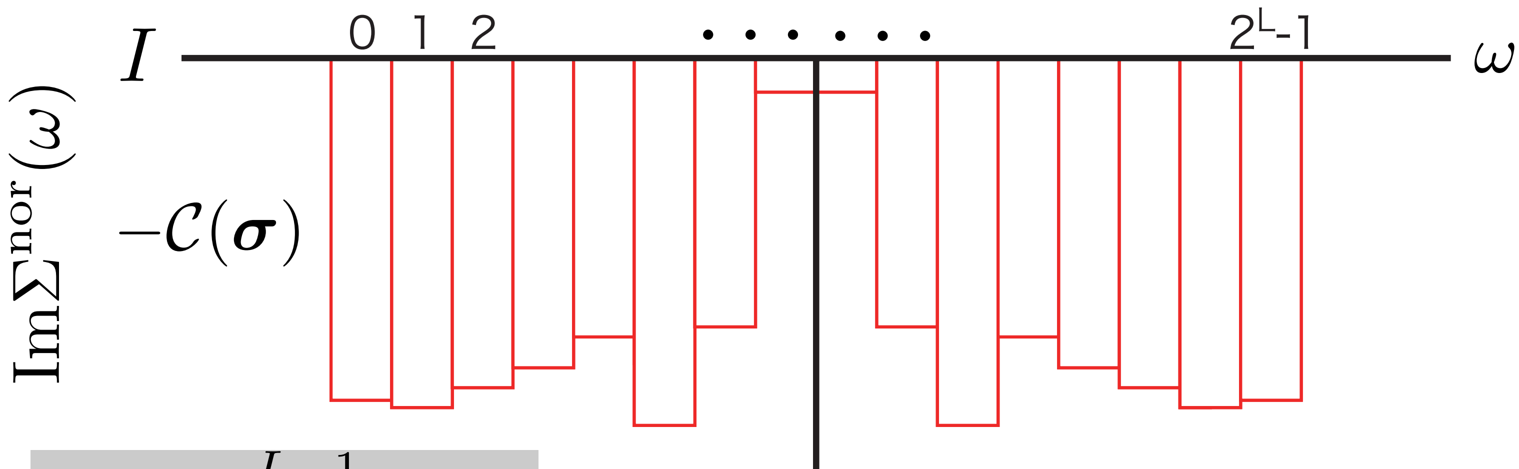
- Physically reasonable Initial guess:
  Σ^{ano} is confined in a finite range of ω

- Fraction of electron observed:
  Determined afterwards self-consistently

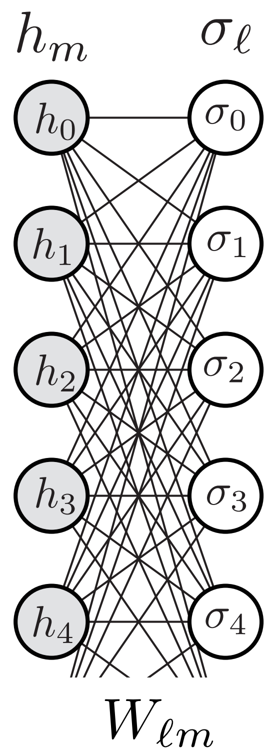


Flexible Representation of Σ^{nor} to Solve the Underdetermined Problem

Rectangular function chosen as basis



$$I(\boldsymbol{\sigma}) = \sum_{\ell=0}^{L-1} \sigma_\ell \cdot 2^\ell \qquad \boldsymbol{\sigma} = (\sigma_0, \sigma_1, \ldots, \sigma_{L-1})$$



Coefficients by restricted Boltzmann machine

$$\mathcal{C}(\boldsymbol{\sigma}) = e^b \sum_{\{h_m = \pm 1\}} e^{\sum_{\ell,m}(2\sigma_\ell - 1) W_{\ell m} h_m}$$

P. Smolensky (1986)

-# of paramters: (# of hidden units) x (# of visible units) = 18 x 9

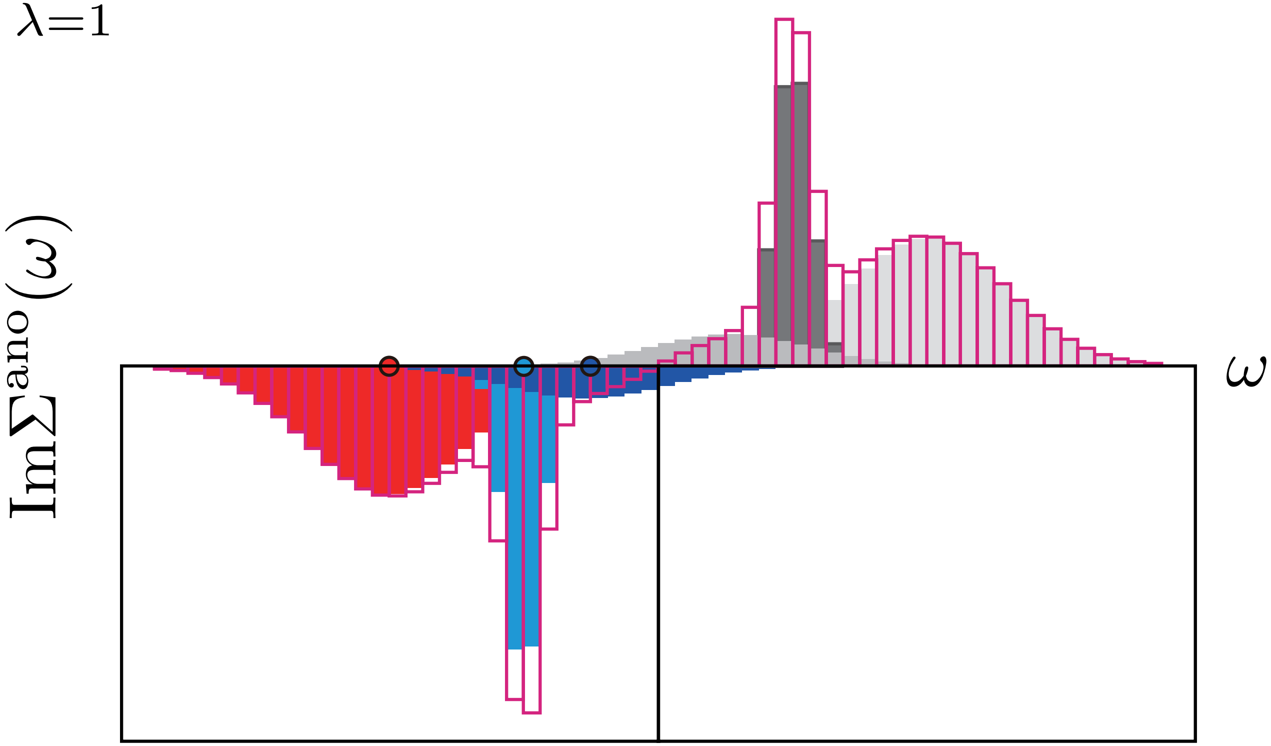
< $2^{\text{\# of visible units}} = 2^9 = 512$

Flexible Representation of Σ^{ano} to Solve the Underdetermined Problem

Mixture distribution of Boltzmann Machine

D. H. Ackley, G. E. Hinton, & T. J. Sejnowski (1985)

$$\mathcal{D}(\boldsymbol{\sigma}) = \sum_{\lambda=1}^{M} w_\lambda e^{\sum_{\ell,m}(2\sigma_\ell - 1)V_{\ell m}^{\lambda}(2\sigma_m - 1) + \sum_\ell (2\sigma_\ell - 1) b_\ell^\lambda}$$

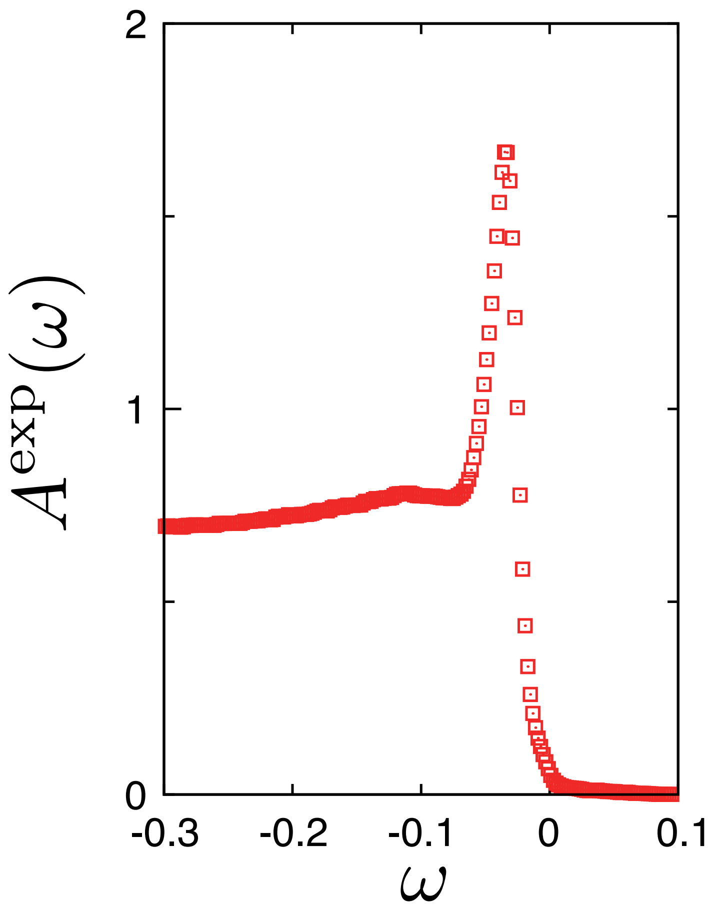


-# of paramters: (# of visible units)^2 + # of visible units = $9^2 + 9$

< $2^{\text{\# of visible units}}$ = 2^9 = 512

Optimizing Self-Energies to Solve the Underdetermined Problem

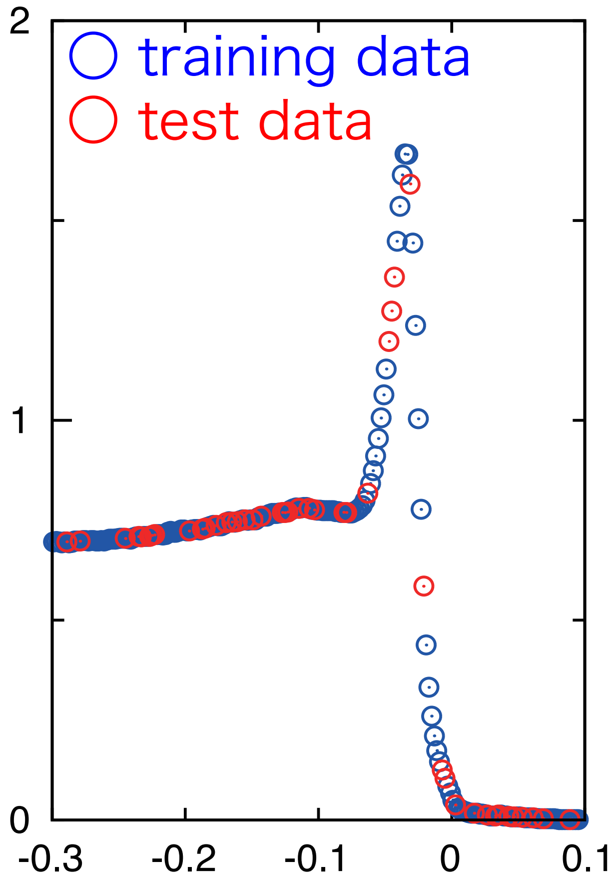
$$\chi^2 = \frac{1}{2N_{\mathrm{data}}} \sum_{j=1}^{N_{\mathrm{data}}} \{A^{\mathrm{exp}}(\omega_j) - A[\Sigma](\omega_j)\}^2$$



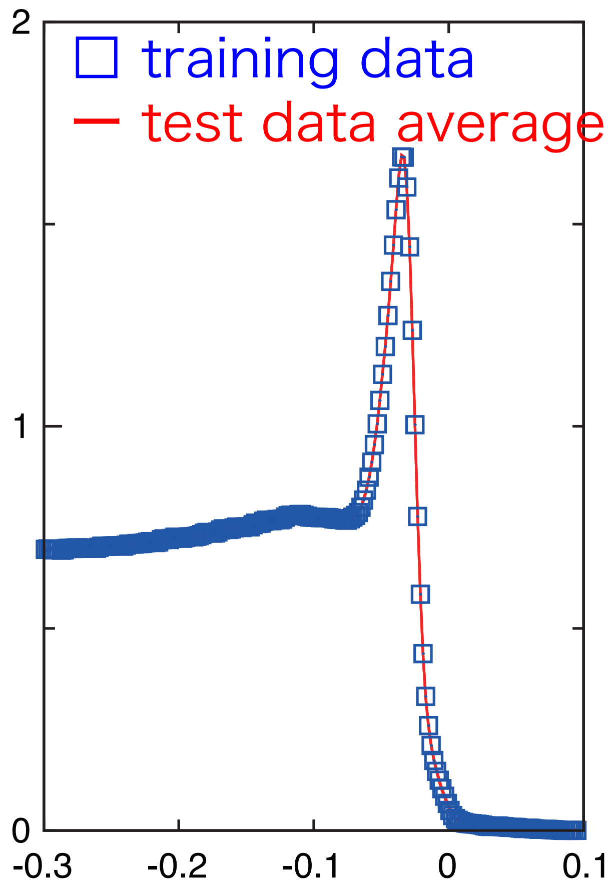
By minimizing the cost function with prior knowledge, optimize Σ^{nor} and Σ^{ano}

Avoiding Overfitting: Cross Validation

1. Dividing data into 2 sets



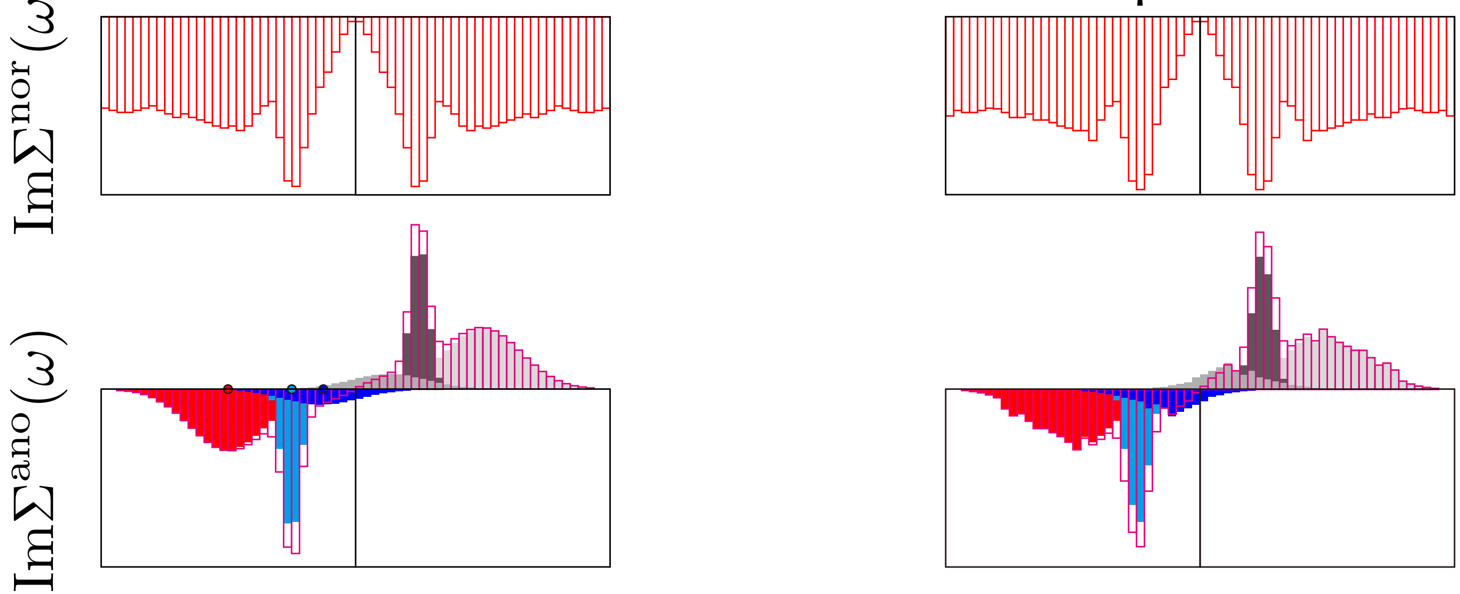
2. Test data generated by maximum likelihood approach



Bayesian Optimization Steps to Optimize Σ

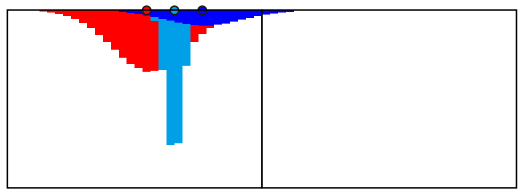
1. Optimizing Σ with training data

Initial conditions　　　　　　　　　　optimized



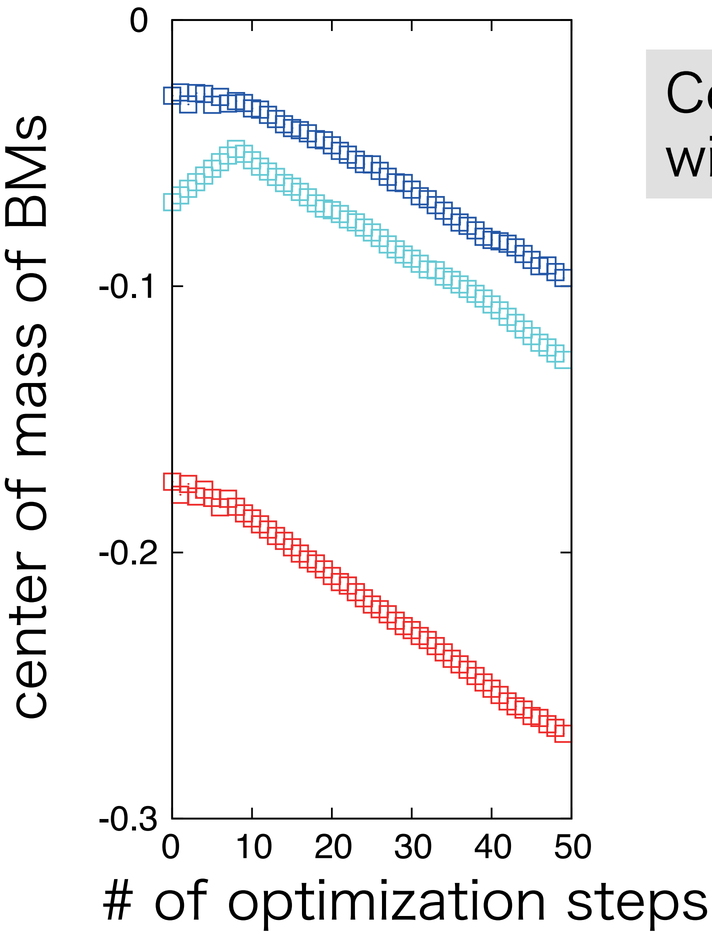
2. Measuring cost function with test data

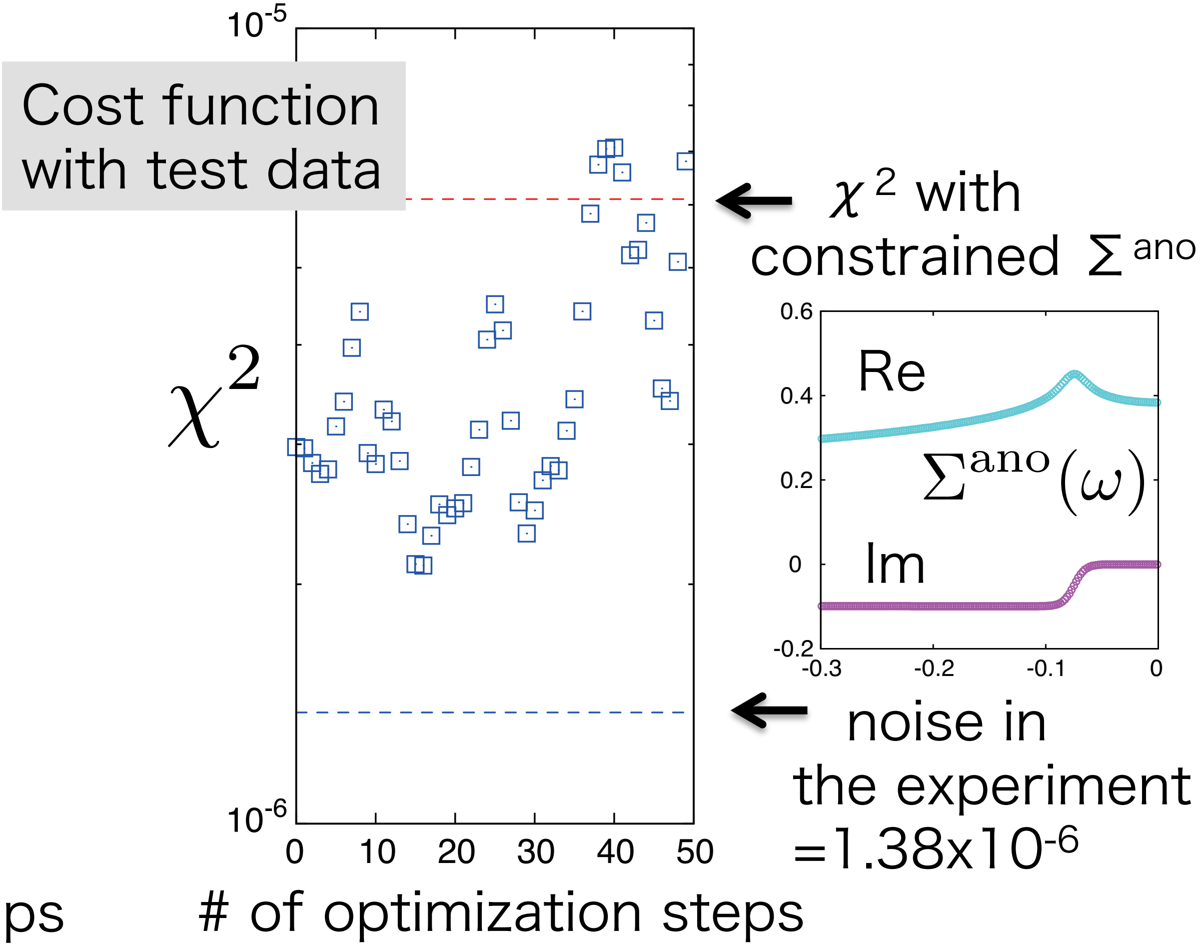
3. Shifting the centers of mass in Σ^{ano}



Go back to 1.

Bayesian Optimization Process to Optimize Σ



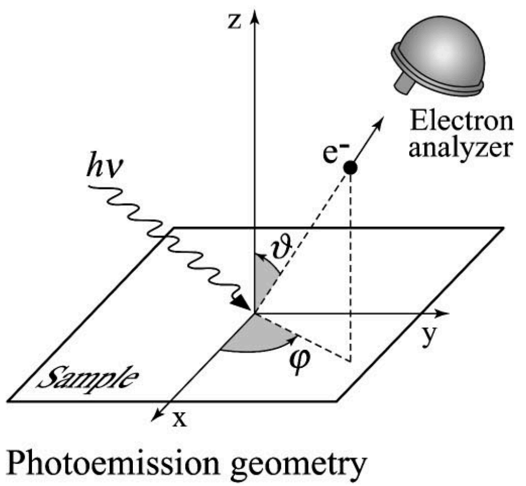


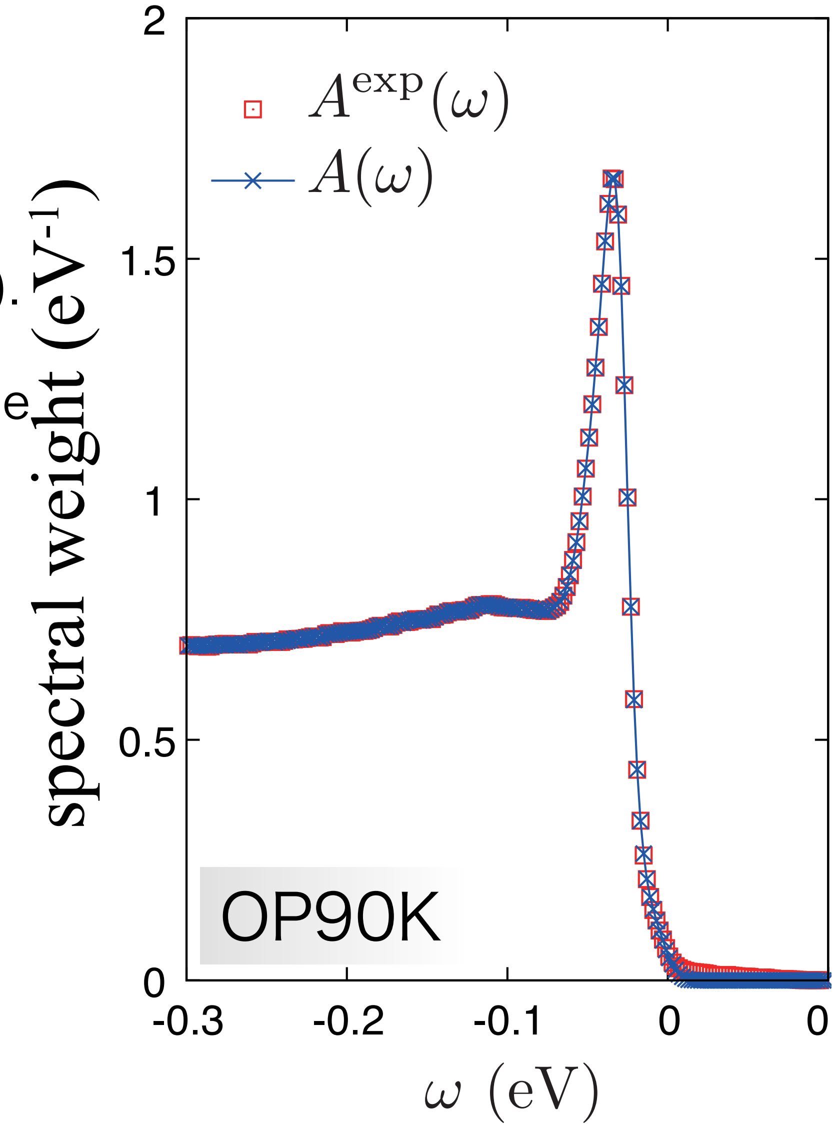
- The cost function χ^2 becomes 1/3 of χ^2 with constrained $\Sigma^{\rm ano}$ by Li *et al.* (2018)
- Optimization is robust against noise

Reproduced Spectrum of SC Cuprates for $T < T_c$

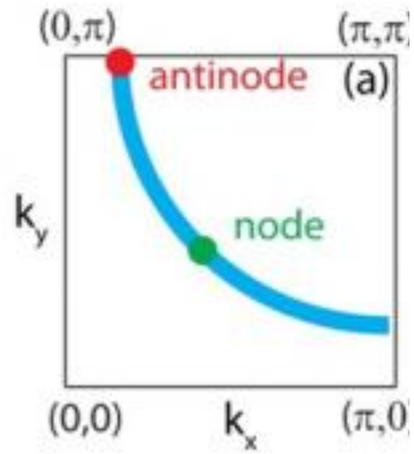
Angle-resolved photoemission

T. Kondo, *et al.*,
Nat. Phys. 7, 21 (2011).
$Bi_2Sr_2CaCu_2O_{8+\delta}$
Optimally doped sample
(T_c=90K)



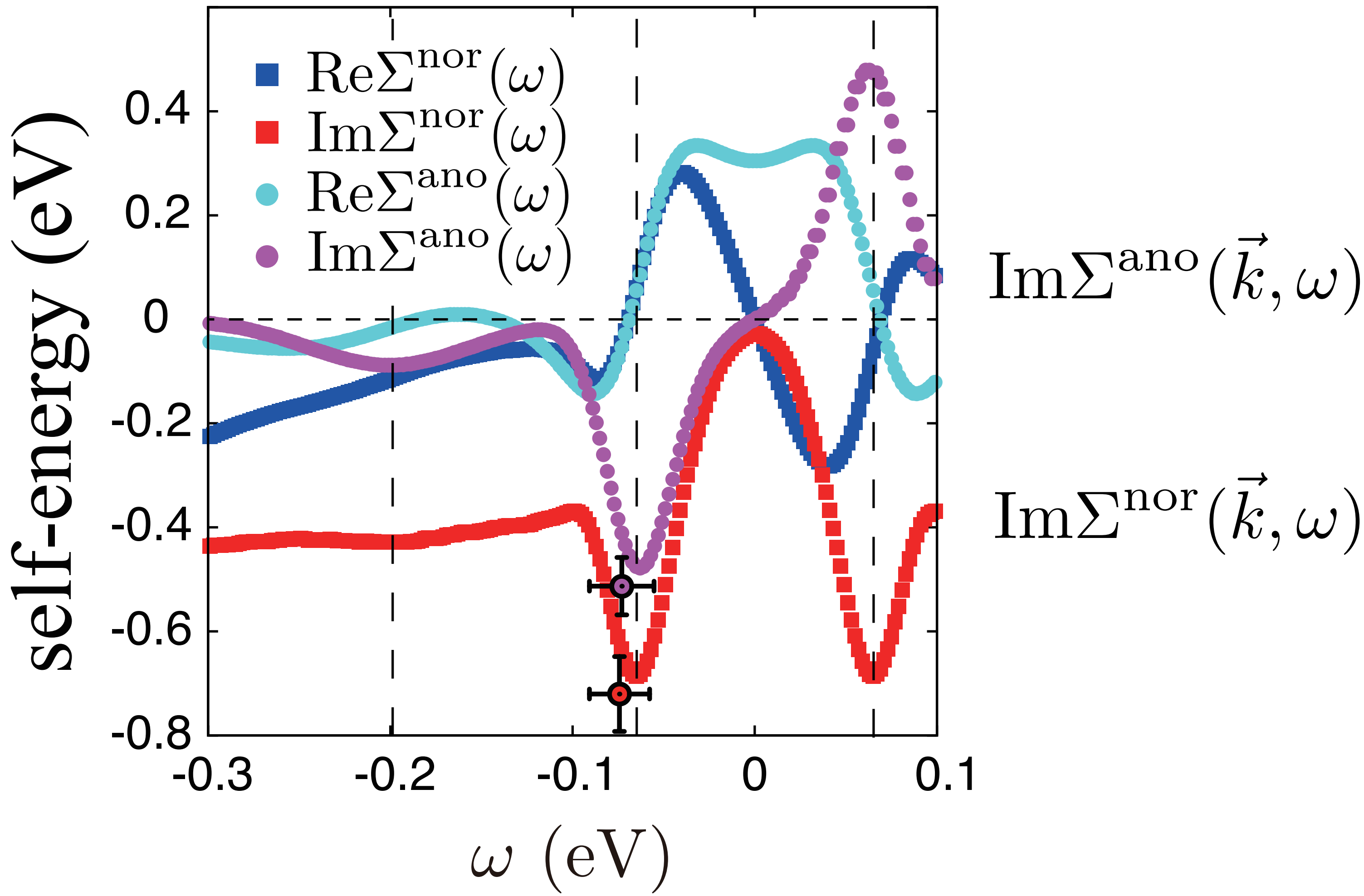


$\vec{k} = \vec{k}_{\mathrm{AN}}$



$A(\omega)$ by optimized Σ precisely reproduces $A^{\mathrm{exp}}(\omega)$

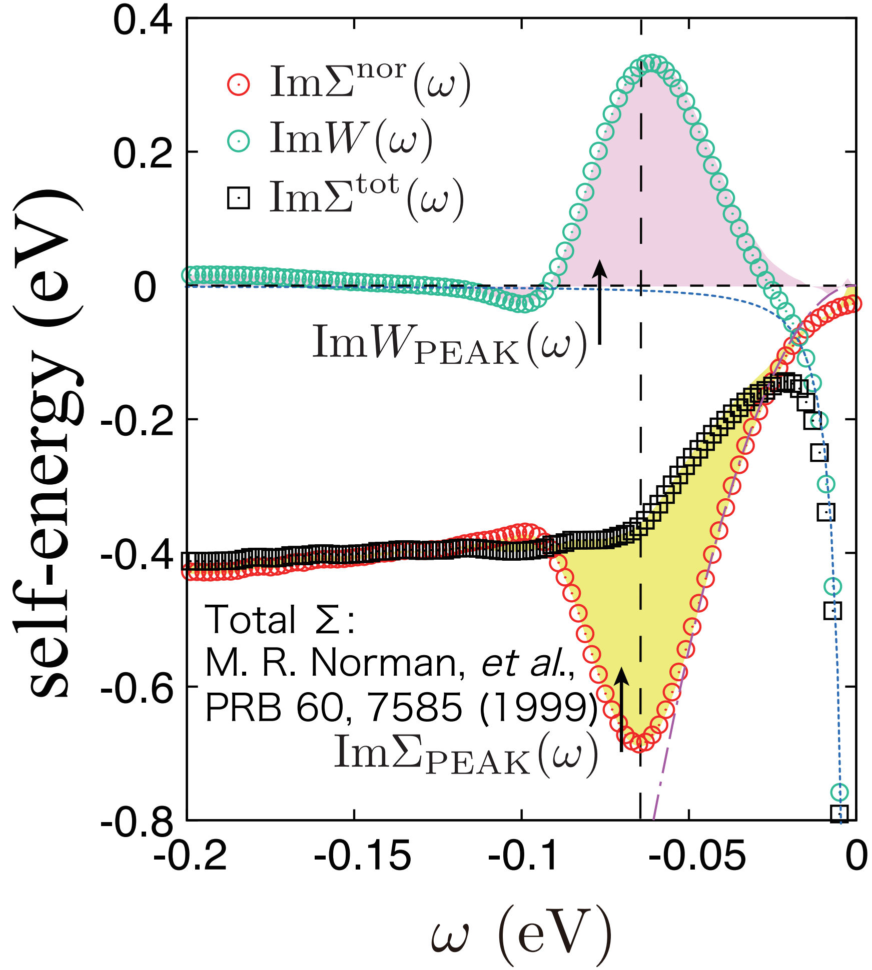
Self-Energy Obtained by the Bayesian Optimization Process



Promiment peaks found in both Σ^{nor} and Σ^{ano}
at the same ω (∼65 meV)

Hidden Peak Structure in Σ Revealed

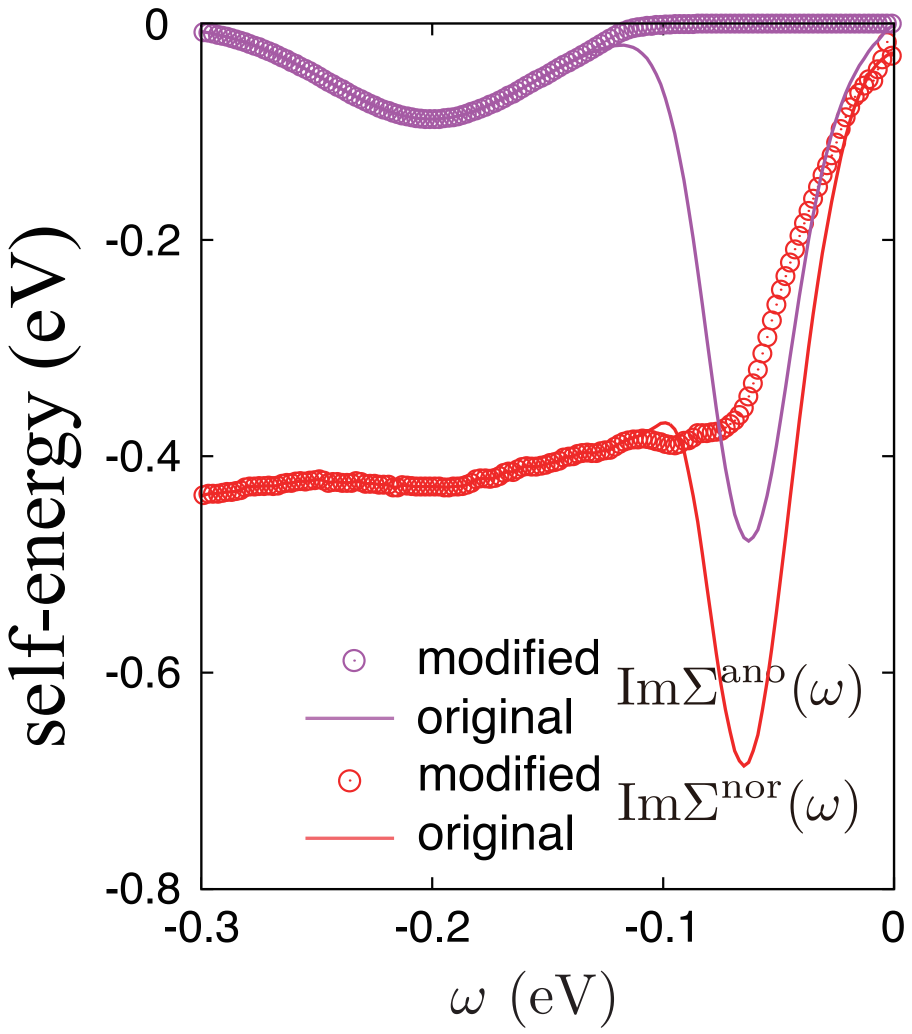
$$\Sigma(\vec{k},\omega) = \Sigma^{\rm nor}(\vec{k},\omega) + \frac{\Sigma^{\rm ano}(\vec{k},\omega)^2}{\omega + i\delta \cdots}$$



Universal ω-linear Im$\Sigma^{\rm nor}$ due to the peak structure: Planckian dissipation, Possible holographic fluid

Peaks exactly canceled and invisible in total Σ: Reason why it has been overlooked for 30 years

Peak structures in Σ and SC: T. Maier, D. Poilblanc, D. Scalapino, PRL 100, 237001 (2008).



Hidden peaks in $\Sigma^{\mathrm{nor/ano}}$ indeed generate SC gap and explain large gap with small anomalies in spectra

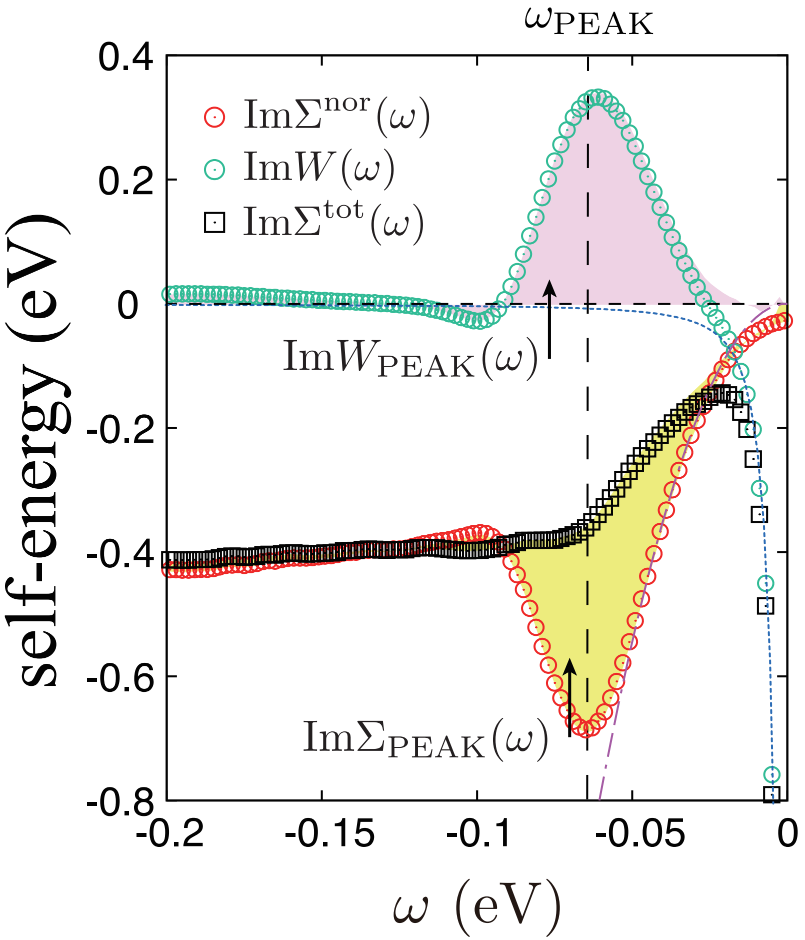
What Determines T_c ?: Attractive Interaction Estimated from Im W_{PEAK}

Effective attractive interaction:

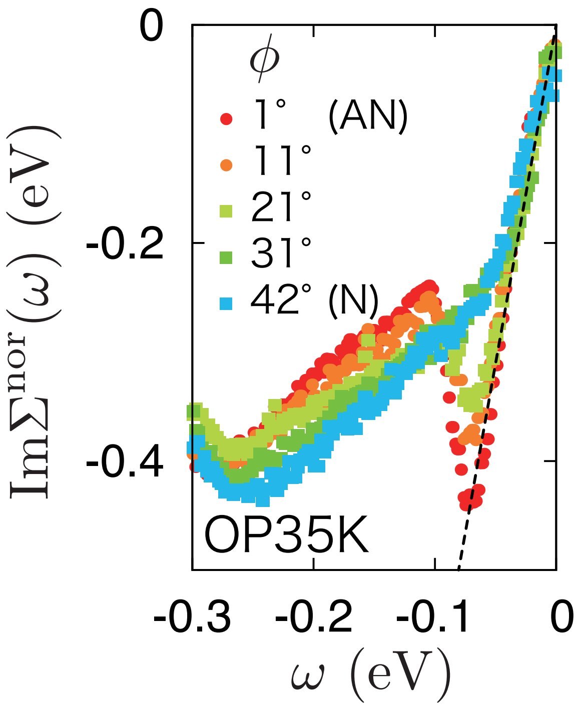
$$g(k) = \frac{\int d\omega \mathrm{Im} W_{\mathrm{PEAK}}(k,\omega) Q(k,\omega)}{\omega_{\mathrm{PEAK}}(k)}$$

Normalization function:

$$Q(k,\omega) = \frac{1}{1 - \frac{\Sigma^{\mathrm{nor}}(k,\omega+i\delta) - \Sigma^{\mathrm{nor}}(k,-\omega-i\delta)^*}{2(\omega+i\delta')}}$$



What Determines T_c ?: Planckian Dissipation from Im Σ_{PEAK}



ARPES of $Bi_2Sr_2CuO_{6+\delta}$
T. Kondo, *et al.*,
Nature 457, 296 (2009).

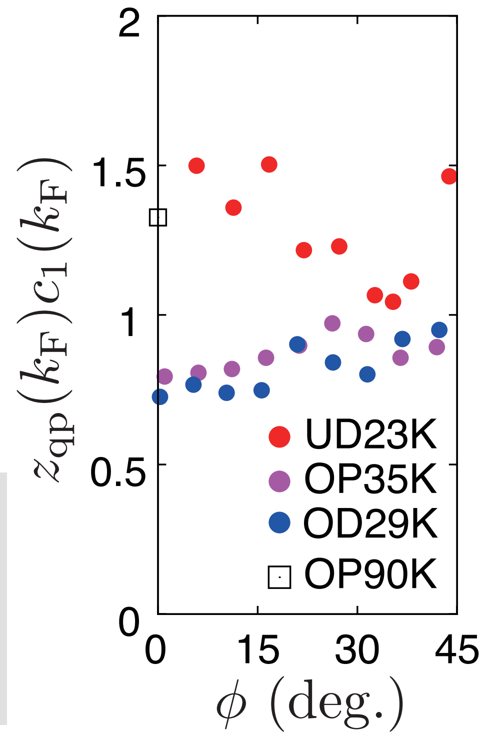
Inelastic relaxation rate:

cf.) Marginal FL: C. Varma *et al.*, PRL 63, 1996 (1990).

$$\mathrm{Im}\Sigma^{\mathrm{nor}}(k,\omega) \sim c_0(k) + \mathrm{sign}(\omega)c_1(k)\omega$$

$$z_{\mathrm{qp}}^{-1}(k) = 1 - \partial\mathrm{Re}\Sigma^{\mathrm{nor}}(k,\omega)/\partial\omega|_{\omega\to 0}$$

$$\Gamma(k) = z_{\mathrm{qp}}(k)c_1(k)$$



Planckian dissipation with universal Γ:

J. Zaanen, Nature 430, 512 (2004).

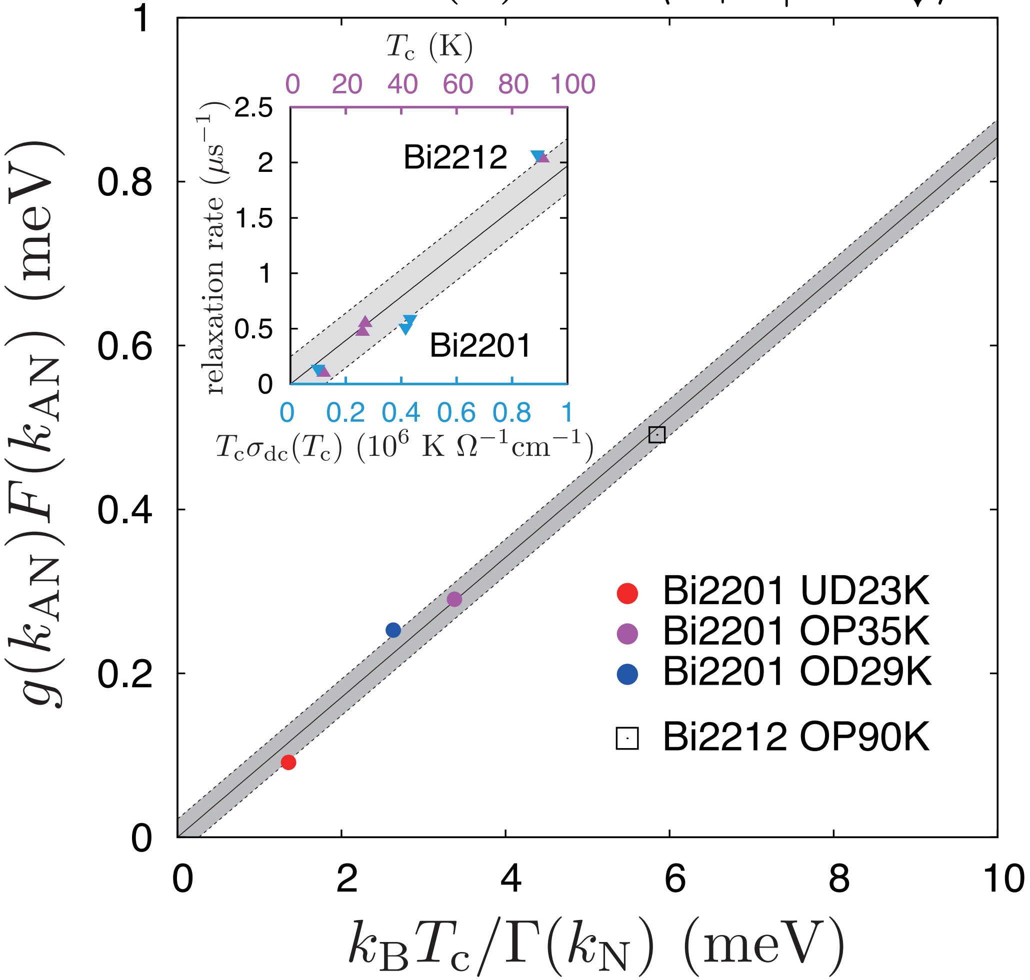
$$\tau^{-1}(k) = \Gamma(k)k_BT/\hbar$$

-Even in SC phase, electrons form fluid
-Im Σ PEAK generates both high-T_c &
Planckian dissipation

What Determines T_c ?

SC order parameter $F(k) = 2\langle \hat{c}_{+k\uparrow}\hat{c}_{-k\downarrow}\rangle$

$$g(k) = \frac{\int d\omega \, \mathrm{Im} W_{\mathrm{PEAK}}(k,\omega) Q(k,\omega)}{\omega_{\mathrm{PEAK}}(k)}$$



$$\Gamma(k) = z_{\mathrm{qp}}(k)c_1(k)$$

Effective interaction — Dissipation

$$k_B T_c = g(k_{AN}) \times F(k_{AN}) \times \Gamma(k_N)$$

-Uemura plot

$T_c \propto$ superfluid density

-Homes plot

$\sigma(T_c)T_c$

$\propto$ superfluid density

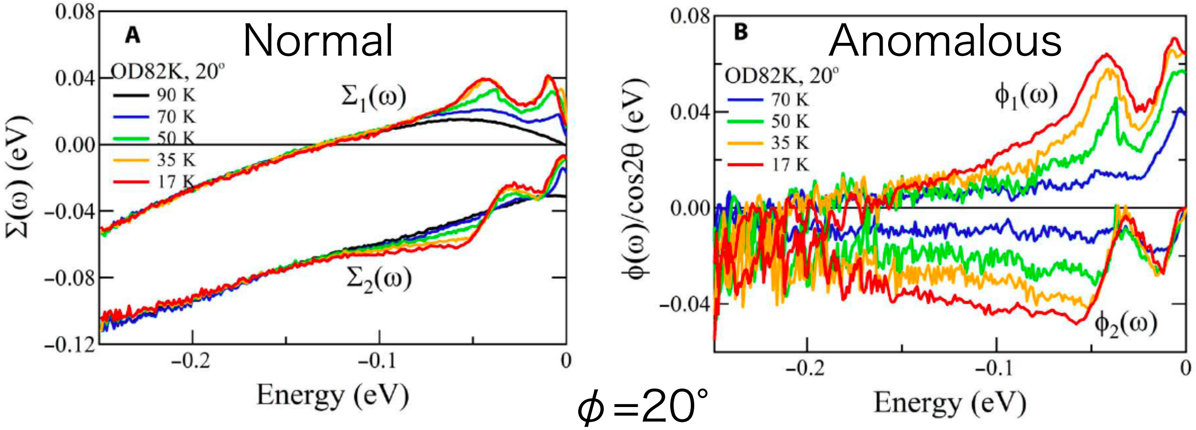
Y. J. Uemura, *et al.*, PRL 62, 2317 (1989).

C. C. Homes *et al.*, Nature 430, 539 (2004).

Comparison with Previous Studies

Compared with J. M. Bok, *et al.*, Sci. Adv. **2**, e1501329 (2016).

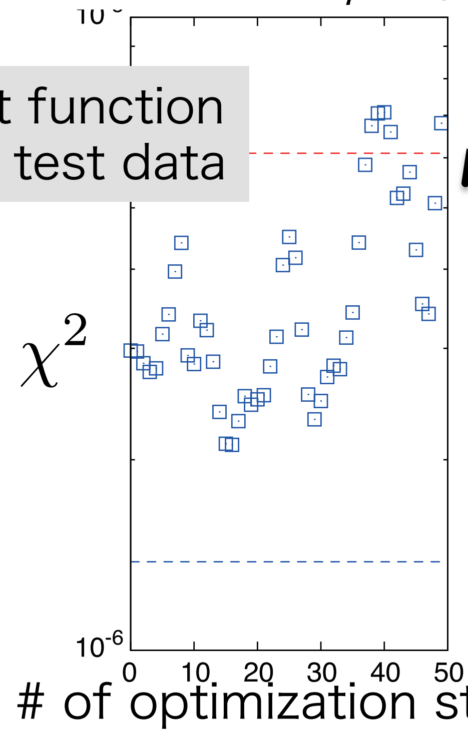
The present method
- obtained Σ^{nor} and Σ^{ano} separately at both N and AN regions for UD, OP, and UD cuprates
- revealed cancellation of peaks in both Σ^{nor} and Σ^{ano}

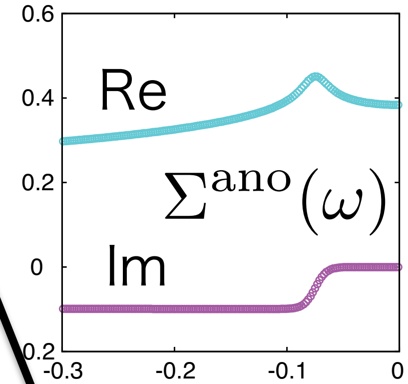


$\phi = 20^\circ$

Compared with H. Li, *et al.*, Nat. Commun. **9**, 26 (2018).

The present method
- showed χ^2 is 2/3 smaller
- revealed peak structure responsible for SC
- revealed that the peak intensity is involved in T_c determination





χ^2 with constrained Σ^{ano} by Li *et al.*

Summary

Y. Yamaji, T. Yoshida, A. Fujimori, and M. Imada, arXiv:1903.08060.

$$A(\vec{k},\omega) = -\frac{1}{\pi}\mathrm{Im}G[\Sigma](\vec{k},\omega)$$

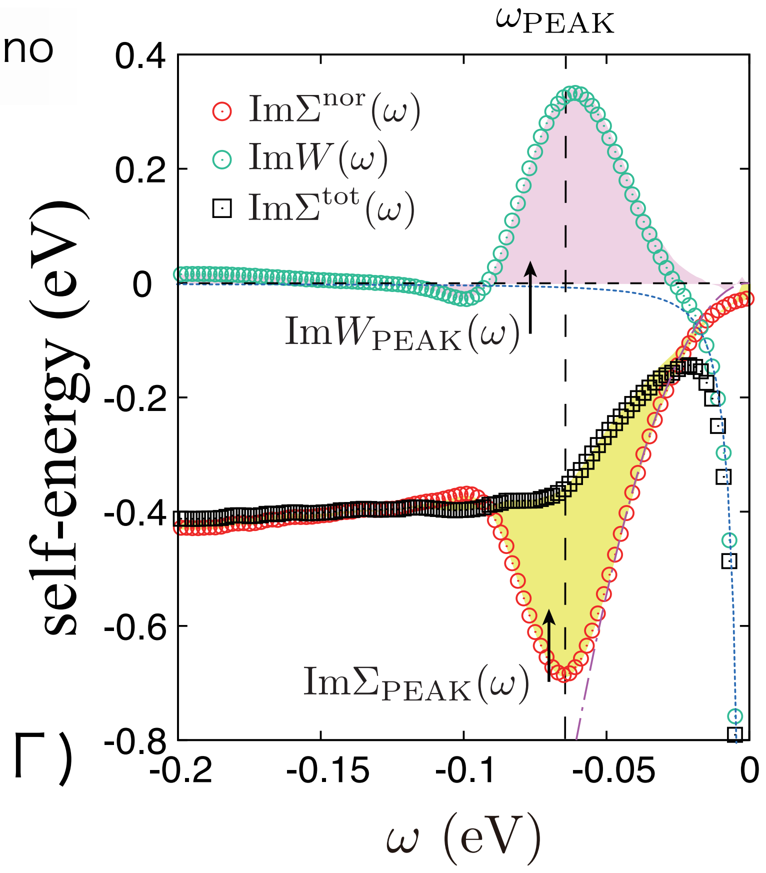
Hidden peaks in both Σ^{nor} and Σ^{ano}

-Origin of both high-T_c SC

-Cancelled each other and invisible in total Σ

Possible origin of the peak structure:
Dark fermion scenario

S. Sakai, M. Civelli, M. Imada, PRL 116, 057003 (2016).
cf.) Singularities in Σ in normal state
T. D. Stanescu & G. Kotliar, PRB 74, 125110 (2006).



What determine T_c ?

-Peak intensity ($\sim g$) & dissipation ($\sim \Gamma$)

$k_B T_c = g(k_{AN}) \times F(k_{AN}) \times \Gamma(k_N)$

Spectroscopy of hidden physics