Beyond DMFT: Spin fluctuations, Pseudogaps and Superconductivity

Karsten Held (TU Wien)

Jülich, Oct. 7th 2022

- Motivation
- Synopsis: dynamical vertex approximation (DΓA)
- 2D Hubbard model, cuprates and nickelates
- Spin fluctuations
- Pseudogap
- Superconductivity

Rev. Mod. Phys. 90, 025003 (2018)

Please ask questions

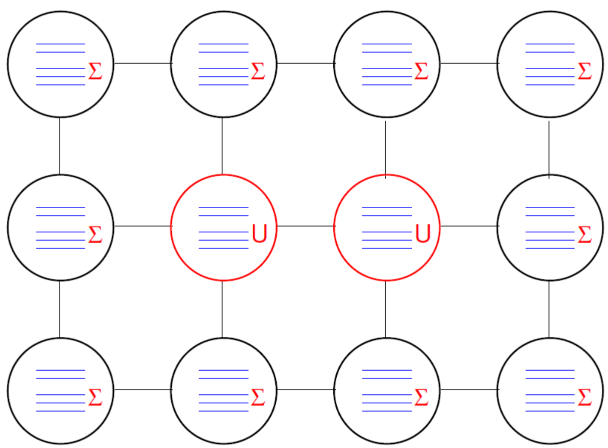
Motivation I: 2 routes beyond DMFT:

Correlations beyond DMFT:

d-, p-wave superconductivity, pseudogaps, (para-)magnons, quantum criticality

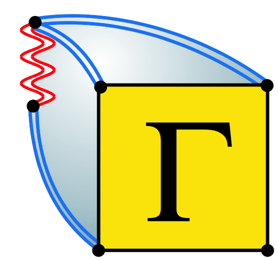
beyond DMFT

cluster extensions



Hettler et al.'98, Lichtenstein, Katsnelson'00
Kotliar et al.'01, Potthoff et al.'03, Maier et al.'05

diagrammatic extensions

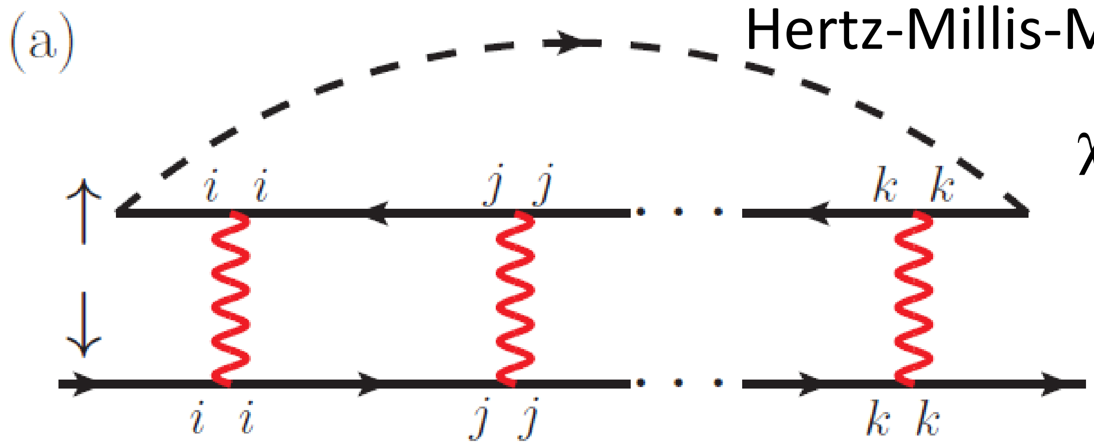


DΓA: Toschi, Katanin, KH'07
DF: Rubtsov et al.'08
1PI, TRILEX ...

RMP'18

Motivation II

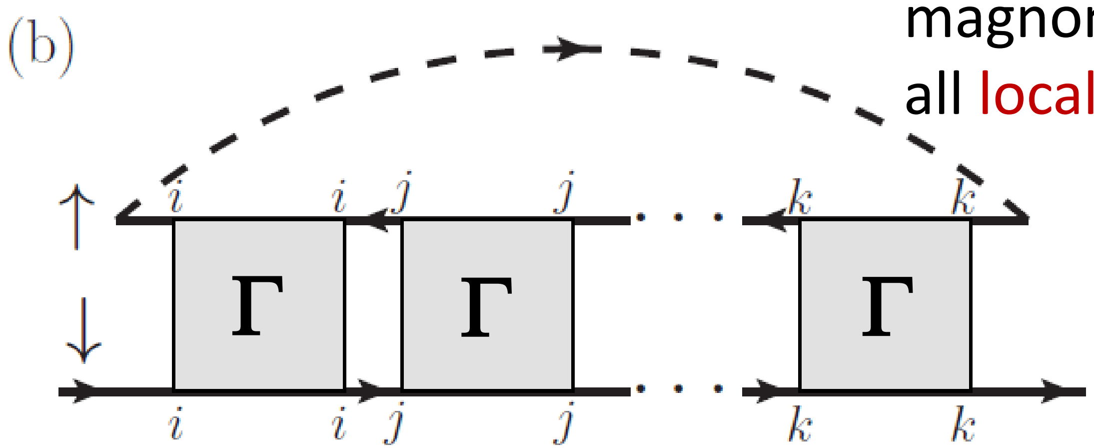
Take spin fluctuations



magnon self-energy Edwards-Hertz

Hertz-Millis-Moriya theory for QCP

$$\chi_{q\omega} = \chi^0_{q\omega}/(1-U\chi^0_{q\omega})$$



magnons but now including all local DMFT physics

$$\chi_{q\omega} = \chi^0_{q\omega}(1-\Gamma_q\chi^0_{q\omega})^{-1}$$

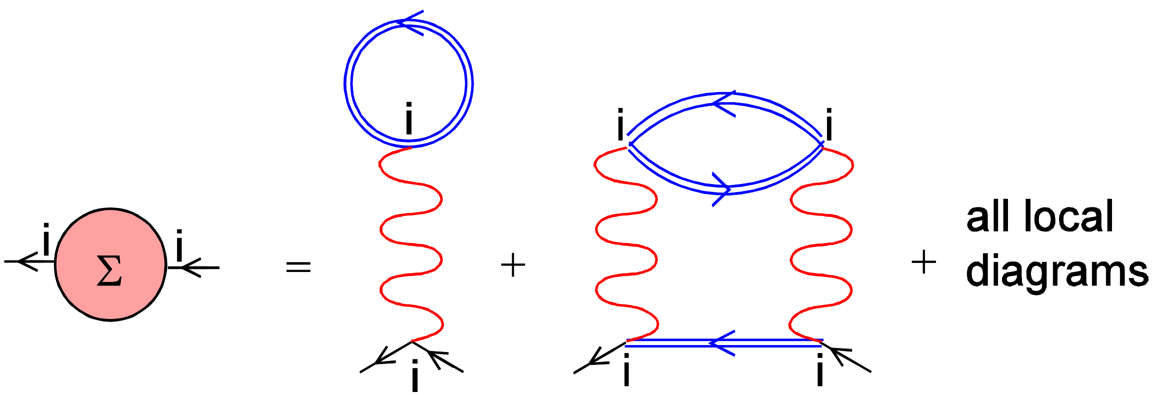
matrices in ν,ν'

Dynamical vertex approximation (DΓA)

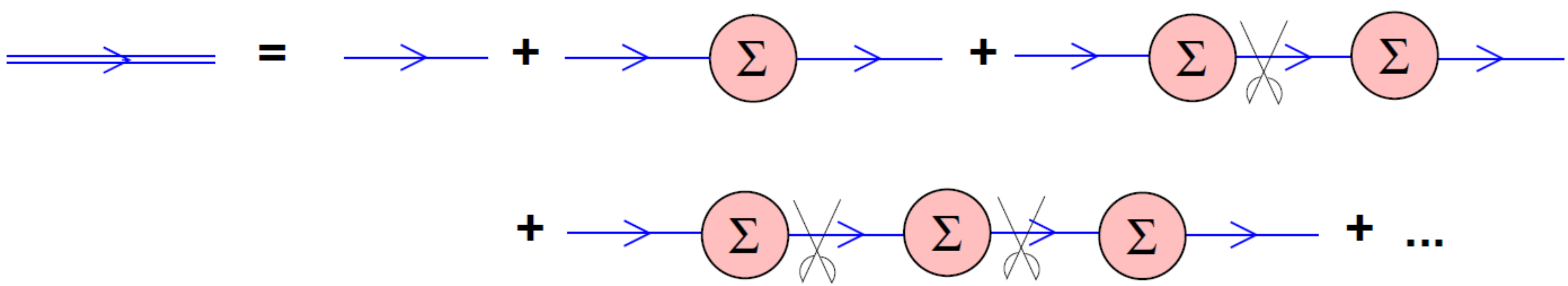
Resummation of Feynman diagrams in terms of locality

n-particle fully irreducible vertex *approximated as local*

n=1: DMFT - **local 1-particle fully irreducible vertex Σ**



Σ: one-particle irreducible one-particle vertex



Dynamical vertex approximation (DΓA)

Resummation of Feynman diagrams in terms of locality

n-particle fully irreducible vertex *approximated as local*

n=1: DMFT - local 1-particle fully irreducible vertex Σ

n=2: DΓA - local 2-particle fully irreducible vertex Λ

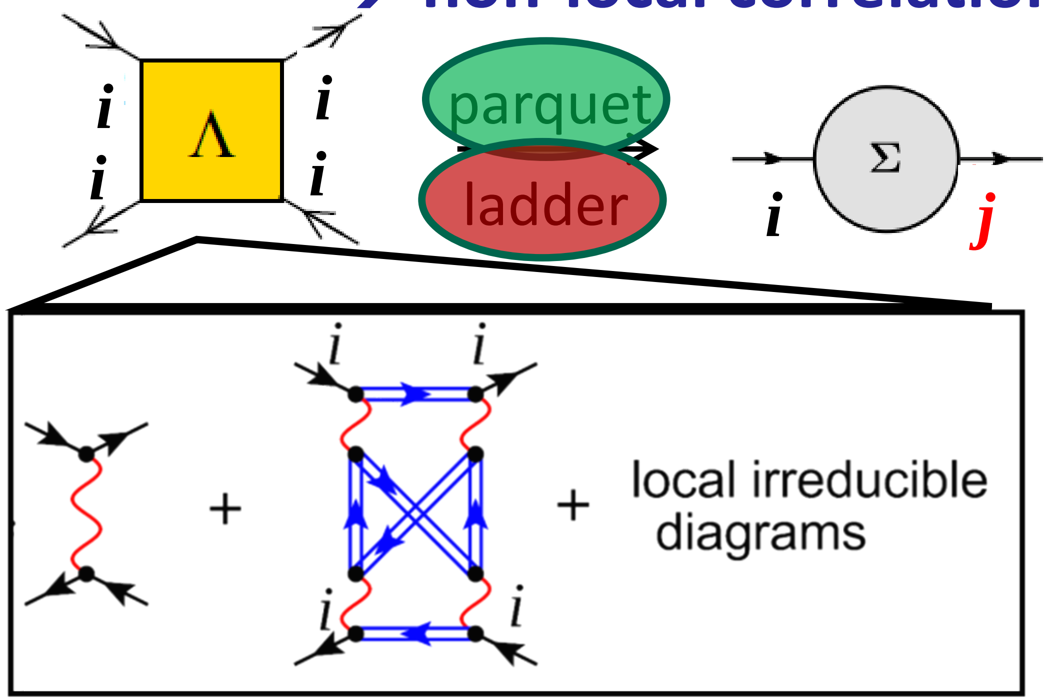
→ non-local correlations

n=3: error estimate

Ribic et al. PRB'17, 18

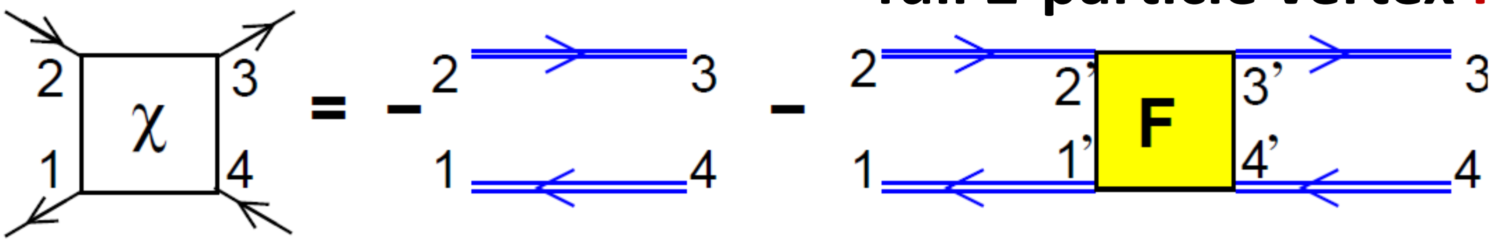
...

n→∞: exact

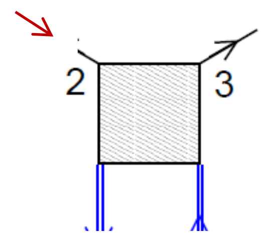


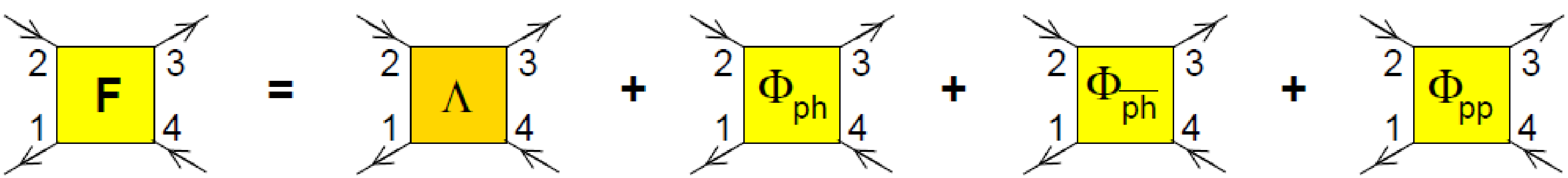
Two-particle irreducibility

full 2-particle vertex **F**



3 ways (channels) to cut two lines

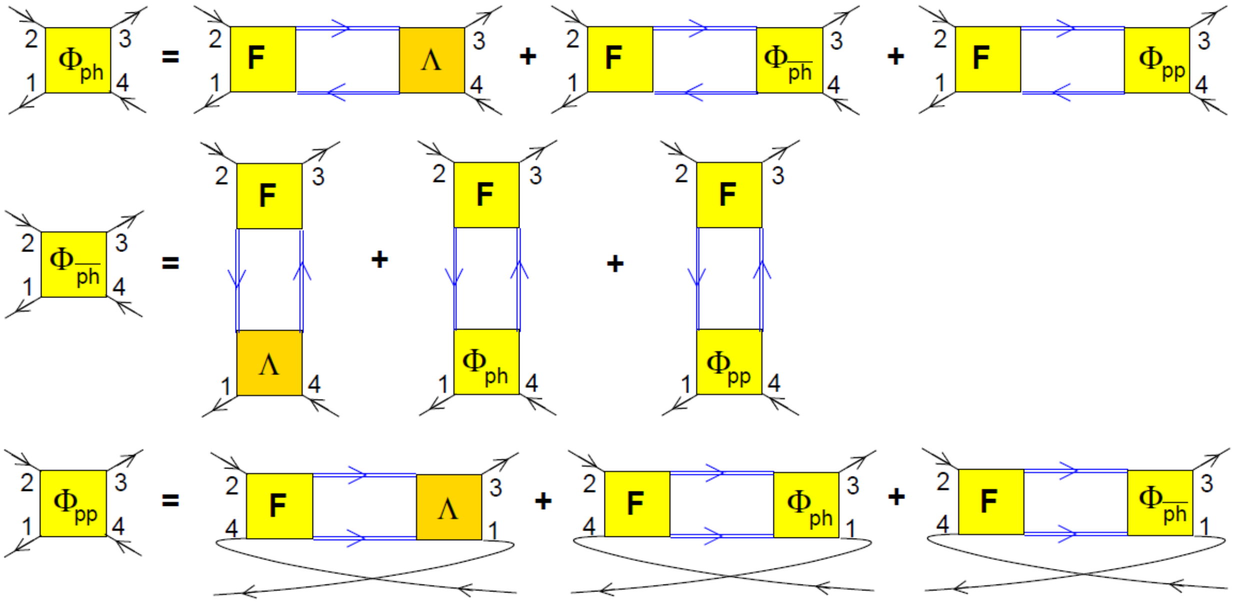




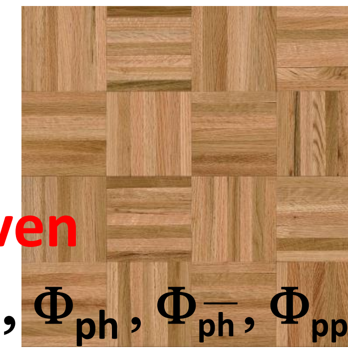
full vertex Λ Φ_{ph} $\Phi_{\overline{ph}}$ Φ_{pp}

parquet equation

Parquet equations

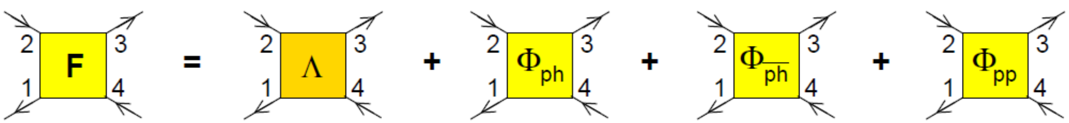


3 Bethe-Salpeter eq.



Λ given

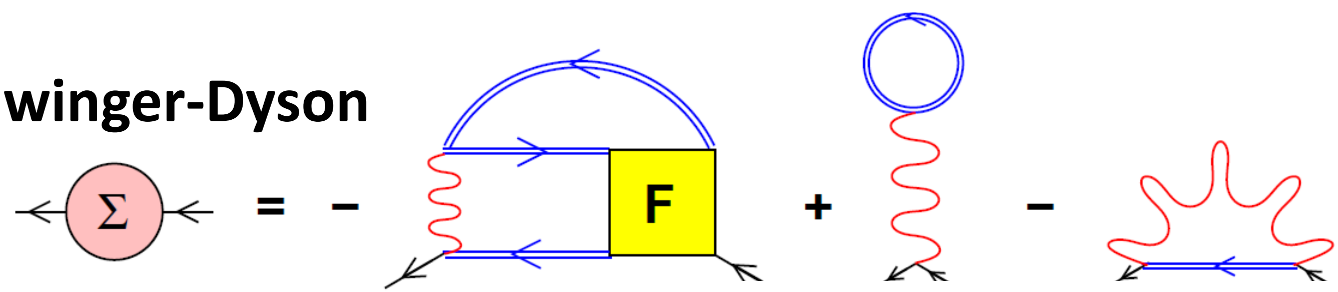
$\rightarrow$ F, Φ_{ph}, $\Phi_{\overline{ph}}$, Φ_{pp}, Σ, G



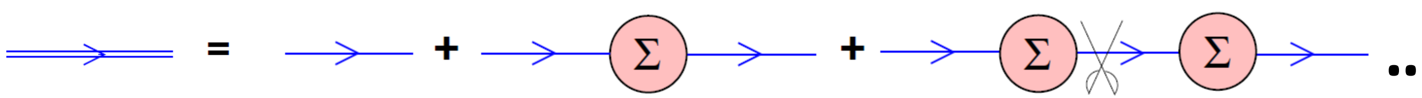
Λ = U (parquet approx.)

$\Lambda = \Lambda_{loc}$ (DΓA)

Schwinger-Dyson



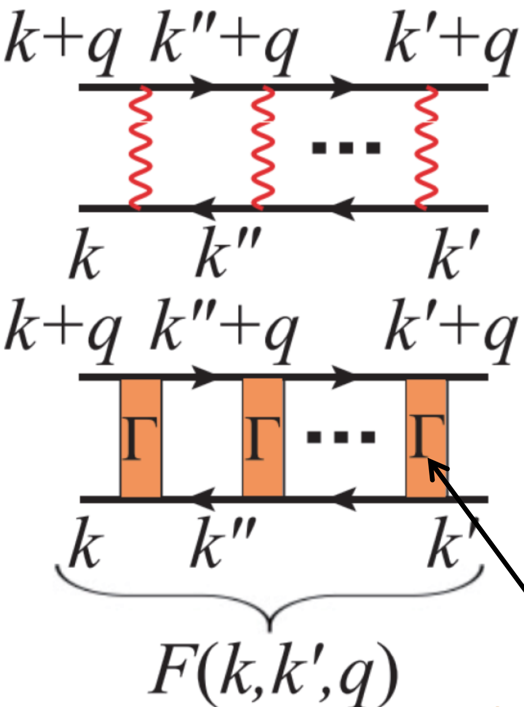
Dyson equation

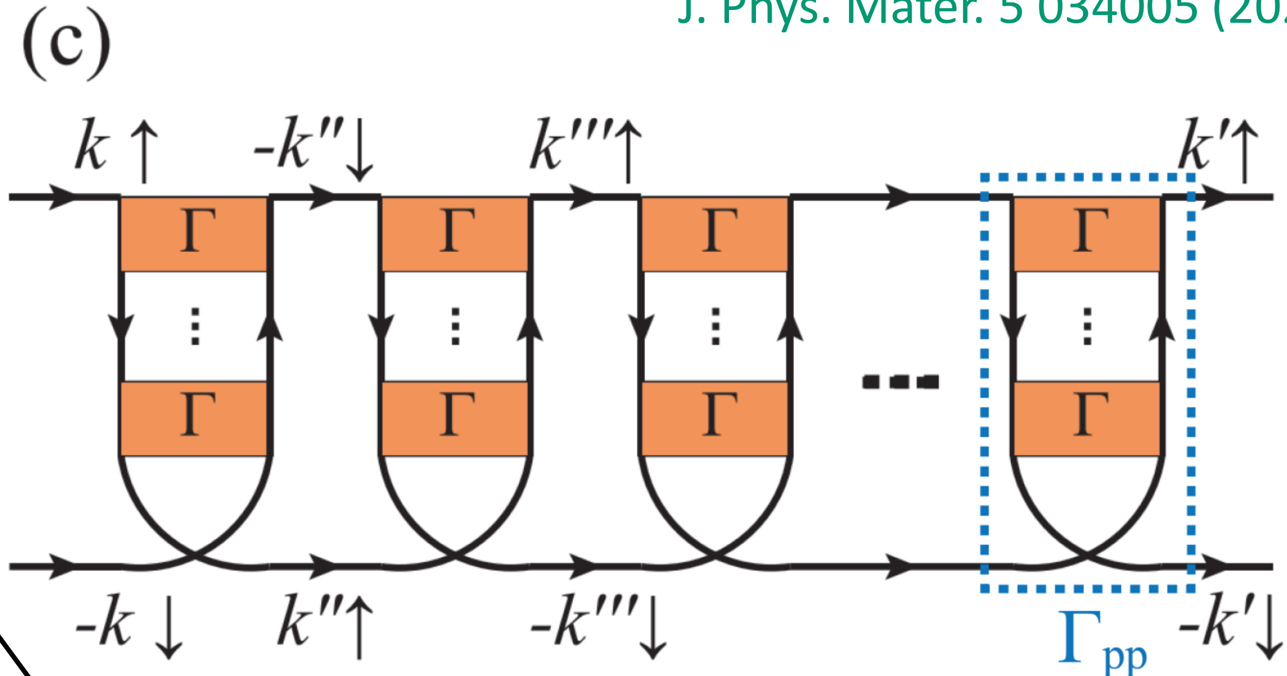


Ladder DΓA

Calculations using ladder DΓA (with λ-correction)

details: Kitatani ... KH arXiv:2203.12844,
J. Phys. Mater. 5 034005 (2022)

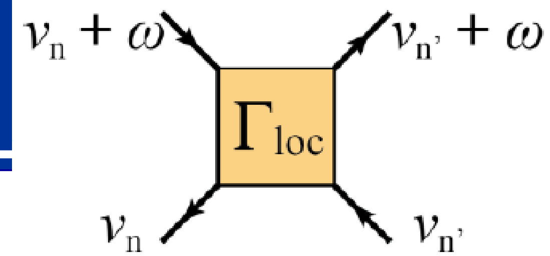




local from AIM, fully frequency dependent

Unbiased: spin and charge fluctuations, quantum critical fluct.
excellent agreement with diag. MC ... Schäfer et al. PRX'21

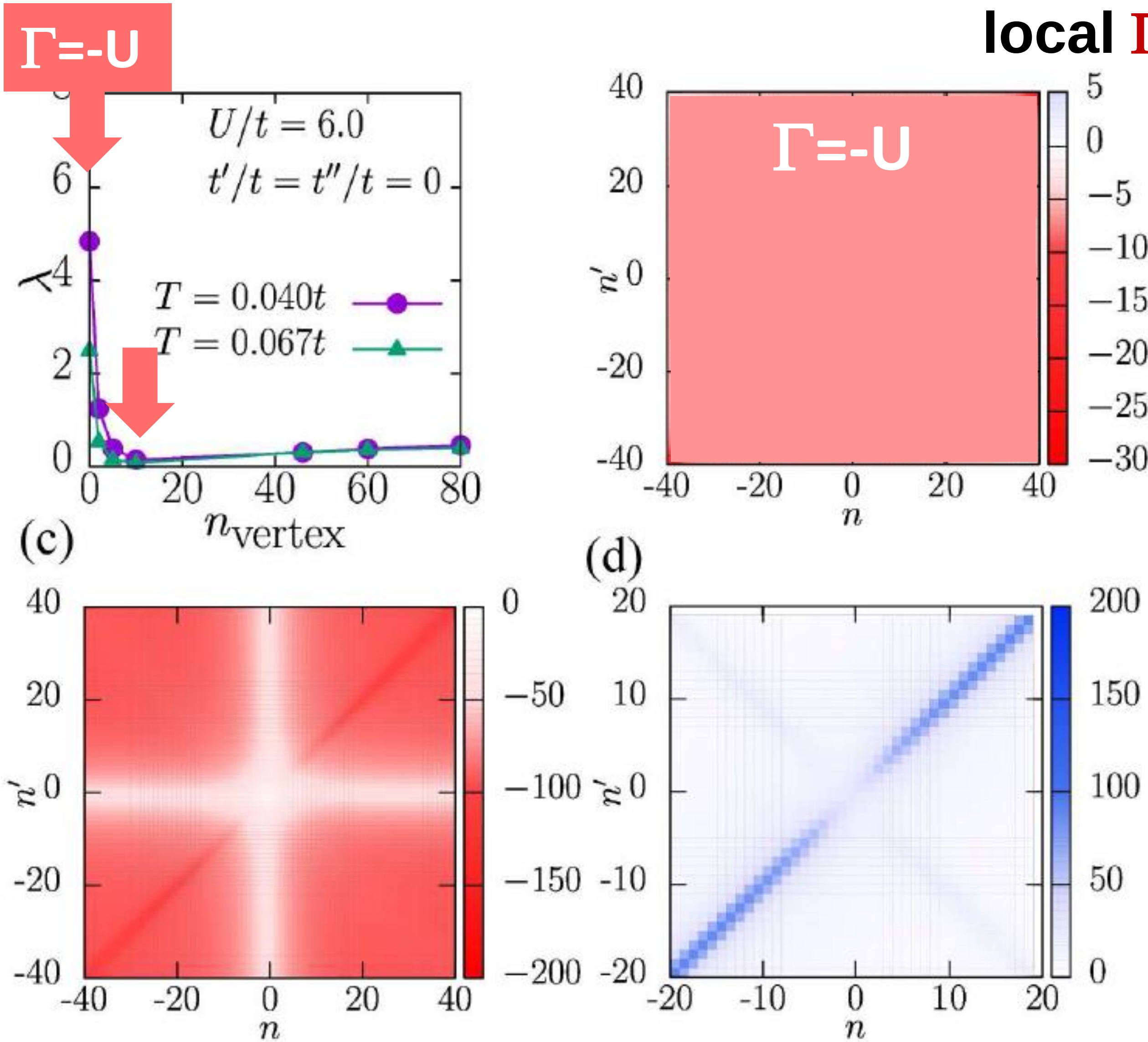
Importance of vertex dynamics



local $\Gamma_m(\nu_n, \nu_{n'}, \omega)$

U=6t

ω=0



nonlocal **F**

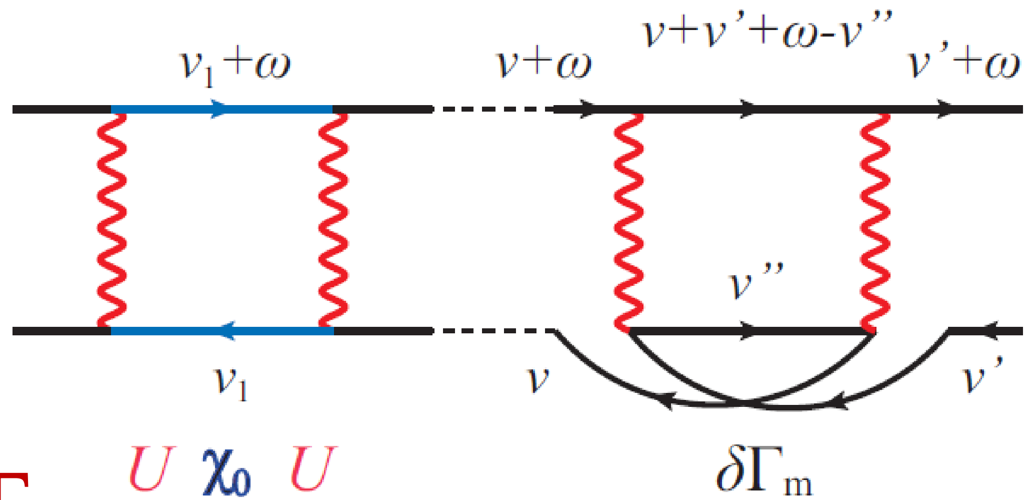
pairing interaction Γ_{pp}

Importance of vertex dynamics

spin fluctuations

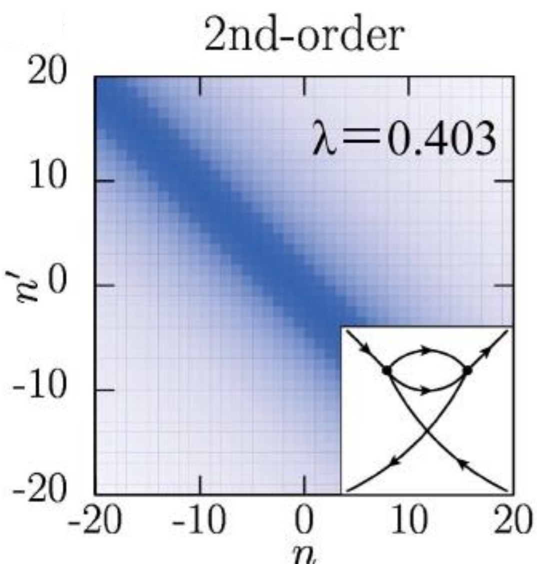
$\chi = \chi_0 + \chi_0 U \chi_0 + \chi_0 U \chi_0 U \chi_0 + \ldots$

$= \chi_0/(1 - \chi_0 U)$



suppressed by pp channel $\delta\Gamma_m$

2nd order



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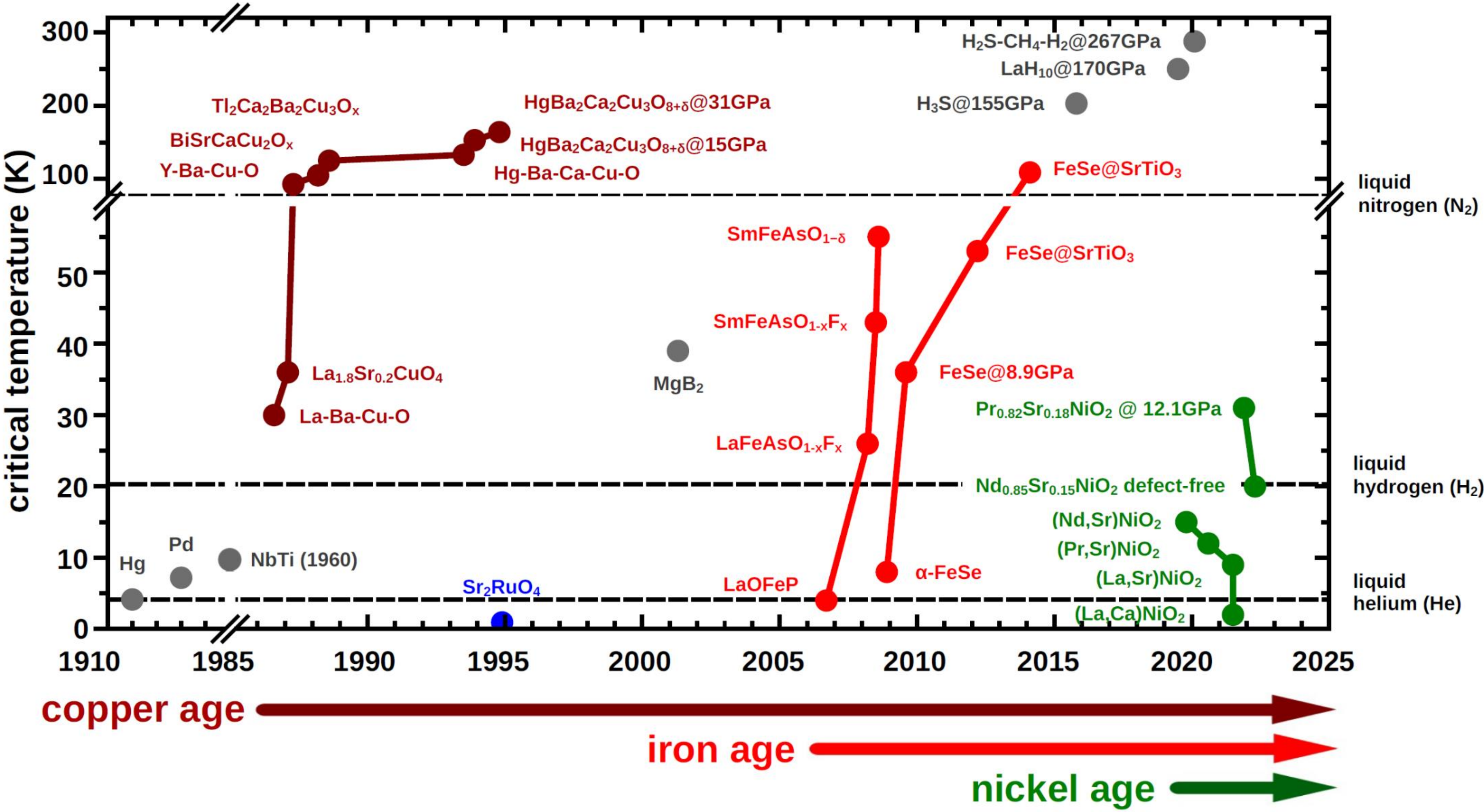
New age of superconductivity: nickel age

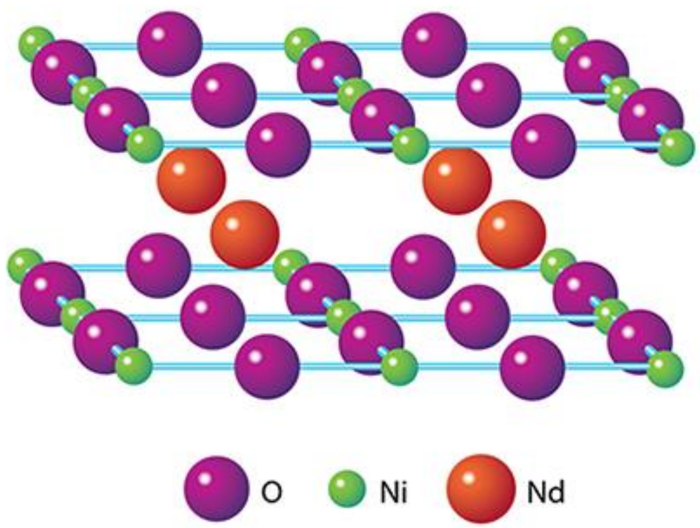


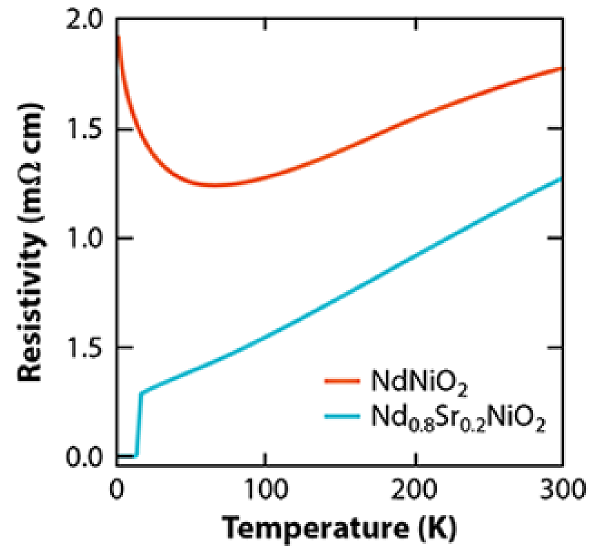
KH et al. Physik Journal Feb. 2022

similar & different to cuprates → better understand high T_c supercond.

Nickelates & cuprates - similarities & differences

Anisomov et al. PRB'99 DFT+U: nickelates are cuprate analog





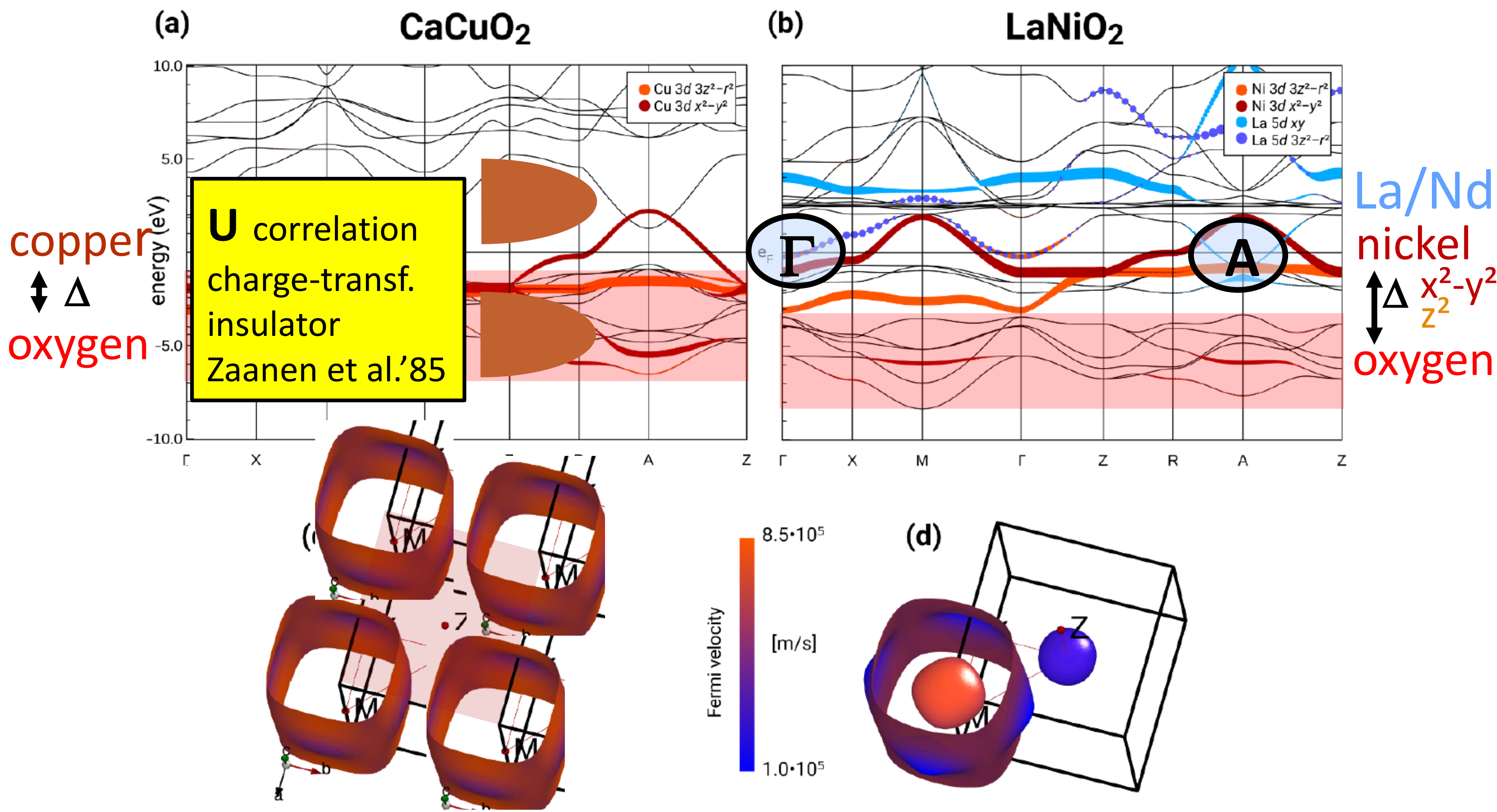
Li et al. Nature'19

$Nd^{3+}Ni^{1+}O_2^{4-}$

isoelectric: $3d^9$
isostructural
to $Ca^{2+}Cu^{2+}O_2^{4-}$

$Nd_{1-x}Sr_xNiO_2$ Zeng et al. PRL'20
$Pr_{1-x}Sr_xNiO_2$ Osada et al. Nano Lett'20
$La_{1-x}Ca_xNiO_2$ Zeng Sci. Adv.'22
$La_{1-x}Sr_xNiO_2$ Osada et al. Adv. Mat.'21
$Nd_6Ni_5O_{12}$ Pan et al. Nature Phys.'21
high quality films, pressure ...

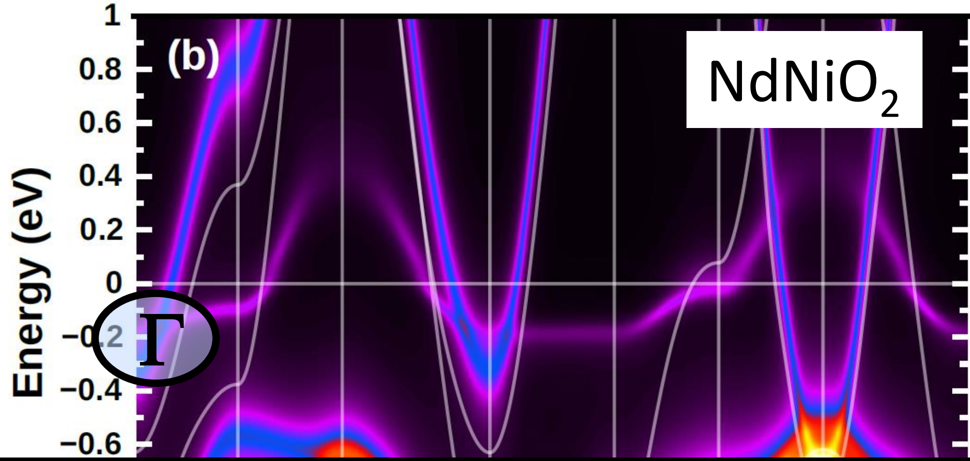
Nickelates & cuprates - similarities & differences

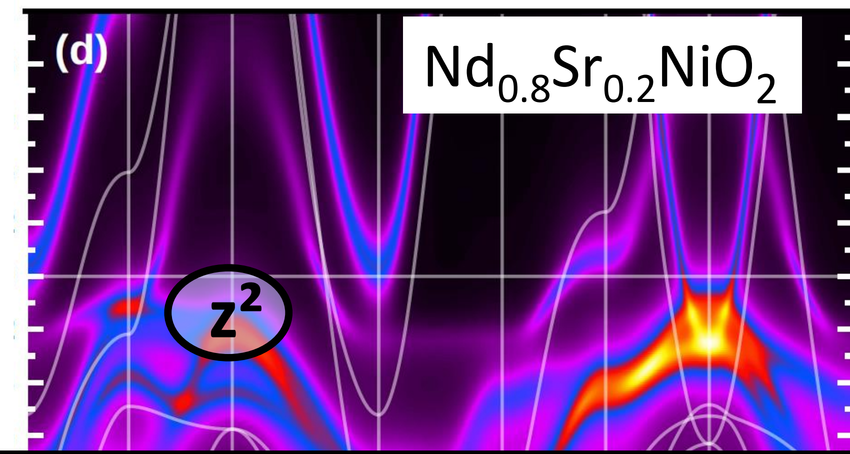


DFT bandstructure

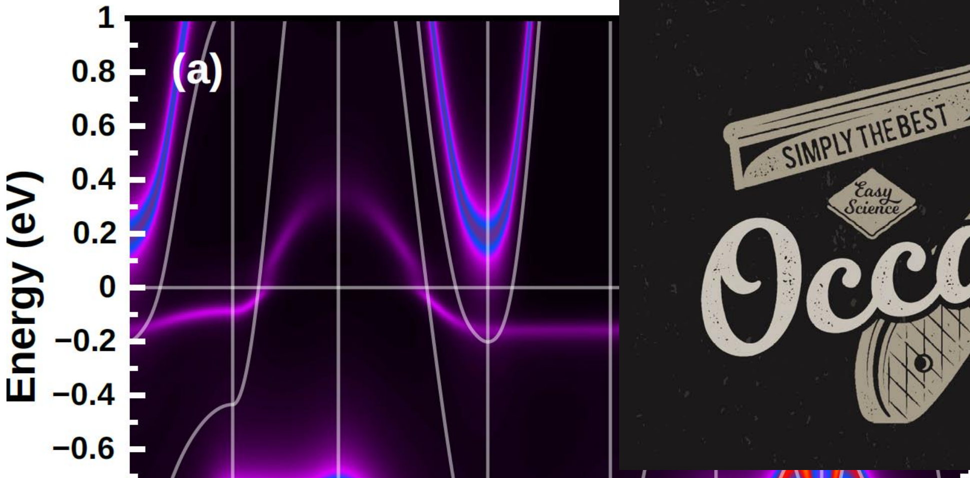
cf. Botana Norman PRX'20 Sakakibara et al. PRB'20
Wu et al. PRB'20, Zhang et al PRB'20, Werner, Hoshino PRB'20 …

DFT+DMFT: Ni x^2-y^2 + A pocket





Occam's razor: Ni x^2-y^2 + A pocket



pocket

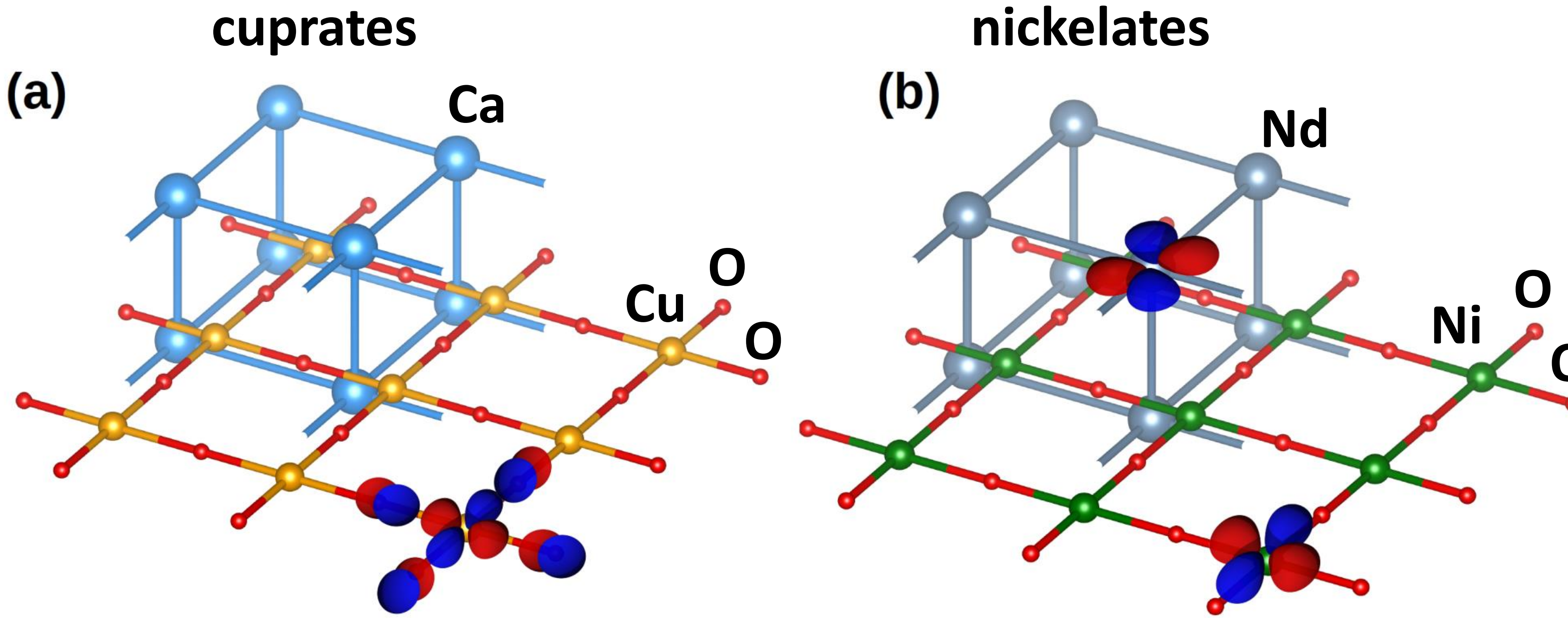
with U on La/Nd

for $LaNiO_2$

with doping

inverse Occam's razor Mazin Nature Phys.'22

Cuprates & nickelates - similarities & differences

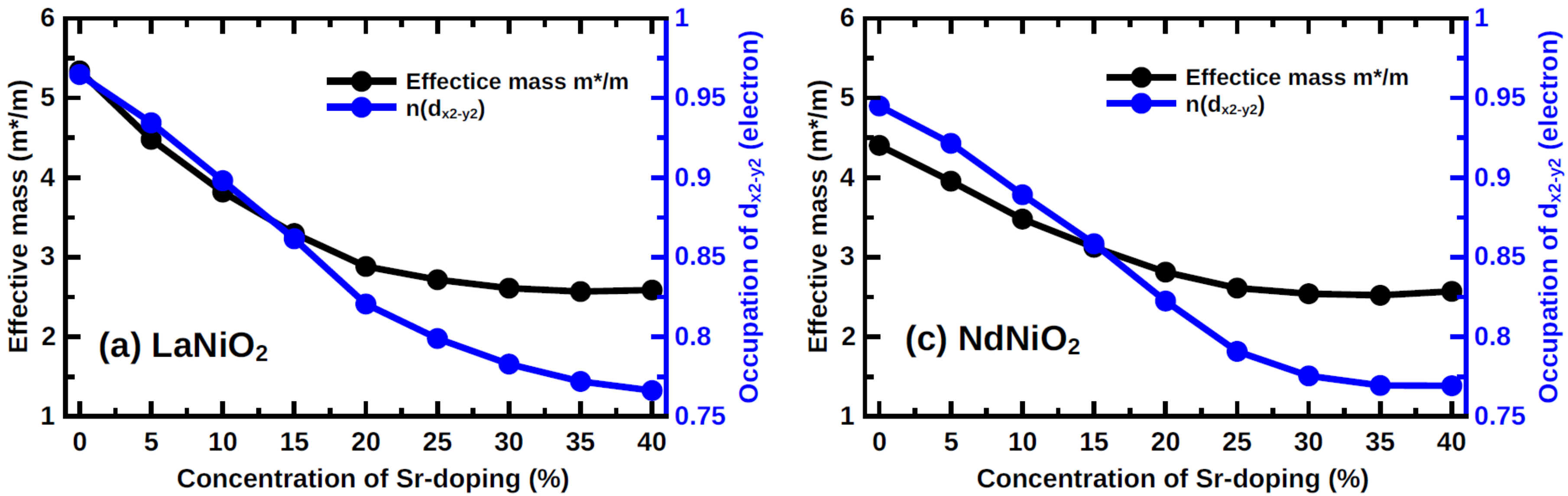


oxygen orbitals important
holes → oxygen orbitals
Emery model
(Hubbard model at most mimics Zhang-Rice singlet)

A pocket only electron reservoir
holes ½ A pocket ½ Ni x^2-y^2

Hubbard model
w properly calculated doping

Γ pocket as electron reservoir → Hubbard model



$NdNiO_2$:

1-band Hubbard model with

U=8t (cRPA: U = 2.6eV = 6.7 t)

t = 395 meV, t'/t = -0.25, t''/t = 0.12

and doping from above Fig.

Kitatani ... KH npj QM'20

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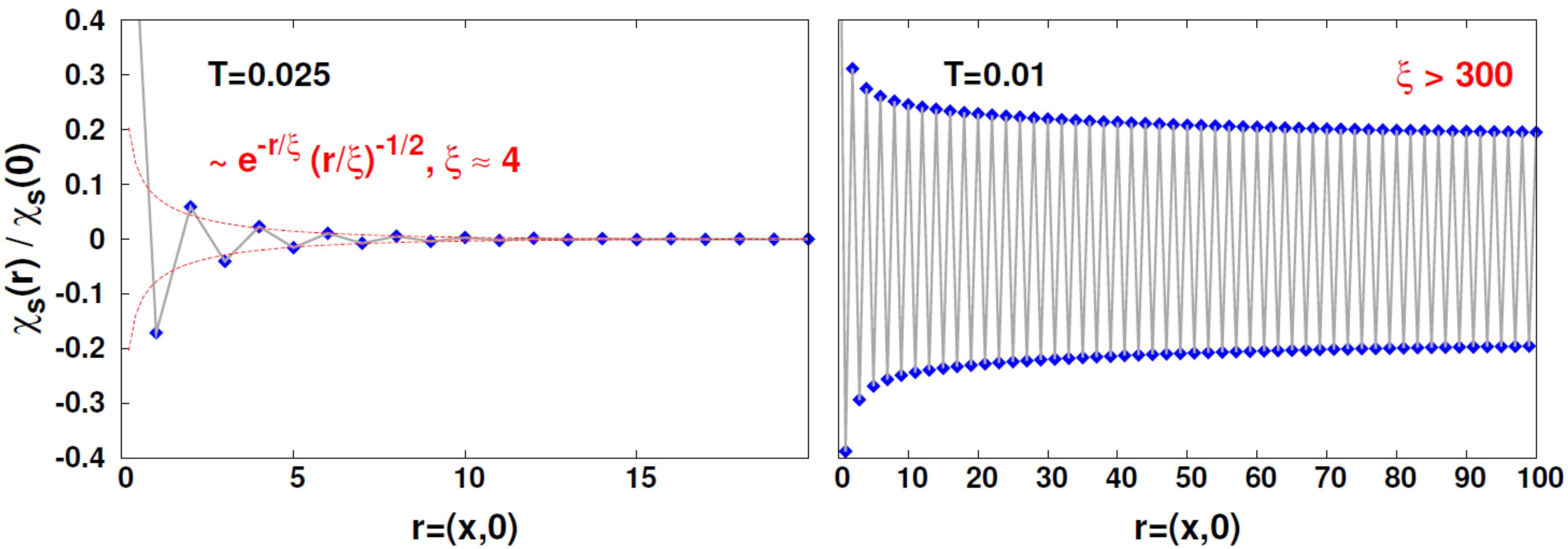
Spin fluctuations

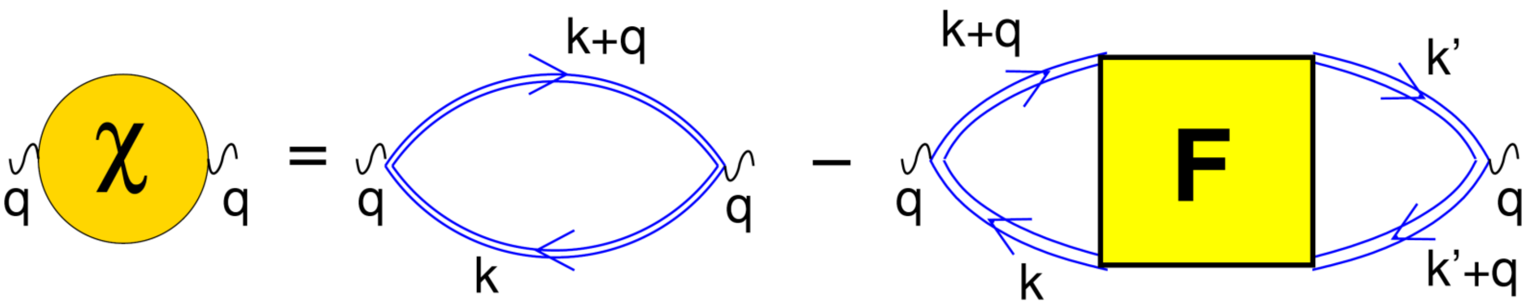


$$\chi(r) = \langle S(r)S(0)\rangle \sim (r/\xi)^{-1/2}\, e^{-r/\xi}$$

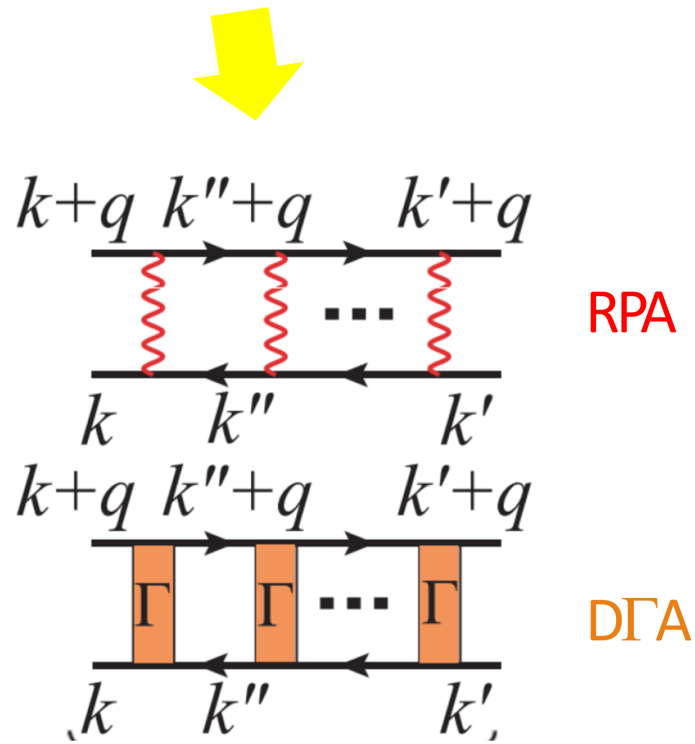
in practice: Ornstein-Zernike form

$$\chi_{\omega=0\ q} \sim 1/[\,(q-Q)^2 + \xi^{-2}]$$

Spin fluctuations



$$\chi_{r,\mathbf{q}\omega} = \underbrace{\sum_{\mathbf{k}\nu} G_{\mathbf{k}\nu} G_{(\mathbf{k}+\mathbf{q})(\nu+\omega)}}_{\equiv \chi^0_{\mathbf{q}\omega}} - \sum_{\mathbf{k}\mathbf{k}'\nu\nu'} G_{\mathbf{k}\nu} G_{(\mathbf{k}+\mathbf{q})(\nu+\omega)} F^{\nu\nu'\omega}_{r,\mathbf{k}+\mathbf{k}'\mathbf{q}} G_{\mathbf{k}'\nu} G_{(\mathbf{k}'+\mathbf{q})(\nu+\omega)}$$

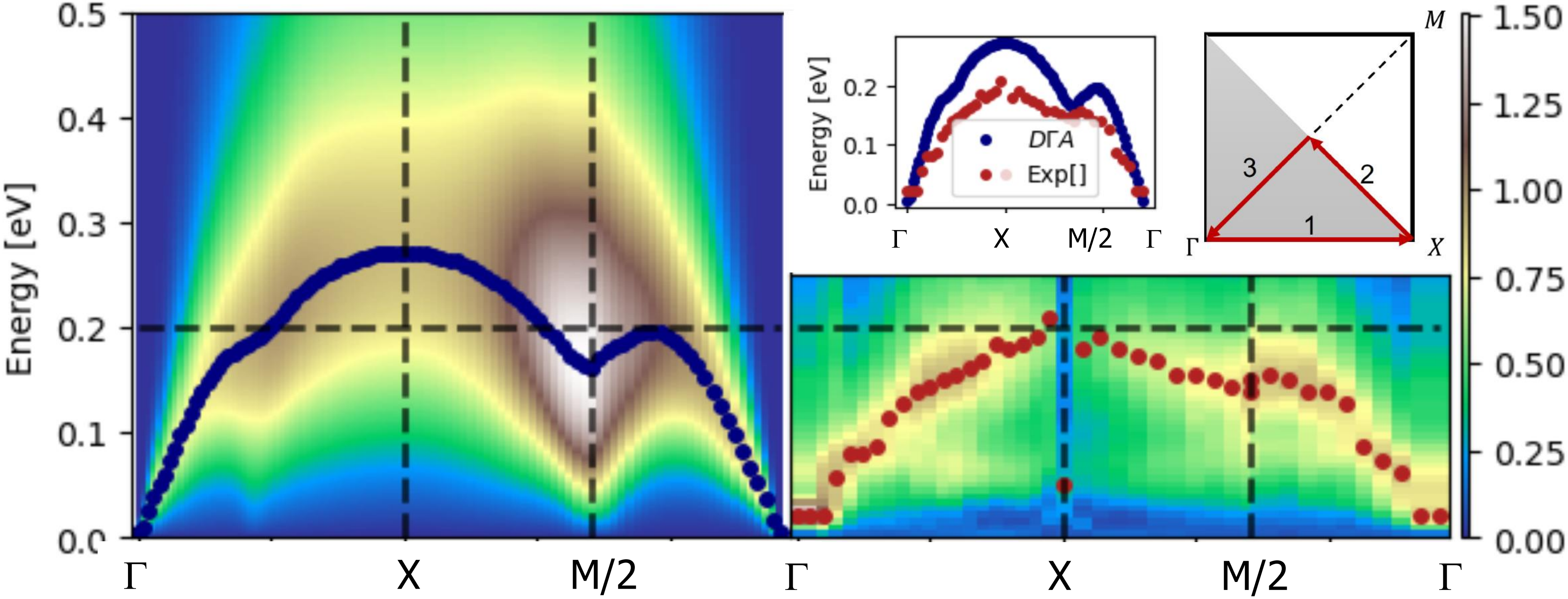


$\chi_{q\omega} = \chi^0_{q\omega}/(1-U\chi^0_{q\omega})$ RPA

$\chi_{q\omega} = \chi^0_{q\omega}(1-\Gamma_q\chi^0_{q\omega})^{-1}$ DΓA matrices in ν,ν'

Spin fluctuations: nickelates

Paramagnon spectrum $NdNiO_2$



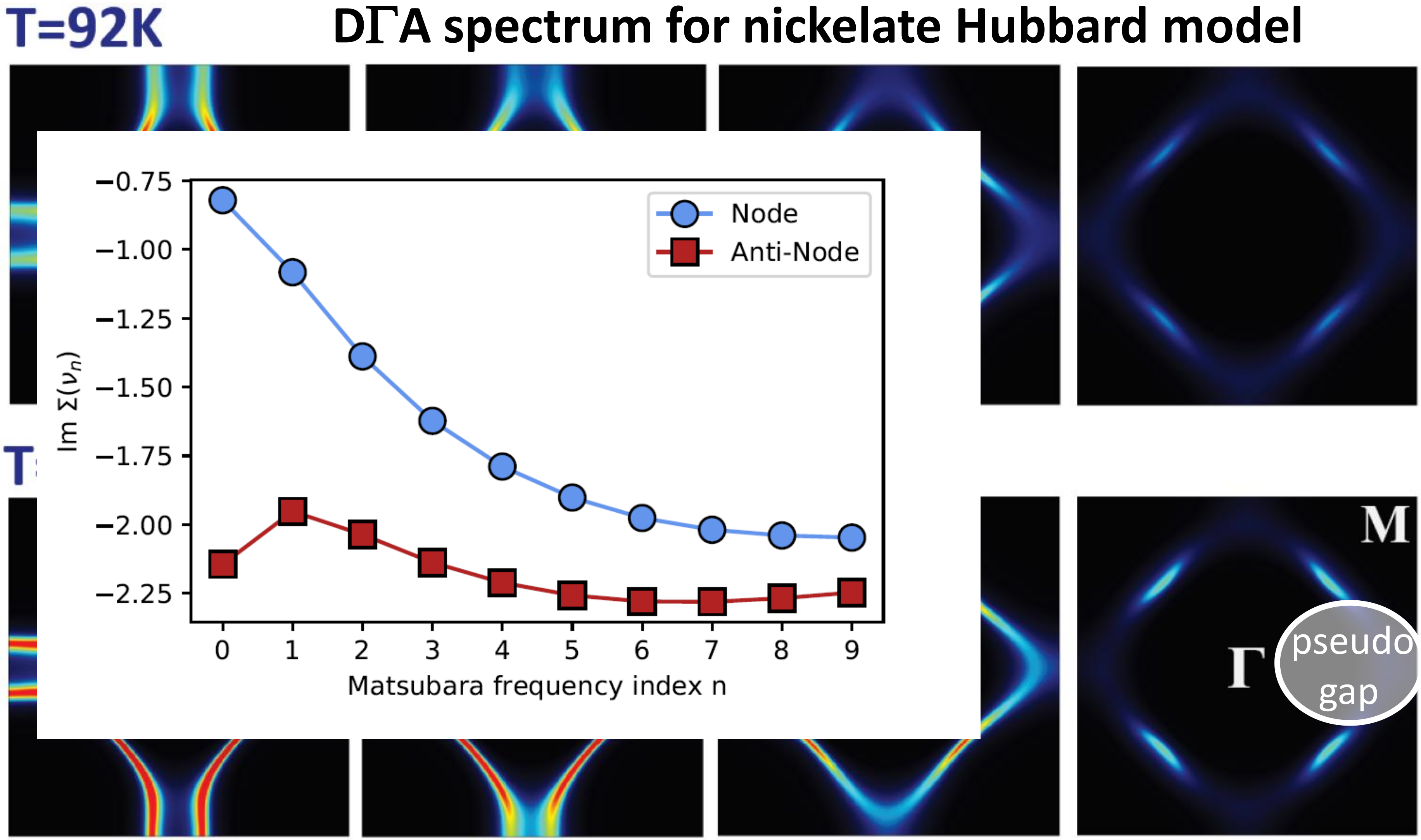
DΓA Theory
Worm ... KH unpublished’22

RIXS exp. Lu et al. Science’21
$NdNiO_2$ on STO (with stacking faults)
better films → better agreement?

Pseudogap

Pseudogap: Nickelates

DΓA spectrum for nickelate Hubbard model



$n_{d_{x^2-y^2}}$=0.80 $n_{d_{x^2-y^2}}$=0.85 $n_{d_{x^2-y^2}}$=0.90 $n_{d_{x^2-y^2}}$=0.95

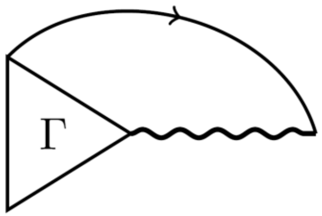
Kitatani ... KH npj QM'20

Pseudogap: Im Γ mechanism

Krien, Worm … KH arXiv:2101.06529

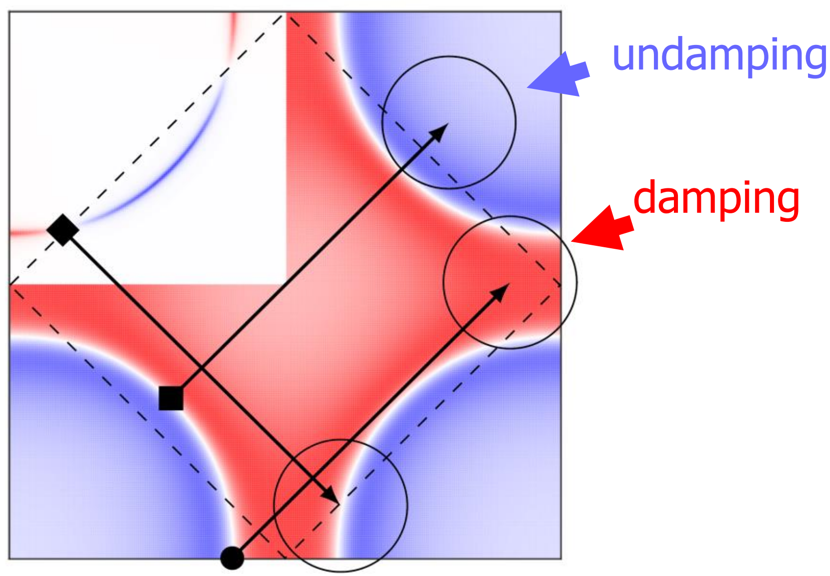
Comm. Phys in print

We can rewrite self-energy as spin-fermion vertex



$$\Sigma''_{\mathrm{sp}}(k,q) \propto -G'_{k+q} W_q \Gamma''_{kq}$$

at strong coupling: contribution from Im Γ (!)



Superconductivity: nickelates

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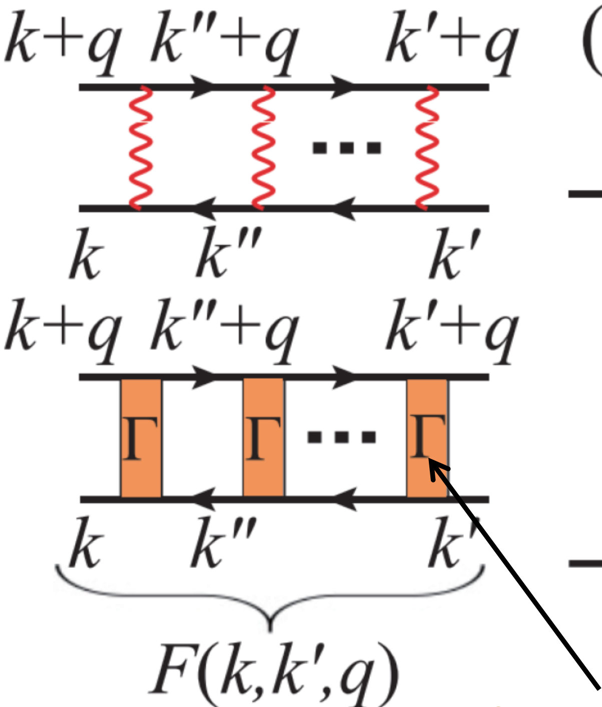
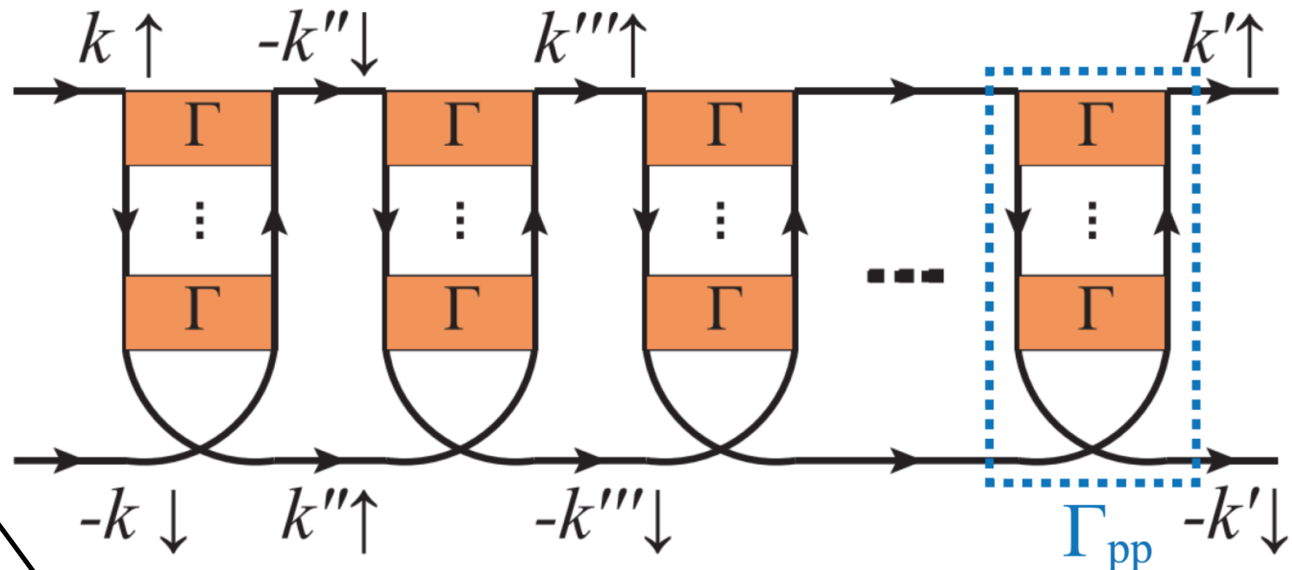
J. Phys. Mater. 5 034005 (2022)



(c)

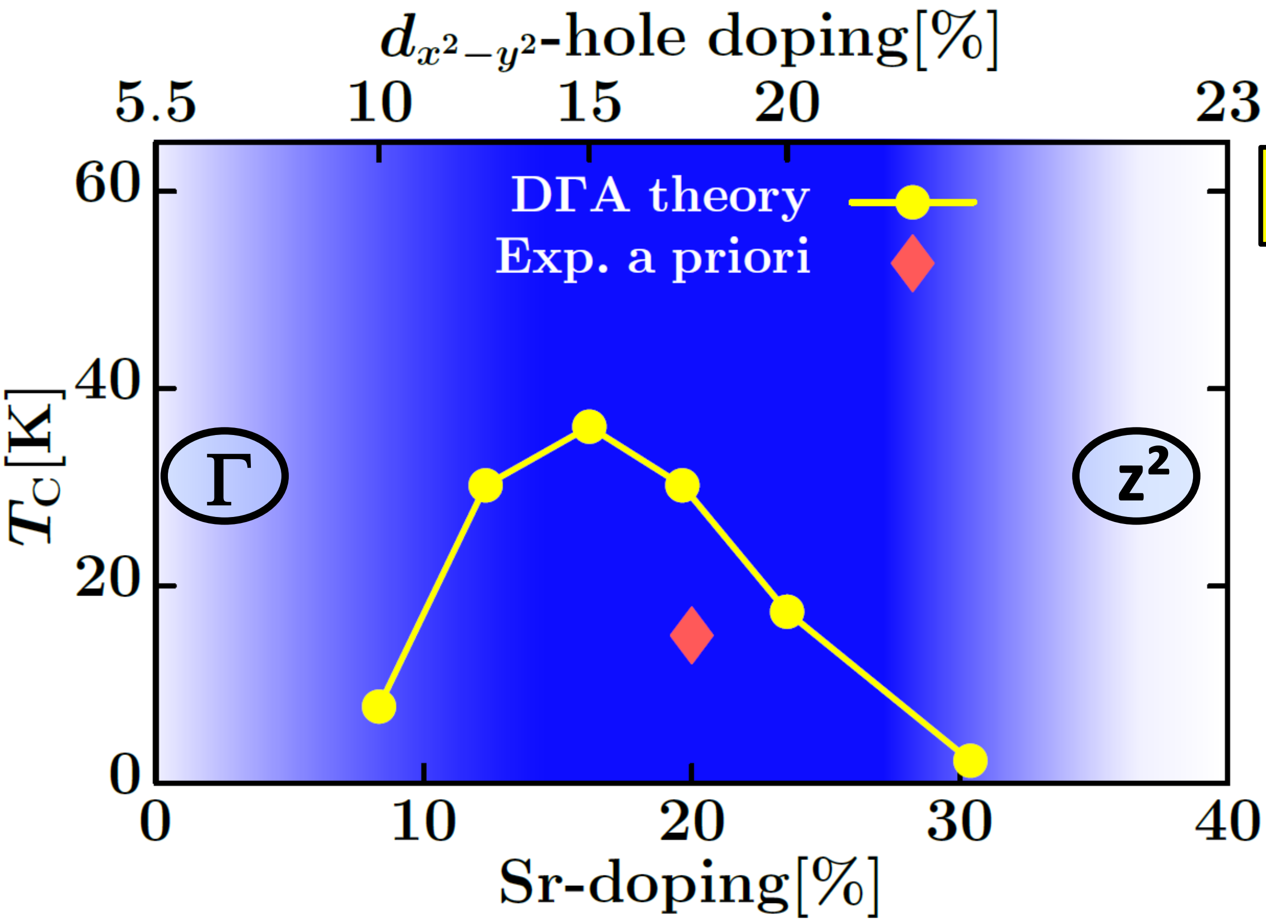


local from AIM, fully frequency dependent

Unbiased: spin and charge fluctuations, quantum critical fluct.
excellent agreement with diag. MC ... Schäfer et al. PRX'21

Superconductivity: nickelates

Superconductivity $Sr_xNd_{1-x}NiO_2$ (d-wave)



no free parameters

Exp:
Li et al. Nature'19

DΓA Kitatani … KH npj QM'20

Superconductivity: nickelates

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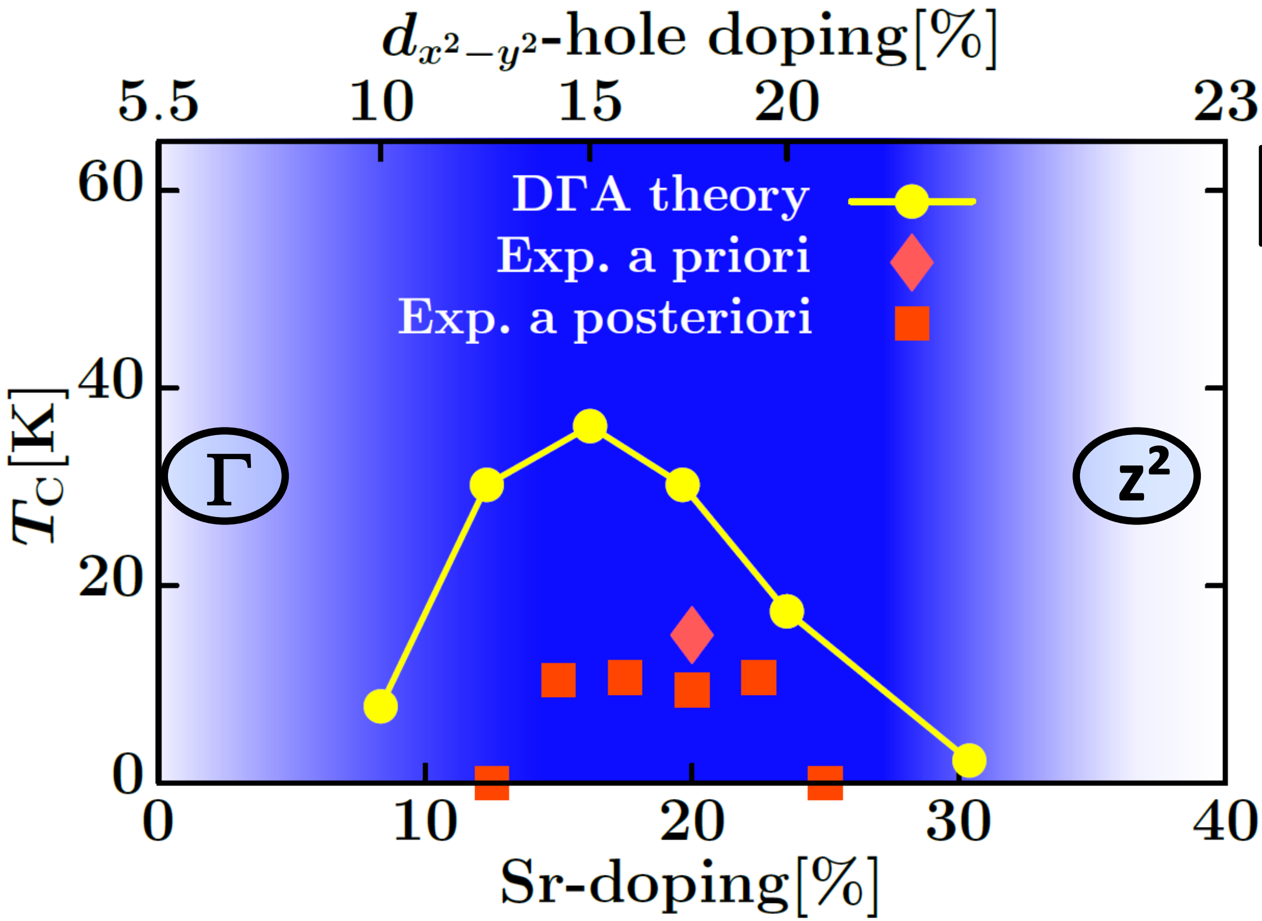

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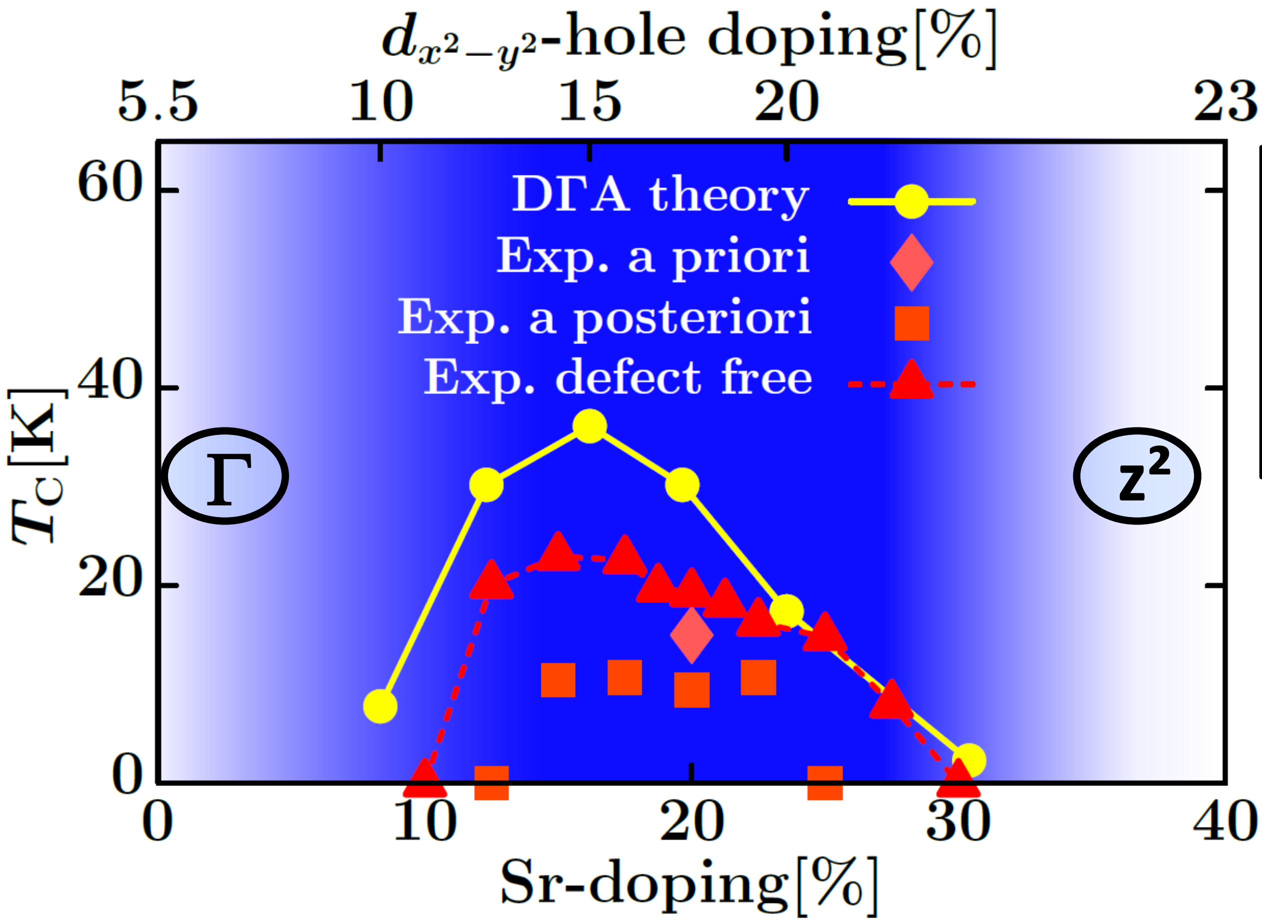


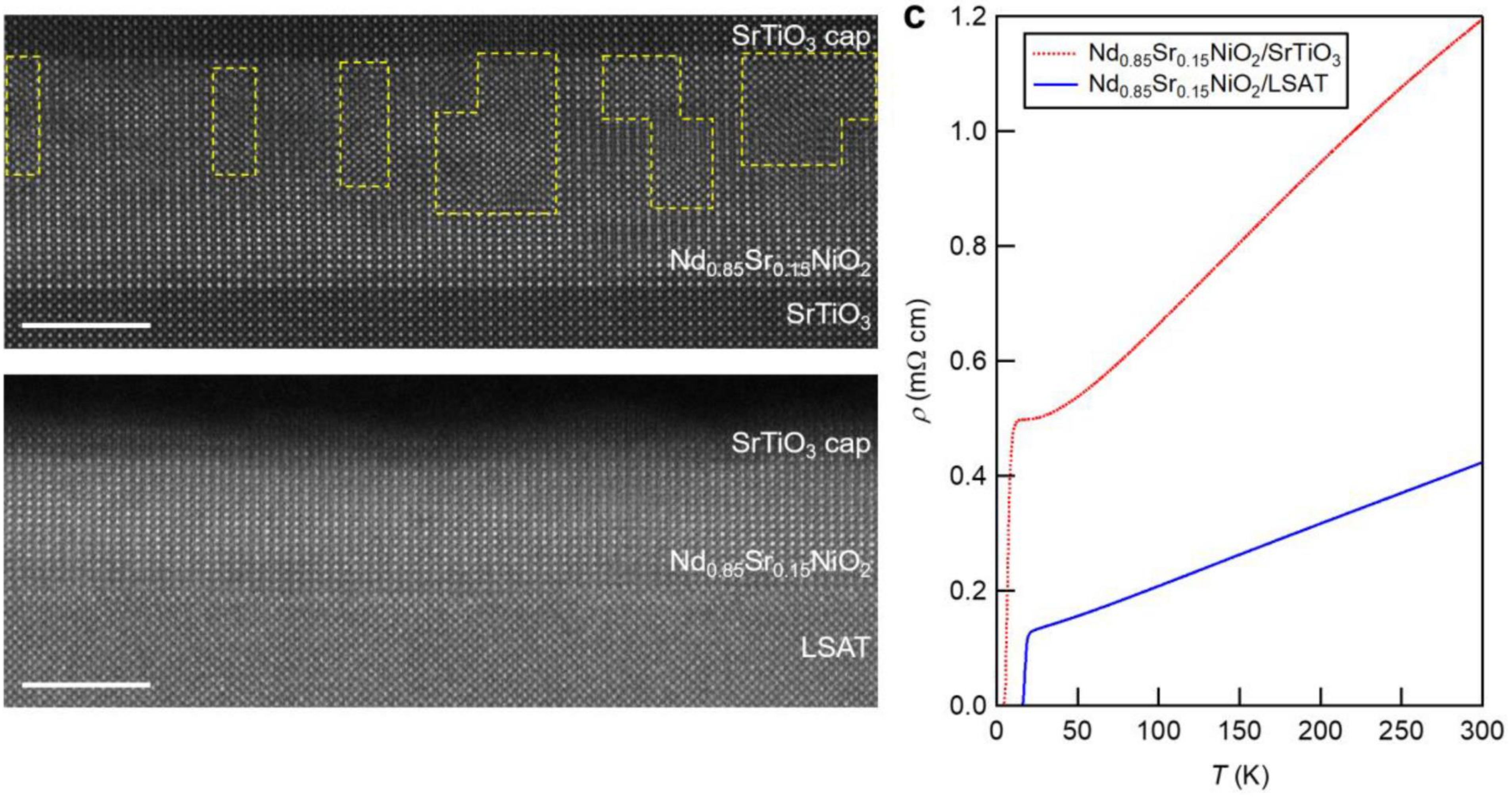
no free parameters

T_c dome astonishingly well predicted

Exp:
Li et al. Nature'19
Li et al. PRL'20
Lee et al. arXiv:2203.02580

DΓA Kitatani … KH npj QM'20

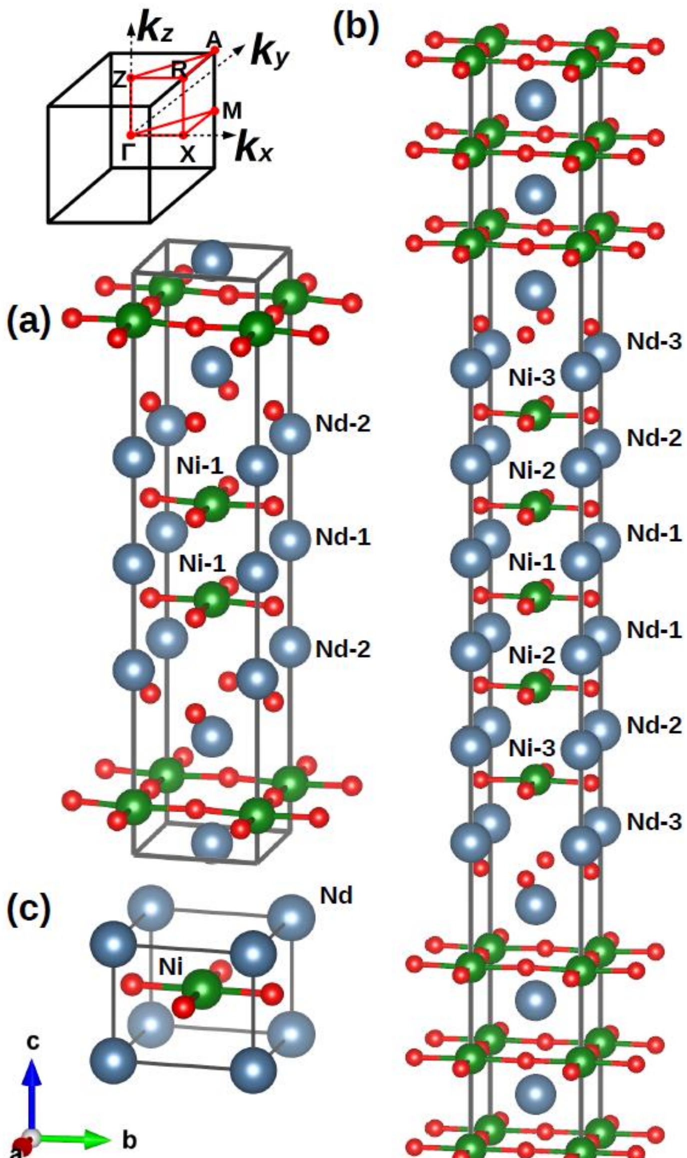
New, cleaner (NdSr)NiO_2 films



LSAT: 3.890 Å instead of STO: 3.905 Å

Lee et al. arXiv:2203.02580

From infinite layer to finite layer



$Nd_6Ni_5O_{12}$

Pan et al. Nature Phys.'21

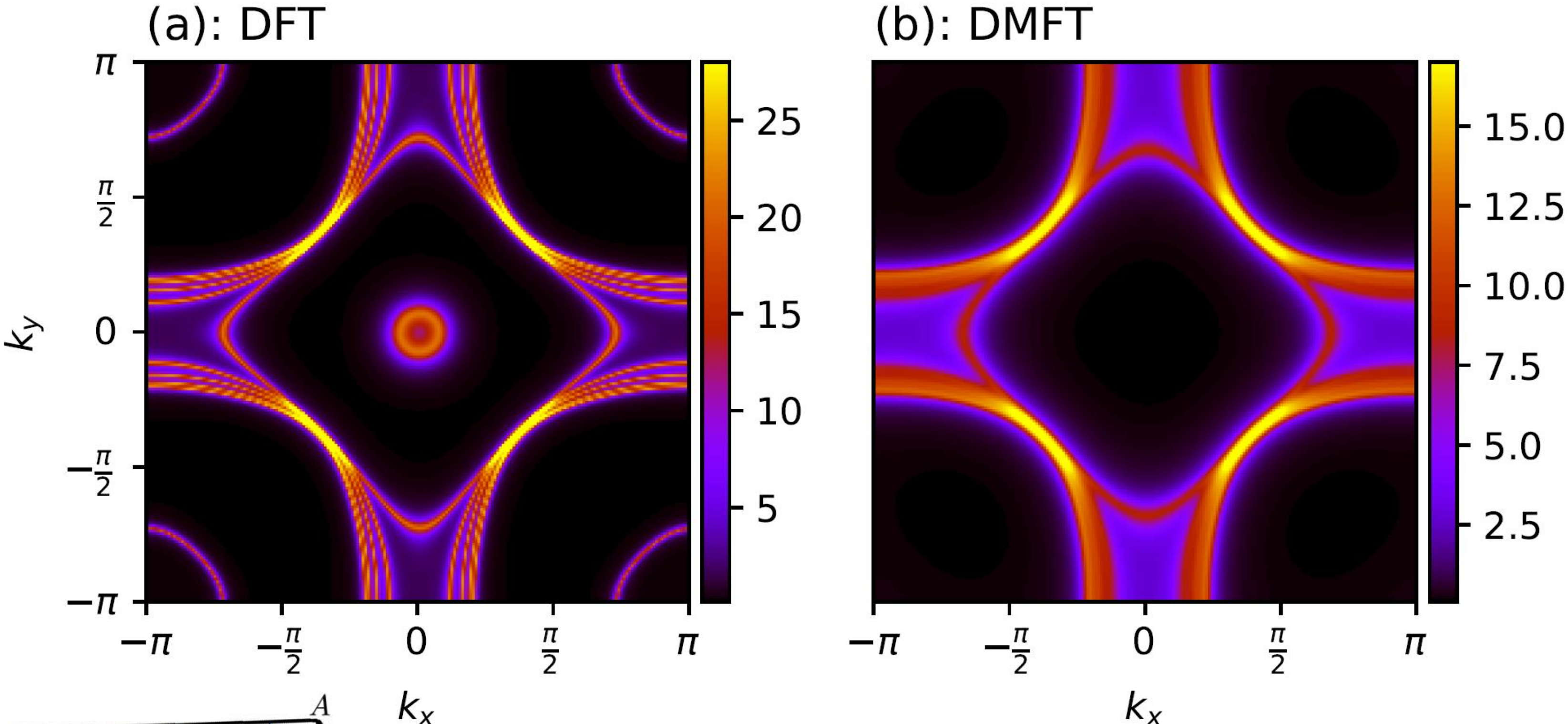
essentially same hopping just cut-off after 5 layers

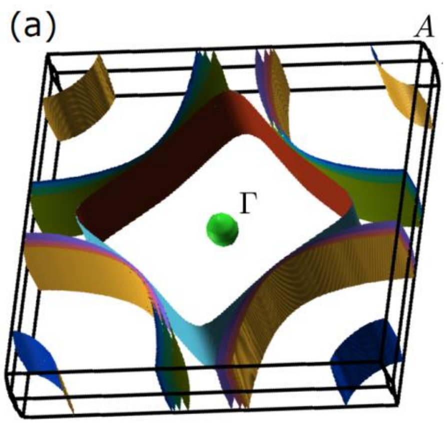
System	t	t'	t''
$NdNiO_2$	-0.395	0.095	-0.047
$Nd_3Ni_2O_6$	-0.414	0.092	-0.055
$Nd_6Ni_5O_{12}$: Ni-1	-0.395	0.098	-0.050
$Nd_6Ni_5O_{12}$: Ni-2	-0.392	0.097	-0.050
$Nd_6Ni_5O_{12}$: Ni-3	-0.398	0.097	-0.049

Worm ... KH arXiv'21

Pentalayer nickelate

$Nd_6Ni_5O_{12}$





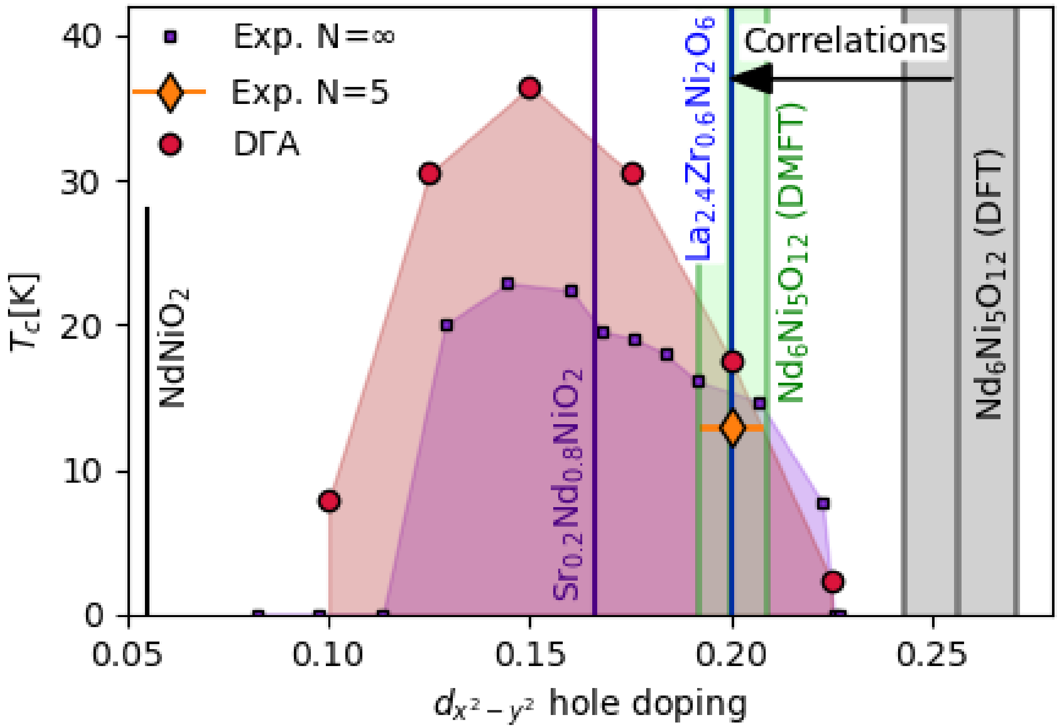
x^2-y^2-orbital system Ni $3d^{8.8}$

no pockets/tubes in DMFT

Worm ... KH arXiv'21

Pentalayer

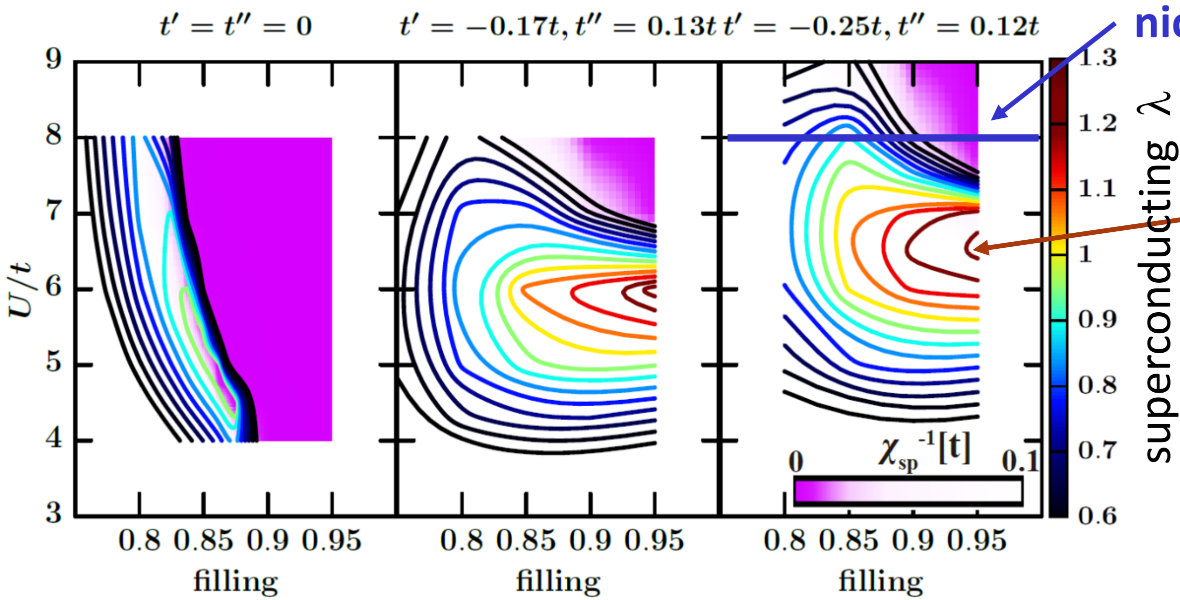
$Nd_6Ni_5O_{12}$



correlations → no pockets/tubes
T_c consistent with infinite layer nickelate at proper $d_{x^2-y^2}$ doping
exp. evidence: positive Hall coef. ✔

Worm … KH arXiv'21

How to increase T_c ?



nickelates

Kitatani … KH unpubl.'22

T=0.01 t

soft spot for SC

strong AFM fluct → pseudogap
→ no SC

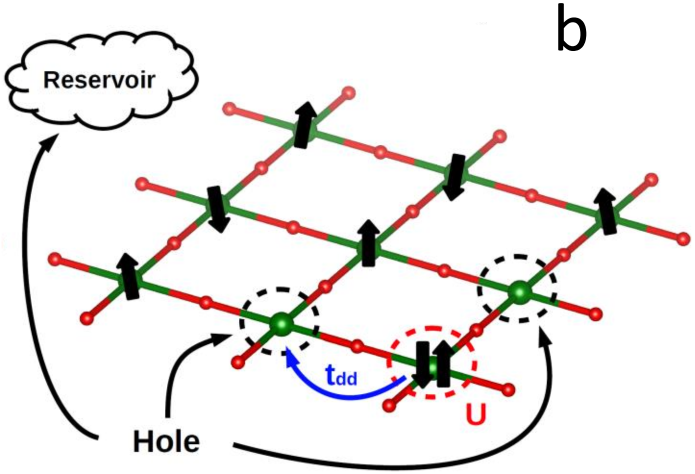
cf. DCA Chen et al. PRL'15

(a) pressure or compressive strain
(b) substrate different from $SrTiO_3$
(c) palladates with 4d instead of 3d

exp. confirmed: $Pr_{1-x}Sr_xNiO_2$ under 12GPa with T_c>30K
Wang et al. arXiv:2109.12811

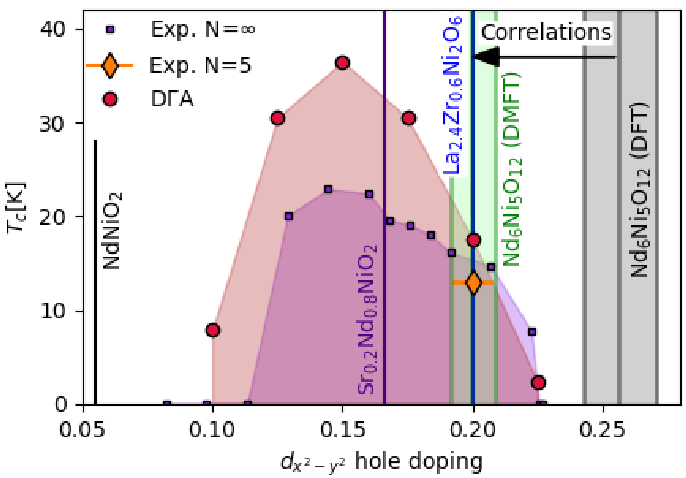
Conclusion

- Diagrammatic extensions of DMFT such as DΓA allow us to describe the physics beyond DMFT such as spin fluctuations superconductivity …

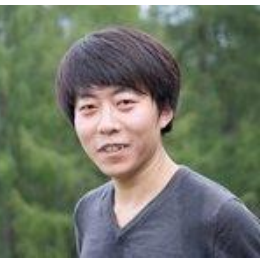


- Nickelates
  Hubbard model: Ni x^2-y^2 orbital
  + electron reservoir: A pocket

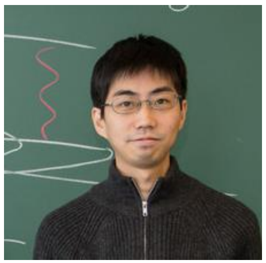
- good DΓA prediction of
  superconducting phase diagram
  consistent picture



Thanks to …



Liang
Si



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Si et al. Phys. Rev. Lett. 124, 166402 (2020)
Kitatani et al. npj Qu. Materials 5, 59 (2020)
Worm et al. arXiv:2111.12687
Held et al. Frontiers in Phys. 9, 810394 (2022)

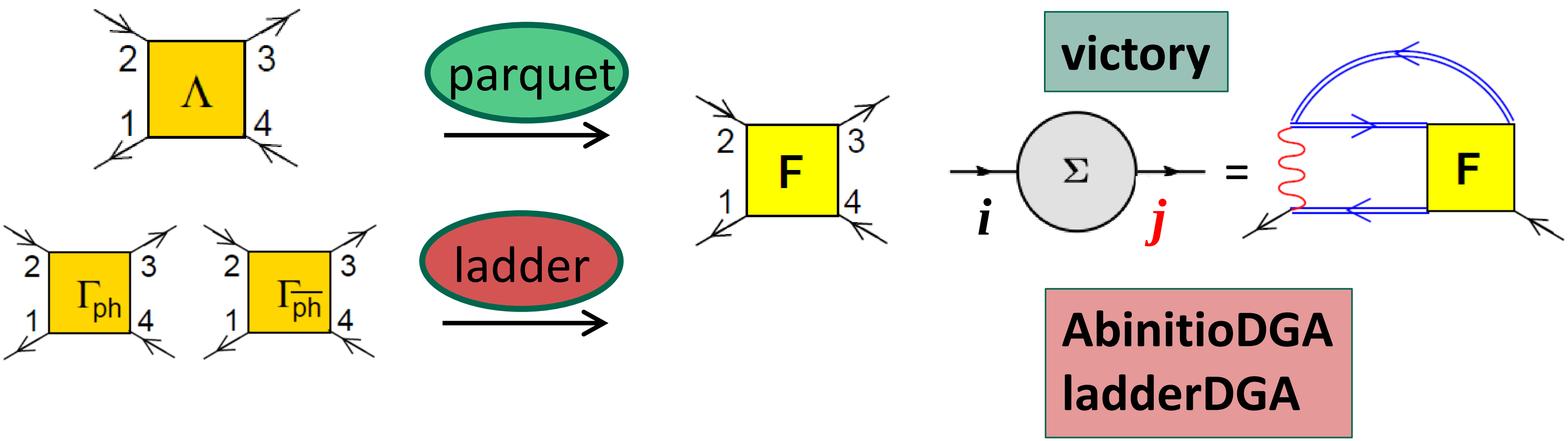
$D\Gamma A$ Rohringer et al. Rev.Mod.Phys. 90, 025003 (2018)

Conclusion: method

DΓA: Resummation of Feynman diagrams in terms of locality

n-particle fully irreducible vertex *approximated as local*

local → non-local



includes local **DMFT** correlations

and non-local correlations

(e.g. spin fluctuations)