Is spin and charge degree of freedom effectively decoupled in the 2D Hubbard model?

Krzysztof Wohlfeld

UNIVERSITAS VARSOVIENSIS

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Papers / collaborators / institutions

Persistent spin excitations in doped antiferromagnets revealed by resonant inelastic light scattering

Nature Communications **5**, 3314 (2014)

C. J. Jia, E. A. Nowadnick, K. Wohlfeld, C.-C. Chen, S. Johnston, T. Tohyama, B. Moritz, and T. P. Devereaux

Origin of strong dispersion in Hubbard insulators

Phyical. Review B **92**, 075119 (2015)

Y. Wang, K. Wohlfeld, B. Moritz, C.J. Jia, M. van Veenendaal, K. Wu, C.-C. Chen, and T. P. Devereaux

SLAC NATIONAL ACCELERATOR LABORATORY

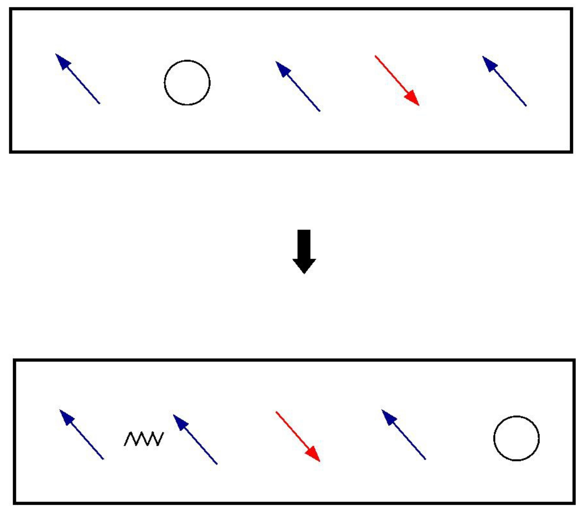
LELAND STANFORD JUNIOR UNIVERSITY

U.S. DEPARTMENT OF ENERGY

Office of Science

Motivation: separation of spin and charge in 1D

Putting 1 hole into the **1D** antiferromagnet (=ground state of the undoped 1D Hubbard model):



→ hole (~holon) + domain wall (~spinon) separate

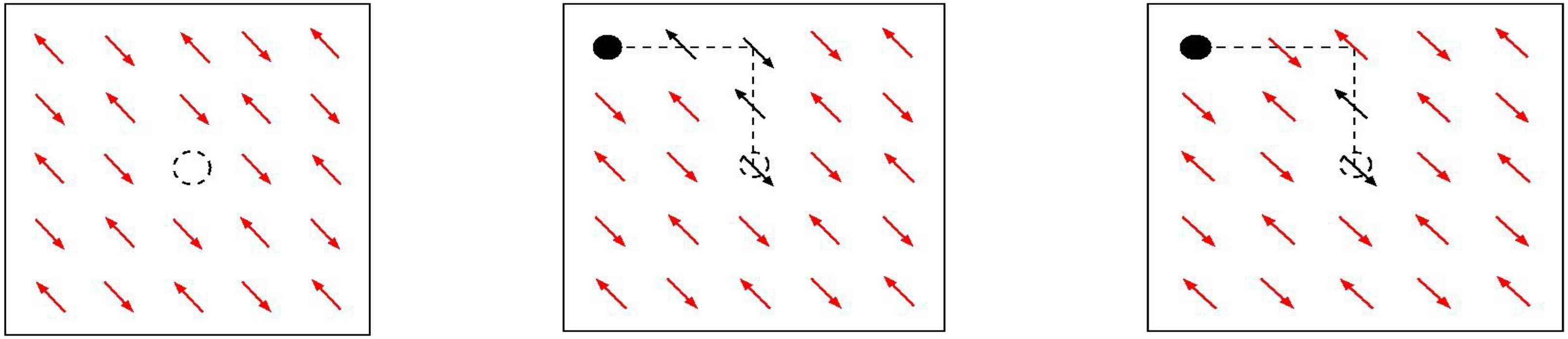
→ spin-charge separation [T. Giamarchi, *Quantum Physics in One Dimension* (2004)]

→ also seen in ARPES on cuprates [C. Kim *et al.*, PRL **77**, 4054 (1996)]

→ cf. spin-orbital separation story [J. Schlappa *et al.*, Nature **485**, 82 (2012)]

Motivation: confinement of spin and charge in 2D

Putting 1 hole into the **2D** antiferromagnet (=ground state of the undoped 2D Hubbard model):



→ hole (~holon) excites collective magnetic excitations (~magnons) when moving

→ not only spin and charge does *not* separate but even...

→ …holon motion hindered by magnons = spin polaron [G. Martinez & P. Horsch, PRB **44**, 317 (1991)]

→ also seen in a *number* of ARPES on cuprates [A. Damascelli, Z. Hussain, & Z.-X. Shen, RMP **75**, 473 (2003)]

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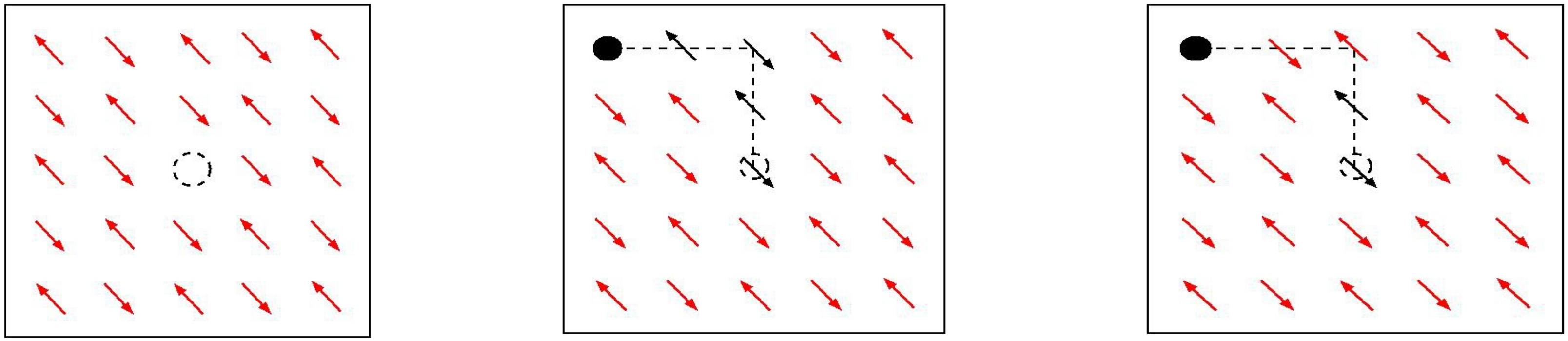

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But is this the whole story?

→ also seen in a *number* of ARPES on cuprates [A. Damascelli, Z. Hussain, & Z.-X. Shen, RMP **75**, 473 (2003)]

Outline

1. Persistence of spin excitations (in doped cuprates / 2D Hubbard model):

   – experiment

   – theory

2. Origin of strong dispersion of a hole (in undoped cuprates / 2D Hubbard model):

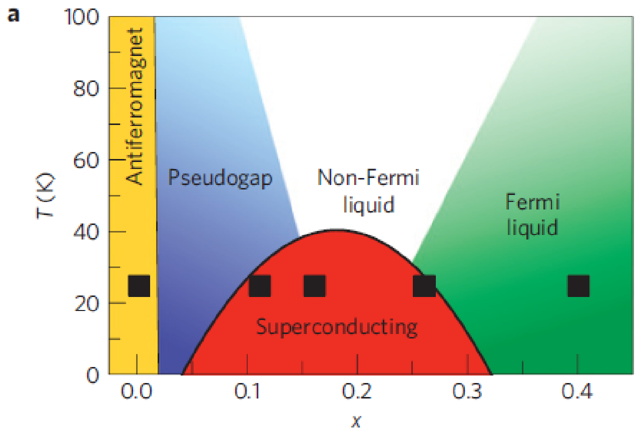
   – experiment

   – theory

3. Conclusions: what connects these 2 stories?

1. Persistence of spin excitations: experiment

$La_{2-x}Sr_xCuO_4$ (LSCO)



→ Phase diagram of LSCO:

antiferromagnet (AF) and superconductivity (SC)

→ "Magnons" measured by RIXS in LSCO

M. Le Tacon *et al,* Nature Phys. **7**, 725-730 (2011); M. P. M. Dean *et al.*, Nature Materials **12**, 1019-2023 (2013); M. Le Tacon *et al.*, Phys. Rev. B **88**, 020501(R) (2013); M. P. M. Dean *et al*., Phys. Rev. Lett. **110**, 147001 (2013); M. Guarise *et al*., Nature Communications **5**, 5760 (2014).

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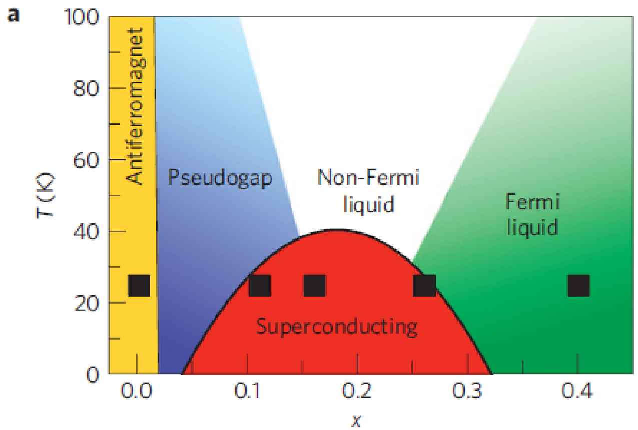

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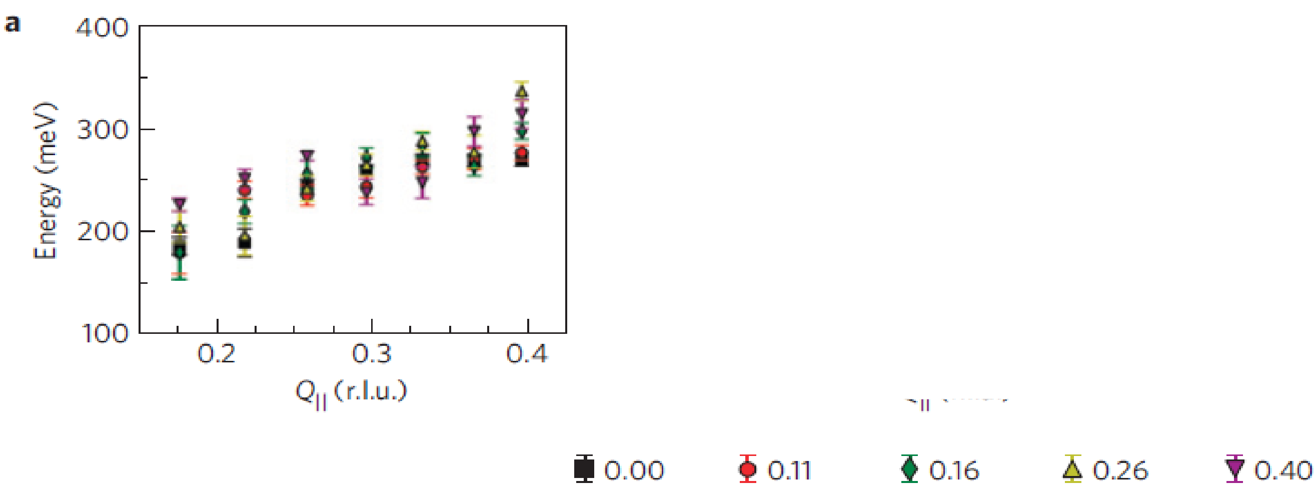

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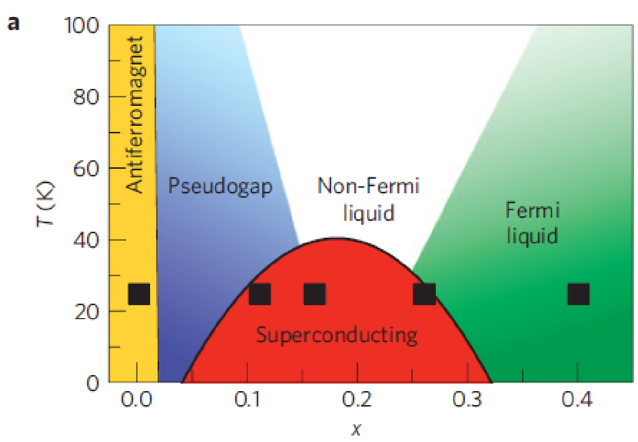

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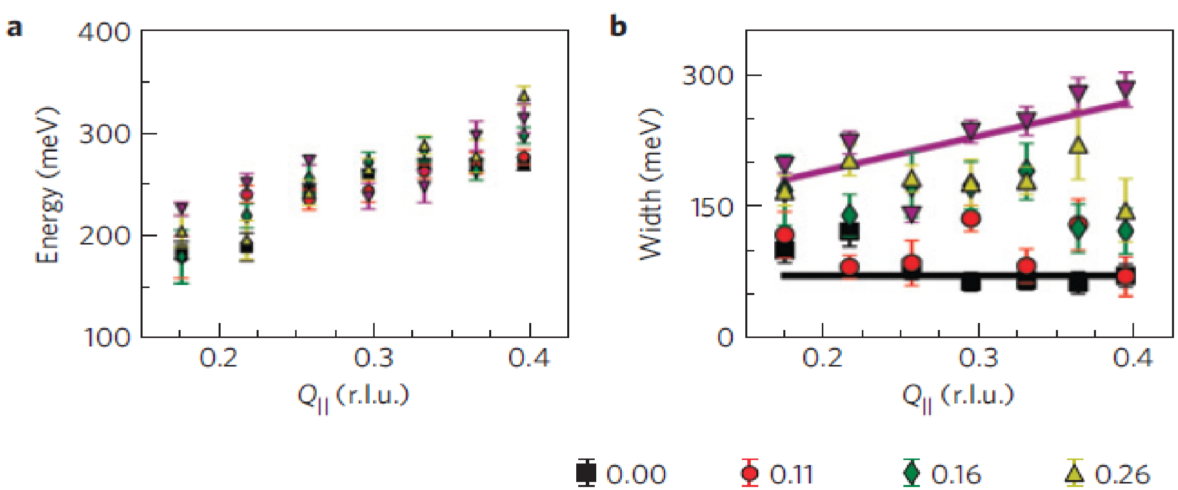

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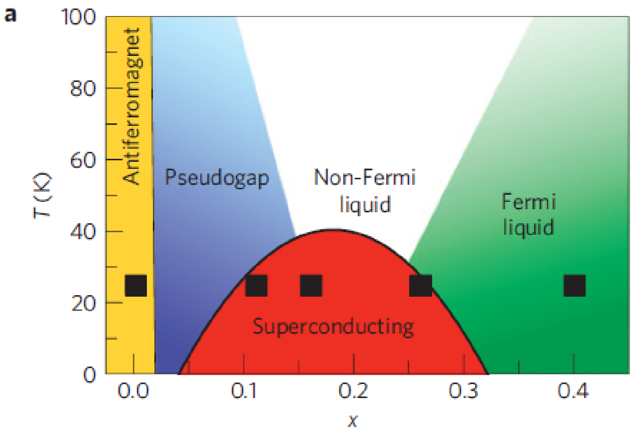


→ Phase diagram of LSCO:

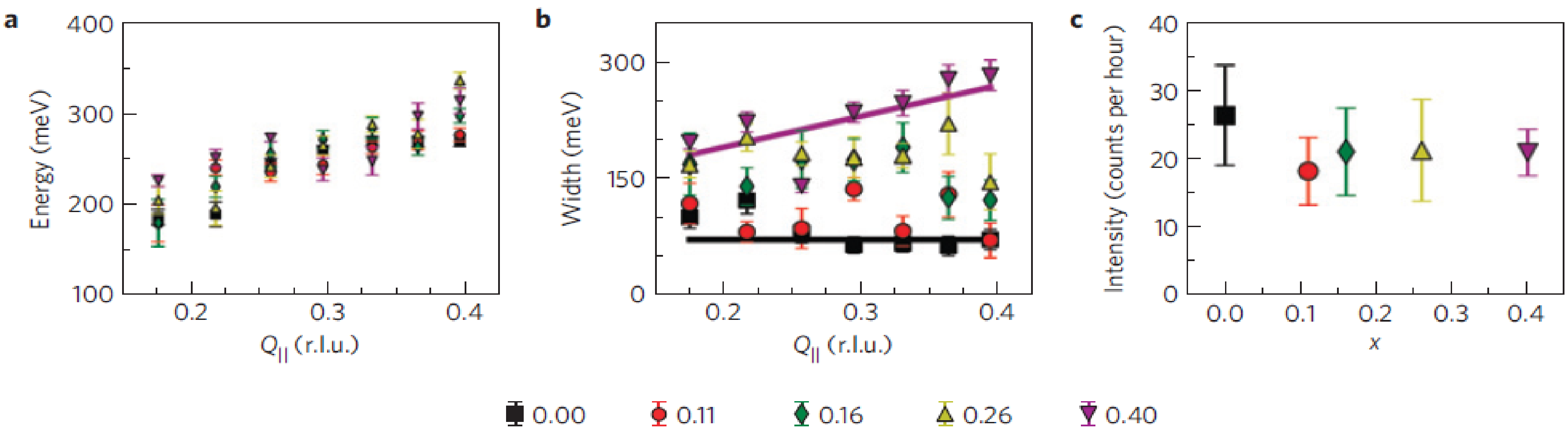
antiferromagnet (AF) and superconductivity (SC)

→ “Magnons” measured by RIXS in LSCO

→ Lack of changes of dispersion upon doping

→ Increase in FWHM of “magnons” upon doping

→ Small changes in the intensities of “magnons”



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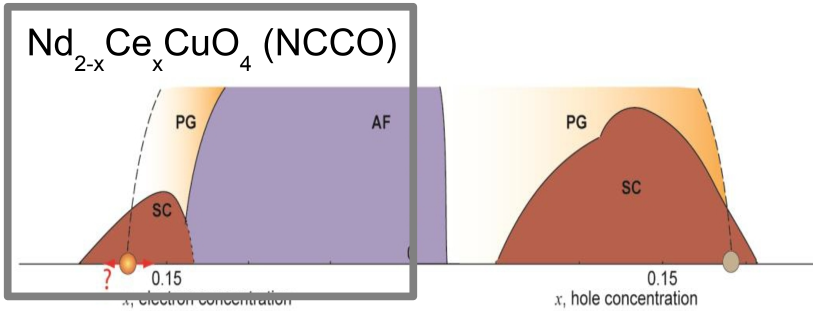
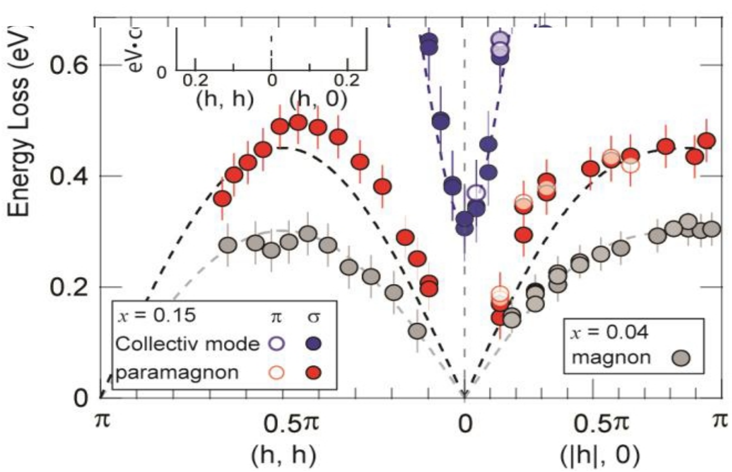


→ NCCO: electron doping

→ upon doping: robust antiferromagnet (AF)

→ "magnon" velocity... increases with doping

[magnon energy for q~(0, π) increases]

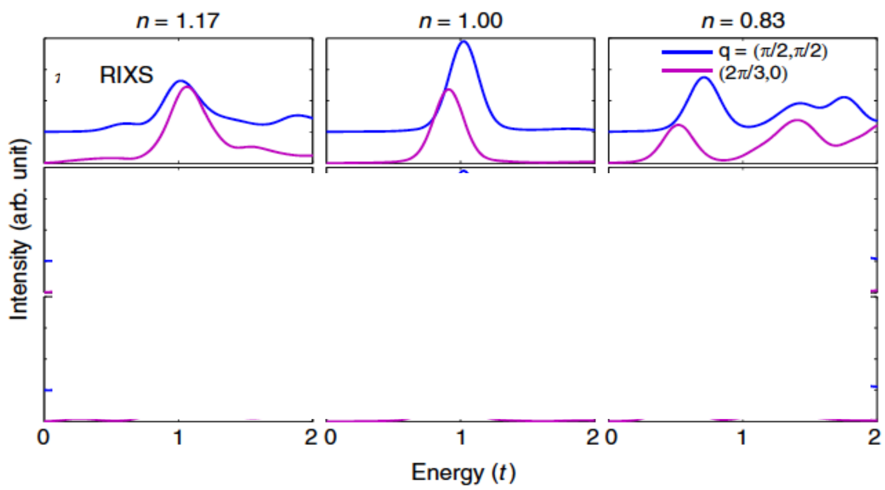


W. S. Lee *et al*, Nature Physics **10**, 883 (2014); K. Ishii *et al.*, Nature Communications **5**, 3714 (2014)

Intermezzo: RIXS ~ **S(q, ω)**

Exact diagonalization for 3 doping levels:

– RIXS for the Hubbard model (+t' + core)



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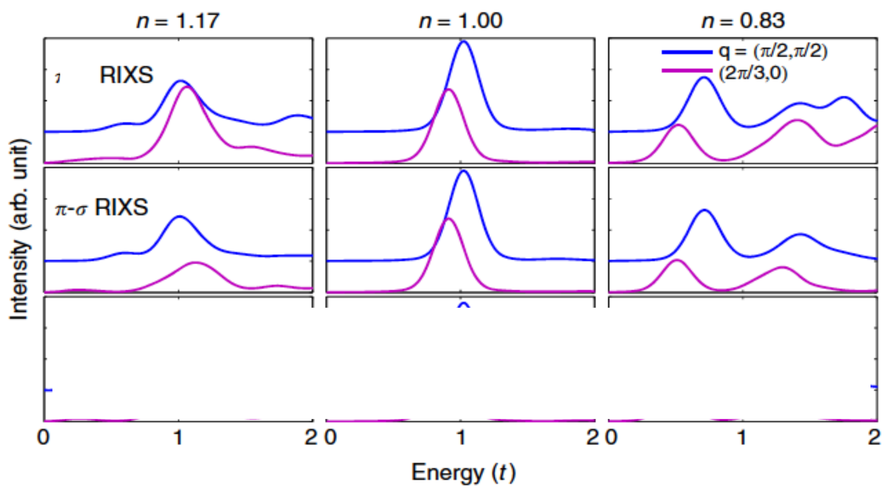

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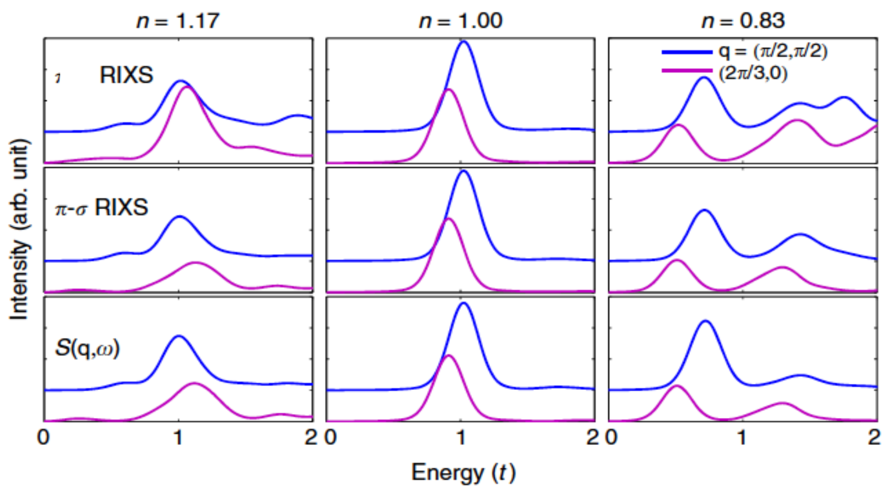
– S(**q**, ω), i.e. spin dynamical structure factor, for the Hubbard model (+t')



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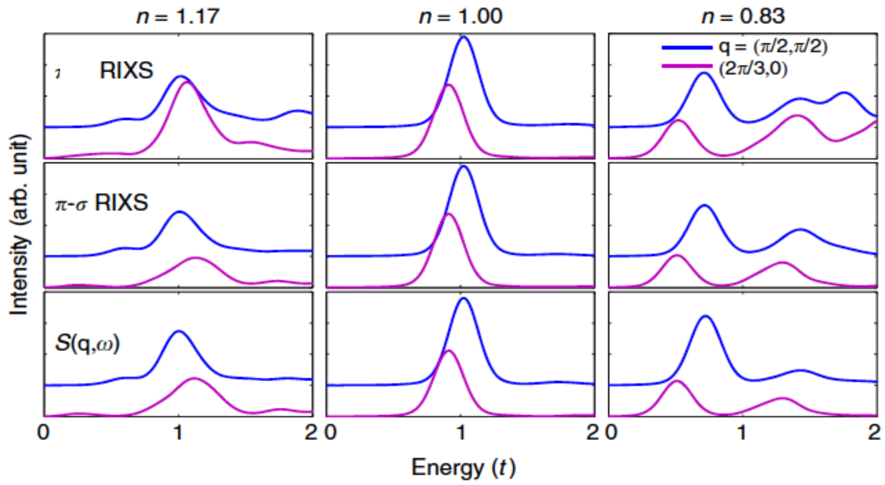


→ Line shapes: π-σ RIXS = S(**q**, ω) upon doping

→ Line shapes: <u>low energy part of full</u> RIXS ~ S(**q**, ω)

Intermezzo: RIXS ~ S(**q**, ω)

Exact diagonalization for 3 doping levels:

– RIXS for the Hubbard model (+*t'* + core)

– π-σ R

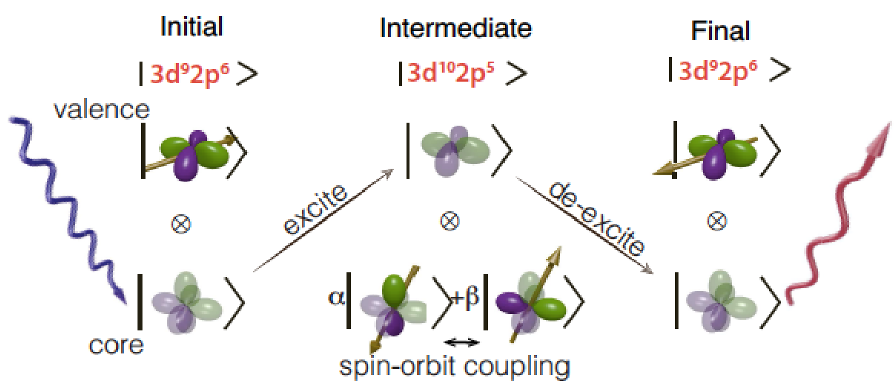
– S(**q**,

Large spin-orbit coupling in the 2p core levels

+ not fully occupied 2p core levels in the intermediate state of RIXS

→

RIXS can trigger spin excitations



Energy (*t*)

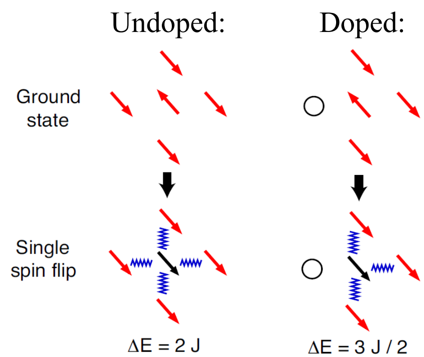
→ Line shapes: π-σ RIXS = S(**q**, ω) upon doping

→ Line shapes: <u>low energy part of full</u> RIXS ~ S(**q**, ω)

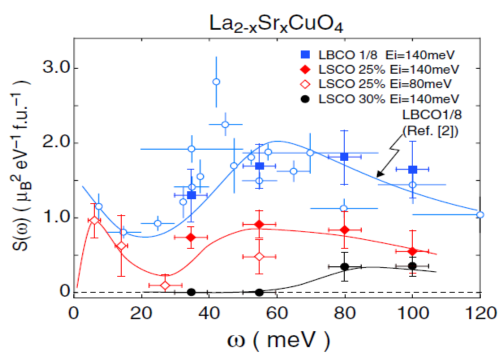
1. Persistence of spin excitations: theory

These results are counterintuitive and relatively novel:

(1) "Magnon" energy: should decrease with doping?!



(2) "Magnon" spectral weight: should decrease with doping?!



S(**q**, ω), i. e. spin dynamical structure factor measured by Inelastic Neutron Scattering

[PRL **98**, 247003 (2007)]

1. Persistence of spin excitations: theory

→ Questions:

(A) Can the **spectral weights** of "magnons" be persistent upon doping?

(B) Can the **energy** of "magnons" be persistent upon doping?

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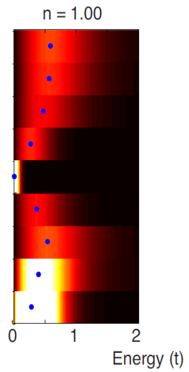

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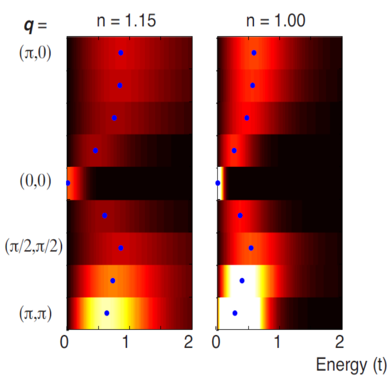

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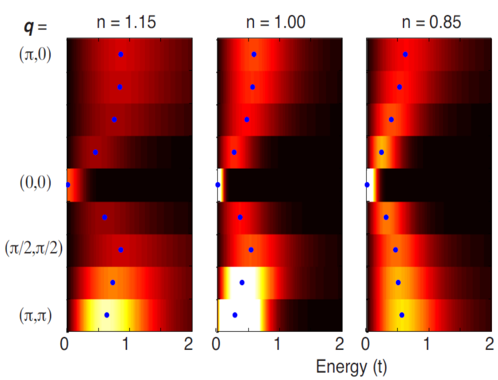

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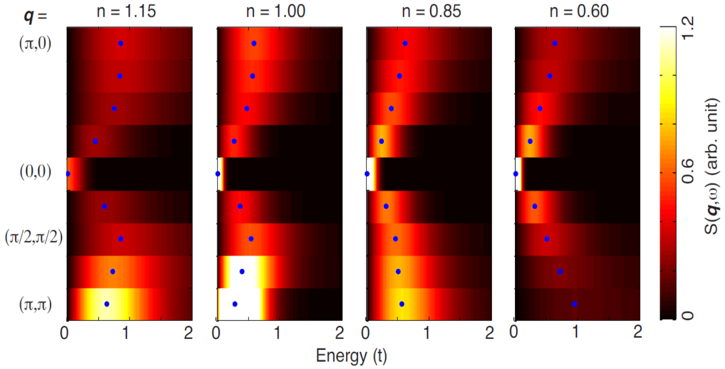

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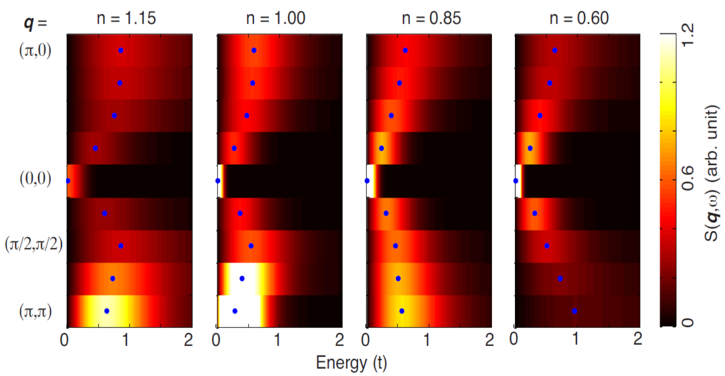

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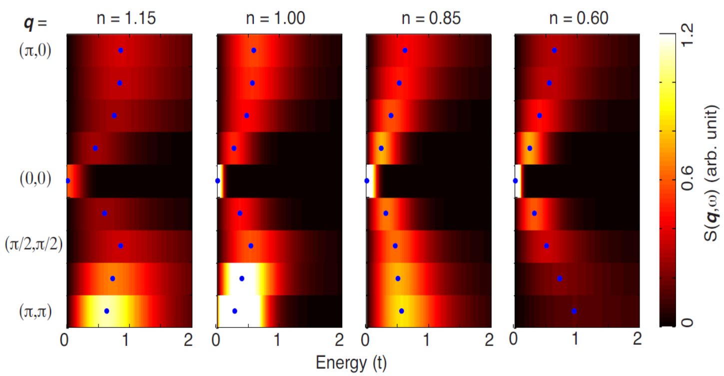

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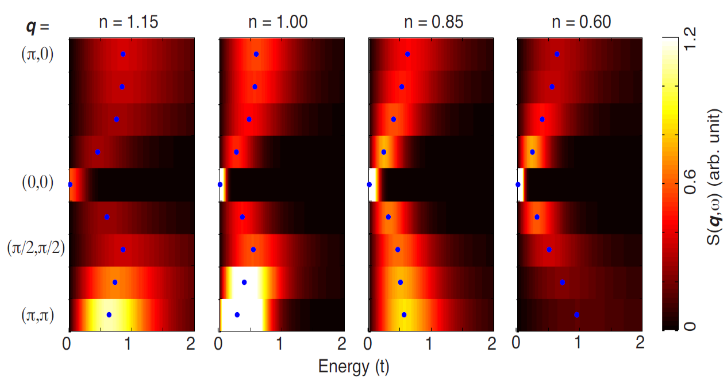

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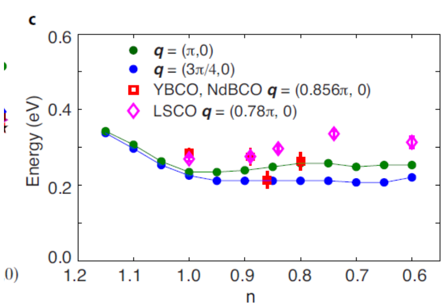

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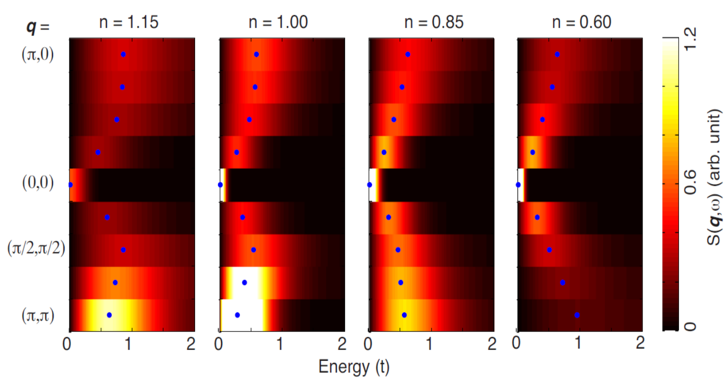

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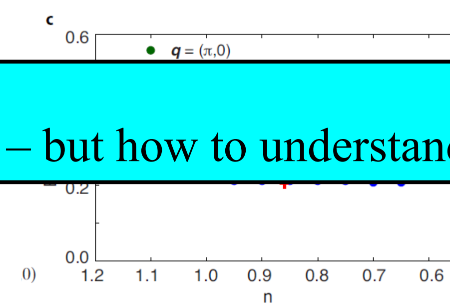
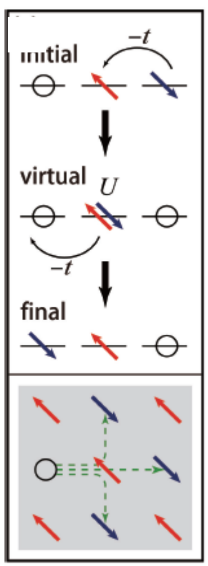


OK... – but how to understand it?

1. Persistence of spin excitations: theory

(A) Introducing the "three-site" terms

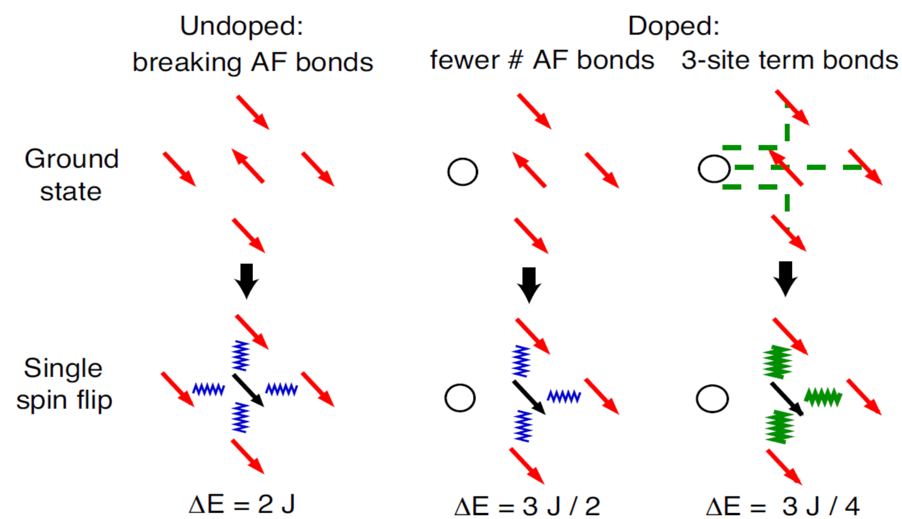
(often neglected but *a priori* present in *t-J*)



$$\mathcal{H}_{3s} = -\frac{J_{3s}}{4} \sum_{\substack{\langle \mathbf{i},\mathbf{j}\rangle,\langle \mathbf{i},\mathbf{j}'\rangle \\ \mathbf{j}\neq\mathbf{j}',\sigma}} \left(\tilde{c}^{\dagger}_{\mathbf{j}'\sigma} \tilde{n}_{\mathbf{i}\bar{\sigma}} \tilde{c}_{\mathbf{j}\sigma} + \tilde{c}^{\dagger}_{\mathbf{j}'\sigma} \tilde{c}^{\dagger}_{\mathbf{i}\bar{\sigma}} \tilde{c}_{\mathbf{i}\sigma} \tilde{c}_{\mathbf{j}\bar{\sigma}} \right)$$

(B) These terms are to a large extent

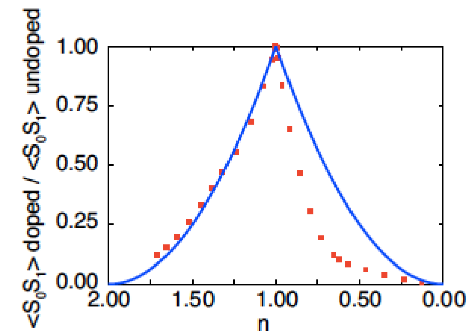
responsible for the lack of softening of "magnons"



1. Persistence of spin excitations: theory

Verifying that the 3-site terms are responsible for the persistence of "magnons":

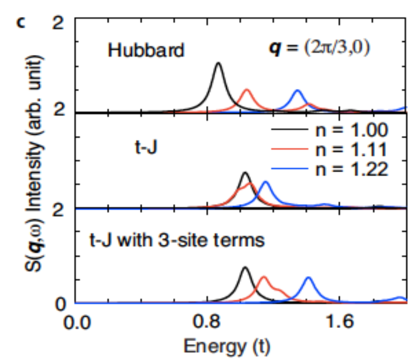
(A) Can such a 'static' picture apply to our situation?



→ Yes: on the electron-doped side (hole-doped side: more complex...)

(B) Do the 3-site terms support the hardening

on the el-doped side?



→ Yes, they seem to play a crucial role in hardening

1. Persistence of spin excitations: conclusions

Conclusions:

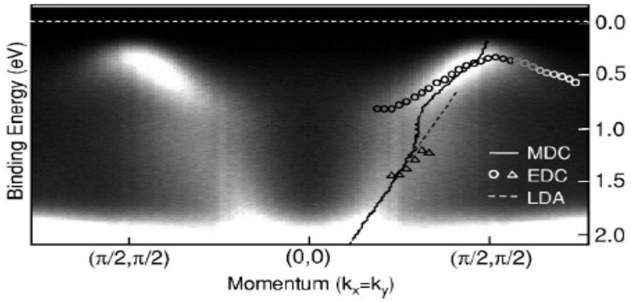
(1) “Magnons” survive doping in some parts of $\mathbf{q}$–ω phase space

(2) 3-site terms are important

What are the consequences of these findings for the electronic properties of cuprates?

2. Origin of strong dispersion of a hole: experiment

Basic features found in ARPES spectra on undoped cuprates...



ARPES spectrum of $Ca_2CuO_2Cl_2$ [PRB **71**, 094518 (2005)]

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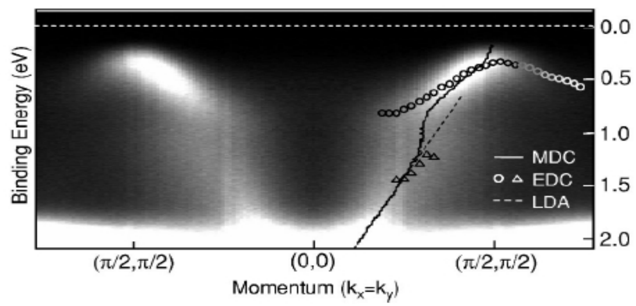

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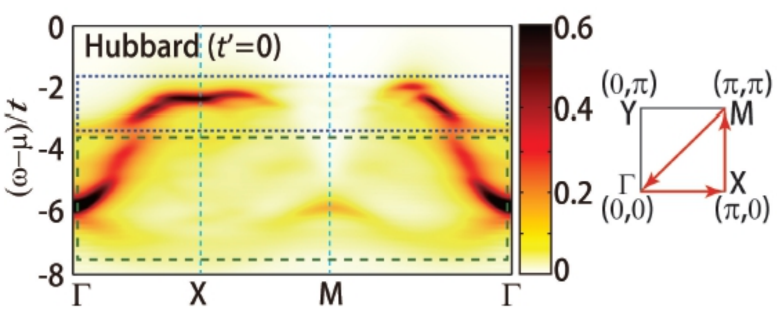

Cluster perturbation theory (CPT) + exact diagonalization (ED) for the Hubbard model

[for more on the method, see PRL **84**, 522 (2000)]

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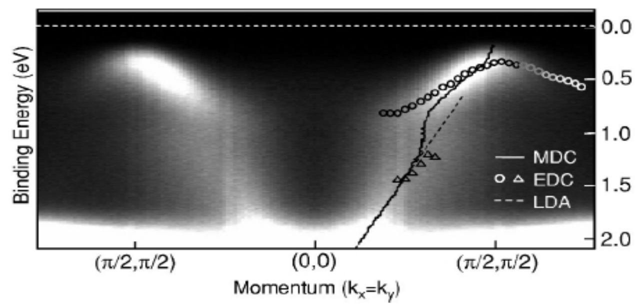

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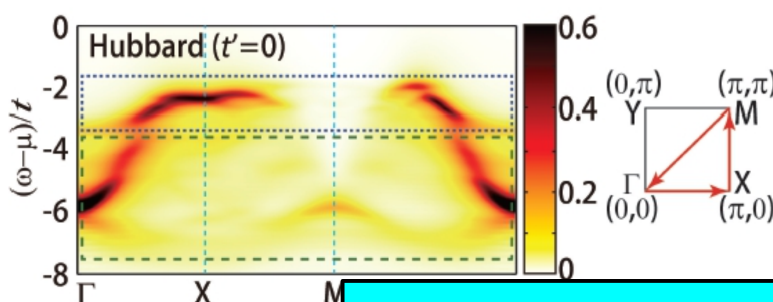

Cluster perturbation theory (CPT) + exact

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But how to understand this spectrum?

2. Origin of strong dispersion of a hole: theory

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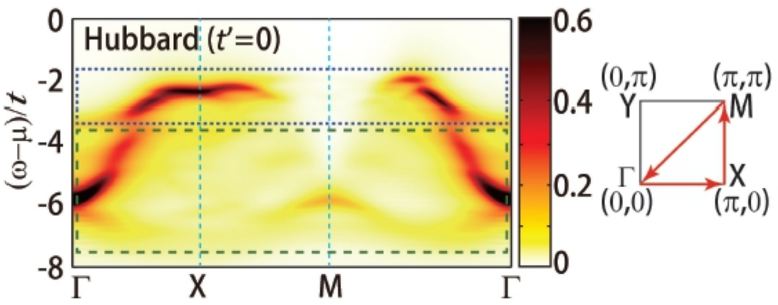

→ Understanding spectral function of undoped Hubbard:

2. Origin of strong dispersion of a hole: theory

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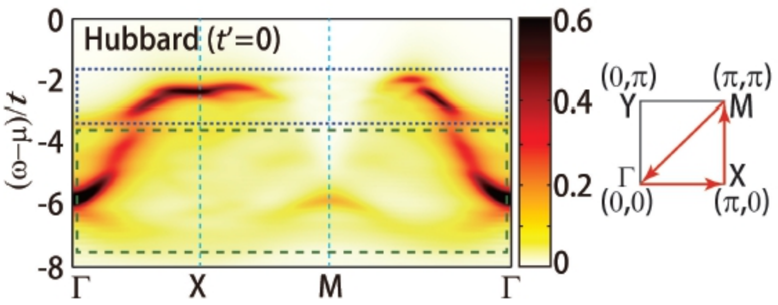
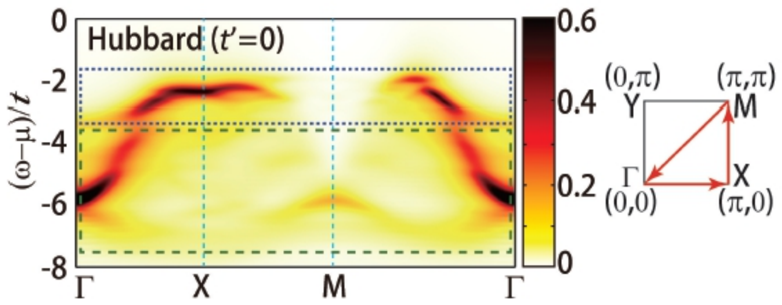


→ Understanding spectral function of undoped Hubbard:

– low binding energy: spin polaron

2. Origin of strong dispersion of a hole: theory

→ Hubbard spectrum:



→ Understanding spectral function of undoped Hubbard:

– low binding energy: spin polaron → OK

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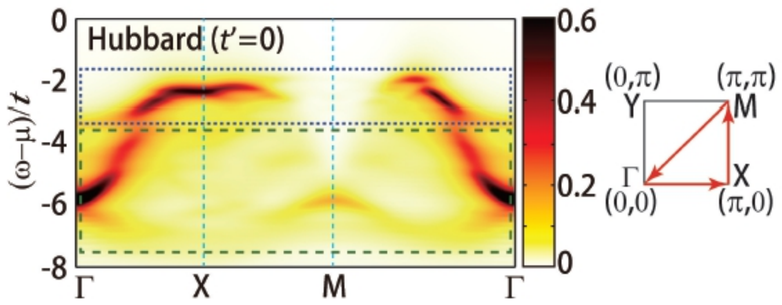

→ Understanding spectral function of undoped Hubbard:

– low binding energy: spin polaron

– high binding energy: SDW? spin-charge separation? *t*-physics?

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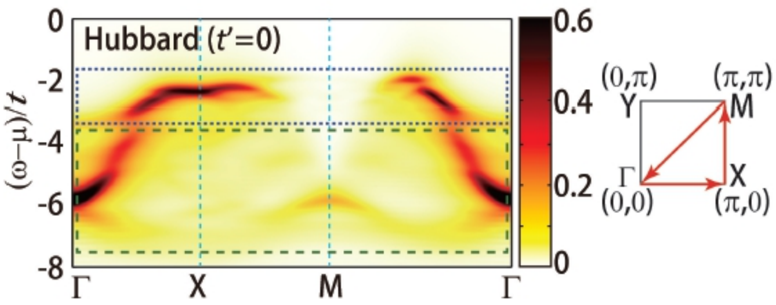


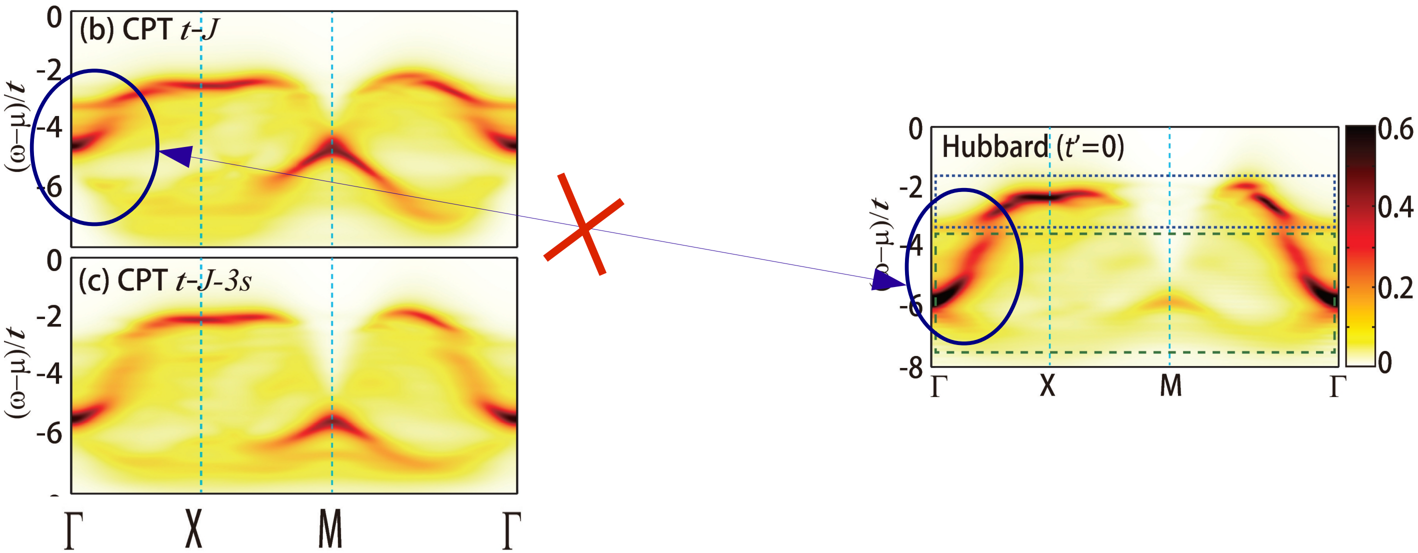
→ Understanding spectral function of undoped Hubbard:

– low binding energy: spin polaron

– high binding energy: SDW? spin-charge separation? *t*-physics?

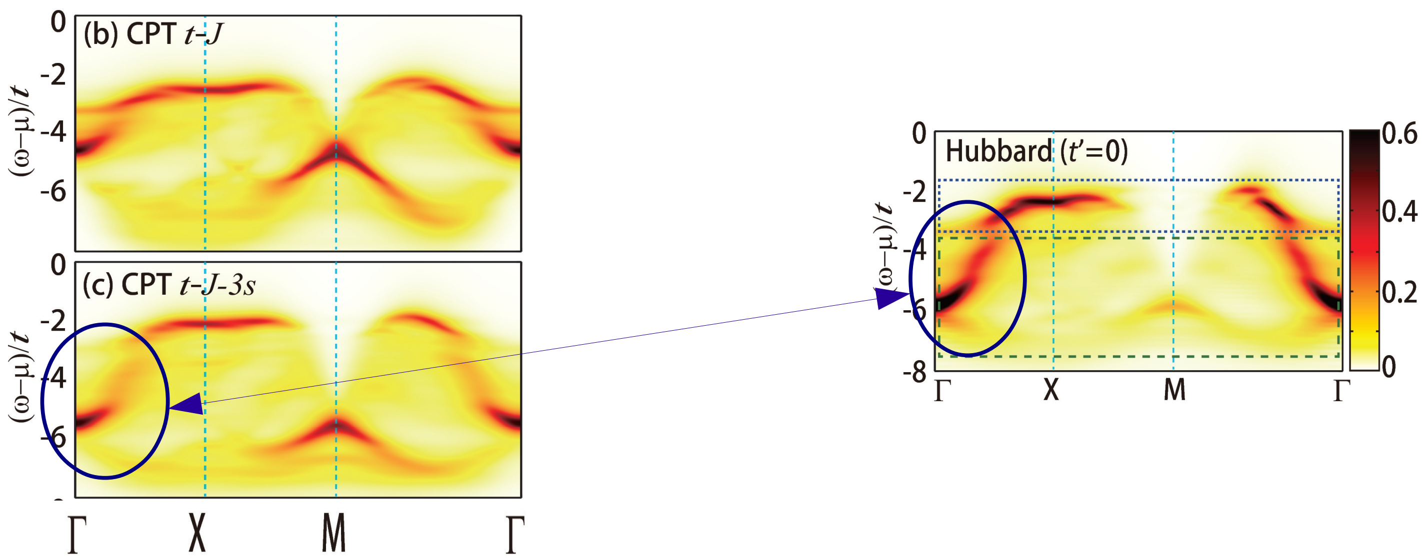
– why at all high and low binding energy ("waterfall")?

In fact: *t-J* model does not reproduce the Hubbard spectrum:



2. Origin of strong dispersion of a hole: theory

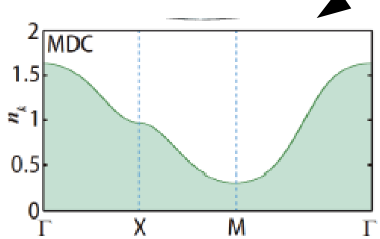
But <u>*t-J*-3-site</u> model basically reproduces the <u>Hubbard</u> model:

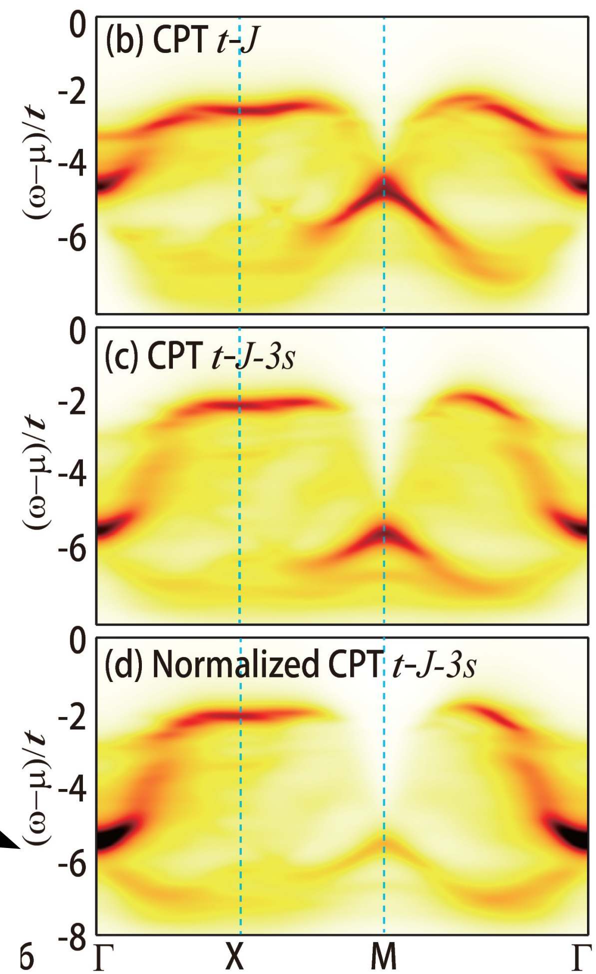


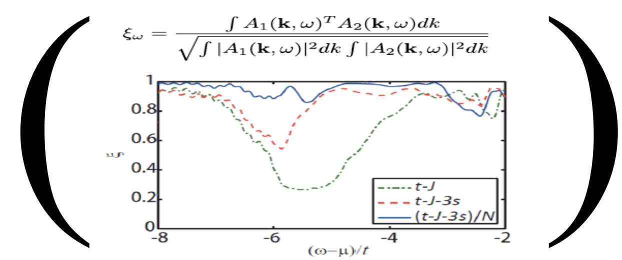
(BTW: different spectral weight sum rules → the remaining differences between these models)

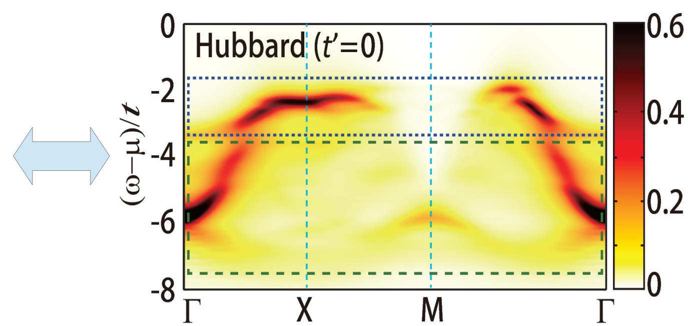
Intermezzo: detailed comparison of the models

Perfect agreement between *t-J-3s* and Hubbard after 'normalization'



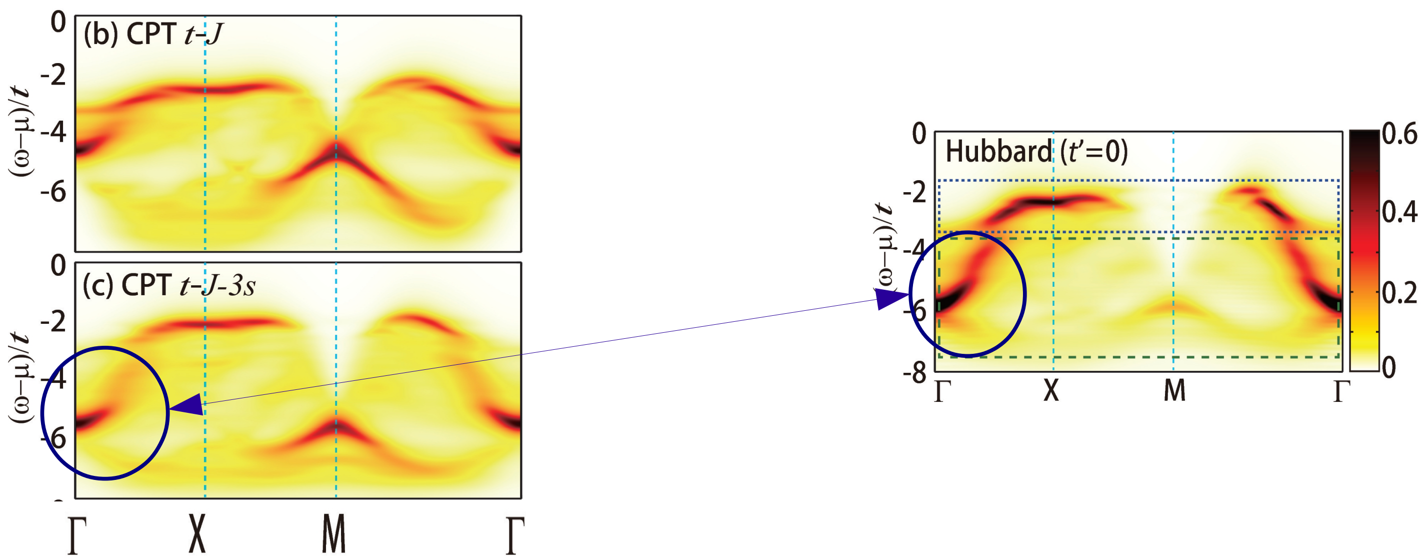






2. Origin of strong dispersion of a hole: theory

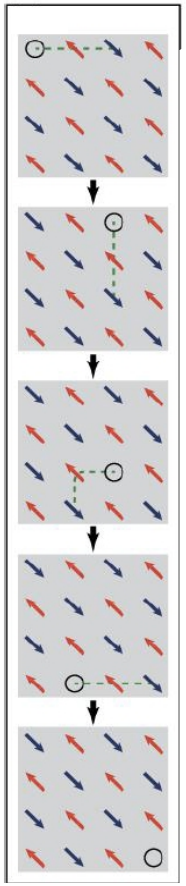
3-site terms responsible for the onset of the high binding energy part of the spectrum...

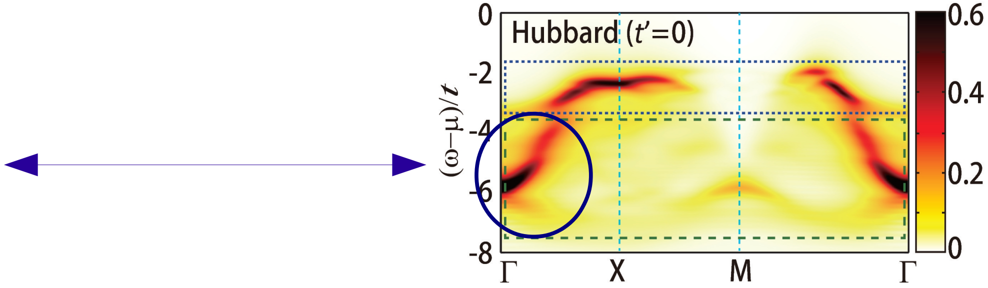


… and for the apparent dispersion

2. Origin of strong dispersion of a hole: theory

3-site terms → strong dispersion in the high binding energy part of the spectrum...

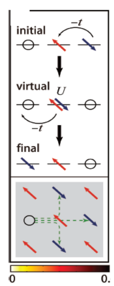


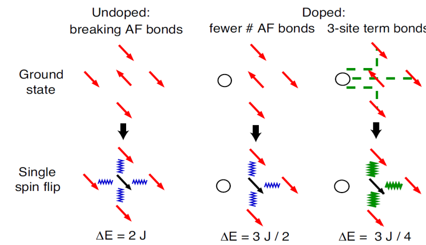


… which was also verified in detail using SCBA and is the main conclusion of 2.

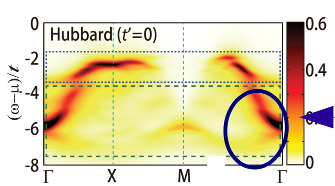
3. Conclusions

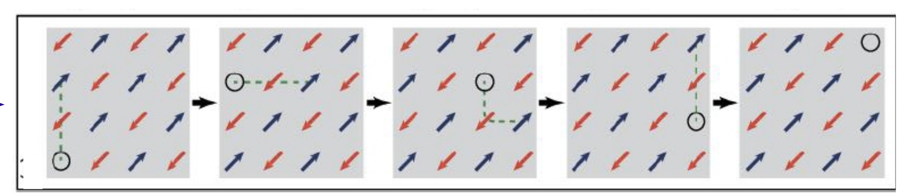
1. 3-site terms → persistence of magnetic excitations upon doping the cuprates:





2. 3-site terms → strong dispersion of a hole in the undoped cuprates:





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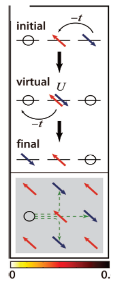

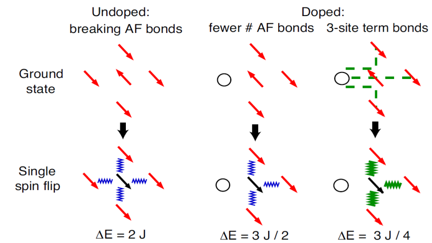

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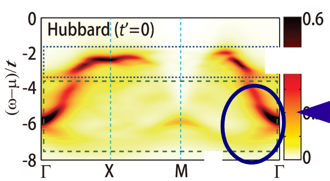
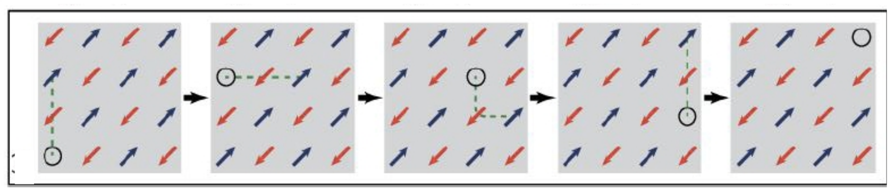




3. What connects these 2 stories:

→ 3-site terms play an important role in the cuprate / 2D Hubbard physics

→ 2 sides of the same phenomenon =

holes & "magnons" are <u>not "fighting with each other"</u> (in some part of **q**–ω space)

Appendix: 3-site terms → dispersion in the spectrum

But do we observe a real

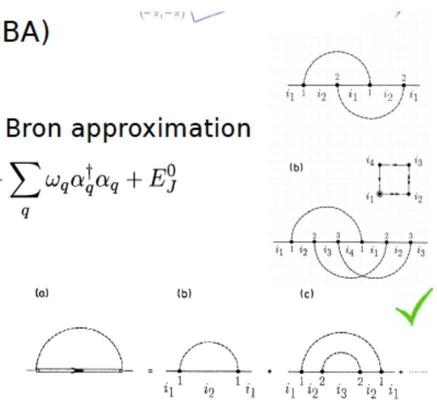
dispersion?

→ use another method – SCBA

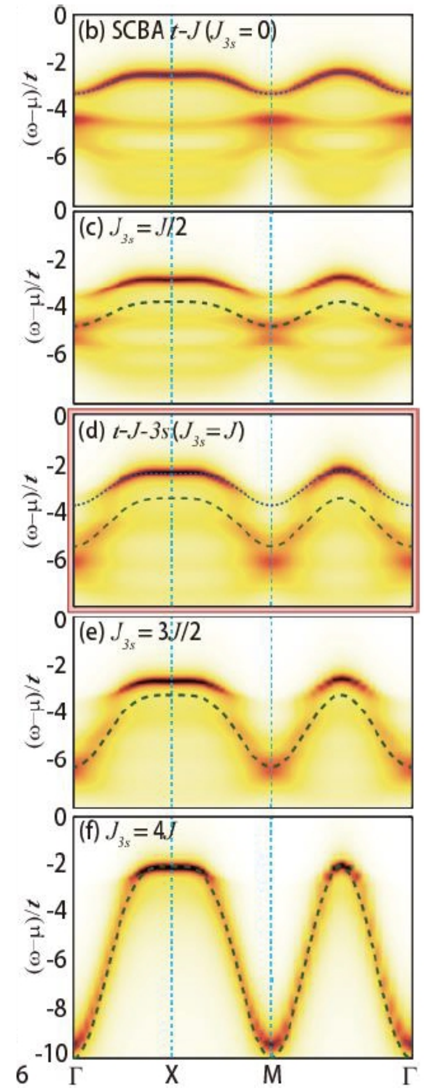
- Self-Consistent Born Approximation (SCBA)
  - Linear Spin Wave (LSW) theory
  - Polaronic Hamiltonian and Self-consistent Bron approximation

$$H_{tJ} = \frac{zt}{\sqrt{N}} \sum_{k,q} \left[h_k^\dagger h_{k-q} \alpha_q (u_q \gamma_{k-q} + v_q \gamma_k) + h.c. \right] + \sum_q \omega_q \alpha_q^\dagger \alpha_q + E_J^0$$

$$\Sigma(k,\omega) = \frac{z^2 t^2}{N} \sum \frac{M^2(k,q)}{\omega - \omega_q - \Sigma(k-q, \omega - \omega_q)}$$



Sénéchal *et al.* *Phys. Rev. Lett.* **84**, 522 (2000)
Martinez *et al.* *Phys. Rev. B* **44**, 317 (1991)

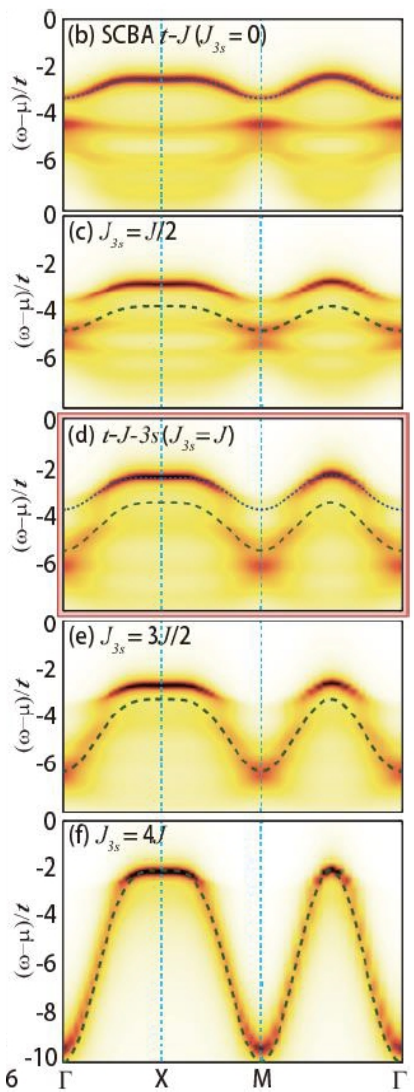


→ indeed – 'dispersion' survives

→ tune 3-site terms

→ indeed – it is a dispersion

Appendix: 3-site terms → dispersion in the spectrum



Finally:

→ this dispersion is *not* renormalized

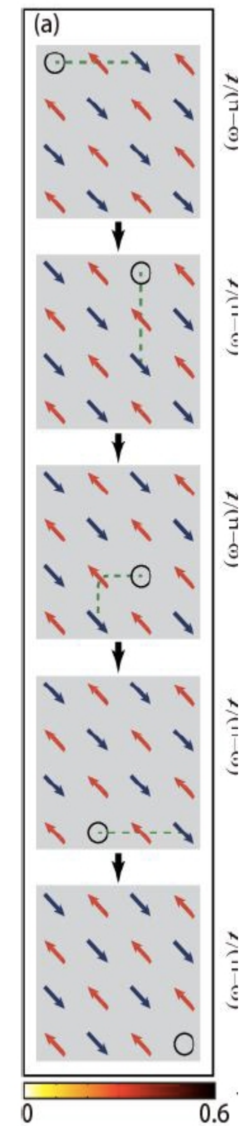
by coupling to magnons:

$$\epsilon_{\mathbf{k}}^{\mathrm{IASH}} = -\frac{U}{2} - \frac{J_{3s}}{2}\left[\cos 2k_x + \cos 2k_y + 4\cos k_x \cos k_y\right]$$

→ so the hole moves as in this cartoon

→ for experts: if bosons were immobile,

this would be different



Appendix: 3-site terms → dispersion in the spectrum

If magnons immobile (*t-J* 'Ising' model),

free dispersion due to 3-site strongly renormalized:

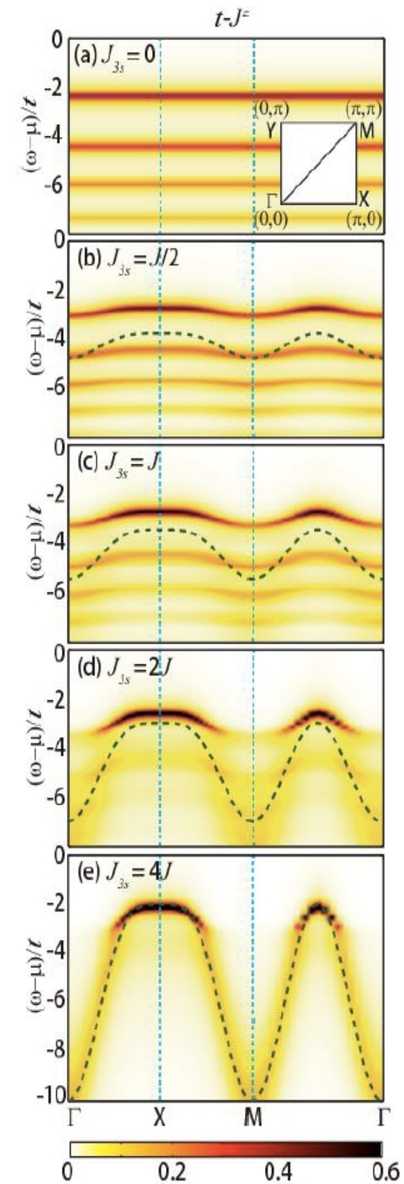
→ similar to the story of the orbital model

[cf. PRL **100**, 066403 (2008); PRB **78**, 214423 (2008)]

→ this would be the same for any polaronic model:

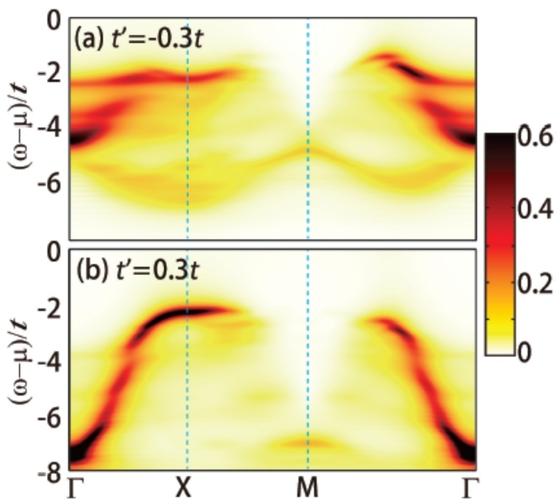
bosons immobile → free fermionic dispersion renormalized

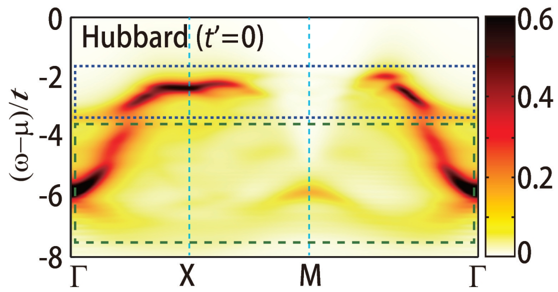
bosons dispersive → free fermionic dispersion shows up freely



Appendix: insight from tuning t'

→ let us add t':





→ indeed: low and high binding features separate

→ low binding part little affected by t'

→ high binding part: huge changes with t'

Appendix: insight from tuning t'

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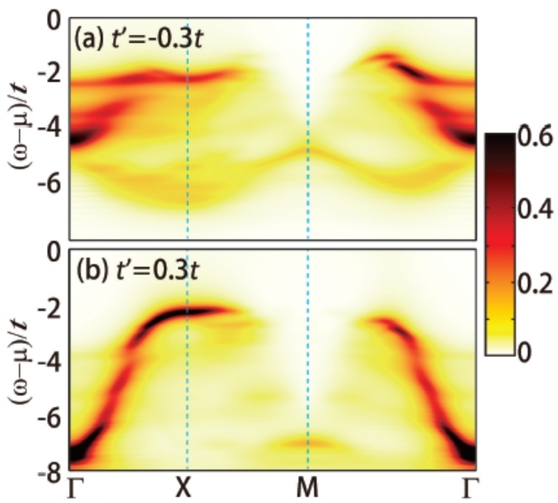

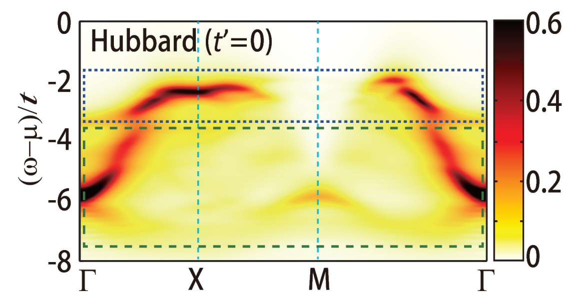

→ high binding part: huge changes with t'

→ high binding feature due to NNN hopping?

→ but can this happen even when t'=0?