“New Frontiers of Strongly Correlated Electron Materials” workshop
KITS Beijing

Rejuvenated Understanding of Cuprate High-T_c Superconductors

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Open post dotoral fellow position

computational approach to
strongly correlated electron systems

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Outline

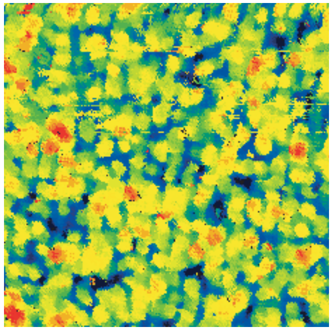
1. **Competing Orders**
   Stripes and *d*-wave superconductivity in Hubbard studied by the state of the art numerical methods

2. ***ab initio* Hamiltonian for cuprate superconductors ($HgBa_2CuO_4$) and its solution**

3. **New concept & mechanism emerging from numerics**
   Emergent fermions; dark fermion theory
   cDMFT and machine learning of ARPES

4. **Summary and outlook**

Charge inhomogeneity vs. superconductivity



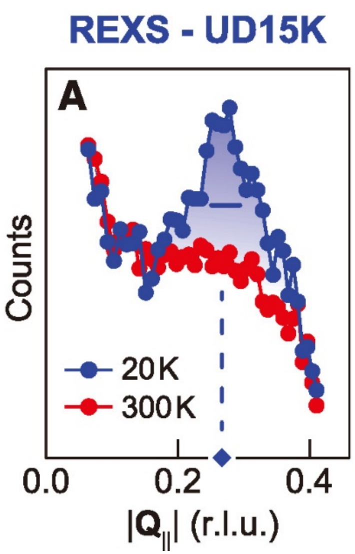
Lee *et al.* Nature 442, 546 (2006)

patch structure,

stripes

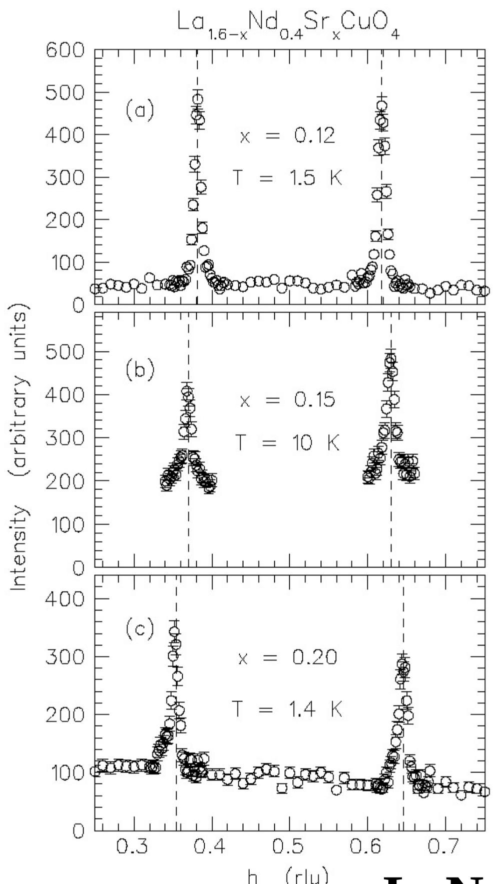
Tranquada(1995),

.....



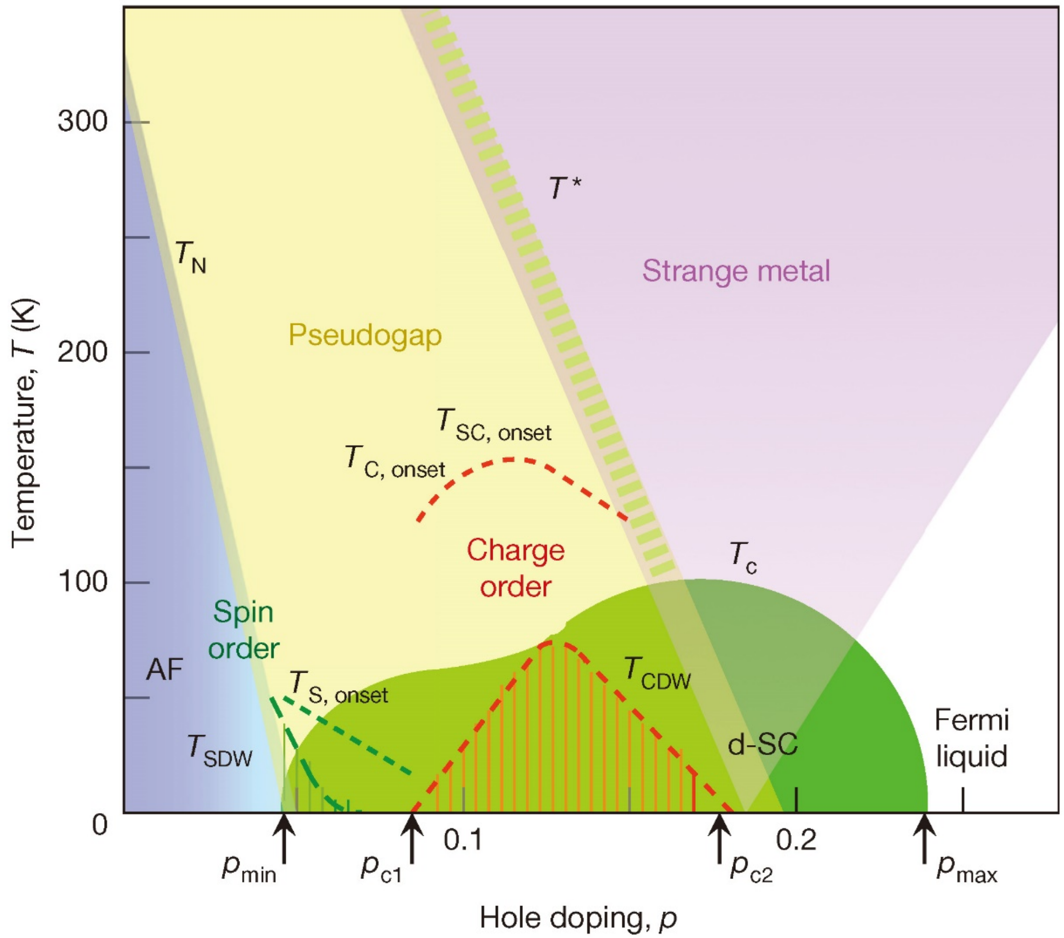
Bi2201

Comin *et al.* 2014



LaNdSrCuO

Tranquada *et al.* 1996



Keimer *et al.* Nature 2015

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Variational Monte Carlo

Tahara, MI
JPSJ 77 (2008), 114701

$$|\psi\rangle = \mathcal{L}_L \mathcal{P}_{\mathrm{J}} \mathcal{P}^{\mathrm{ex.}}_{\mathrm{d\text{-}h}} \mathcal{P}_{\mathrm{G}} \mathcal{L}^{S=0} |\phi_{\mathrm{pair}}\rangle$$

$$\left|\Phi_{\mathrm{pair}}\right\rangle = \left[\sum_{ij\sigma\tau} f_{ij\sigma\tau} c^{\dagger}_{i\sigma} c^{\dagger}_{j\tau}\right]^{N/2} |0\rangle$$

f_{ij} : pair-dependent variational parameter

optimization of 1000-10000 variables to overcome bias

Represent strong entanglement in the real space representation

Various Correlation Factors and Quantum Number Projection

Tahara, MI
JPSJ 77 (2008) 114701

$$|\psi\rangle = \mathcal{L}_L \mathcal{P}_{\rm J}\mathcal{P}_{\rm d\text{-}h}^{\rm ex.}\mathcal{P}_{\rm G}\mathcal{L}^{S=0}|\phi_{\rm pair}\rangle$$

Gutzwiller factor

$$\mathcal{P}_{\rm G} = \exp\left[-g\sum_i n_{i\uparrow}n_{i\downarrow}\right]$$

doublon-holon correlation factor

Yokoyama *et al.*

$$\mathcal{P}_{\rm d\text{-}h}^{\rm ex.} = \exp\left[-\sum_{m=0}^{2}\sum_{\ell=1,2}\alpha_{(m)}^{(\ell)}\sum_i \xi_{i(m)}^{(\ell)}\right]$$

$$\xi_{i(0)}^{(1)} = d_i\prod_\tau^{\rm n.n.}(1-h_{i+\tau}) + h_i\prod_\tau^{\rm n.n.}(1-d_{i+\tau})$$

long-ranged Jastrow factor

Sorella *et al.*
Giamarchi *et al.*

$$\mathcal{P}_{\rm J} = \exp\left[-\frac{1}{2}\sum_{i\neq j}v_{ij}n_in_j\right]$$

quantum number projection

$$\mathcal{L}^S = \frac{2S+1}{8\pi^2}\int d\Omega\, P_S(\cos\beta)\hat{R}(\Omega)$$

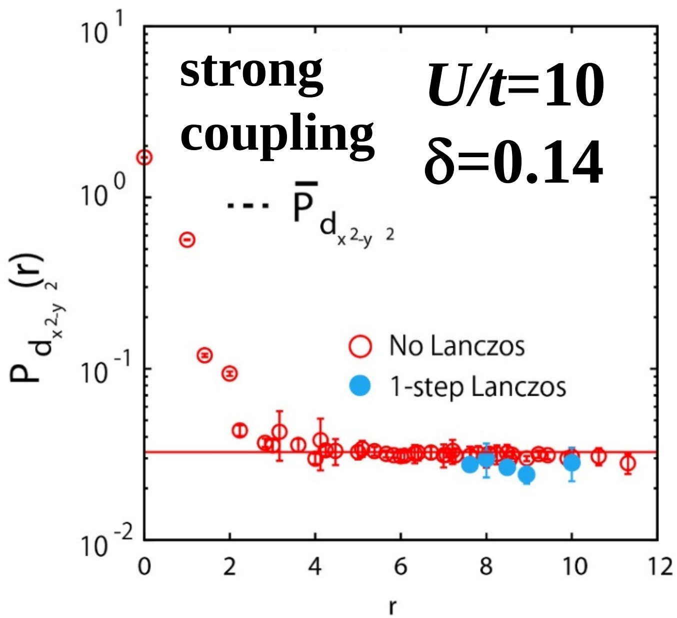
Lanczos operation $\mathcal{L}_L = (1+\alpha H)$

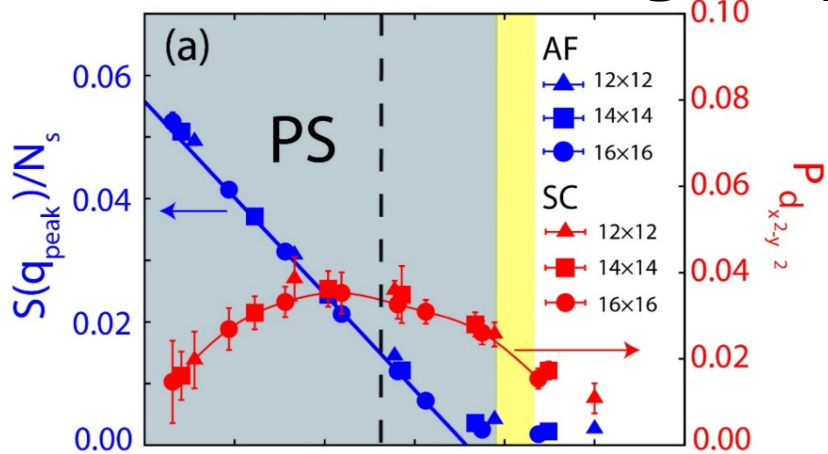
Phase separation and SC

Hubbard models: VMC

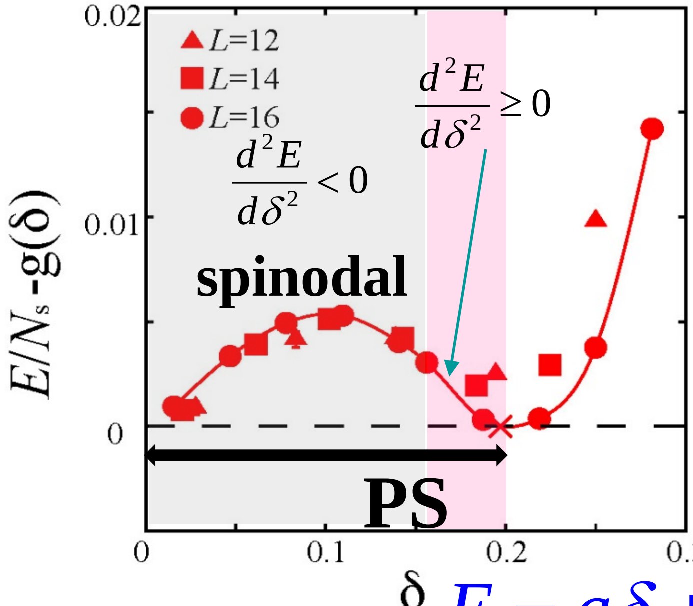
Misawa & Imada Phys. Rev. B 90, 115137 (2014)

$U/t = 10$: strong coupling

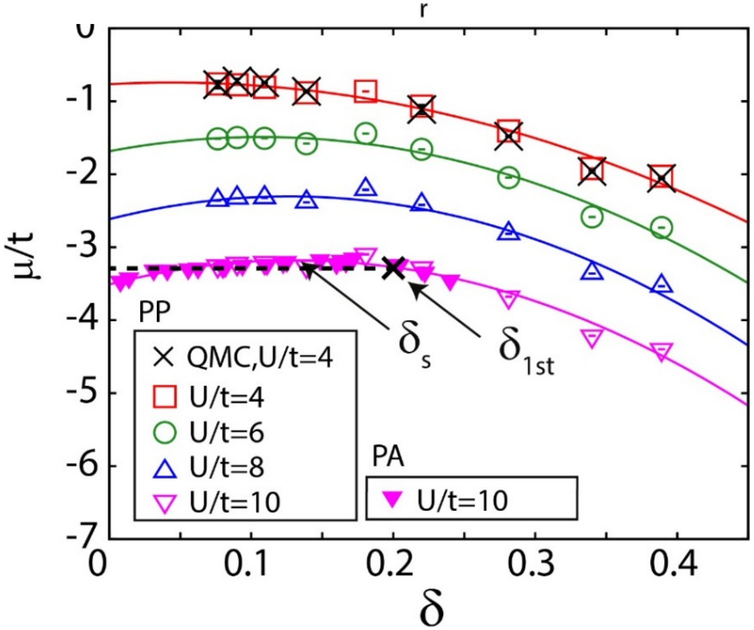




$\bar{P}_{dx2-y2}$: squared SC order parameter



see also
Capone, Kotliar (2009)
Aichhorn *et al.* (2007)
Sordi *et al.*(2012)
Yokoyama *et al.* (2012)
Neuscamman *et al.* (2012)
Chang *et al.* (2010)



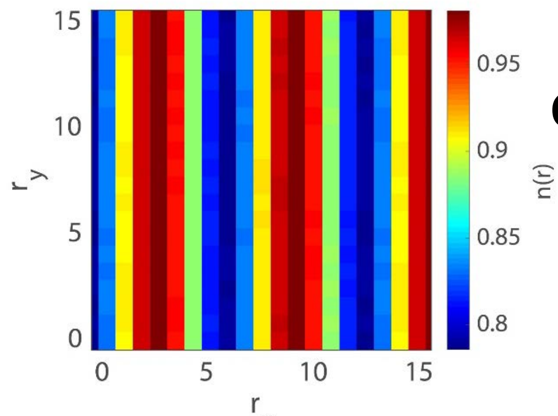
$$E = a\delta + b\delta^2 + \cdots, \quad b < 0$$

PS (inhomogeneity) is universally unavoidable for strong coupling SC

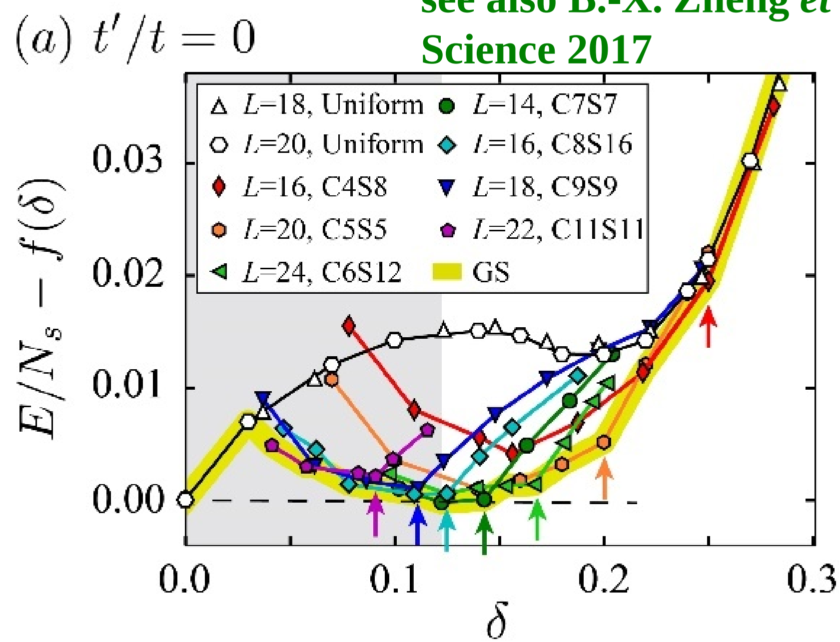
If long-period stripe is allowed: severe competition of dSC and stripes

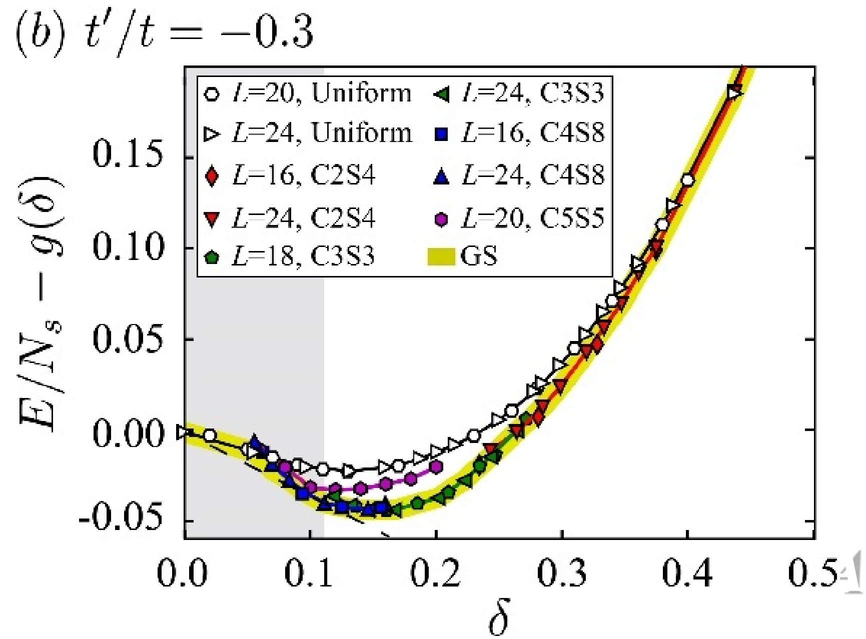
Ido, Ohgoe, Imada
Phys. Rev. B 97, 045138 (2018)
see also B.-X. Zheng *et al.* Science 2017

U/t=10 Hubbard δ~0.11



c8s16





uniform dSC metastable
stripe (weak dSC) GS
energy difference ~ 0.01t

FTTN combined with VMC

Zhao *et al.* PRB 96, 085103 (2017)

$$|\Psi\rangle = \mathcal{P}(\mathcal{L}^{K=0}\mathcal{L}^{C_4}\mathcal{M})\mathcal{L}^{K=0}\mathcal{L}^{S=0}|\phi_{\text{pair}}\rangle$$

$$\Rightarrow \mathcal{P}(\mathcal{L}^{K=0}\mathcal{L}^{C_4}\mathcal{M}) \sum_{\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N} |\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N\rangle\langle\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N|\mathcal{L}^{K=0}\mathcal{L}^{S=0}|\phi_{\text{pair}}\rangle$$

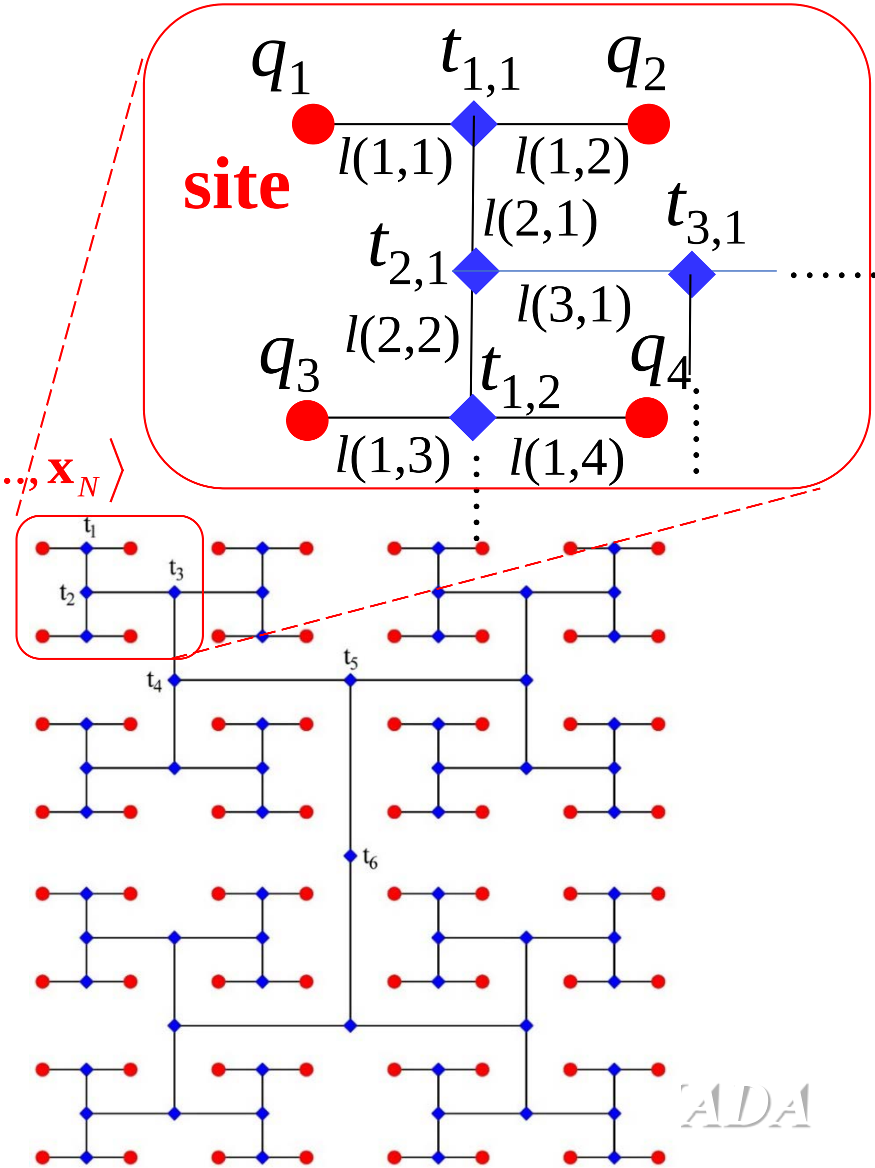
1. exact contraction, variational principle
2. lattice symmetry preserving
3. guaranteed convergence for $D\rightarrow\infty$

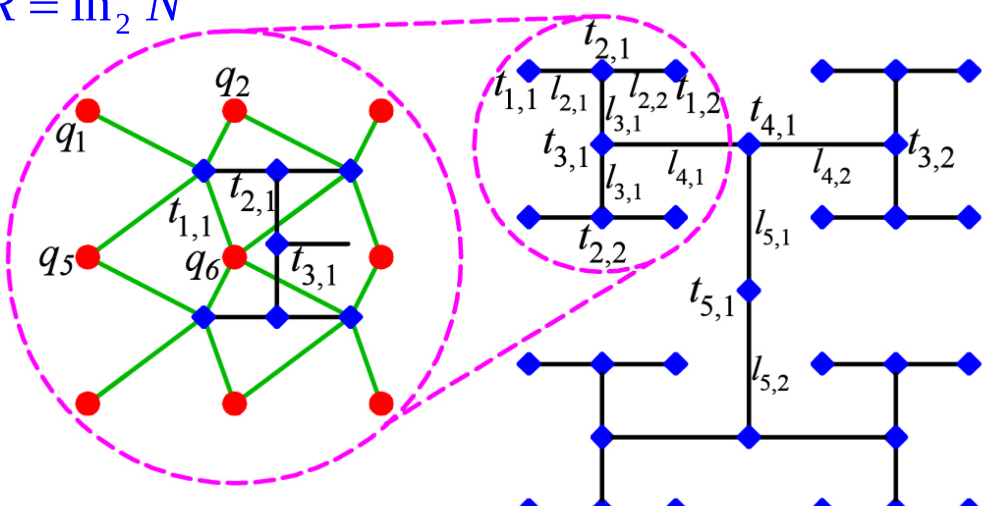
$$\mathcal{M}|q_1,q_2,\ldots,q_N\rangle = \sum_{\{l(j,i)\}=1}^{D}\prod_{i=1}^{N/2}\left[t_{1,i}(q_{2i-1},q_{2i},l_{2,i})\right]$$

$$\times\prod_{j=2}^{R-1}\prod_{i=1}^{N/2^j}\left[t_{j,i}(l_{j,2i-1},l_{j,2i},l_{j+1,i})\right]t_{R,1}(l_{R,1},l_{R,2})|\mathbf{x}_1,\mathbf{x}_2,\ldots,\mathbf{x}_N\rangle$$

$R = \ln_2 N$

TTN



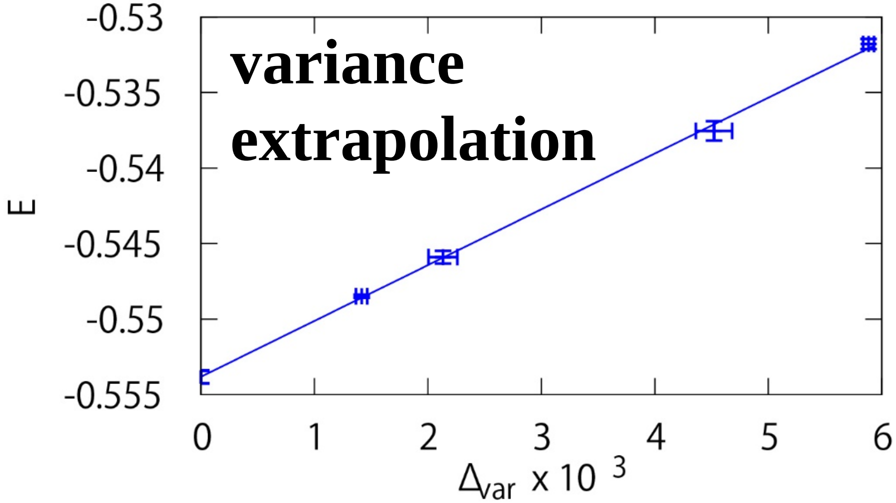


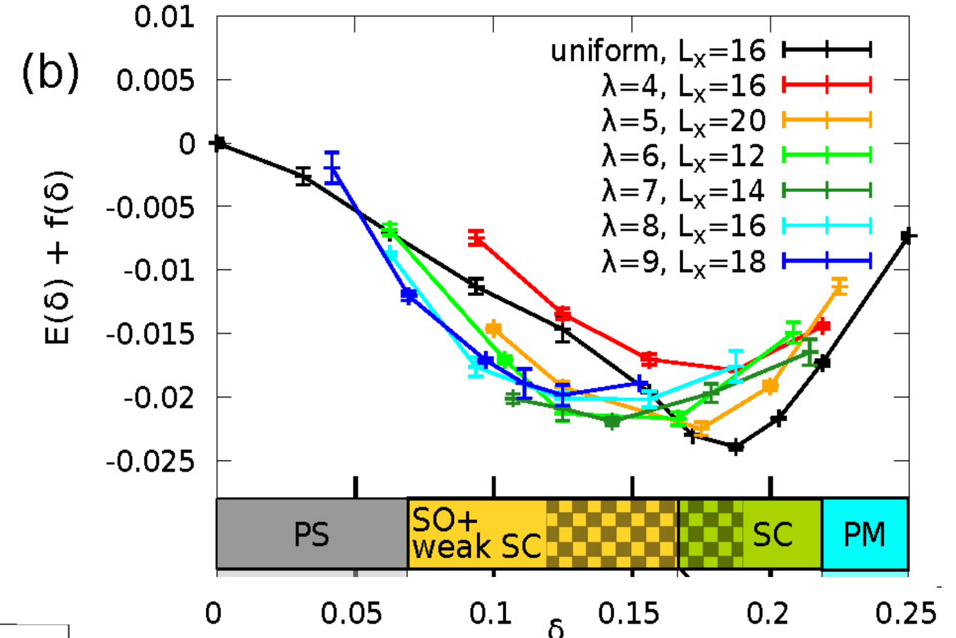
Fat tree tensor network

VMC+ tensor network+ Lanczos with variance extrapolation: Phase diagram of Hubbard

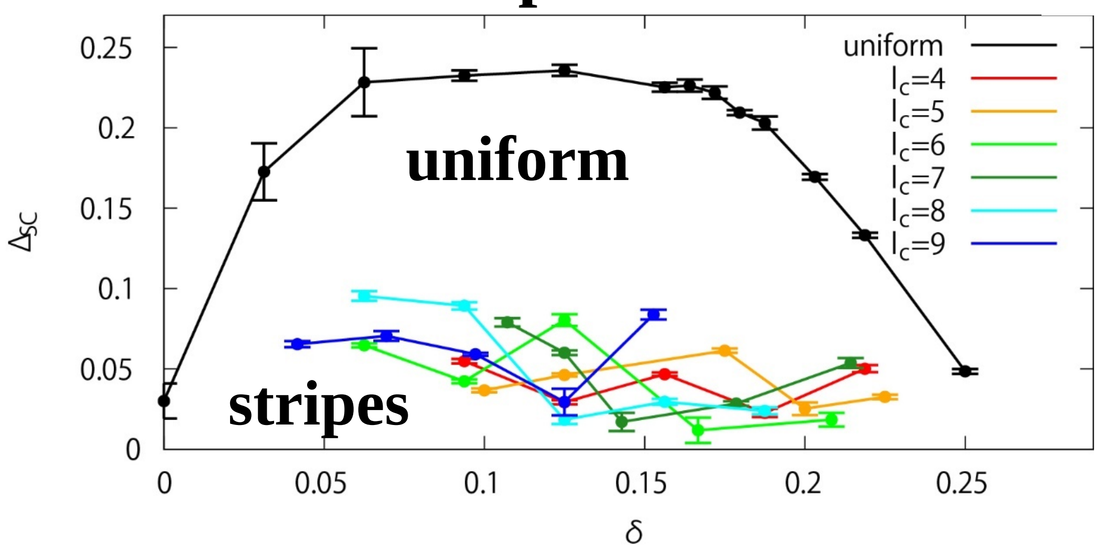
VMC, FTTN, Lanczos U/t=10

Darmawan, Yamaji, Nomura, Imada

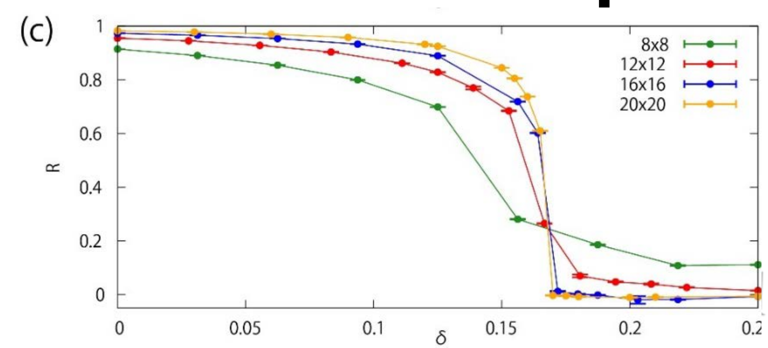




d-wave SC order parameter



AF quantum critical at δ~0.17 for uniform phase



Outline

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   Stripes and *d*-wave superconductivity in Hubbard studied by the state of the art numerical methods

2. ***ab initio* Hamiltonian for cuprate superconductors ($HgBa_2CuO_4$) and its solution**

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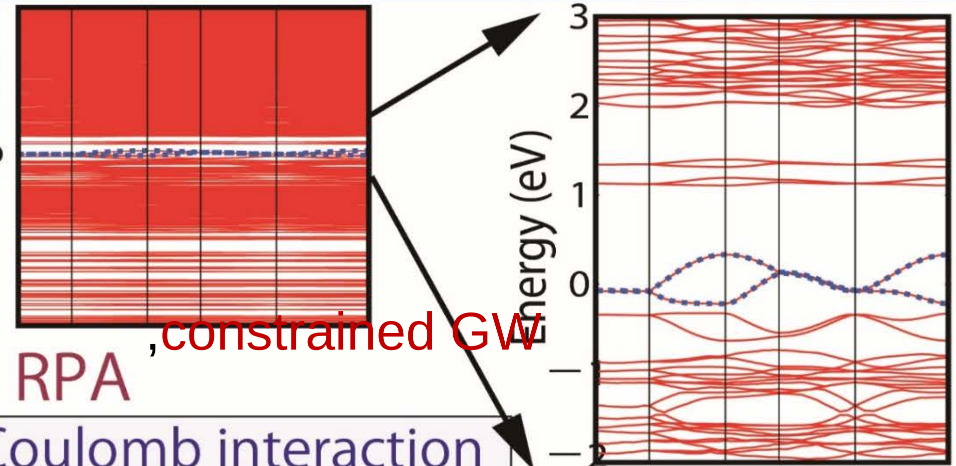
4. Summary and outlook

Basic Scheme of MACE
(multi-scale *ab initio* scheme for correlated electrons)

1. Global electronic structure by DFT。

far from Fermi level

tens eV



,constrained GW

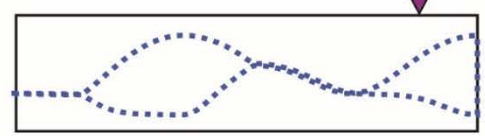
2. downfolding constrained RPA

(1) Screened Coulomb interaction

(2) Self-energy

Low-energy effective Hamiltonian

1/10-1/100 eV



"target band"

3. Low-energy solver

variational Monte Carlo (VMC),

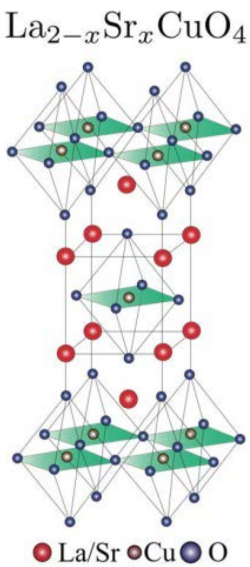
path-integral renormalization group (PIRG) ,

(cluster) dynamical mean-field theory (DMFT),

………

remove double counting by LDA+cRPA → cGW

1st-principles effective Hamiltonian for curates



Hirayama *et al.*
arXiv:1708.07498

Aryasetiawan *et al.* PRB 2004
MACE scheme for *ab initio* hamiltonian

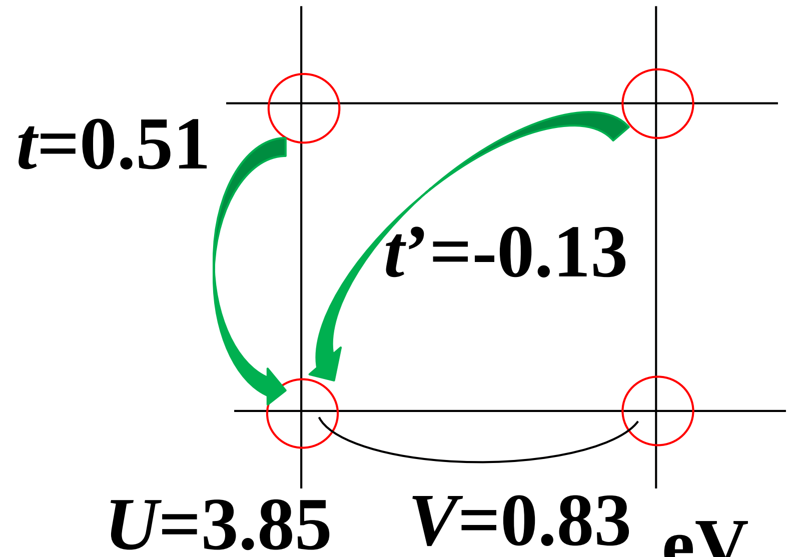
$HgBa_2CuO_4$
La_2CuO_4
1band (x^2-y^2)
2band (x^2-y^2, $3z^2$-r^2)
3band (x^2-y^2,$2p_\sigma$)
Hamiltonians

improved cGW-SIC method
$2p\sigma$ level feedback to satisfy
$n_{GW} = n_{VMC}$

$HgBa_2CuO_4$ 1-band Hamiltonian eV

One-body	t_1	t_2	t_3	t_4	t_5
parameters (eV)	0.509	-0.127	0.077	-0.018	-0.004
Two-body	U	V_1	V_2	V_3	V_4
parameters (eV)	3.846	0.834	0.460	0.318	0.271

U/t~7.6



VMC+FTTN+LCZS for *ab initio* Hamiltonian of $HgBa_2CuO_4$

fully *ab initio* results with long-ranged transfer and interaction

Uniform SC state is stabilized for *ab intio* case

V_3 partially cancels V_1

experiments: $0.09<\delta<0.12$, q~0.25
W. Tabis, Y. Li, M. L. Tacon,
et al., Nat. Commun. 5, 5875 (2014).
G. Campi, A. Bianconi, et al.
S. M. Kazakov, et al., Nature 525,
359 (2015).

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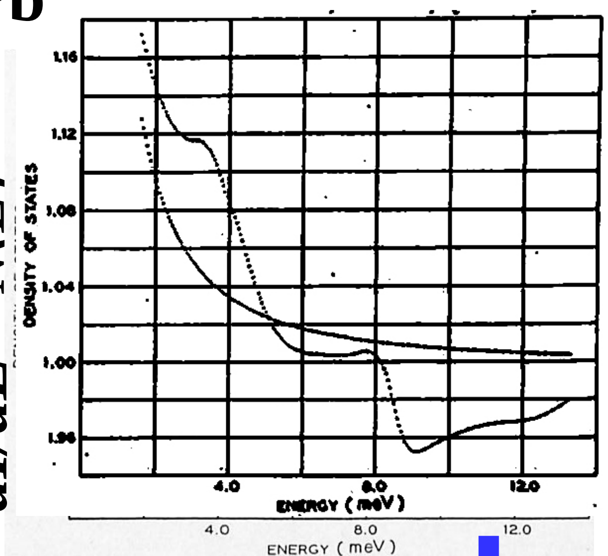
Introduction
How did the BCS el-ph mechanism become convincing?

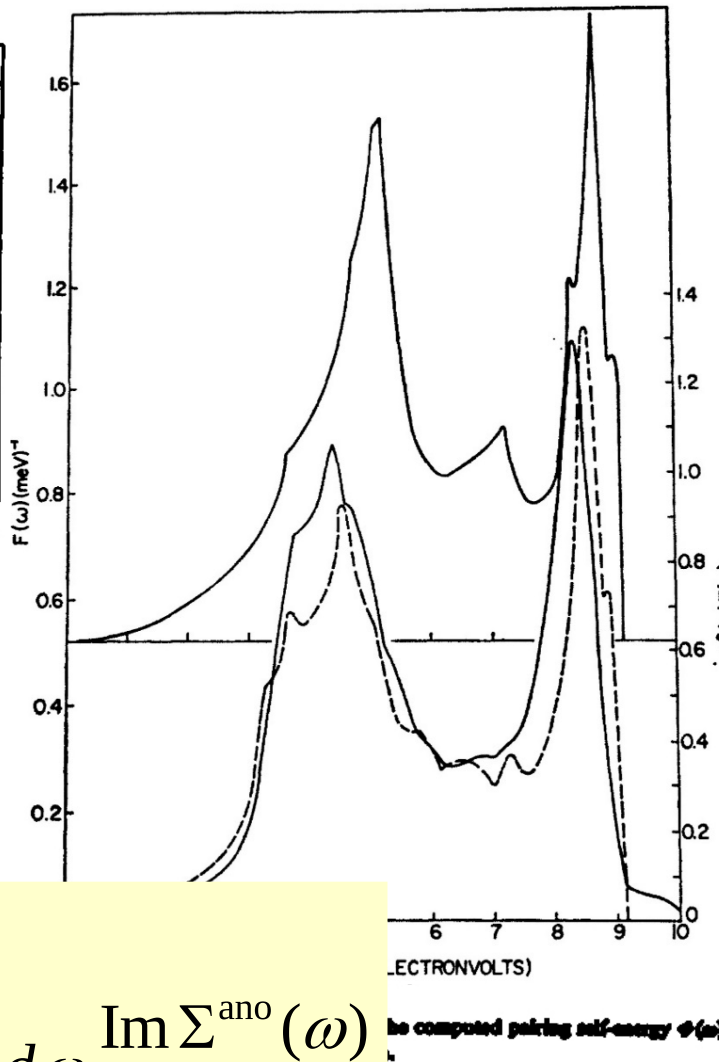
strong-coupling superconductivity

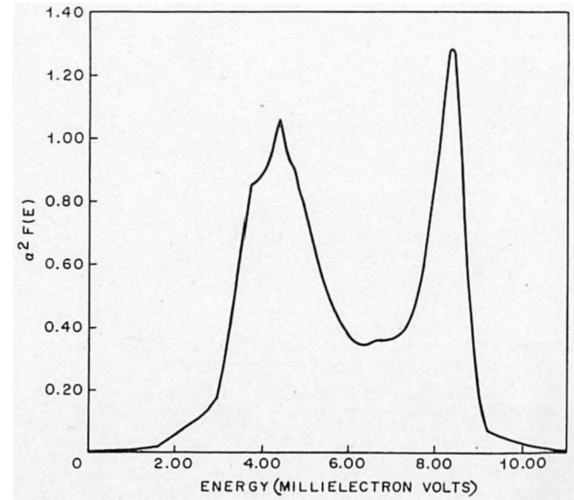
Pb

dI/dE N(E)



E





E

measured phonon density of states

neutron scattering data

$$N(\omega) = \int dk \,\mathrm{Im}\, G(k,\omega)$$

$$G(k,\omega) \Rightarrow \Sigma^{\mathrm{ano}}$$

$$\Delta\,(E) = z\Sigma^{\mathrm{ano}}$$

Kramers Kronig

$$\Delta \propto \mathrm{Re}\,\Sigma^{\mathrm{ano}}(\omega = 0) = \frac{2}{\pi}\int_0^\infty d\omega \frac{\mathrm{Im}\,\Sigma^{\mathrm{ano}}(\omega)}{\omega}$$

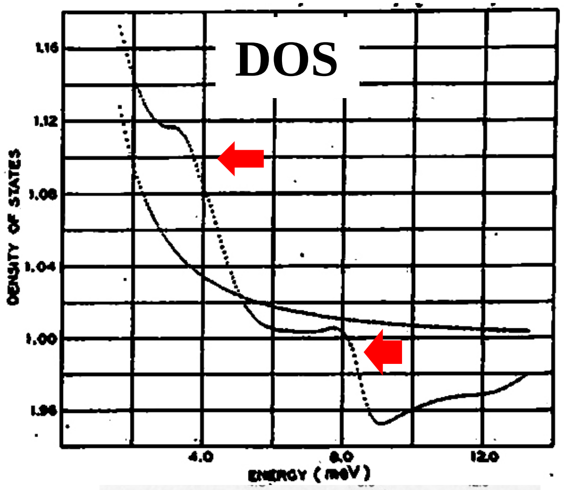
Bosonic (phonon) glue makes peaks

High resolution ARPES data for cuprates

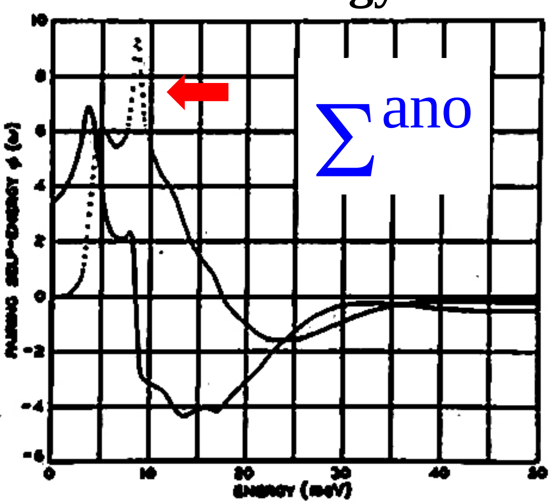
Kondo *et al.*
Nature 457, 296 (2009)
Nat. Phys. 5, 21 (2010)

Pb

McMillan-Rowell
1965, 1969



self-energy



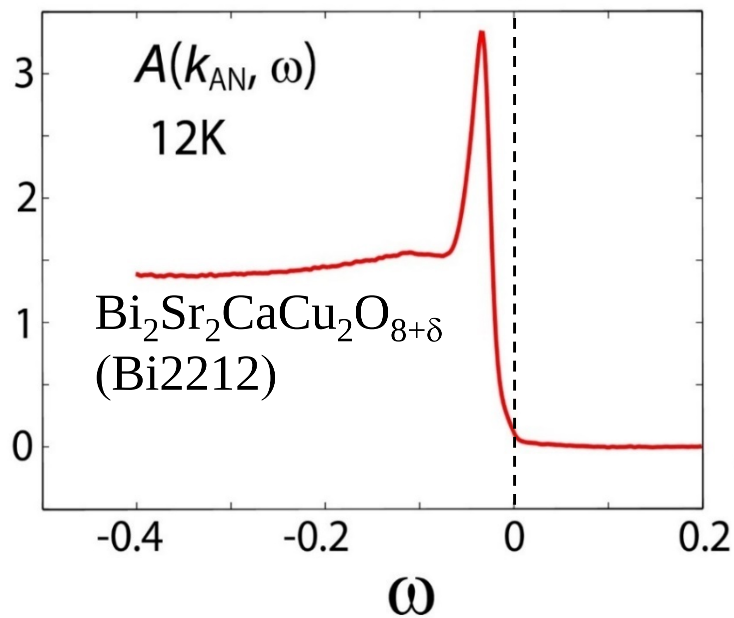
Real (——) and imaginary (···) parts of the computed pairing self-energy $\phi(\omega)$ for Pb vs. $\omega - \Delta_0$.

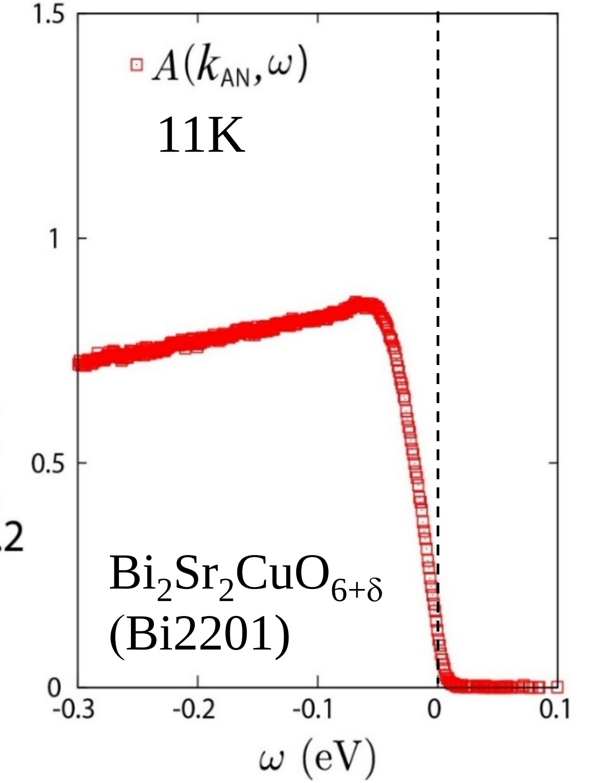
BCS superconductors

ARPES data

spectral func. $A(k,\omega)=\mathrm{Im}\,G(k,\omega)$

optimal doping T_c~90K underdoped T_c~29K





antinodal point
mild peak-dip-hump

Can we infer SC mechanism from $A(k,\omega)$?
Thirty-years-long puzzle & challenge

Green's function and self-energy in Nambu representation

$$G=\begin{pmatrix}\omega-\varepsilon_{\mathbf{k}}-\Sigma^{\text{nor}} & -\Sigma^{\text{ano}}\\ -\Sigma^{\text{ano}} & \omega+\varepsilon_{\mathbf{k}}+\Sigma^{\text{nor}}\end{pmatrix}^{-1}$$

Nambu representation

$$G(\mathbf{k},\omega)=\left[\omega+\mu-\varepsilon_{\mathbf{k}}-\left(\Sigma^{\text{nor}}(\mathbf{k},\omega)+W(\mathbf{k},\omega)\right)\right]^{-1}$$

$$W(\mathbf{k},\omega)=\frac{\Sigma^{\text{ano}}(\mathbf{k},\omega)^2}{\omega-\mu+\varepsilon_{\mathbf{k}}+\Sigma^{\text{nor}}(\mathbf{k},-\omega)^*}$$

$A(k,\omega)=\text{Im}\, G(k,\omega)$

Re Σ is given from Im Σ through K.K. transformation

$$A(k,\omega)\quad\Leftrightarrow\quad\mathcal{A}\left(\left\{\text{Im}\,\Sigma^{\text{nor}}(k,\omega),\text{Im}\,\Sigma^{\text{ano}}(k,\omega)\right\}\right)$$

$A(k,\omega)$ is functional of Im $\Sigma^{\text{nor}}(k,\omega)$ and Im $\Sigma^{\text{ano}}(k,\omega)$

Experimentally, only $A(k,\omega)$ is known

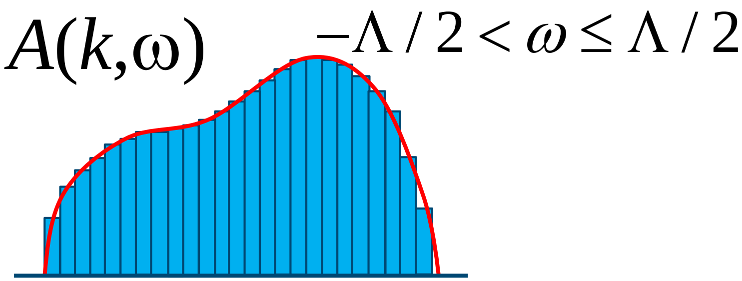
How to estimate (infer)

Im $\Sigma^{\text{nor}}(k,\omega)$ and Im $\Sigma^{\text{ano}}(k,\omega)$ separately?

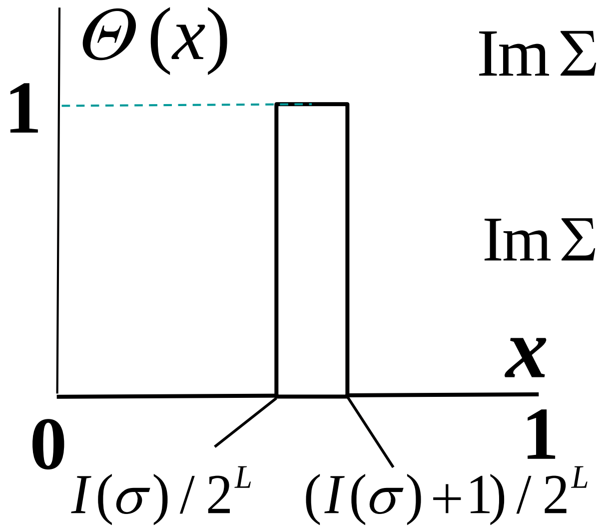
inverse problem

⇒ machine learning

Boltzmann Machine Representation



dividing up into grids with block function fit



$$\mathrm{Im}\,\Sigma^{\mathrm{nor}}(\boldsymbol{k},\omega) = -\sum_{\boldsymbol{S}} \mathcal{C}(\boldsymbol{S})\Theta_{\sigma}^{L}\left(\frac{\omega+\Lambda/2}{\Lambda}\right)$$

$$\mathrm{Im}\,\Sigma^{\mathrm{ano}}(\boldsymbol{k},\omega) = -\sum_{\boldsymbol{S}} \mathcal{D}(\boldsymbol{S})\left[\Theta_{\sigma}^{L}\left(\frac{\omega+\Lambda/2}{\Lambda}\right) - \Theta_{\sigma}^{L}\left(\frac{\Lambda/2-\omega}{\Lambda}\right)\right]$$

+ real parts from K.K. trans.
physical constraints from symmetry

$\mathcal{C}, \mathcal{D}$ ⟷ $A(k,\omega)$

Boltzmann machine

minimize $\chi^2 = \dfrac{1}{2N_d}\sum_{j}\left[A^{\mathrm{exp}}(\omega_j) - A^{\mathrm{BM}}(\omega_j)\right]^2$

Normal and anomalous self-energies; peaks and cancellation

optimal Bi2212

underdoped Bi2201

prominent peaks in Σ^{nor} and Σ^{ano} at $\pm$45 meV(OP)
$\pm$55 meV (UD)

secondary weak peaks at $\pm$130meV (OP), $\pm$160 meV (UD)

Cancellation of Σ^{nor} and *W* in $\Sigma^{tot} = \Sigma^{nor} + W$

The reason why overlooked in experiments for decades

Agreement with dark fermion theory

existence of *dark fermion*

Sakai *et al.* PRL 116, 057003 (2016)

Peaks are the origin of SC

$$\mathrm{Re}\,\Sigma^{\mathrm{ano}}(\mathbf{k},\omega=0)\propto \mathrm{Re}\Delta(\mathbf{k},\omega=0)$$

; SC gap

truncated K.K. transform

$$I_{\Sigma}(\Omega)\equiv\frac{2}{\pi}\frac{\left|\int_0^{\Omega}d\omega\frac{\mathrm{Im}\,\Sigma^{\mathrm{ano}}(\omega)}{\omega}\right|}{\mathrm{Re}\,\Sigma^{\mathrm{ano}}(\omega=0)}$$

90% of Re $\Sigma^{\mathrm{ano}}(\omega=0)$ is from the first negative peaks in Im $\Sigma^{\mathrm{ano}}(\omega)$

Cutting the first peaks leads to the disappearance of SC and to a good normal metal

QP width ~ exp. resolution 10 meV

Why ML teaches us cancellation? Black box?
We are led to physical intuition

large SC gap around ω=0 in $A(k,\omega)$ → prominent peak structure in Im Σ^{ano} at $|\omega|$ > gap

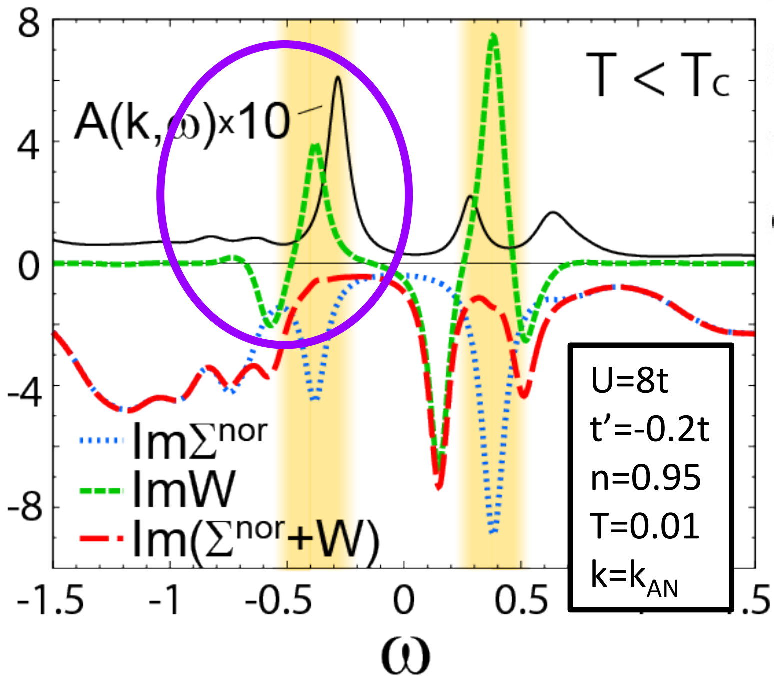
No prominent structure in $A(k,\omega)$ at $|\omega|$> gap → Cancellation of normal and anomalous constribution in $A(k,\omega)$

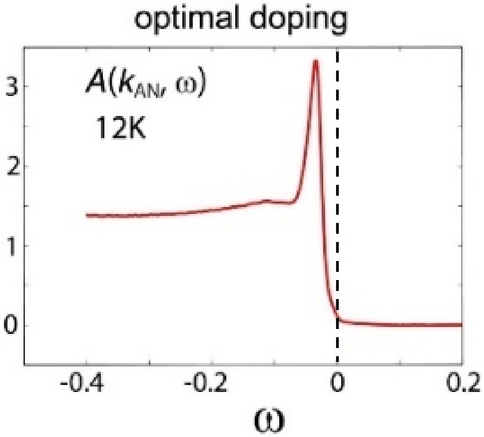
quantum coherence only at $|\omega|$< ω* → Peak must be in the region $|\omega|$< ω*

Pole cancellation between Σ^{nor} and Σ^{ano} in CDMFT of Hubbard

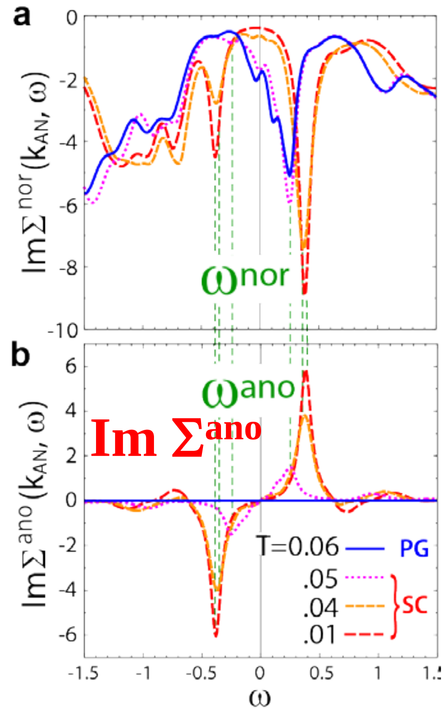
Sakai *et al.*
Phys. Rev. Lett.
116 (2016) 057003

A(**k**,ω) similar to exp.





Σ^{nor} cancels with W in $\Sigma^{tot} = \Sigma^{nor} + W$!



Perfect agreement with the machine learning result obtained purely from the experimental data

sharp peaks in Σ^{nor} , Σ^{ano} , W !

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How is the cancellation understood?
As far as we know, the only way is the dark fermion (two-component) theory.
What is TCFM (two-component fermion model — dark fermion model) ?

$$H = \sum_k [\varepsilon_c(k) c_{k\sigma}^\dagger c_{k\sigma} + \Lambda_k (c_{k\sigma}^\dagger d_{k\sigma} + \mathrm{H.c.}) + \varepsilon_d(k) d_{k\sigma}^\dagger d_{k\sigma}]$$

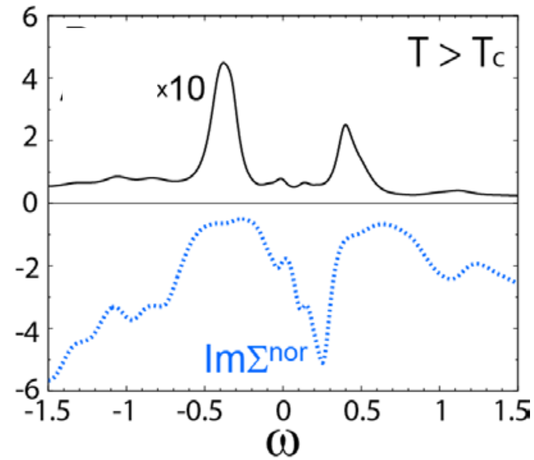
$$G = (\omega - H)^{-1} = \begin{pmatrix} \omega - \varepsilon_c & -\Lambda \\ -\Lambda & \omega - \varepsilon_d \end{pmatrix}^{-1}$$

CDMFT

Sakai *et al.*

$$G_c = \frac{1}{(\omega - \varepsilon_c(k)) - \Sigma^{\mathrm{nor}}(k,\omega)}$$

$$\Sigma_c^{\mathrm{nor}}(k,\omega) = \frac{\Lambda_k^{\ 2}}{\omega - \varepsilon_d}$$



hybridization gap = pseudogap

***cf*. RVB**
Yang, Rice, Zhang (2006)
Konig, Rice, Tsvelik (2006)
for two-leg laddres

How to understand the cancellation; Dark fermion theory

Sakai *et al.* Phys. Rev. Lett. 116 (2016) 057003

Two-component fermion model at $T<T_c$

***d*; dark fermion**

$$H = \sum_k [\varepsilon_c(k) c_{k\sigma}{}^{\dagger} c_{k\sigma} + \Lambda_k (c_{k\sigma}{}^{\dagger} d_{k\sigma} + \text{H.c.}) + \varepsilon_d(k) d_{k\sigma}{}^{\dagger} d_{k\sigma}$$

$$\boxed{+(\Delta_c c_{k\sigma}{}^{\dagger} c_{k\sigma}{}^{\dagger} + \Delta_d d_{k\sigma}{}^{\dagger} d_{k\sigma}{}^{\dagger} + \text{H.c.})]}$$

Nambu representation 4x4 matrix

$$\Sigma_c^{\text{nor}}(k,\omega) = G_d \Lambda_k{}^2 = \frac{\Lambda_k{}^2}{(\omega - \varepsilon_d) - \dfrac{\Delta_d{}^2}{\omega + \varepsilon_d}}$$

$$G(\mathbf{k},\omega) = \left[\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma_c^{\text{nor}}(\mathbf{k},\omega) - W(\mathbf{k},\omega)\right]^{-1}$$

$$W(\mathbf{k},\omega) = \frac{\Sigma_c^{\text{ano}}(\mathbf{k},\omega)^2}{\omega - \mu + \varepsilon_{\mathbf{k}} + \Sigma_c^{\text{nor}}(\mathbf{k},-\omega)^*}$$

$$\Sigma_c^{\text{ano}}(k,\omega) = \Delta_c + G_d \Lambda_k{}^2 = \Delta_c + \frac{\Lambda_k{}^2 \Delta_d (\omega + \varepsilon_d)}{(\omega - \varepsilon_d) - \dfrac{\Delta_d{}^2}{(\omega + \varepsilon_d)}}$$

For $T > T_c$, pole at $\omega = \varepsilon_d$ generates pseudogap

The residue of W has the same amplitude with that of Σ^{ano} but with the opposite sign
$\Rightarrow$ The poles cancel in $\Sigma^{\text{nor}} + W$ smoking gun

Bosonic excitations such as spin fluctuations would not cause the cancellation.

Emergent hybridization as the universal origin of gap generation

Hybridization gap of TCFM is the universal origin of gap formation

$$H = \sum_{k\sigma\sigma'} [\varepsilon(k) c_{k\sigma}{}^{\dagger} c_{k\sigma} + \varepsilon'(k) d_{k\sigma'}{}^{\dagger} d_{k\sigma'} + \Lambda(k)(c_{k\sigma}{}^{\dagger} d_{k\sigma'} + h.c)]$$

(1) fermion symmetry breaking **ex. AF, CO** $d_k = c_{k+Q}$

$$c^{\dagger} c d^{\dagger} d \Rightarrow \langle d^{\dagger} c \rangle c^{\dagger} d$$

CO, AF, BCS-SC, QCD mass (Nambu-Jona-Lasinio)

(2) bose condensation

$$c^{\dagger} d \left(b + b^{\dagger}\right) \Rightarrow c^{\dagger} d \left(\langle b \rangle + \langle b^{\dagger} \rangle\right)$$

weak interaction (W-, Z-boson condensation),
QCD gluon condensation

Nambu-Goldstone
⬍
Higgs mechanism

They require always spontaneous symmetry breaking.
How about the pseudogap and Mott gap
where apparent SSB is absent?

⇒ML and cDMFT tell us electron fractionalization into
***c* and dark fermion *d* without SSB**

How about Mott gap?

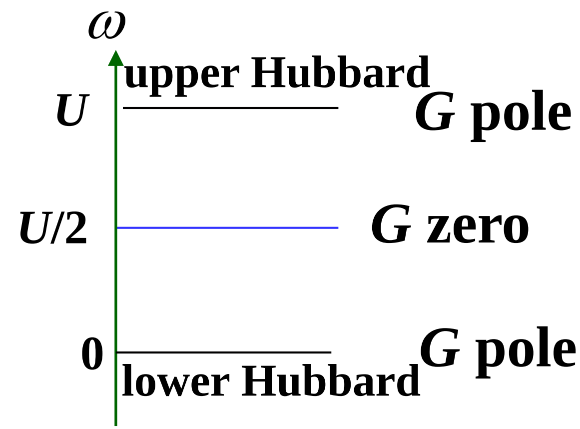
Zhu, Zhu PRB 87, 085120 (2013)
Sakai *et al.* PRB 94, 115130 (2016)
Imada, Suzuki arXiv:1804.05301

$$H = Uc_{\uparrow}^{\dagger}c_{\uparrow}c_{\downarrow}^{\dagger}c_{\downarrow}$$

***t*→0 atomic limit; exact**

$$G = \frac{1}{2}\frac{1}{\omega} + \frac{1}{2}\frac{1}{\omega - U} \Leftrightarrow G = \frac{1}{\omega - \Sigma}, \quad \Sigma = \frac{\frac{1}{4}U^2}{\omega - \frac{U}{2}}$$

lower Hubbard **upper Hubbard**



$$\tilde{d}_{\sigma} \equiv c_{\sigma}(1 - 2n_{-\sigma})$$
$$\tilde{c}_{\sigma} \equiv c_{\sigma}$$

$$H_{\mathrm{TCFM}} = \sum_{\sigma}[\varepsilon_{\tilde{c}}\tilde{c}_{\sigma}^{\dagger}\tilde{c}_{\sigma} + \varepsilon_{\tilde{d}}\tilde{d}_{\sigma}^{\dagger}\tilde{d}_{\sigma} + \Lambda(\tilde{c}_{\sigma}^{\dagger}\tilde{d}_{\sigma} + h.c)]$$

$$\varepsilon_{\tilde{c}} = \varepsilon_{\tilde{d}} = -\Lambda = \frac{U}{2}$$

***no* symmetry breaking**

$\tilde{d}_{\sigma}$; Mott gap fermion

exact fractionalization

mapping between single-component interacting system (Hubbard)
and two-component noninteracting system (TCFM)

Electron fractionalization in Mott insulator
Emergent Mott gap fermion

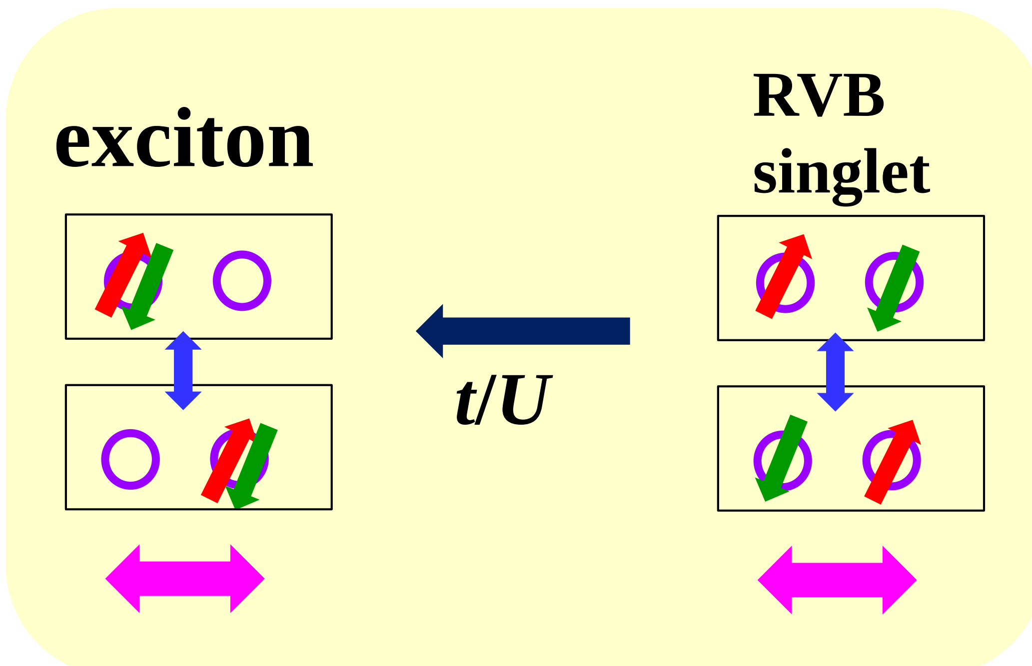
When t/U is nonzero,

Mottgap fermion $\tilde{d}_\sigma = c_\sigma(1-n_{-\sigma}) - c_\sigma n_{-\sigma}$ is interpreted as a fermion extracted from an antiresonant state of UHB and LHB, namely doublon-holon bound state (exciton) in the insulator

$c^\dagger_\sigma n_{-\sigma}$ **upper Hubbard creation (doublon generation)**

$c^\dagger_\sigma (1-n_{-\sigma})$ **lower Hubbard creation (singlon generation)**

"cradle" of Mott gap fermion =

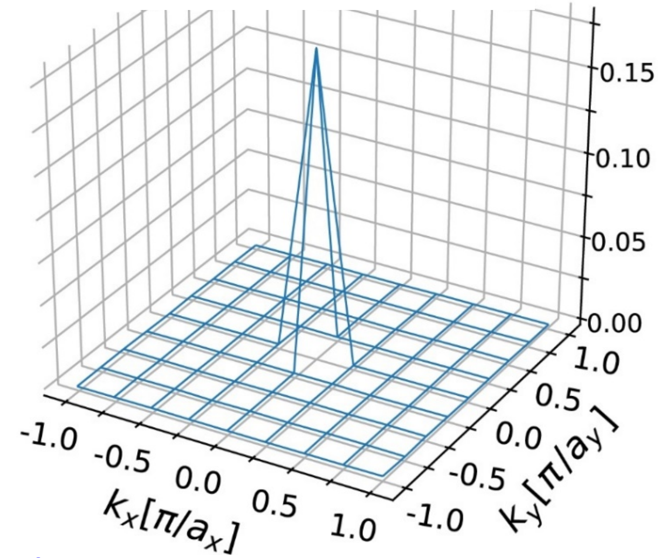


singlet-exciton resonant state

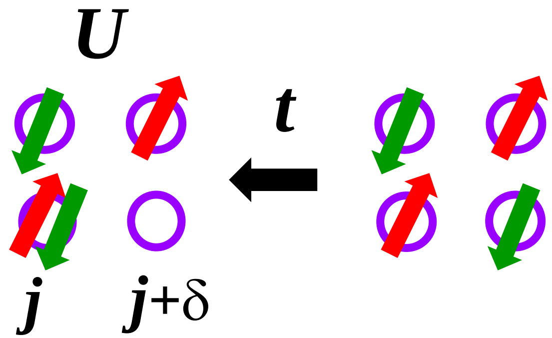
Imada, Suzuki
arXiv:1804.05301

Bose-Einstein condensation of excitons

$$\langle b(k)_\sigma{}^\dagger \rangle = \langle b(k)_\sigma \rangle$$



case of nonzero *t*



exciton dynamics

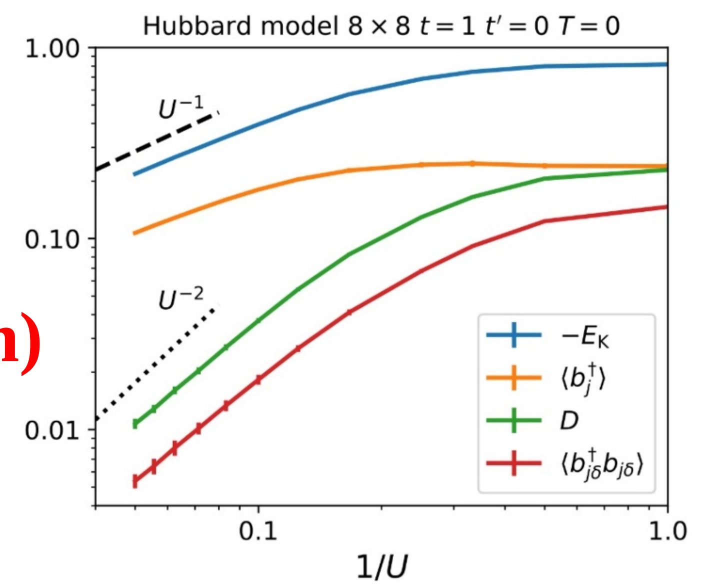
exciton creation

$$b_{j,\delta}{}^\dagger = \sum_\sigma g_{b\delta} c_{j,\sigma}{}^\dagger c_{j+\delta,\sigma} n_{j,-\sigma} (1 - n_{j+\delta,-\sigma})$$

$$H_b = \zeta \sum_{j,\delta} (b_{j,\delta}{}^\dagger + b_{j,\delta}) + \sum_{k,\delta,\delta'} \varepsilon_{b\delta,\delta'}(k) b^\dagger{}_{k,\delta} b_{k,\delta'} + \sum_{i,j,\delta,\delta'} V_b(i,j,\delta,\delta') n_{bi,\delta} n_{bj,\delta'}$$

ζ : symmetry breaking field, $\zeta \ll \varepsilon_b$

vacuum fluctuation



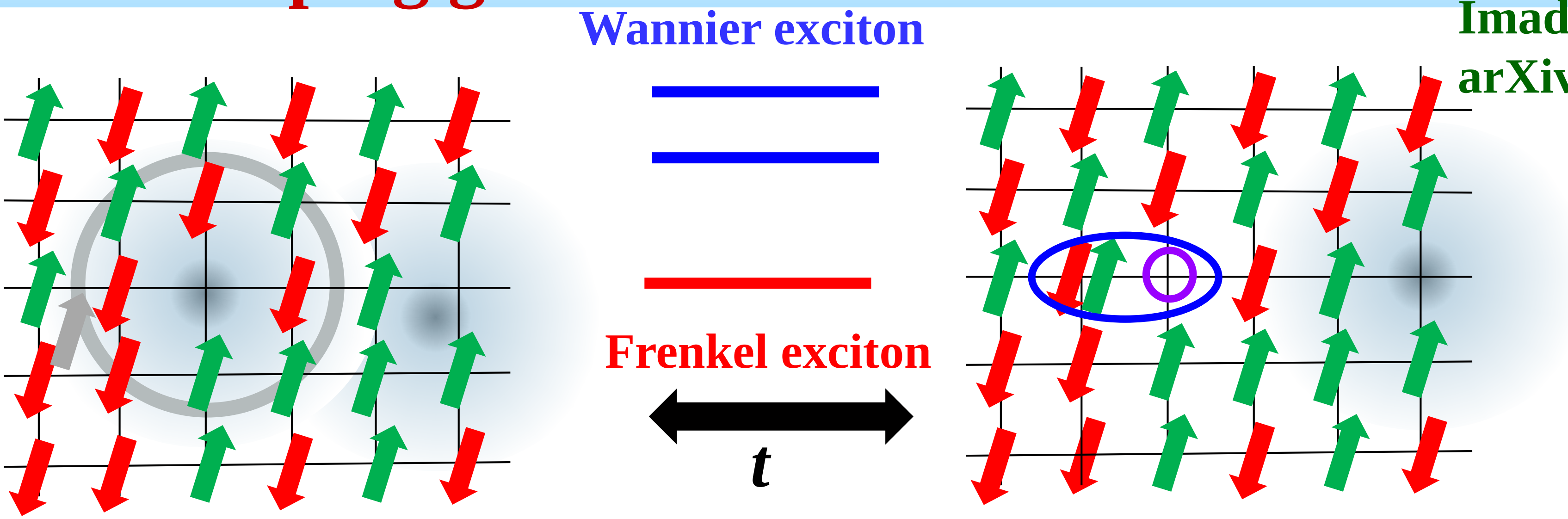
$$b_{ij,\sigma}{}^\dagger \Rightarrow \langle b_{ij,\sigma}{}^\dagger \rangle \neq 0$$

Frenkel-type exciton

BEC (trivial condensation)

Carrier doping generates several excitonic bound states

Imada, Suzuki
arXiv:1804.05301

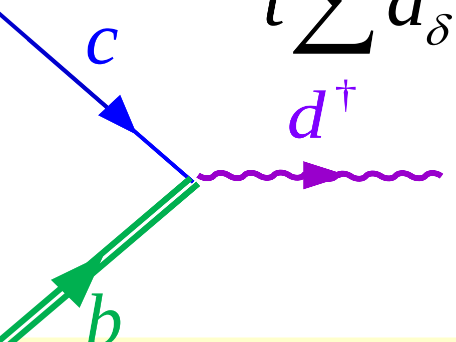


||

dark fermion +hole

Mott gap fermion

$$t\sum a_\delta d^\dagger{}_{j,\delta,\sigma} c_{k\sigma} b_{j,\delta} + \mathrm{H.c.} \Longrightarrow \boxed{t\sum_\delta d^\dagger{}_{j,\delta,\sigma} c_{k\sigma} \left\langle b_{j,\delta}\right\rangle + \mathrm{H.c.}}$$



$$\left\langle b_{j,\delta}\right\rangle \sim t/U$$

hybridization gap ~ t^2/U

bistability/fractionalization between dark fermion and electron
⇒ charge inhomogeneity & phase separation

Summary

1. ***ab intio* results support dominant uniform dSC ⇔ Hubbard**

2. **Boltzmann machine and cDMFT; completely different approaches give consistent self-energy structure;**
   - **★ anomalous peaks, dominating the SC**
   - **★ cancellation of Σ^{nor} and Σ^{ano} contributions**

Summary

3. **supports dark fermion and 2-component hybridization mechanism resulting in**

★ **peak cancellation on the self-energies &**

★ **gap generation without spontaneous symmetry breaking inTCFM**

$$H=\sum_k[\varepsilon_c(k)c_{k\sigma}{}^{\dagger}c_{k\sigma}+\Lambda_k(c_{k\sigma}{}^{\dagger}d_{k\sigma}+\mathrm{H.c.})+\varepsilon_d(k)d_{k\sigma}{}^{\dagger}d_{k\sigma}$$
$$+(\Delta_c c_{k\sigma}{}^{\dagger}c_{k\sigma}{}^{\dagger}+\Delta_d d_{k\sigma}{}^{\dagger}d_{k\sigma}{}^{\dagger}+\ \mathrm{H.c.})]$$

4. **origin of cuprate pseudogap and superconductivity**

★ **Interpreted from electron fractionalization in Mott insulator, giving associated Frenkel excitons and Mott gap fermions**

★**Possible further fractionalization in the doped Mott insulator whose hot bed is Wannier excitons**

Dark fermions arising from Wannier excitons boost up SC and generates pseudogap

⇒ experimental detection