Evidences for significant electron-phonon coupling in high Tc cuprates: Fermi blockade of the coupling with doping: results and Stochastic Method of Analytic Continuation

# Andrey S. Mishchenko

# RIKEN Center for Emergent Matter Science (CEMS)

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Physical results (by Diagrammatic Monte Carlo and numeric analytic continuation)



Stochastic Optimization Consistent Constrains method (SOCC)

### Not serious: OPTIMISTIC INTEREST DIAGRAMM





# **RIKEN, CEMS**



### A. S. Mishchenko

#### **RIKEN** (Institute of Physical and Chemical Research), Japan



### A. S. Mishchenko RIKEN (Institute of Physical and Chemical Research), Japan



### 1994-1999: Kondo, Spin Liquid



Trieste, 70<sup>th</sup> anniversary © Darya Zelentsova

### 1986-1987: Polaron, Lang-Firsov

### Don Quixote and Sancho Panza

Trieste, 70<sup>th</sup> anniversary © Darya Zelentsova



1986-1987: Polaron, Lang-Firsov

One can treat polaron either in weak or srong coupling limit only!

**1. DMC** 

2. Analytic continuation ARPES, OC, etc.



Evidences for significant electron-phonon coupling in high Tc cuprates: Fermi blockade of the coupling with doping: results and Stochastic Method of Analytic Continuation

# Andrey S. Mishchenko

# RIKEN Center for Emergent Matter Science (CEMS)

### Electron-phonon coupling in underdoped cuprates A S Mishchenko



George Sawatzky, Vancouver



Naoto Nagaosa, Tokyo



Giulio de Filippis



Vittorio and Cataudella Napoli



Z.-X. Shen, Stanford



Jan Zaanen, Leiden



Christian Bernhard, Kyungwan Kim Freiburg



Kyle Shen, Cornell University



Tom Devereaux, Stanford

Are <u>Hubbard-related models</u> enough to describe the physics of high T<sub>c</sub> materials or one needs an additional coupling to some extra bosonic field which is not included into Hubbard model?

## Hubbard-related models





# Large U>>t $\rightarrow$ t-J model

### additional coupling to some

### extra bosonic field

# Motivation and model



- 2. Naively, experimental data indicate that increase of doping decreases manifestations of the electron-boson coupling
- 3. We solve famous sign-problem in Mote Carlo for many-particle Fermi-polarons system and explain what happens with electron-boson coupling when doping of high  $T_c$  cuprates increases.

#### 1. Explanation of

# (a) ARPES; (b) optical conductivity; (d) pump-probe evolution of the optical conductivity in underdoped cuprates requires strong electron-boson coupling



There is no considerable manifestation of electron-boson coupling in spectroscopy of doped compounds. 2. Naively, experimental data indicate that increase of doping decreases manifestations of the electron-boson coupling





Fermi screening in finite density Fermi system?

Famous **Diagrammatic Monte Carlo** for many-particle Fermi system





### Naoto Nagaosa RIKEN, U. Tokyo

### Nikolay Prokof'ev UMASS

# **Funeral of**

# electron-phonon interaction in doped cuprates



**Funeral of** electron-phonon interaction in doped cuprates



Why we need additional electron-boson interaction on top of Hubbard model to explain

# ARPES

# (in undedoped)

# ARPES

Damascelli, Hussain, and Shen: Photoemission studies of the cuprate superconductors



FIG. 3. Angle-resolved photoemission spetroscopy: (a) geometry of an ARPES experiment in which the emission direction of the photoelectron is specified by the polar ( $\vartheta$ ) and azimuthal ( $\varphi$ ) angles; (b) momentum-resolved one-electron removal and addition spectra for a noninteracting electron system with a single energy band dispersing across  $E_F$ ; (c) the same spectra for an interacting Fermi-liquid system (Sawatzky, 1989; Meinders, 1994). For both noninteracting and interacting systems the corresponding ground-state (T=0 K) momentum distribution function  $n(\mathbf{k})$  is also shown. (c) Lower right, photoelectron spectrum of gaseous hydrogen and the ARPES spectrum of solid hydrogen developed from the gaseous one (Sawatzky, 1989).

ARPES experiments), one can relate the kinetic energy and momentum of the photoelectron to the binding energy  $E_B$  and crystal momentum  $\hbar \mathbf{k}$  inside the solid:

$$E_{kin} = h\nu - \phi - |E_B|, \qquad (1)$$

$$\mathbf{p}_{\parallel} = \hbar \mathbf{k}_{\parallel} = \sqrt{2mE_{kin}} \cdot \sin \vartheta.$$
<sup>(2)</sup>

Here  $\hbar \mathbf{k}_{\parallel}$  is the component parallel to the surface of the electron crystal momentum in the *extended* zone scheme. Upon going to larger  $\vartheta$  angles, one actually

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# ARPES

Damascelli, Hussain, and Shen: Photoemission studies of the cuprate superconductors



FIG. 3. Angle-resolved photoemission spetroscopy: (a) geometry of an ARPES experiment in which the emission direction of the photoelectron is specified by the polar ( $\vartheta$ ) and azimuthal ( $\varphi$ ) angles; (b) momentum-resolved one-electron removal and addition spectra for a noninteracting electron system with a single energy band dispersing across  $E_F$ ; (c) the same spectra for an interacting Fermi-liquid system (Sawatzky, 1989; Meinders, 1994). For both noninteracting and interacting systems the corresponding ground-state (T=0 K) momentum distribution function  $n(\mathbf{k})$  is also shown. (c) Lower right, photoelectron spectrum of gaseous hydrogen and the ARPES spectrum of solid hydrogen developed from the gaseous one (Sawatzky, 1989).

to obtain the one-particle spectral function 
$$A(\mathbf{k},\omega)$$
  
= $A^{+}(\mathbf{k},\omega) + A^{-}(\mathbf{k},\omega) = -(1/\pi) \operatorname{Im} G(\mathbf{k},\omega)$ , with  
 $A^{\pm}(\mathbf{k},\omega) = \sum_{m} |\langle \Psi_{m}^{N\pm1} | c_{\mathbf{k}}^{\pm} | \Psi_{i}^{N} \rangle|^{2} \delta(\omega - E_{m}^{N\pm1} + E_{i}^{N})$ 
(11)

and  $G(\mathbf{k},\omega) = G^+(\mathbf{k},\omega) + [G^-(\mathbf{k},\omega)]^*$ , which defines the *retarded Green's function*. Note that  $A^-(\mathbf{k},\omega)$  and  $A^+(\mathbf{k},\omega)$  define the one-electron removal and addition spectra which one can probe with direct and inverse photoemission, respectively. This can be seen, for the

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### **Typical ARPES of interacting system**



**Fig. 10.** Sketch of the polaron spectral function  $A(\omega, \mathbf{k})$  at low electron excitation energy  $E(\mathbf{k}) - E_F$ . The characteristic peak-dip-hump (PDH) spectral shape is formed by the quasiparticle (QP) peak followed by the phonon sideband tail corresponding to a sequence of optical phonons with frequency  $\omega_0$ .

#### **Typical ARPES of interacting system**



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# Typical ARPES of interacting system



Standard t-J model (Hubbard large U) where hole moves in the antiferrromagnet. Extended t-J model well describes the dispersion of the quasiparticle



Wells et al, PRL (1995)



T. Xiang and J.M. Whetley, PRB, vol.54, R12653 (1996)

### Standard t-J model .....



# String of the overturned pins prevent hole from free movement.

### **Theory: spectral function**

**Diagrammatic Monte Carlo** 

# 

ASM, B.V. Svistunov and N.V. Prokof'ev, PRB, vol. 64, 033101 (2001)



T. Xiang and J.M. Whetley, PRB, vol.54, R12653 (1996)

### **Experiment: ARPES**

### Extended t-J model gives wrong description of the peak width in ARPES



Wells et al, PRL (1995) 33

### **Theory: spectral function**

**Diagrammatic Monte Carlo** 

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ASM, B.V. Svistunov and N.V. Prokof'ev, PRB, vol. 64, 033101 (2001)



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### **Experiment: ARPES**

### Extended t-J model gives wrong description of the peak width in ARPES



Wells et al, PRL (1995) 34

# Standard spin-wave approximation for a hole in the t-J model.

Hole with dispersion  $\varepsilon(k)$  in the field magnons and **EXTRA BOSONS**  $H^{(0)}_{tt't"-J} = \sum_{k} \varepsilon(k) h_{k}^{+} h_{k} + \sum_{k} \upsilon(k) \alpha_{k}^{+} \alpha_{k}^{-} + \sum_{k} \omega_{ph} b_{k}^{+} b_{k}^{-}$ 

Scattering on magnons:  $H_{h-m} = N^{-1} \Sigma_{k,q} M_{k,q} [h_k^+ h_{k-q} \alpha_q + h.c.]$ 

... and on EXTRA bosons:  $H_{h-ph} = N^{-1} \sum_{k,q} \gamma [h_k^+ h_{k-q} b_q + h.c.]$ 

Dimensionless coupling constant :  $\lambda = \gamma^2 / 4t\omega_{ph}$  $g = \lambda / 2$ 

Crossover to strong-coupling regime usually happens at  $\lambda$ =1

### ARPES: dependence on the el-boson coupling



ASM and N. Nagaosa, Phys. Rev. Lett. 93, 036402 (2004)


#### **Dispersion of the Franck-Condon peak**

g=0.23



ASM and N. Nagaosa, Phys. Rev. Lett. 93, 036402 (2004)



**Surprise: dispersion of wide peak** <u>exactly</u> reproduces result of the t-J model.

#### **Dispersion of the Franck-Condon peak**

g=0.23



ASM and N. Nagaosa, Phys. Rev. Lett. 93, 036402 (2004)



It is difficult to see real quasiparticle because of small weight.

#### **Dispersion of the Franck-Condon peak**

g=0.23



ASM and N. Nagaosa, Phys. Rev. Lett. 93, 036402 (2004)



It is difficult to see real quasiparticle because of small weight.

**Chemical potential !!!!!** 



Chemical potential must be separated from the "fake" QP



ASM and N. Nagaosa, Phys. Rev. Lett. 93, 036402 (2004)



0,0

Relative Energy (eV)

-0,5

0,0

-0,5

0,0

K. M. Shen et al Phys. Rev. Lett. 93, 267002 (2004)

-0,5

0,0

(0,2π,0,2π) -0,5 Linewidth ratio  $W(x,x)/W(\pi/2,\pi/2)$  exactly reproduces experiment



The ratio  $W(x,x) / W(\pi/2,\pi/2)$ is **universal** in theory for any  $\lambda$  in strong coupling regime (λ=0.7,1.0) and **Universal** in experiment for different compounds (Sr,Ca)<sub>2</sub>CuO<sub>2</sub>Cl<sub>2</sub>

Why we need additional electron-boson interaction on top of Hubbard model to explain OPTICAL CONDUCTIVITY

## (underdoped !!!)

#### Optical conductivity: Are there some contributions from both magnetic (Hubbard) and EXTRA bosonic systems ?

#### **MIR in experiment**



FIG. 10. In-plane  $(E \perp c)$  optical conductivity  $\sigma(\omega)$  obtained from a Kramers-Kronig analysis of the reflectivity data for various compositions of YBa<sub>2</sub>Cu<sub>3</sub>O<sub>6+x</sub>. Adapted from Cooper, Reznik, *et al.*, 1993.



FIG. 9. Doping dependence of  $YBa_2Cu_3O_x$  at 4 K (100 K for the superconducting samples with x=6.4 and 6.92). From Gruninger, 1999.



Basov

FIG. 5. (Top panel) Doping dependent  $\sigma_1(\omega)$  at 10 K or at  $T \simeq T_c$  for y=6.30, 6.35, 6.43, 6.50, 6.55, and 6.75. For clarity, the sharp phonon structures are removed. Inset shows the  $\sigma_1(\omega)$  up to 30 000 cm<sup>-1</sup> for y=6.30 and 6.75. (Bottom panel) Doping dependences of the peak position of mid-IR absorption  $\omega_{mid}$  (solid square) and the pseudogap onset temperature  $T^*$  (open square) quoted from Ref. 22. The  $\omega_{mid}/k_B T^*$  values are estimated to be 7–9.

Cooper, Reznik et al 1993

**Gruninger 1999** 

#### **MIR** – contradiction with experiment No 1

#### **Pure t-J model**



**Experiment:** MIR = 0.5 eVat low doping

#### **Experiment**



FIG. 10. In-plane  $(E \perp c)$  optical conductivity  $\sigma(\omega)$  obtained from a Kramers-Kronig analysis of the reflectivity data for various compositions of YBa2Cu3O6+r. Adapted from Cooper, Reznik, et al., 1993.

#### MIR – contradiction with experiment No2

#### Pure t-J model



Experiment: MIR energy decreases with with doping.

Theory: other way around.

Extra bosons?

#### Experiment



Evolution of the OC with electron-boson coupling (Hubbard-Holstein model, i.e. electron-boson coupling on top of Hubbard model).



Diagrammatic Monte Carlo and SOCC

ASM, N. Nagaosa, Z.-X. Shen, G. De Filippis, V. Cataudella, T. P. Devereaux, C. Bernhard, K.W. Kim, and J. Zaanen, Phys. Rev. Lett. 100, 166401 (2008) 46

#### Two peaks in OC



ASM, N. Nagaosa, Z.-X. Shen, G. De Filippis, V. Cataudella, T. P. Devereaux, C. Bernhard, K.W. Kim, and J. Zaanen, Phys. Rev. Lett. 100, 166401 (2008) <sub>47</sub>

#### **Diagrammatic Monte Carlo**



Note: for 2-peak structure of the optical conductivity both magnetic system and a coupling to an extra magnetic mode is required.

> Ellipsometry: 1.5% hole doped (Eu<sub>1-x</sub>Ca<sub>x</sub>)Ba<sub>2</sub>Cu<sub>3</sub>O<sub>6</sub>

ASM, N. Nagaosa, Z.-X. Shen, G. De Filippis, V. Cataudella, T. P. Devereaux, C. Bernhard, K.W. Kim, and J. Zaanen, Phys. Rev. Lett. 100, 166401 (2008) 48

Why we need <u>additional</u> electron-boson interaction <u>on top of Hubbard model</u> to explain

TEMPERATURE DEPENDENCE (underdoped !!)

#### **Temperature dependence of ARPES**



George Sawatzky

#### The linewidth, seems, extrapolates to zero .....



Kyle Shen and Z.-X. Shen et al



K.M. Shen, Phys. Rev. B 75, 075115 (2007)

#### **Temperature dependence of ARPES**



V. Cataudella et al, Phys. Rev. Lett. 99, 226402 (2007)

#### **Temperature dependence of ARPES**



George Sawatzky

The linewidth, as seems, extrapolates to zero .....



V. Cataudella et al, Phys. Rev. Lett. 99, 226402 (200



#### Kyle Shen and Z.-X. Shen et al



#### K.M. Shen, Phys. Rev. B 75, 075115 (2007)

N>0.4 is already strong coupling

Why we need <u>additional</u> electron-boson interaction on top of Hubbard model to explain

PUMP-PROBE PHENOMENA (undoped !!) Novel kind of pump-probe phenomenon

# Witnessing the formation and relaxation of dressed quasi-particles in a strongly correlated electron system

Fabio Novelli<sup>1,2</sup>, Giulio De Filippis<sup>3</sup>, Vittorio Cataudella<sup>3</sup>, Martina Esposito<sup>1</sup>, Ignacio Vergara<sup>4</sup>, Federico Cilento<sup>2</sup>, Enrico Sindici<sup>1</sup>, Adriano Amaricci<sup>5</sup>, Claudio Giannetti<sup>6,7</sup>, Dharmalingam Prabhakaran<sup>8</sup>, Simon Wall<sup>9</sup>, Andrea Perucchi<sup>2,10</sup>, Stefano Dal Conte<sup>11</sup>, Giulio Cerullo<sup>11</sup>, Massimo Capone<sup>5</sup>, Andrey Mishchenko<sup>12,13</sup>, Markus Grüninger<sup>4</sup>, Naoto Nagaosa<sup>12,14</sup>, Fulvio Parmigiani<sup>1,2,4</sup> & Daniele Fausti<sup>1,2</sup>

#### NATURE COMMUNICATIONS | 5:5112 | DOI: 10.1038/ncomms6112

### Pump-probe phenomena.





General understanding: To change the electronic state and watch how system evolves with time.





### Witnessing the formation and relaxation of dressed quasi-particles in a strongly correlated electron system

Fabio Novelli<sup>1,2</sup>, Giulio De Filippis<sup>3</sup>, Vittorio Cataudella<sup>3</sup>, Martina Esposito<sup>1</sup>, Ignacio Vergara<sup>4</sup>, Federico Cilento<sup>2</sup>, Enrico Sindici<sup>1</sup>, Adriano Amaricci<sup>5</sup>, Claudio Giannetti<sup>6,7</sup>, Dharmalingam Prabhakaran<sup>8</sup>, Simon Wall<sup>9</sup>, Andrea Perucchi<sup>2,10</sup>, Stefano Dal Conte<sup>11</sup>, Giulio Cerullo<sup>11</sup>, Massimo Capone<sup>5</sup>, Andrey Mishchenko<sup>12,13</sup>, Markus Grüninger<sup>4</sup>, Naoto Nagaosa<sup>12,14</sup>, Fulvio Parmigiani<sup>1,2,4</sup> & Daniele Fausti<sup>1,2</sup>

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#### Undoped La₂CuO₄

### Novel phenomenon



#### **Over-gap pulse**



Daniel Fausti



Sub-gap pulse shows fast component in comparison with over-gap pulse.

Effect is normalized to the absorbed energy. Hence, fast component is not connected to absorption!

What is peculiarity of the sub-gap pulse?

#### Sub-gap pulse

No absorption of real energy when the pulse is over!



picoseconds

**Bosonic field** 



There is a red shift of the variation of the optical conductivity which survives only several tenth of femtoseconds after the pump pulse is over.

This effect is present in theoretical results ONLY if considerable electron-boson coupling is assumed in the Hubbard-Holstein model.



# Physical picture of fast component in sub-gap pulse.



In the absence of electron-boson coupling the distortion of ground state by the electric field of pump exists only few femtoseconds after the pulse is over (electron characteristic times are h/t ~ 2 fs).

However, memory of slower bosonic filed prolongs the memory of the pulse and the red shift is observed for some time when the pump pulse is already over. Sub-gap pump-probe spectroscopy: A novel tool to probe electron-boson coupling.



Why we need <u>additional</u> electron-boson interaction <u>on top of Hubbard model</u> to <u>explain</u>

# RAMAN and Optical conductivity (undoped !!)

#### Joint description of RAMAN and optical conductivity: extended Hubbard versus Hubbard-Holstein



#### Joint description of RAMAN and optical conductivity: extended Hubbard versus Hubbard-Holstein



We need considerable electron-boson coupling on top of the Hubbard model to explain all spectroscopy **IN UNDERDOPED** compounds



George Sawatzky, Vancouver



Naoto Nagaosa, Tokyo



Giulio de Filippis



Vittorio and Cataudella Napoli



Z.-X. Shen, Stanford



Jan Zaanen, Leiden



Christian Bernhard, Kyungwan Kim Freiburg



Kyle Shen, Cornell University



Tom Devereaux, Stanford



 $\mathbf{K}$ 



Z.-X. Shen, Stanford



Tom Devereaux, Stanford

# What happens with hole doping?

It looks like in experiments that the manifestations of the electron-phonon coupling decreases with doping as if effective  $\lambda$  decreases when holes concentration increases.

Let us determine effective  $\lambda$  from:

1.Optical conductivity 2.ARPES

### Dependence of effective electron-phonon coupling from MIR position in optical conductivity.



ASM, N. Nagaosa, Z.-X. Shen, G. De Filippis, V. Cataudella, T. P. Devereaux, C. Bernhard, K.W. Kim, and J. Zaanen, Phys. Rev. Lett. 100, 166401 (2008)



FIG. 5. (Top panel) Doping dependent  $\sigma_1(\omega)$  at 10 K or at  $T \equiv T_c$  for y = 6.30, 6.35, 6.43, 6.50, 6.55, and 6.75. For clarity, the sharp phonon structures are removed. Inset shows the  $\sigma_1(\omega)$  up to 30 000 cm<sup>-1</sup> for y = 6.30 and 6.75. (Bottom panel) Doping dependences of the peak position of mid-IR absorption  $\omega_{mid}$  (solid square) and the pseudogap onset temperature  $T^*$  (open square) quoted from Ref. 22. The  $\omega_{mid}/k_BT^*$  values are stimated to be 7–9.

Lee at al 2005 <sup>70</sup>



Reuze 1: Quasiparticle dispersion in the direction  $(0, 0) - (\pi, \pi)$  in the compounds  $L_{2,2}$  spc\_20x<sub>0</sub> (LSCO), BL<sub>2</sub>Sr<sub>2</sub>CuC<sub>0</sub>, (B1221), and BL<sub>2</sub>Sr<sub>2</sub>CuC<sub>4</sub>, (B1221), and dopings. Panel (f) shows the value 1 +  $\lambda'$ , evaluated by the change of the dispersion ingle in the weak coupling theory for noninteraciting electrons in metal, after Lanzara et al. [64].

#### Lanzara et al, 2001

Effective EPI strength is defined from comparison of experimental and theoretical kink's angle.



A. S. M., N. Nagaosa, K. M. Shen, Z.-X. Shen, X. J. Zhou, and T. P. Devereaux, EPL, 95 (2011) 57007



#### **Dependence of effective electron-phonon coupling:**

#### **From MIR position**



#### From kink angle in ARPES




Of course there is no decrease of material parameter  $\lambda$  with increase of doping.

However, one can show that manifestations of strong electron-phonon coupling are suppressed with doping as if  $\lambda$  is small.



#### **Conventional Diagrammatic Monte Carlo**

Green function: 
$$G(p,\tau) = \left\langle a_p(0) a_p^+(\tau) \right\rangle = \left\langle a_p e^{-\tau H} a_p^+(\tau) \right\rangle$$

Sum of all Feynman diagrams  $\vec{p}, au$  representation





Graph-to-math correspondence:

$$G\left(\vec{p},\tau\right) = \sum_{n=0}^{\infty} \sum_{\xi} \iiint d\vec{x}_1 d\vec{x}_2 \dots d\vec{x}_n \ D_n\left(\xi; \vec{x}_1, \vec{x}_2, \dots, \vec{x}_n, \vec{p}, \tau\right) \text{ where } \vec{x}_i = (\vec{q}_i, \tau_i, \tau_i')$$
  
is a product of

Positive definite series in the  $(p, \tau)$  representation

# One polaron

## Sign problem Sign blessing



ASM, N. Nagaosa and N. Prokof'ev, Phys. Rev. Lett. 113, 166402 (2014) – finite density polaron gas







Holstein,  $\lambda$ =0.45, 2D, 128x128  $\gamma = \omega_0 / \epsilon_F$ 

- Converge even for γ≈1
   On-site DMFT good for GS
  - large density
- 3. Not good for excited states

ASM, N. Nagaosa and N. Prokof'ev, Phys. Rev. Lett. 113, 166402 (2014)

### Strong coupling.

### Spin-polarized fermion gas = holes in t-J model



### Polaronic spectral function: Z-factor



**Fig. 10.** Sketch of the polaron spectral function  $A(\omega, \mathbf{k})$  at low electron excitation energy  $E(\mathbf{k}) - E_F$ . The characteristic peak-dip-hump (PDH) spectral shape is formed by the quasiparticle (QP) peak followed by the phonon sideband tail corresponding to a sequence of optical phonons with frequency  $\omega_0$ .

Explanation of

 (a) ARPES;
 (b) optical conductivity;
 (c) T-dependence of the spectral properties;
 (d) pump-probe evolution of the optical conductivity
 (e) Raman
 in underdoped cuprates
 requires considerable electron-boson coupling

- 2. Naively, experimental data indicate that increase of doping decreases manifestations of the electron-boson coupling in specroscopy
- 3. We solve famous sign-problem in Mote Carlo for many-particle Fermi-polarons system and explain what happens with electron-boson coupling when doping in high  $T_c$  cuprates increases.

#### **PART I: Further reading for details:**

Phys. Rev. Lett., vol. 86, 4624 (2001): Pseudo-Jahn-Teller polaron Phys. Rev. Lett., vol. 91, 236401 (2003) : Optical cond-ty of Frohlich polaron Phys. Rev. Lett., vol. 93, 036402 (2004) : ARPES in high T<sub>c</sub> cuprates Phys. Rev. Lett., vol. 99, 146405 (2007) : Nonlocal el-ph in high T<sub>c</sub> cuprates Phys. Rev. Lett., vol. 99, 226402 (2007) : ARPES in high T<sub>c</sub> cuprates Phys. Rev. Lett., vol. 100, 166401 (2008) : Optical cond-ty in high T<sub>c</sub> cuprates Phys. Rev. Lett., vol. 107, 076403 (2011) : Optical cond-ty of Holstein polaron Phys. Rev. Lett., vol. 109, 176402 (2012) : Time dependent Holstein-Hubbard Nature Commun. 5:5112 (2014) : Pump-probe in optics of LaCuO4 Phys. Rev. Lett., vol. 113, 166402 (2014) : Finite density polaron gas Phys. Rev. Lett., vol. 114, 146401 (2015) : Unbiased mobility of Holstein polaron Nature Commun. 7:10386 (2016) : Polarons in LAO-STO interface

New advances in analytic continuation method: well posed answers to ill posed questions.

Andrey S. Mishchenko RIKEN CEMS (Center for Emergent Matter Science)

- 1. Analytic continuation.
- 2. Why difficult.
- 3. Why SOM successful and what are drawbacks.
- 4. Consistent constraints cure.
- 5. Playing with linear combinations of solutions.
- 6. Which additional information we can get with new ideology.

Physical properties under interest: absorption by polaron.

Such relation between imaginary-time function and spectral properties is rather general:

$$G_{\mathbf{k}}(\tau) = \int_0^\infty d\omega \, L_{\mathbf{k}}(\omega) \, e^{-\omega\tau}$$

### ARPES

Current–current corelation function is related to optical absorption by polarons by the same expression:

$$\langle J_{\beta}(\tau) J_{\delta} \rangle$$

$$\sigma_{\beta\delta}(\omega) = \pi \hat{\mathcal{F}}_{\omega}^{-1} \left[ \langle J_{\beta}(\tau) J_{\delta} \rangle \right] / \omega$$

Optical absorption

### $\mu = \sigma (\omega \rightarrow 0)/en$

Mobility

G(m) = $d\omega \ \mathcal{K}(m,\omega) \ A(\omega)$ 

There are a lot of problems where one has to solve Fredholm integral equation of the first kind

### Optical conductivity at finite T in imaginary times representation

$$G(m) = \int_{-\infty}^{\infty} d\omega \ \mathcal{K}(m,\omega) \ A(\omega)$$

$$\mathcal{G}(i\omega_m) = \int_0^\beta d\tau \ e^{i\omega_m\tau} \ G(\tau)$$

$$G(\tau) = \frac{1}{\beta} \sum_{\omega_m} e^{-i\omega_m \tau} \mathcal{G}(i\omega_m)$$

$$\mathcal{K}(\tau_m, \omega) = \frac{1}{\pi} \frac{\omega \exp(-\tau_m \omega)}{1 - \exp(-\beta \omega)}$$

Equation for many problems

### Image deblurring with e.g. known 2D noise K(m,ω)

 $G(m) = \int_{-\infty}^{\infty} d\omega \ \mathcal{K}(m,\omega) \ A(\omega)$ 

### m and ω are 2D vectors

#### Original



Blurred & noisy



one  $\lambda$ 



three  $\lambda$ 's



### K(m,ω) is a 2D x 2D noise distributon function

### Tomography image reconstruction (CT scan)



G(m) $d\omega \ \mathcal{K}(m,\omega) \ A(\omega)$ 

### m and $\omega$ are 2D vectors

### K(m,ω) is a 2D x 2D distribution function





$$G(m) = \int_{-\infty}^{\infty} d\omega \ \mathcal{K}(m,\omega) \ A(\omega)$$



Ill-posed!  $G(m) = \int d\omega \ \mathcal{K}(m,\omega) \ A(\omega)$ 

We cannot obtain an exact solution not because of some approximations of our approaches.

Instead, we have to admit that the exact solution does not exist at all!



$$G(m) = \int_{-\infty}^{\infty} d\omega \ \mathcal{K}(m,\omega) \ A(\omega)$$

1. No unique solution in mathematical sense No function A to satisfy the equation

2. Some additional information is required which specifies which kind of solution is expected. In order to chose among many approximate solutions.



Regularization



ridge regression

Tikhonov Regularization

$$G(m) = \int_{-\infty}^{\infty} d\omega \ \mathcal{K}(m,\omega) \ A(\omega)$$
$$G(m) = \sum_{n=1}^{N} \mathcal{K}(m,\omega_n)A(\omega_n) \ , \ m = 1, \dots, M$$

Because of noise present in the input data G(m) there is no unique A( $\omega_n$ )=A(n) which exactly satisfies the equation. Hence, one *Can* search for the *least-square* fitted solution A(n) which minimizes:

$$\|\widehat{\mathcal{K}}\overrightarrow{A} - \overrightarrow{G}\|^2 = \sum_{m=1}^{M} \left| \sum_{n=1}^{N} \mathcal{K}(m, \omega_n) A(\omega_n) - G(m) \right|^2$$

$$\left\| \widehat{\mathcal{K}} \vec{A} - \vec{G} \right\|^2 = \sum_{m=1}^{M} \left| \sum_{n=1}^{N} \mathcal{K}(m, \omega_n) A(\omega_n) - G(m) \right|^2$$

### Saw tooth noise instability due to small singular values.

#### **Explicit expression:**





$$\|\widehat{\mathcal{K}}\overrightarrow{A} - \overrightarrow{G}\|^2 = \sum_{m=1}^{M} \left|\sum_{n=1}^{N} \mathcal{K}(m,\omega_n)A(\omega_n) - G(m)\right|^2$$

### III-posed!

Tikhonov regularization to fight with the **saw tooth noise** instability.



### TIKHONOW-SAMARSKY







All existing methods are biased and over-smoothing!

### New player:

Stochastic optimization method

Particular solution L<sup>(i)</sup>(ω) for LSF is presented as a sum of a number K of rectangles with some width, height and center.

Continuous-ω parametrization !!



**Fig. 2:** An example of configuration with K = 4. Panel (b) shows how the intersection of rectangles in panel (a) is treated.

- Particular solution L<sup>(i)</sup>(ω) for LSF is presented as a sum of a number K of rectangles with some width, height and center.
- Initial configuration of rectangles is created by random number generator (i.e. number K and all parameters of of rectangles are randomly generated).



**Fig. 2:** An example of configuration with K = 4. Panel (b) shows how the intersection of rectangles in panel (a) is treated.

- Particular solution L<sup>(i)</sup>(ω) for LSF is presented as a sum of a number K of rectangles with some width, height and center.
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Final solution is obtained after M steps of such procedure

 $L(\omega) = M^{-1} \sum_{i} \alpha(i) L^{(i)}(\omega)$ 

Particular solution L<sup>(i)</sup>(ω) for LSF is presented as a sum of a number K of rectangles with some width, height and center.



Each particular basic solution has saw tooth noise

### Abandon Tikhonov regularization



- Particular solution L<sup>(i)</sup>(ω) for LSF is presented as a sum of a number K of rectangles with some width, height and center.
- Initial configuration of rectangles is created by random number generator (i.e. number K and all parameters of of rectangles are randomly generated).
- Each basic solution L<sup>(i)(ω)</sup> is obtained by a naïve method without regularization (though, varying number K).

Final solution is obtained after M steps of such procedure

 $L(\omega) = M^{-1} \sum_{i} \alpha(i) L^{(i)}(\omega)$ 

Each particular basic solution has saw tooth noise

Final averaged solution L(ω) has no saw tooth noise though not regularized with sharp peaks/edges!!!!

#### Self-averaging of the saw-tooth noise.



Fig. 7. Comparison of the actual spectral function (dashed line) with the results of spectral analysis after averaging over (a) M = 4, (b) M = 28, and (c) M = 500 particular solutions.

#### Self-averaging of the saw-tooth noise.



Fig. 7. Comparison of the actual spectral function (dashed line) with the results of spectral analysis after averaging over (a) M = 4, (b) M = 28, and (c) M = 500 particular solutions.
### Self-averaging of the saw-tooth noise.



**Fig. 7.** Comparison of the actual spectral function (dashed line) with the results of spectral analysis after averaging over (a) M = 4, (b) M = 28, and (c M = 500 particular solutions.

### Stochastic Optimization method: update procedures.

**Objectuve** K+M chain is accepted if final objective is smaller than initial CONFIGURATON

Shake-off two-step strategy: Step 1: Increase of objective function is allowed during M steps with high probability Step 2: Only decrease of objective function is allowed during last K steps.

# Errorbars estimate

### Expectation and standard deviation in every selected bin



Preparing final solutions

### Self-averaging of the saw-tooth noise.



**Fig. 7.** Comparison of the actual spectral function (dashed line) with the results of spectral analysis after averaging over (a) M = 4, (b) M = 28, and (c M = 500 particular solutions.

The formulation of the SOCC method :

1. Finding a large set of solutions  $A_j(z)$   $[j = 1, ..., J \gg 1]$  to Eq. (1) that satisfy the input data within their error bounds. In what follows we call them "basic" solutions. Basic solutions are not biased in any way to be smooth or to satisfy any other requirements based on knowledge about the problem outside of Eq. (1).

2. Using the basic solutions  $A_j(z)$  to determine the final solution by selecting a superposition of basic solutions

$$A_{\text{fin}}(z) = \sum_{j=1}^{J} c_j A_j(z), \qquad \sum_{j=1}^{J} c_j = 1 , \qquad (2)$$

such that A(z) remains non-negative and the coefficients  $c_j$  are optimized to impose smooth behavior or any other "conditional knowledge". Even  $C_j$  the simplest interpretation corresponds to  $c_j = 1/J$ .

The search for basic solutions relies on the minimization of

$$\chi^{2} = N^{-1} \sum_{n=1}^{N} \left( \frac{g_{n} - G[n, A]}{\delta_{n}} \right)^{2}$$
(3)

where  $\delta_n$  is the error of the  $g_n$  value. We choose a maximal tolerance  $\chi_c$  of order unity and search for functions A(z) > 0 with  $\chi^2 < \chi_c^2$ , which are then added to the set of basic solutions for further processing.

Information about the input data is limited to the objective function (3). Truly unbiased methods should not assume anything about A(z) that is not part of exact knowledge, such as the predetermined grid of points, and the number and parameters of peaks/gaps.

2. Using the basic solutions  $A_j(z)$  to determine the final solution by selecting a superposition of basic solutions

$$A_{\text{fin}}(z) = \sum_{j=1}^{J} c_j A_j(z), \qquad \sum_{j=1}^{J} c_j = 1 , \qquad (2)$$

such that A(z) remains non-negative and the coefficients  $c_j$  are optimized to impose smooth behavior or any other "conditional knowledge". Formally, the simplest interpretation corresponds to  $c_j = 1/J$ .

$$\chi^2 = N^{-1} \sum_{n=1}^N \left( \frac{g_n - G[n, A]}{\delta_n} \right)^2$$

Quadratic form with respect to {c<sub>j</sub>}

$$\chi^{2} = \sum_{j,j'=1}^{J} c_{j}c_{j'}\chi_{jj'} \leq \bar{C}^{2}\chi_{c}^{2}, \text{ with } \bar{C} = \sum_{j=1}^{J} |c_{j}|, \quad (10)$$
$$\chi_{jj'} = N^{-1}\sum_{n=1}^{N} \frac{(g_{n} - G[n, A_{j}])(g_{n} - G[n, A_{j'}])}{\delta_{n}^{2}}. \quad (11)$$

If some c-coefficients are negative, the accuracy of the final solution is guaranteed only if  $\bar{C}$  is not large. One may argue that the upper bound  $\chi^2 \leq \bar{C}^2 \chi_c^2$  is substantially overestimating deviations, and the actual accuracy is better. Finally, Eq. (10) is only an upper bound, and superpositions with  $\bar{C}$  as large as 2 may still have  $\chi^2 < \chi_c^2$ .

### What is to minimize?

• To suppress large derivatives we consider the following form

$$D_1 = \sum_{k=2}^{K} \left\{ D_k^2 [A'(z_k)]^2 + B_k^2 [A''(z_k)]^2 \right\} , \qquad (12)$$

where  $\{z_k\}$  is the grid of points used to define the first and second discrete derivatives of the function A(z). The sets of coefficients  $D_k$  and  $B_k$  are adjusted under iterations self-consistently in such a way that contributions of all  $z_k$ -points to  $O_1$  are similar.

• The unity-sum constraint on the sum of all coefficients in the superposition is expressed as

$$O_2 = \mathcal{U}\left(\sum_{j=1}^J c_j - 1\right)^2 , \qquad (13)$$

with a large constant  $\mathcal{U}$ .

• Since  $O_1 + O_2$  does not constrain the amplitudes and signs of all  $c_j$  the minimization cannot proceed by matrix inversion. To improve matrix properties we add a "soft" penalty for large deviations of  $c_j$  from the equal-weight superposition

$$O_3 = \sum_{j=1}^{J} (c_j - 1/J)^2 . \tag{14}$$

• To ensure that the spectral function is non-negative (with high accuracy) we need z-dependent penalties (to be set self-consistently) that suppress the development of large negative fluctuations:

$$O_4 = \sum_{k=1}^{K} Q_k A(z_k)^2 .$$
 (15)

• Finally, we can introduce a penalty for the solution to deviate from some "target" function (or "default model")  $A_T(z_k)$ :

$$O_5 = \sum_{k=1}^{K} T_k \left[ A(z_k) - A_T(z_k) \right]^2 \,. \tag{16}$$

The main purpose of  $O_5$  is to address subtle multi-point correlations between allowed shapes: by forcing the solution to be close to a certain target function one can monitor how the solution starts developing additional sawtooth-instability-related features or violates the unitysum constraint. This penalty is zero when preparing  $A_{\text{fin}}$ in the absence of any target function.

### Self-consistent protocol.

After the quadratic form for the objective function O is minimized, the new set of *c*-coefficients is used to define a new solution A(z), penalties for derivatives are increased,  $\mathcal{D} \to f\mathcal{D}, D_k \to fD_k, B_k \to fB_k$  by some factor f > 1, and then all penalties in in  $O_1$  and  $O_4$  are adjusted self-consistently as follows:

• If  $D_k|A'(z_k)| > \mathcal{D}$ , we assign  $D_k = \mathcal{D}/|A'(z_k)|$ ;

• If 
$$B_k|A''(z_k)| > \mathcal{D}$$
, we assign  $B_k = \mathcal{D}/|A''(z_k)|$ ;

 If A(z<sub>k</sub>) < 0, we assign a large penalty suppressing the amplitude of the solution at this point, Q<sub>k</sub> = Q, where Q is a large constant; otherwise the value of Q<sub>k</sub> is increased by two orders of magnitude.

In this work we use  $\mathcal{U} = 10^6$ ,  $\mathcal{Q} = 10^6$ , and f = 2. This sets the stage for the next iteration of the *O*-optimization protocol. The final solution (2) is based on the last set of *c*-coefficients that satisfied the condition  $\chi^2 < \chi_c^2$ .







A

### Valid Transformation?







### Blind tests: how much we can say about second peak



O. Goulko et al, Phys. Rev. B 95, 014102 (2017)

# Noise level $\delta = 10^{-3}$



FIG. 3. (Color online.) Results for test 1, featuring two peaks of finite width with noise level  $10^{-3}$ . Shown is the compari-

# Noise level $\delta = 10^{-5}$



FIG. 6. (Color online.) Results for test 2, featuring two peaks of finite width with noise level  $10^{-5}$ . Shown is the com-

# Noise level $\delta = 10^{-5}$ First peak -> $\delta$ function



FIG. 8. (Color online.) Results for test 3, characterized by a  $\delta$ -function at low frequency and a peak of finite width at high frequency with noise level 10<sup>-5</sup>. Shown is the comparison be-

## **Conclusions.** Numeric analytic continuation :

well posed answers to the ill posed problems.

 $g_n - given MC data,$  K[n,z] - known kernel  $G[n,A] = \int dz K[n,z] A(z)$ A(z) - spectral function to find





#### **Objectives:**

1.Stochastic optimization method (SOM) can quickly find a lot of [J>1000] solutions {A<sub>j</sub>(z)} each having good objective function ( $\delta_n$  – error bars) ...  $O_1 = \chi^2 = N^{-1} \sum_{n=1}^{N} [ (g_n - G[n,A_j]) / \delta_n ]^2 < \chi_c^2 = 1$ 

Usually, final solution is obtained as average

$$< A(z) > = J^{-1} \sum_{j=1}^{J} A_{j}$$

which removes saw tooth instability. However, one can search solution as

$$A_{fin}(z) = J^{-1} \sum_{j=1}^{J} c_j A_j$$
 where  $\sum_{j=1}^{J} c_j = 1$ 

where Cj<0 are possible untill  $\chi^2 < \chi_c^2$ .

Results

1. One can introduce one more part of objective function  $O_5 = \sum_{k} T(k) [A_{fin}(z_k) - A_T(z_k)]^2$ 

which characterizes deviation from target function  $A_T(z)$ .

2. It is legal to satisfy  $O_5$  until  $\chi^2 < \chi_c^2$ .

3. This approach can verify which features of result are robust and which can be an artefact at given error bars  $\delta_n$ . (see example where high energy peak can be made very narrow (green) or very wide (blue) in comparison with actual peak (red) without compromising the error bars). Hence, peak width is undefined.

O. Goulko et al, arXiv: 1609.01260

# Polaron mobility:

5 different regimes  $\mu = \sigma(\omega \rightarrow 0) / eN$ 

A.S.M., N. Nagaosa, G. De Filippis, A. de Candia, and V. Cataudella, Phys. Rev. Lett., vol. 114, 146401 (2015)

## Hamiltonian

$$\mathcal{H} = \sum_{k} \left( \varepsilon_k c_k^{\dagger} c_k + \omega_0 b_k^{\dagger} b_k \right) + \frac{g}{\sqrt{N}} \sum_{k,q} c_{k-q}^{\dagger} c_k \left( b_q^{\dagger} + b_{-q} \right)$$

#### Analytic continuation

$$\Pi(\tau) = \int_{-\infty}^{\infty} d\omega \ \frac{1}{\pi} \frac{\omega \exp[-\tau\omega]}{1 - \exp[-\beta\omega]} \ \sigma(\omega) \equiv \mathcal{F}[\tau, \sigma(\omega)]$$

# Regimes

Metallic

$$u_{\rm metal}(T) \sim T^{-\delta}$$

þ

Activation  

$$\mu_{\text{hop}}(T) \sim T^{-\kappa} \exp(-\varepsilon_a/T)$$

 $\sim a$ 

$$\mu_{\lambda}(\omega, T) = \sigma_{\lambda}(\omega, T)/(eN_e)$$

# $\lambda$ =0.5, weak copling



# $\mu_{\lambda}(\omega,T) = \sigma_{\lambda}(\omega,T)/(eN_e)$ $\lambda=4.0$ , strong coupling











Phys. Rev. Lett., vol. 114, 146401 (2015)



### Part II. Further reading for details:

Phys. Rev. Lett., vol. 86, 4624 (2001): Pseudo-Jahn-Teller polaron Phys. Rev. Lett., vol. 87, 186402 (2001) : Exciton in semiconductors Phys. Rev. Lett., vol. 91, 236401 (2003) : Optical conductivity of Frohlich polaron Phys. Rev. Lett., vol. 93, 036402 (2004) : ARPES in high T<sub>c</sub> cuprates Phys. Rev. Lett., vol. 96, 136405 (2006) : Franck-Condon principle Phys. Rev. Lett., vol. 99, 146405 (2007) : Nonlocal el-ph in high T<sub>c</sub> cuprates Phys. Rev. Lett., vol. 99, 226402 (2007) : ARPES in high T<sub>c</sub> cuprates Phys. Rev. Lett., vol. 100, 166401 (2008) : Optical conductivity in high T<sub>c</sub> cuprates Phys. Rev. Lett., vol. 101, 116403 (2008) : Exciton-polaron in semiconductors Phys. Rev. Lett., vol. 104, 056602 (2010) : ESR in organic transistors Phys. Rev. Lett., vol. 105, 266605 (2010) : SSH polaron in organic compounds Phys. Rev. Lett., vol. 107, 076403 (2011) : Optical conductivity of Holstein polaron Phys. Rev. Lett., vol. 109, 176402 (2012) : Time dependent Holstein-Hubbard Phys. Rev. Lett., vol. 113, 166402 (2014) : Finite density polaron gas Phys. Rev. Lett., vol. 114, 086601 (2015) : Conductivity in organic materials Phys. Rev. Lett., vol. 114, 146401 (2015) : Unbiased mobility of Holstein polaron