Excitons

in the spin-orbital systems

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Acknowledgments

Orbital excitons / cuprates:

Justina Schlappa, Cheng-Chien Chen, Maria Daghofer, Maurits Haverkort, Thorsten Schmitt, Valentina Bisogni, Jeroen van den Brink, *et al.*

Spin-orbital excitons / iridates:

Ekaterina Plotnikova, Maria Daghofer, BJ Kim, Marco Moretti, Jeroen van den Brink, *et al.*

Alexander von Humboldt
Stiftung/Foundation

IFW

Leibniz Institute
for Solid State and
Materials Research
Dresden

SLAC
NATIONAL ACCELERATOR
LABORATORY

LELAND STANFORD JUNIOR UNIVERSITY
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1891

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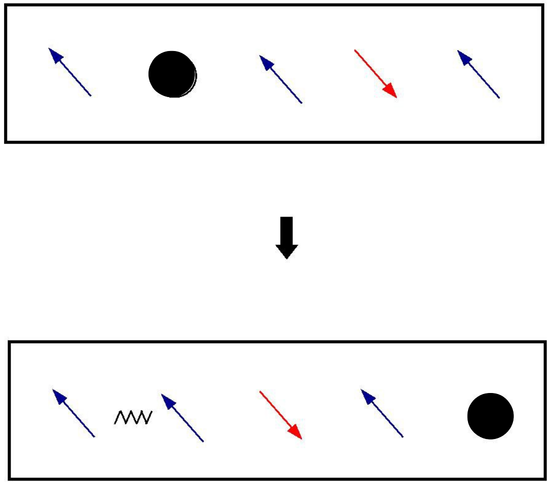
Office of Science

Motivation: single hole in 1D antiferromagnet

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



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

→ **paradigm**: spin-charge separation in 1D [T. Giamarchi, *Quantum Physics in One Dimension* (2004)]

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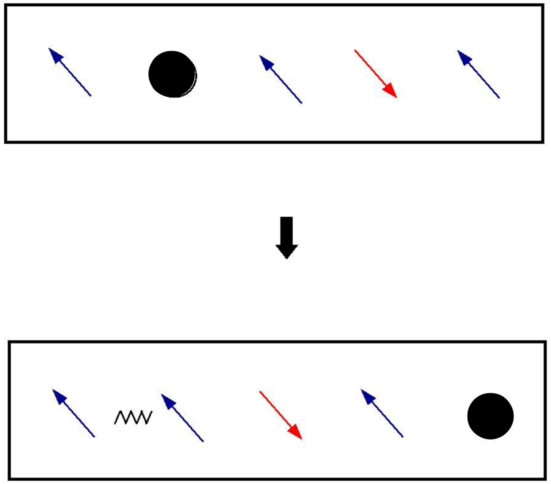

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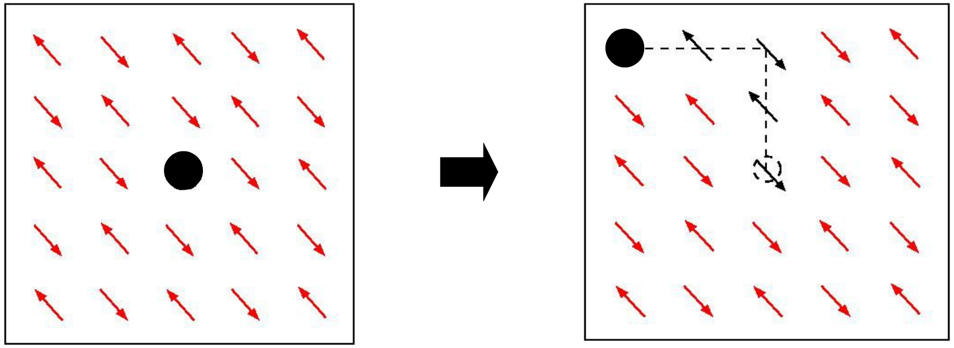
→ observed by ARPES on undoped quasi-1D cuprates [C. Kim *et al.*, PRL **77**, 4054 (1996)]

Motivation: single hole in 2D antiferromagnet

Putting 1 hole into the 2D AF (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

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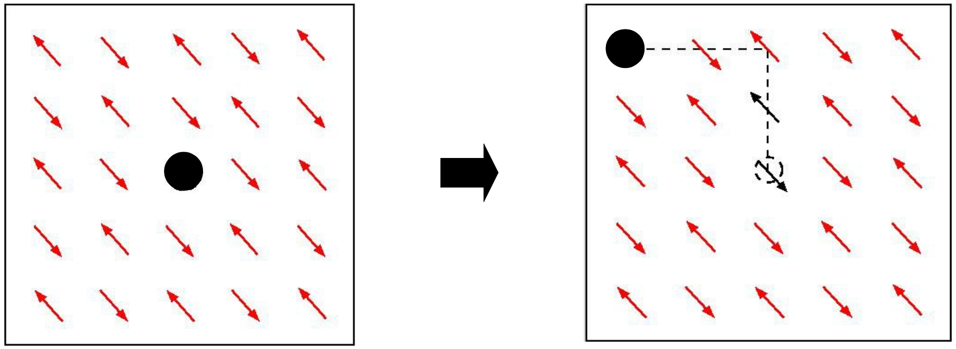

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→ **paradigm**: but quantum fluctuations help and spin polaron formed in 2D

[G. Martinez & P. Horsch, PRB **44**, 317 (1991)]

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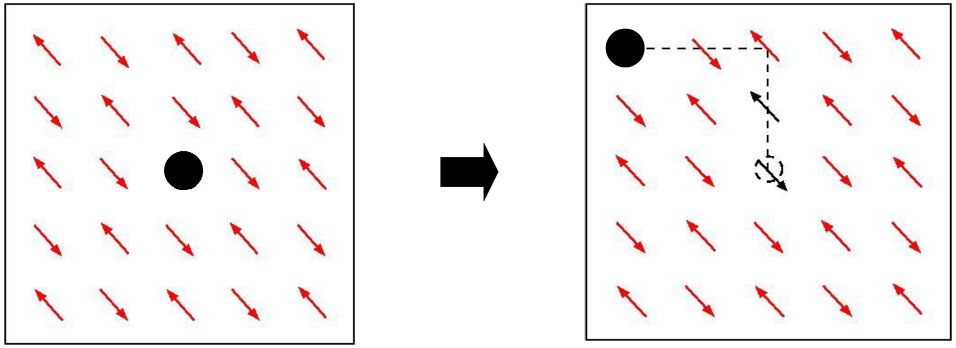

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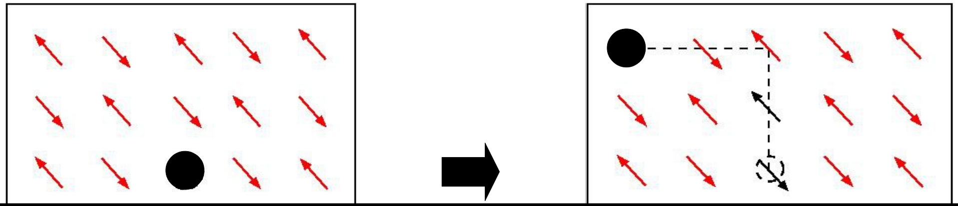

How generic are these paradigms?

Can we find similar physics in other correlated systems?

→ hole (~hol

ving

→ not only spin and charge does *not* separate but even... holon motion hindered by magnons

→ **paradigm**: but quantum fluctuations help and spin polaron formed in 2D

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Outline

1. Spin-orbital separation in quasi-1D cuprates:

   – theory

   – experiment

   – postsciptum (PS)

2. Polaronic motion of j=3/2 spin-orbital excitons in quasi-2D iridates:

   – theory

   – experiment

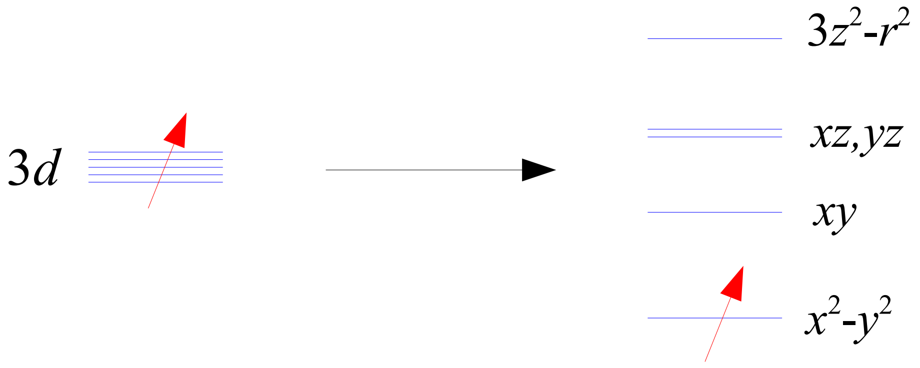
   – postscriptum (PS)

3. Conclusions

1. Spin-orbital separation in quasi-1D cuprates: theory

Single Cu^{2+} ion in Sr$_2$CuO$_3$ (1 hole in 3*d* orbitals):

crystal field → hole with $s=1/2$ spin in the x^2-y^2 orbital (ground state) & 4 excited orbitals



1D lattice of Sr$_2$CuO$_3$:

hopping + Coulomb repulsion → low energy: Heisenberg superexchange between $s=1/2$ spins

$$\mathcal{H} = J \sum_{\langle ij \rangle} \left(\mathbf{S}_i \mathbf{S}_j + \frac{1}{4} \right)$$

[KW *et al.*, PRL **107**, 147201 (2011); KW *et al.*, PRB **88**, 195138 (2013)]

1. Spin-orbital separation in quasi-1D cuprates: theory

How does orbital excitation move in 1D s=1/2 AF?

1st step: 1D AF and ferroorbital (FO) ground state

[KW *et al.*, PRL **107**, 147201 (2011); KW *et al.*, PRB **88**, 195138 (2013)]

1. Spin-orbital separation in quasi-1D cuprates: theory

How does orbital excitation move in 1D s=1/2 AF?

1st step: 1D AF and FO

2nd step: we create orbital excitation (also called: exciton)

[KW *et al.*, PRL **107**, 147201 (2011); KW *et al.*, PRB **88**, 195138 (2013)]

1. Spin-orbital separation in quasi-1D cuprates: theory

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How does orbital excitation move in 1D $s=1/2$ AF?

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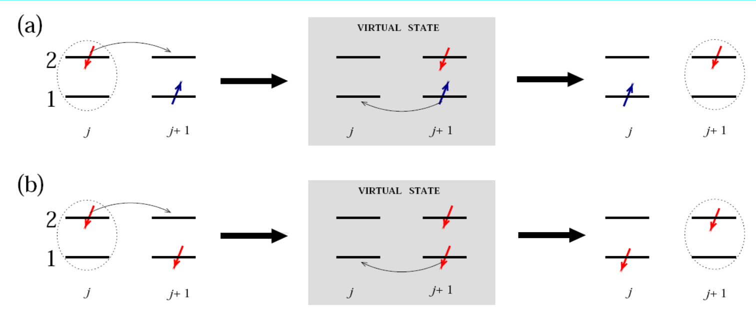
3rd step: orbital excitation moves and creates 1 spinon

Spin of electron in the upper orbital is *conserved*

during this superexchange process

(a rather realistic assumption):



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4th step: further motion does *not* create more spinons

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⬇

$(\Delta T=1, \Delta S=\frac{1}{2}) \rightarrow \Delta T=1 + \Delta S=\frac{1}{2}$

orbital excitation → orbiton + spinon

⬇

spin-orbital separation

[KW *et al.*, PRL **107**, 147201 (2011); KW *et al.*, PRB **88**, 195138 (2013)]

1. Spin-orbital separation in quasi-1D cuprates: theory

How does orbital excitation move in 1D *s*=1/2 AF?

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(ΔT=1, ΔS=½)

orbital excitatio

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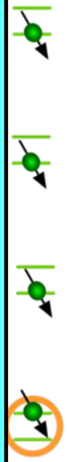


Note:

spin-orbital separation ~ spin-charge separation

In fact:

exact mapping between these two phenomena

(spin-orbital model of Kugel-Khomskii type and *t-J* model)

[KW *et al.*, PRL **107**, 147201 (2011); KW *et al.*, PRB **88**, 195138 (2013)]

1. Spin-orbital separation in quasi-1D cuprates: experiment

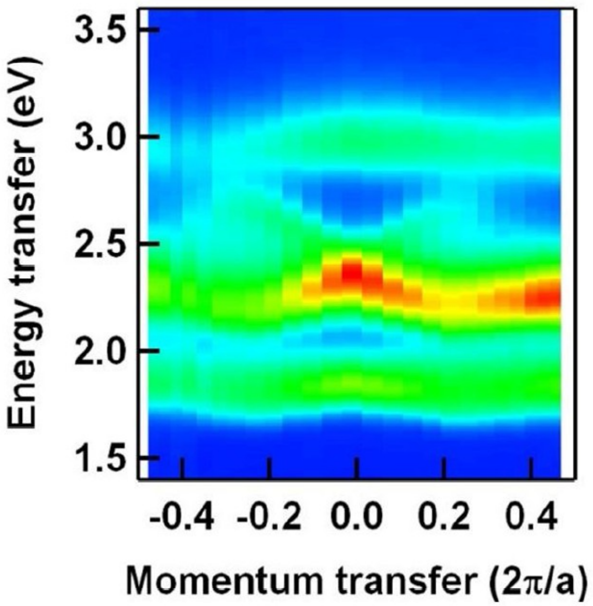
Resonant inelastic x-ray scattering (RIXS) at Cu L_3 edge in $\mathrm{Sr_2CuO_3}$

[J. Schlappa *et al.,* Nature **485**, 82 (2012); V. Bisogni *et al.*, PRL **114**, 096402 (2015)]

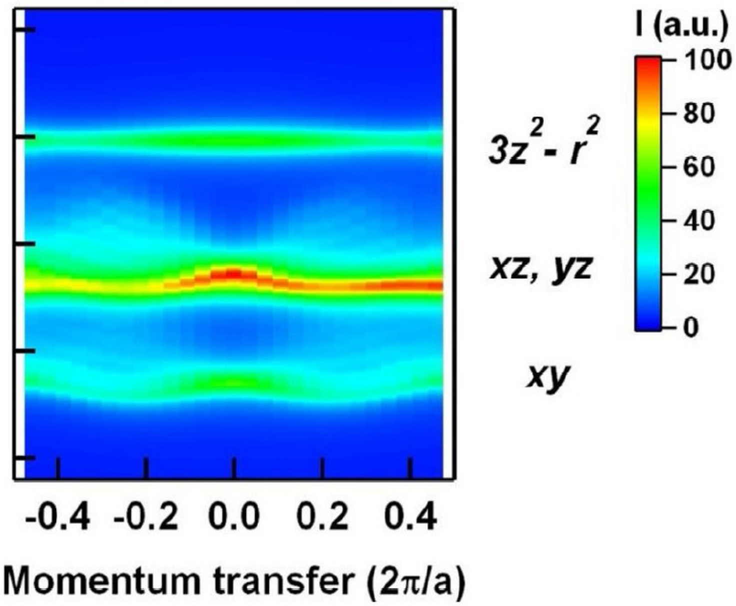
1. Spin-orbital separation in quasi-1D cuprates: experiment

Excellent agreement with the experiment and theory (~spin-orbital model)

RIXS experiment



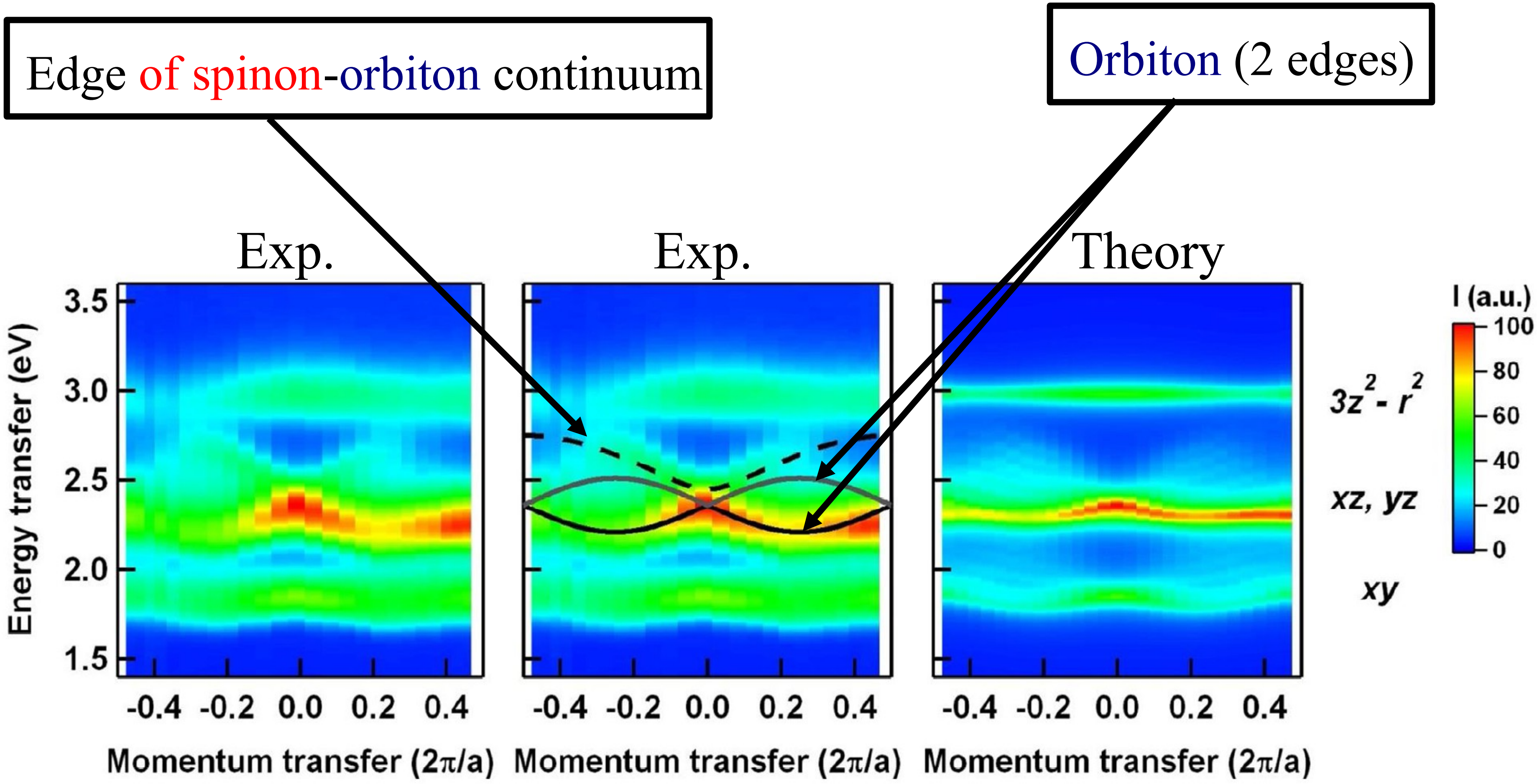
Theory (exact diagonalization)



[J. Schlappa *et al.,* Nature **485**, 82 (2012); V. Bisogni *et al.*, PRL **114**, 096402 (2015)]

1. Spin-orbital separation in quasi-1D cuprates: experiment

But where is the 'pure' orbiton?



Edge of spinon-orbiton continuum

Orbiton (2 edges)

Exp.

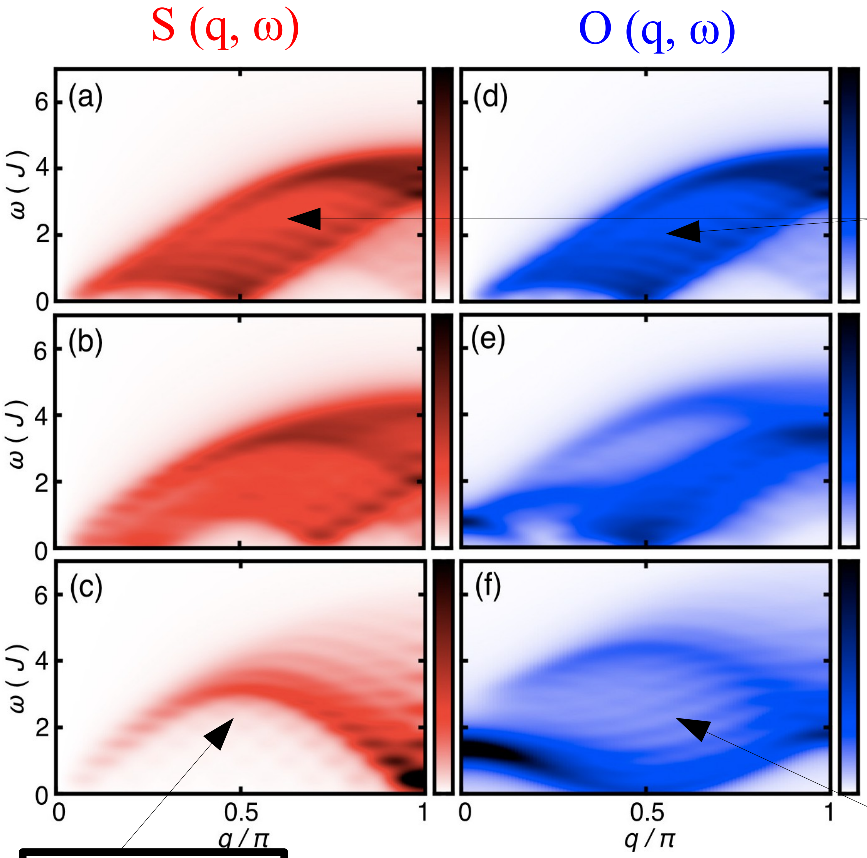
Exp.

Theory

[J. Schlappa *et al.,* Nature **485**, 82 (2012); V. Bisogni *et al.*, PRL **114**, 096402 (2015)]

1. Spin-orbital separation in quasi-1D cuprates: PS

The above physics is *only* valid when strong crystal field fully polarizes the ground state (FO state)



No crystal field ('Bethe' chain, SU(4) symmetry)

identical

Moderate crystal field

Strong crystal field (FO ground state)

spin-orbital separation spectrum

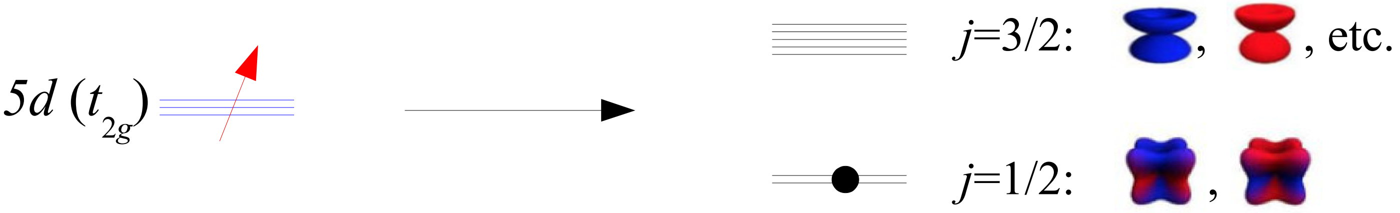
like 1D AF

[C. C. Chen *et al.*, PRB **91**, 165102 (2015)]

2. Polaronic motion of j=3/2 spin-orbital excitons in quasi-2D iridates: theory

Single Ir^{4+} ion in $\mathrm{Sr_2IrO_4}$ (1 hole in 5*d* orbitals):

crystal field + spin-orbit → hole in j=1/2 spin-orbital isospin ground state and j=3/2 excitations



2D lattice of $\mathrm{Sr_2IrO_4}$:

hopping + Coulomb repulsion → low energy: Heisenberg superexchange between j=1/2 isospins

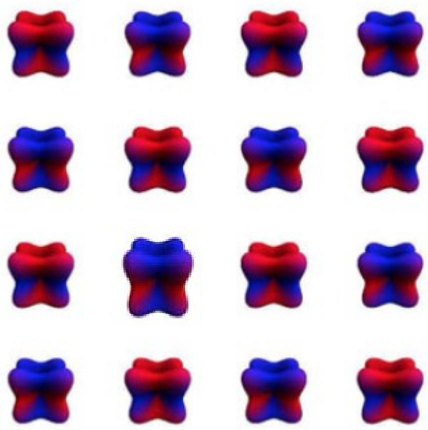
$$\mathcal{H} = J\sum_{\langle ij\rangle}\left(\mathbf{S}_i\mathbf{S}_j+\frac{1}{4}\right)$$

[J. Kim *et al.*, PRL **108**, 177003 (2012); J. Kim *et al.*, Nature Communications **5**, 4453 (2014)]

2. Polaronic motion of *j*=3/2 spin-orbital excitons in quasi-2D iridates: theory

How does *j*=3/2 spin-orbital excitation move in 2D *j*=1/2 AF?

1st : ground state is a 2D AF formed by *j*=1/2 isospins



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2. Polaronic motion of j=3/2 spin-orbital excitons in quasi-2D iridates: theory

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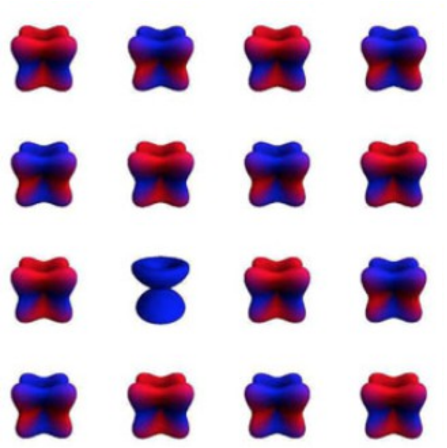
2nd : we create a single j=3/2 excitation in the ground state

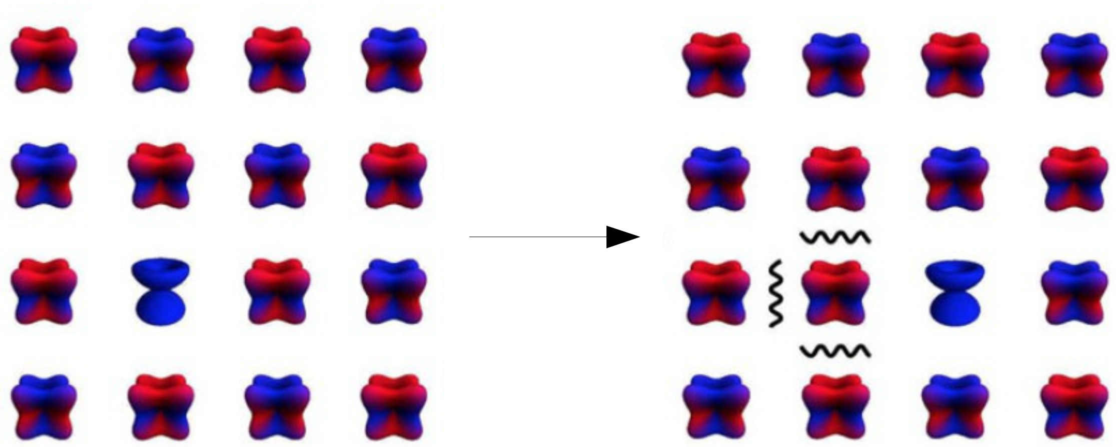


[J. Kim *et al.*, PRL **108**, 177003 (2012); J. Kim *et al.*, Nature Communications **5**, 4453 (2014)]

2. Polaronic motion of j=3/2 spin-orbital excitons in quasi-2D iridates: theory

How does j=3/2 spin-orbital excitation move in 2D j=1/2 AF?

3rd : we propagate it to the *nn* site via superexchange process → a j=1/2 magnon left behind

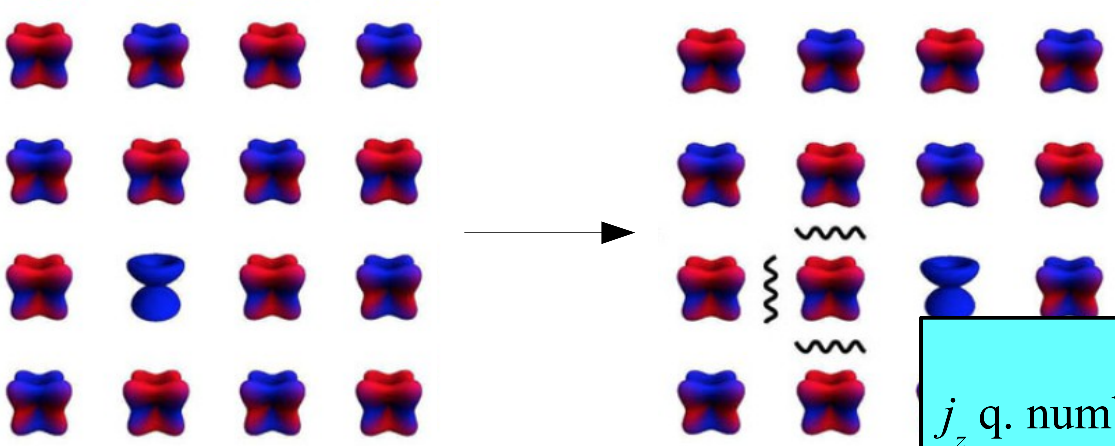


[J. Kim *et al.*, PRL **108**, 177003 (2012); J. Kim *et al.*, Nature Communications **5**, 4453 (2014)]

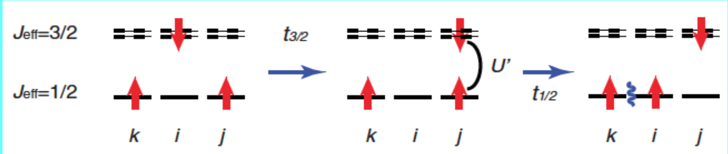
2. Polaronic motion of $j=3/2$ spin-orbital excitons in quasi-2D iridates: theory

How does $j=3/2$ spin-orbital excitation move in 2D $j=1/2$ AF?

3rd : we propagate it to the *nn* site via superexchange process → a $j=1/2$ magnon left behind



j_z q. number of the electron in the j=3/2 state *conserved* during this superexchange process (a rather realistic assumption):

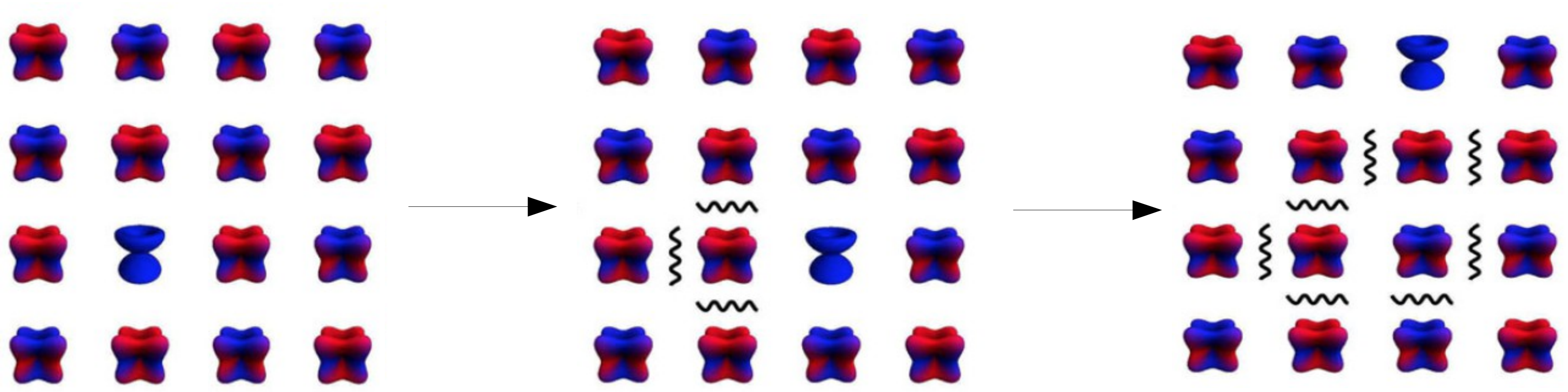


[J. Kim *et al.*, PRL **108**, 177003 (2012); J. Kim *e*

2. Polaronic motion of *j*=3/2 spin-orbital excitons in quasi-2D iridates: theory

How does *j*=3/2 spin-orbital excitation move in 2D *j*=1/2 AF?

4th : we propagate the excitation further → *more* magnons left behind



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2. Polaronic motion of j=3/2 spin-orbital excitons in quasi-2D iridates: theory

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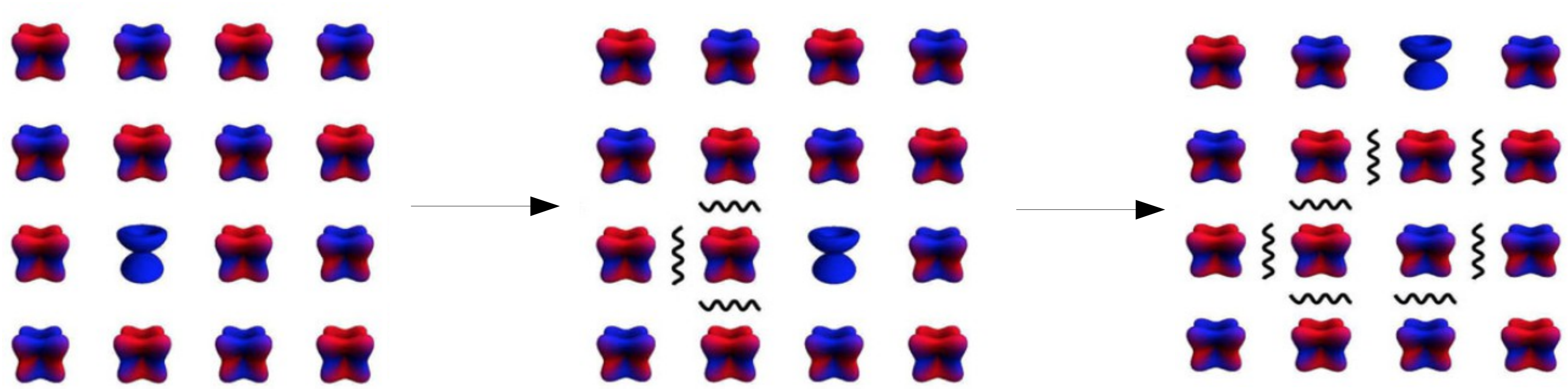


Only motion by coupling to spin fluctuations possible, just like for a hole in 2D AF

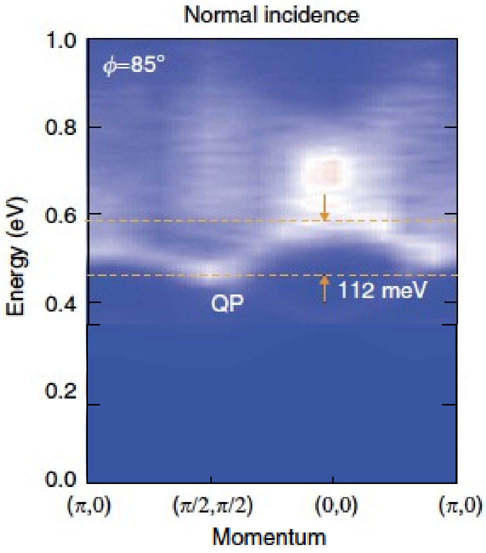
→ also in this case the j=3/2 exciton moves as a polaron

[J. Kim *et al.*, PRL **108**, 177003 (2012); J. Kim *et al.*, Nature Communications **5**, 4453 (2014)]

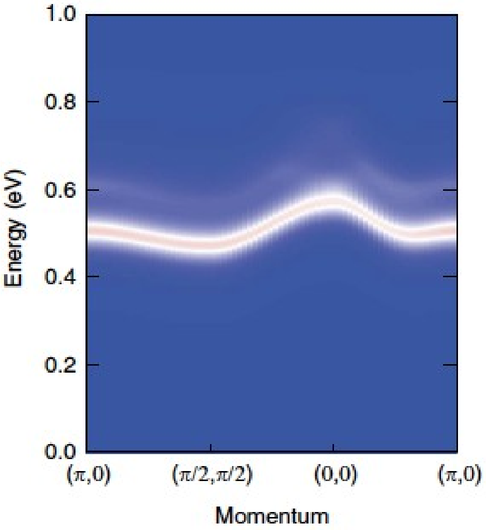
2. Polaronic motion of *j*=3/2 spin-orbital excitons in quasi-2D iridates: experiment

Good agreement between experiment and theory

Ir L_3 edge RIXS on Sr_2IrO_4



Self-consistent Born approximation calculations

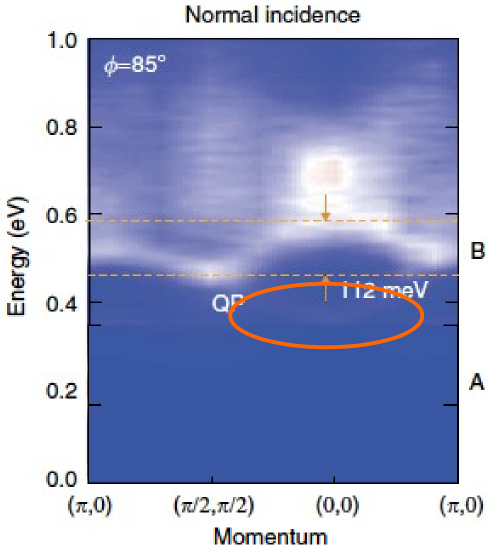


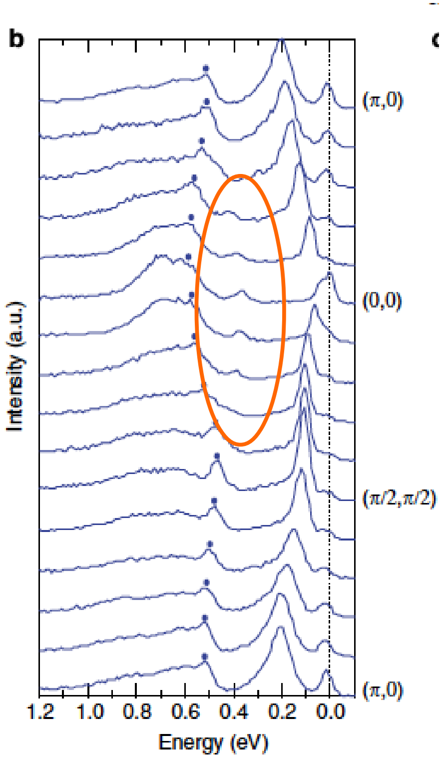
Note: theoretical calculations include the polaronic motion of the *j*=3/2 excitons

[J. Kim *et al*., PRL **108**, 177003 (2012); J. Kim *et al*., Nature Communications **5**, 4453 (2014)]

2. Polaronic motion of j=3/2 spin-orbital excitons in quasi-2D iridates: PS

Is that the full story?



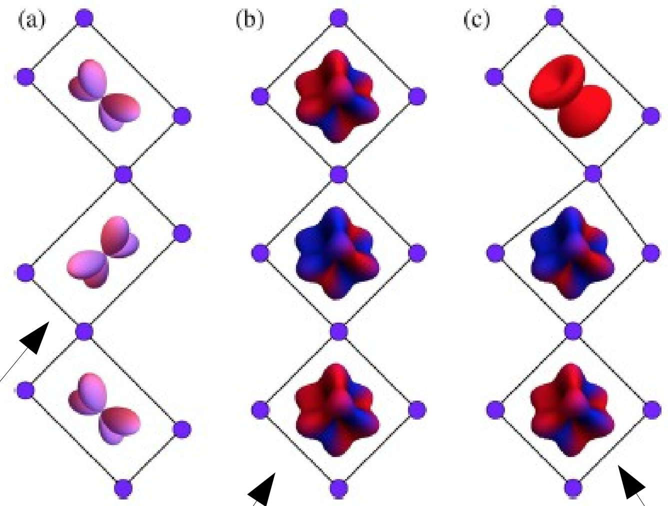


What is the origin of the small branch of the exciton dispersion with the minimum at Γ?

[J. Kim *et al.*, PRL **108**, 177003 (2012); J. Kim *et al.*, Nature Communications **5**, 4453 (2014)]

2. Polaronic motion of *j*=3/2 spin-orbital excitons in quasi-2D iridates: PS

Not in the previous model: the Jahn-Teller interaction between *j*=3/2 and *j*=1/2 isospins



Jahn-Teller for t_{2g} orbitals

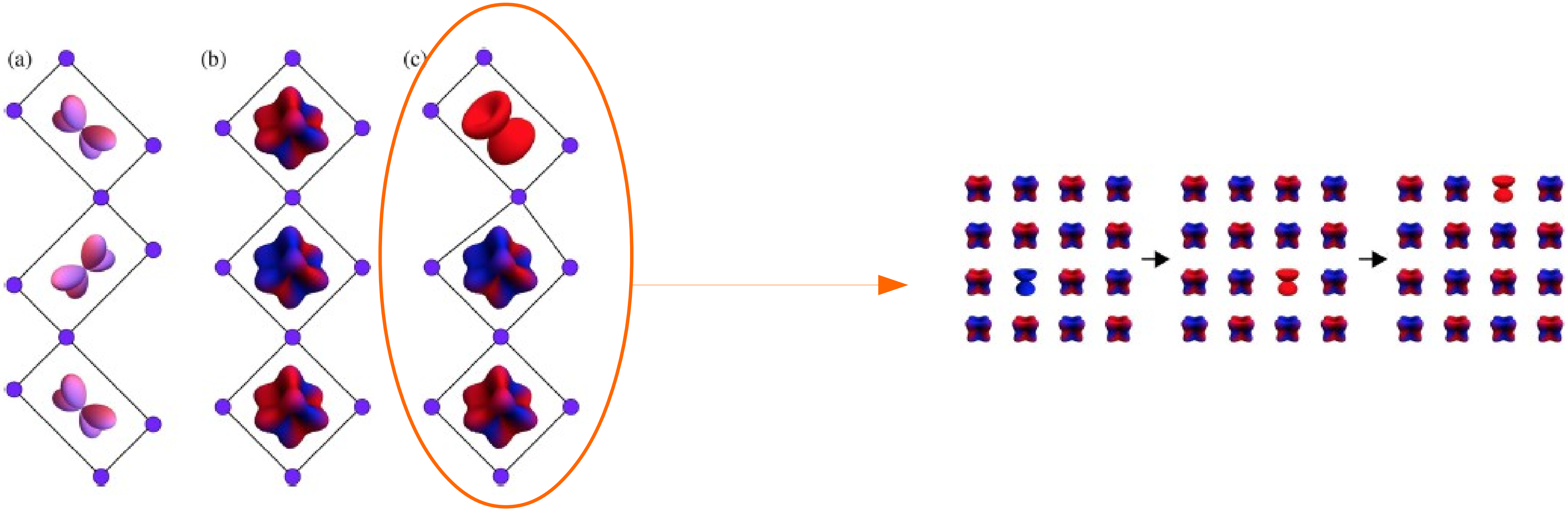
No Jahn-Teller for *j*=1/2

Jahn-Teller for *j*=3/2 and *j*=1/2

[E. M. Plotnikova *et al*.,, Phys. Rev. Lett. **116**, 106401 (2016)]

2. Polaronic motion of *j*=3/2 spin-orbital excitons in quasi-2D iridates: PS

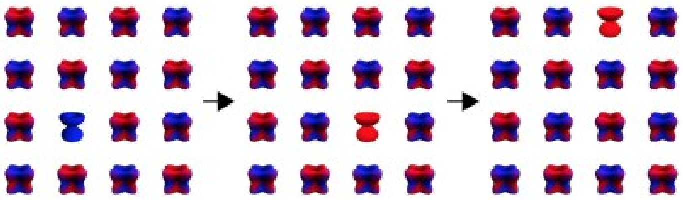
This allows for the hopping of *j*=3/2 exciton which does not introduce defects in AF...

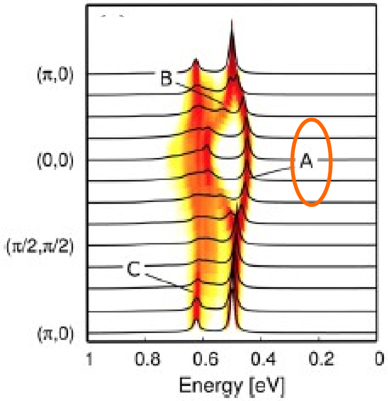


[E. M. Plotnikova *et al*.,, Phys. Rev. Lett. **116**, 106401 (2016)]

2. Polaronic motion of $j=3/2$ spin-orbital excitons in quasi-2D iridates: PS

… and it may explain the extra feature with minimum at Γ in RIXS (peak “A”)





[superexchange and Jahn-Teller;

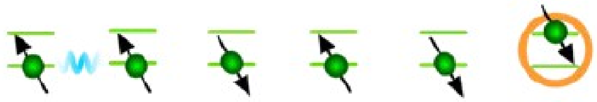
self-consistent Born approximation]

[E. M. Plotnikova *et al*.,, Phys. Rev. Lett. **116**, 106401 (2016)]

3. Conclusions

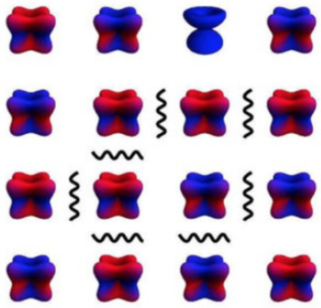
1. Motion of orbital exciton in quasi-1D cuprates:

spin-orbital separation, just like spin-charge separation (note: valid only for strong crystal field)



2. Motion of spin-orbital exciton in quasi-2D iridates:

polaronic type of motion, just like for a hole in 2D AF (though Jahn-Teller changes it a bit)

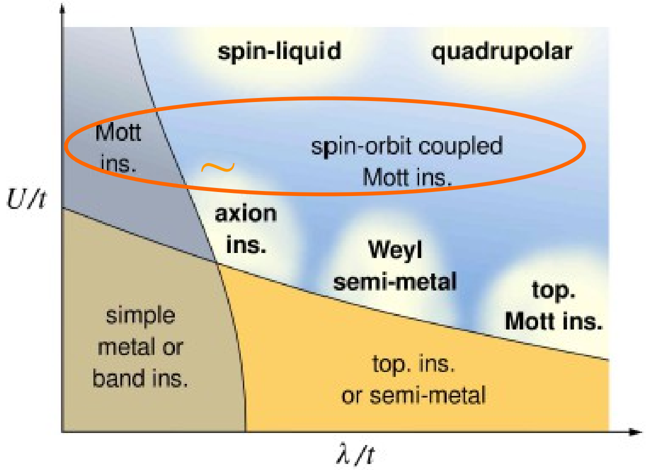


Take-home message

Systems *without* strong on-site spin-orbit coupling ("3d": cuprates, manganites, etc.)

are NOT always very different from

the ones *with* strong on-site spin-orbit coupling ("5d": iridates, osmates, etc.)



[W. Witczak-Krempa, Annual Review of Condensed Matter Physics, **5**, 57 (2014)]