Are spins and orbitals entangled in the Mott insulators with strong spin-orbit coupling?

Krzysztof Wohlfeld

UNIVERSITAS VARSOVIENSIS

Papers & acknowledgments

PHYSICAL REVIEW RESEARCH **2**, 013353 (2020)

How spin-orbital entanglement depends on the spin-orbit coupling in a Mott insulator

Dorota Gotfryd,[1,2] Ekaterina M. Pärschke,[3,4] Jiří Chaloupka,[5,6] Andrzej M. Oleś,[2,7] and Krzysztof Wohlfeld[1]

Condens. Matter **2020**, *5*, 53

Evolution of Spin-Orbital Entanglement with Increasing Ising Spin-Orbit Coupling

Dorota Gotfryd [1,2], Ekaterina Pärschke [3], Krzysztof Wohlfeld [1] and Andrzej M. Oleś [2,4,*]

NATIONAL SCIENCE CENTRE POLAND

Introduction: spin-orbital entanglement

States |*g*> are spin-orbitally entangled:

- "Cannot be written as a product of spin and orbital states":

$$|g\rangle \neq |\mathrm{SPIN}\rangle|\mathrm{ORBITAL}\rangle$$

- Formally – nonzero von Neumann entropy:

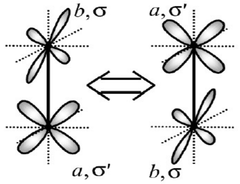
$$\mathcal{S}_{\mathrm{vN}} = -\frac{1}{L}\mathrm{Tr}_S\{\rho_S \ln \rho_S\} \quad \text{where} \quad \rho_S = \mathrm{Tr}_T|g\rangle\langle g|$$

- Example for 1 site:

$$|g\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle|a\rangle \pm |\downarrow\rangle|b\rangle)$$

- An example for 2 sites...

$$|g\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle_B|a\rangle_B|\downarrow\rangle_T|b\rangle_T \pm |\downarrow\rangle_B|b\rangle_B|\uparrow\rangle_T|a\rangle_T))$$



[A. M. Oles *et al.*, PRL **96**, 147205 (2006); Y. Chen *et al.*, PRB **75**, 195113 (2007); G. Khaliullin & S. Maekawa PRL **85**, 3950 (2000)]

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- Example for 1 site:

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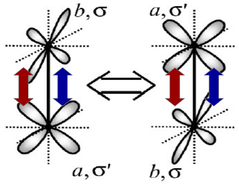
- … another example for 2 sites:

$$|g\rangle = \frac{1}{\sqrt{2}}(|\mathrm{SINGLET}\rangle_{BT}|\mathrm{TRIPLET}\rangle_{BT} \pm |\mathrm{TRIPLET}\rangle_{BT}|\mathrm{SINGLET}\rangle_{BT})$$



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- "Cannot be written as a product of spin and orbital states":

$$|g\rangle \neq |\mathrm{SPIN}\rangle|\mathrm{ORBITAL}\rangle$$

- Formally – nonzero von Neumann entropy:

But is the concept of spin-orbital entanglement useful?

- Examp

$$|g\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle|a\rangle \pm |\downarrow\rangle|b\rangle)$$

- … another example for 2 sites:

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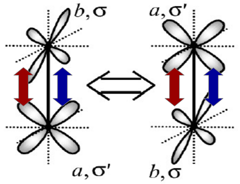

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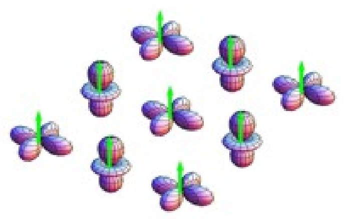
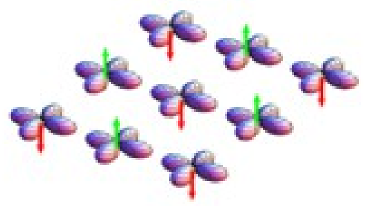
MOTIVATION #1:
spin-orbital entanglement in ground state of 3*d* Mott insulator

Goodenough-Kanamori rules in Mott insulators with partially filled 3*d* orbitals:



Alternating Orbital (AO) → Ferromagnetism (FM)



Ferroorbital (FO) → Antiferromagnetism (AF)

Justification:

– "typical Kugel-Khomskii" spin-orbital model, i.e. (super)exchange & *no* spin-orbit coupling:

$$\mathcal{H} = J \sum_{\substack{\langle i,l \rangle \\ a,b=x,y,z}} (\mathbf{S}_i \cdot \mathbf{S}_l + A) \left(f_{ab} T_i^a T_l^b + B \right)$$

– spins S and orbital pseudospins T decoupled in a mean-field way:

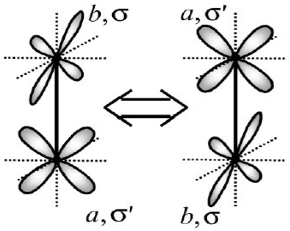
$$\mathcal{H} \sim J \sum_{\substack{\langle i,l \rangle \\ a,b=x,y,z}} f_{ab} \mathbf{S}_i \cdot \mathbf{S}_l \langle T_i^a T_l^b \rangle + f_{ab} T_i^a T_l^b \langle \mathbf{S}_i \cdot \mathbf{S}_l \rangle + \dots$$

– consequently: Goodenough-Kanamori rules, valid e.g. in $LaMnO_3$ or $KCuF_3$

[KI Kugel & DI Khomskii, Sov. Phys. Usp. **25**, 231 (1982); Y. Tokura and N. Nagaosa, Science **288**, 462 (2000)]

MOTIVATION #1:
spin-orbital entanglement in ground state of 3*d* Mott insulator

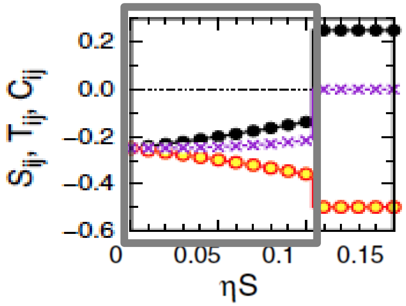
Goodenough-Kanamori rules can be (partially) violated:



– |Orbital Liquid>|AF> in $LaTiO_3$

– |Weak AO>|FM> and anomalously large ferromagnetic $J \,||\, c$ in $LaVO_3$

Origin of the violation:



– spin-orbital correlation nonzero for small Hund's constant η

$$C_{ij} \equiv \langle (\mathbf{S}_i \cdot \mathbf{S}_j)(\mathbf{T}_i \cdot \mathbf{T}_j) \rangle - \langle \mathbf{S}_i \cdot \mathbf{S}_j \rangle \langle \mathbf{T}_i \cdot \mathbf{T}_j \rangle \neq 0$$

→ mean-field decoupling fails

Interestingly:

– spin-orbital correlation correlation = a good proxy for spin-orbital entanglement

– nonzero spin-orbital entanglement → violation of the Goodenough-Kanamori rules

[G. Khaliullin & S. Maekawa, PRL **85**, 3950 (2000); G. Khaliullin *et al.*, PRL **86**, 3879 (2001); A. M. Oles *et al.*, PRL **96**, 147205 (2006); W. L. You *et al.*, PRB **92**, 054423 (2015)]

MOTIVATION #2:
spin-orbital entanglement in excited state of 3*d* Mott insulator

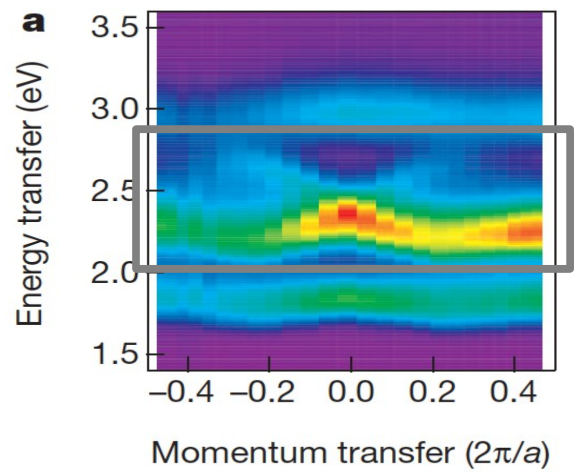
Experiment:

RIXS on quasi-1D (||*x*) cuprate, Sr_2CuO_3

– |GS> = 1D |AF>|FO>, *no* S-O entanglement

– highly dispersive |xz> excitation

– a huge continuum associated with |xz>



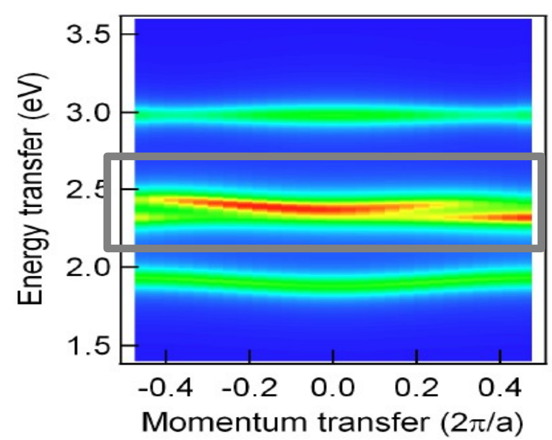
Theory #1:

– "proper" Kugel-Khomskii model

– mean-field decoupling of spin & orbitals

– mostly "single branches", no intrinsic continuum

– <u>failure</u> → S-O entanglement for excitations?



[K. Wohlfeld *et al.*, PRL **107**, 147201 (2011); J. Schlappa *et al.*, Nature **82**, 10974 (2012); CC Chen *et al.*, PRB **91**, 165102 (2015)]

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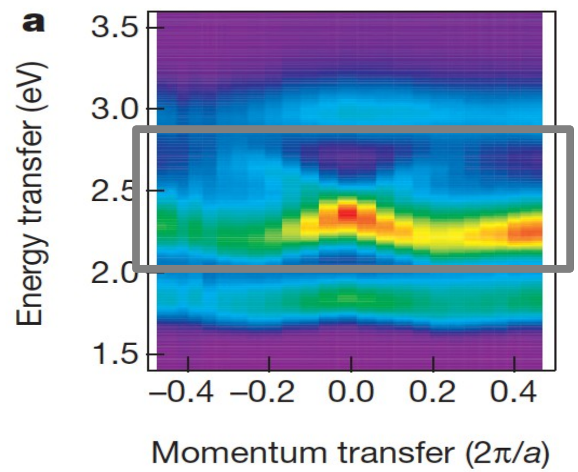
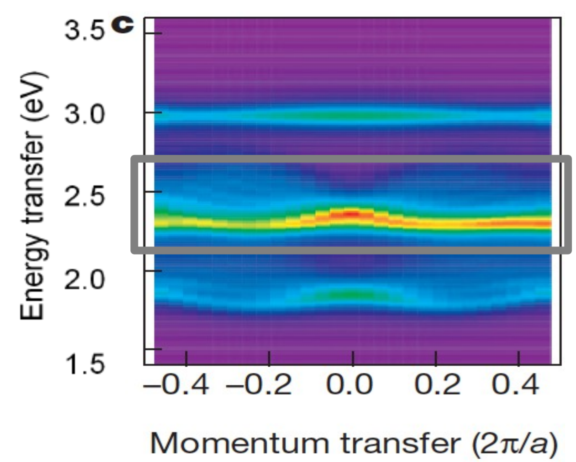


Theory #2:

– "proper" Kugel-Khomskii model

– exact diagonalisation (ED)

– almost perfect agreement → how to understand it?



[K. Wohlfeld *et al.*, PRL **107**, 147201 (2011); J. Schlappa *et al.*, Nature **82**, 10974 (2012); CC Chen *et al.*, PRB **91**, 165102 (2015)]

MOTIVATION #2:
spin-orbital entanglement in excited state of 3*d* Mott insulator

Understanding the continuum in orbital excitation → "large-*N* mean-field":

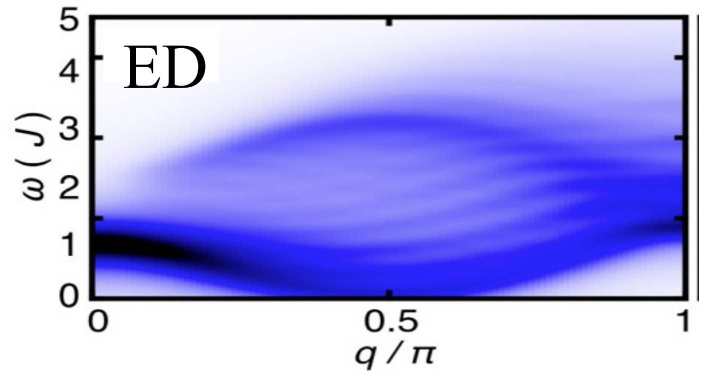
– S and T in terms of $f_{i\,\alpha\sigma}$ constrained fermions

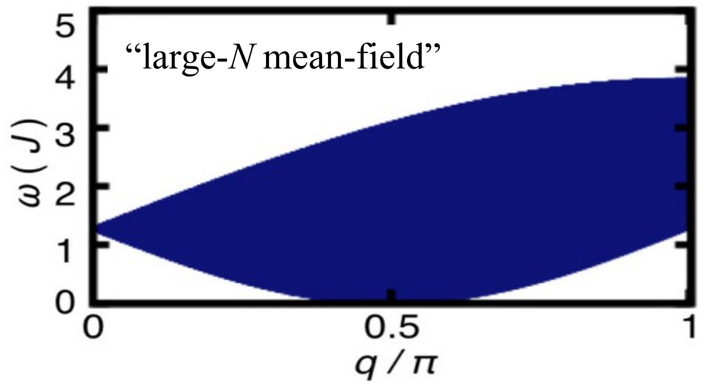
(“back to the derivation of Kugel-Khomskii model”)

– In *k* space: $|f_{k\,\alpha\sigma}>$ = **entangled spin-orbital state**

– Hamiltonian after mean-field = **free $f_{k\,\alpha\sigma}$ fermions**

– **Orbital spectrum ~** $f^{+}_{k+q\,a\sigma} f_{k\,b\sigma}$





[Note: one can choose the basis differently & obtain spin-orbital separation...]

[D. P. Arovas and A. Auerbach, Phys. Rev. B **38**, 316 (1988); CC Chen *et al.*, PRB **91**, 165102 (2015)]

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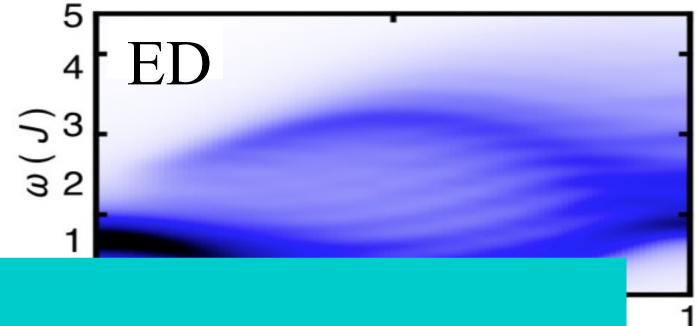
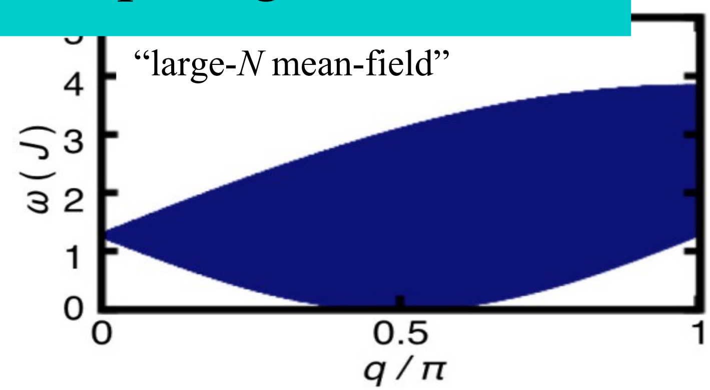


– In k space:

Any other examples where this concept might be useful?

– Hamiltonian after mean-field = **free** $\boldsymbol{f}_{k\,\alpha\sigma}$ **fermions**

– **Orbital spectrum ~** $\boldsymbol{f}^{+}_{k+q\,\alpha\sigma}\boldsymbol{f}_{k\,b\sigma}$



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MOTIVATION #3:
"novel" Mott insulators with strong spin-orbit coupling

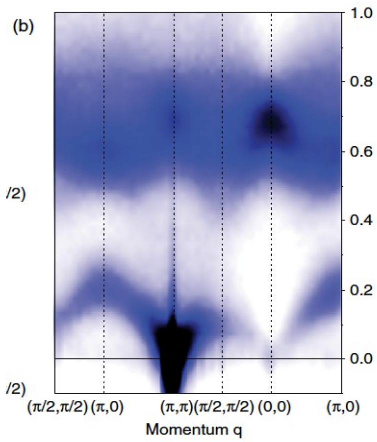
"Novel" Mott insulators found in 5*d* transition metal compounds:

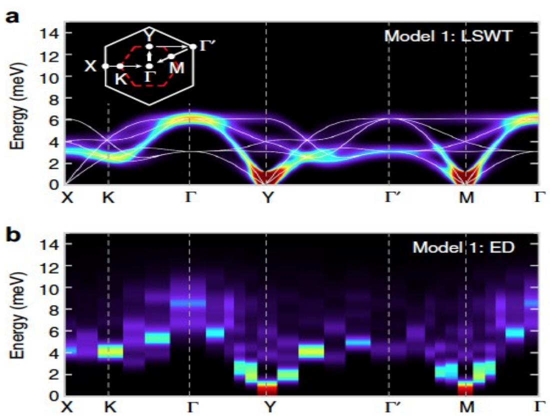
– gained popularity due to PRL by G. Jackeli and G. Khaliullin (2009)

– so far mostly 4 iridates: Sr_2IrO_4, Ba_2IrO_4, Li_2IrO_3, Na_2IrO_3

– no need to introduce them here

– just one point to be stressed on next slide: crucial role of spin-orbit coupling...

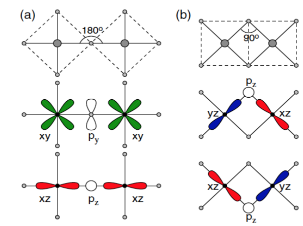




[BJ Kim *et al.*, PRL **108**, 177003 (2012); S. M. Winter *et al.*, Nat. Commun. **8**, 1152 (2017)]

MOTIVATION #3:
“novel” Mott insulators with strong spin-orbit coupling

(1) Basic ingredients:

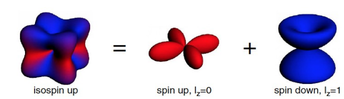


– Kugel-Khomskii spin-orbital exchange

$$\mathcal{H} = J \sum_{\substack{\langle i,l \rangle \\ a,b=x,y,z}} (\mathbf{S}_i \cdot \mathbf{S}_l + A)\left(f_{ab} T_i^a T_l^b + B\right)$$

– on-site spin-orbit coupling λ

$$\mathcal{H}_{\rm SOC} = \lambda \sum_i l_i \cdot \mathbf{S}_i$$



(2) **<u>Crucial role of strong λ</u>** → effective model in terms of *j*=1/2 isospins:

– “**2-1-4**” → square lattice:

$$\mathcal{H} = J \sum_{\langle \mathbf{i},\mathbf{j} \rangle} \mathbf{S_i} \mathbf{S_j}$$

– **physics (almost) like in 2D cuprates**

– “**2-1-3**” → honeycomb lattice:

$$\mathcal{H} = K \sum_{\langle ij \rangle \| \gamma} S_i^\gamma S_j^\gamma + J \sum_{\langle ij \rangle} S_i \cdot S_j$$

– **contain Kitaev isospin liquid physics**

[G. Jackeli & G. Khaliullin, PRL **102**, 017205 (2009)]

SUMMARY OF MOTIVATION:

How about spin-orbital entanglement

in 5*d* Mott insulators with strong spin-orbit coupling?

$\longrightarrow$

MAIN QUESTION:

How spin-orbital entanglement depends on the spin-orbit coupling?

Model and methods

Spin-orbital 1D model

1) Hamiltonian

$$\mathcal{H} = \mathcal{H}_{\mathrm{SE}} + \mathcal{H}_{\mathrm{SOC}}$$

- SU(2)xSU(2) **intersite** spin-orbital super**exchange**

$$\mathcal{H}_{\mathrm{SE}} = J \sum_i \left[\left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} + \alpha \right) \left(\mathbf{T}_i \cdot \mathbf{T}_{i+1} + \beta \right) - \alpha\beta \right]$$

- Ising **onsite** spin-orbit **coupling**

$$\mathcal{H}_{\mathrm{SOC}} = 2\lambda \sum_i S_i^z T_i^z$$

- S=1/2 spin and T=1/2 orbital (pseudospin) operators
- 3 independent parameters: α, β, λ

Model and methods

Spin-orbital 1D model

2) Lanczos **exact diagonalization** (ED) on *L*= 4, 8, 12, 16, 20-site chains

3) Calculated "observables":

- von-Neumann spin-orbital **entanglement entropy** in ground state |GS>:

$$\mathcal{S}_{\rm vN} = -\frac{1}{L}\mathrm{Tr}_S\{\rho_S \ln \rho_S\} \quad \text{where} \quad \rho_S = \mathrm{Tr}_T|\mathrm{GS}\rangle\langle\mathrm{GS}|$$

- simple spin, orbital, and spin-orbital correlators in |GS>...:

$$S^{\gamma\gamma} = \frac{1}{L}\sum_{i=1}^{L}\langle S_i^\gamma S_{i+1}^\gamma\rangle \qquad T^{\gamma\gamma} = \frac{1}{L}\sum_{i=1}^{L}\langle T_i^\gamma T_{i+1}^\gamma\rangle \qquad \mathcal{O}_{\rm SO} = \frac{1}{L}\sum_{i=1}^{L}\langle S_i^z T_i^z\rangle$$

Model and methods

Spin-orbital 1D model

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- ..and a particular **intersite spin-orbital correlation** function:

$$\mathcal{C}_{\rm SO} = \frac{1}{L}\sum_{i=1}^{L}\left[\langle(\mathbf{S}_i\cdot\mathbf{S}_{i+1})(\mathbf{T}_i\cdot\mathbf{T}_{i+1})\rangle - \langle\mathbf{S}_i\cdot\mathbf{S}_{i+1}\rangle\langle\mathbf{T}_i\cdot\mathbf{T}_{i+1}\rangle\right]$$

Model and methods

Spin-orbital 1D model

4) Why study this particular model?

- **Superexchange**:

  simple, yet nontrivial "Kugel-Khomskii physics"

- **Spin-orbit coupling**:

  simplest possible and *relatively realistic* for S=1/2 & T=1/2 case

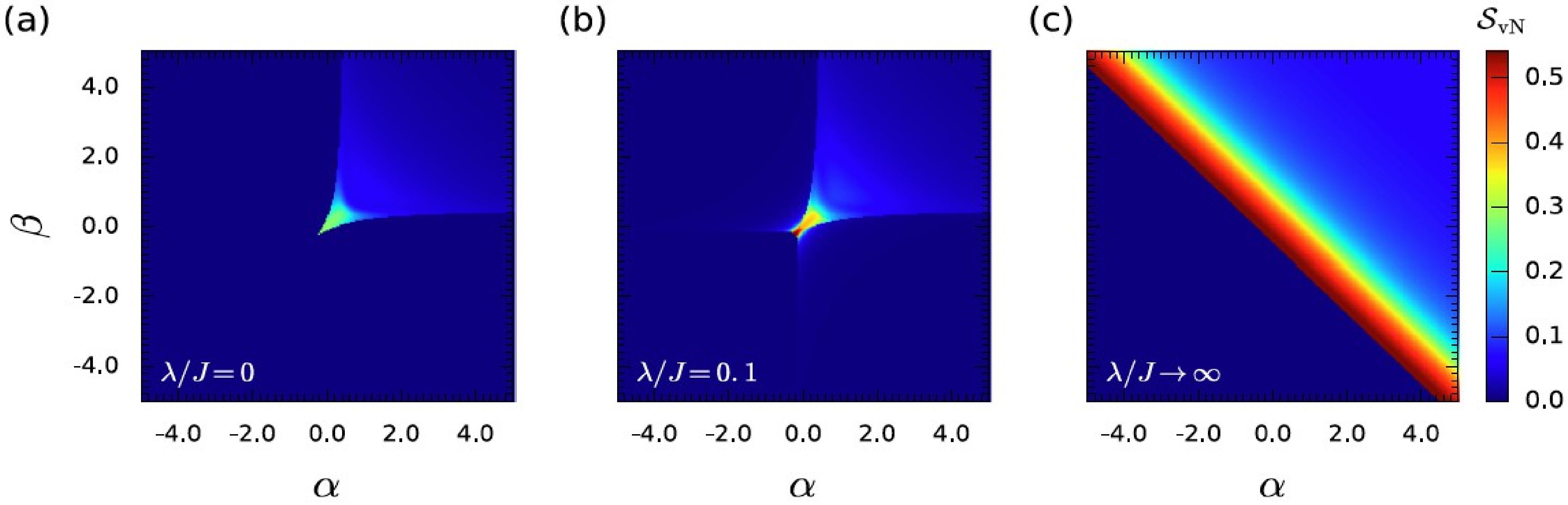
- **1D**:

  small finite size effects & analytic "benchmarking" possible

[*cf.* model for p_x and p_y orbitals RbO_2, KO_2, *etc.* in EPL **96**, 27001 (2011) or PRB **102**, 085129 (2020)]

Results

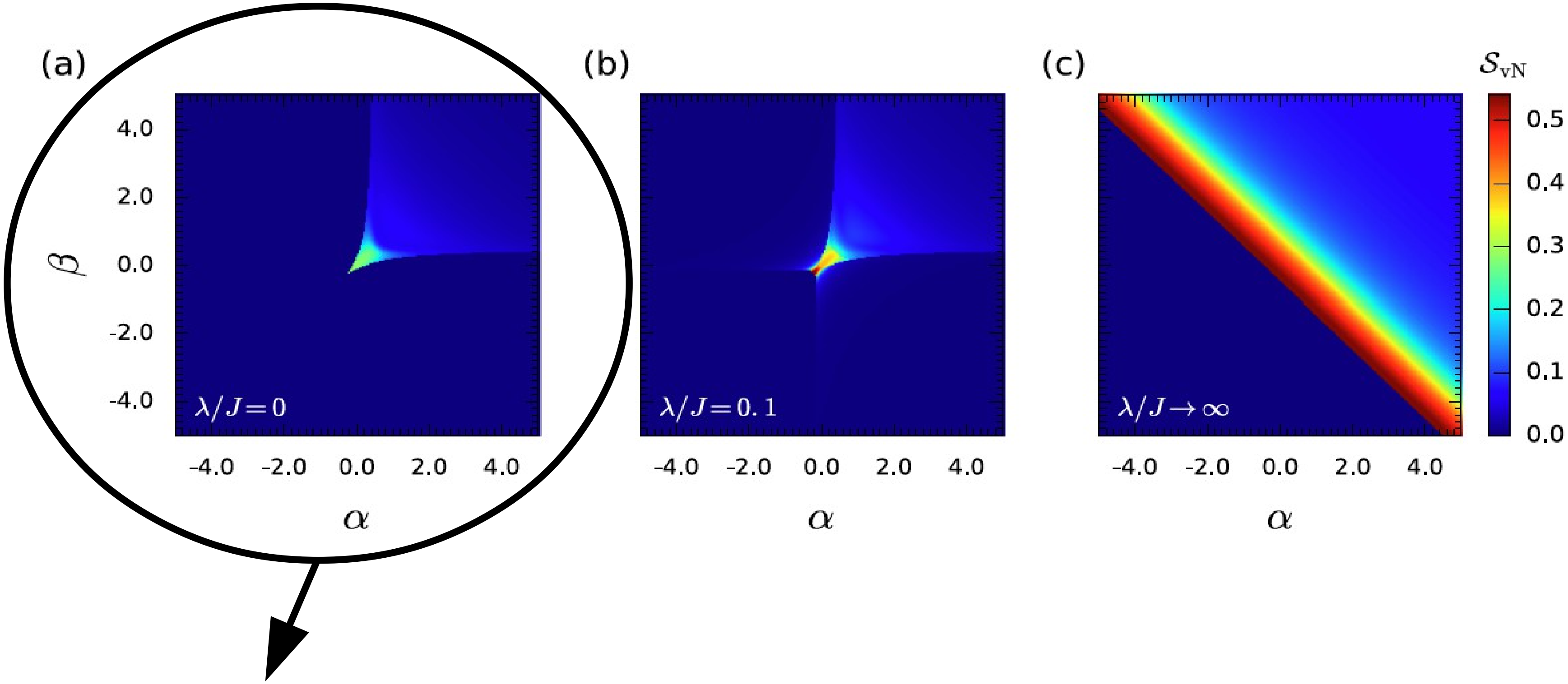
Central result = von-Neumann spin-orbital entanglement entropy



- ED on L=12-site chains
- As function of (α, β) and for **3 distinct values of spin-orbit coupling** λ...

Results

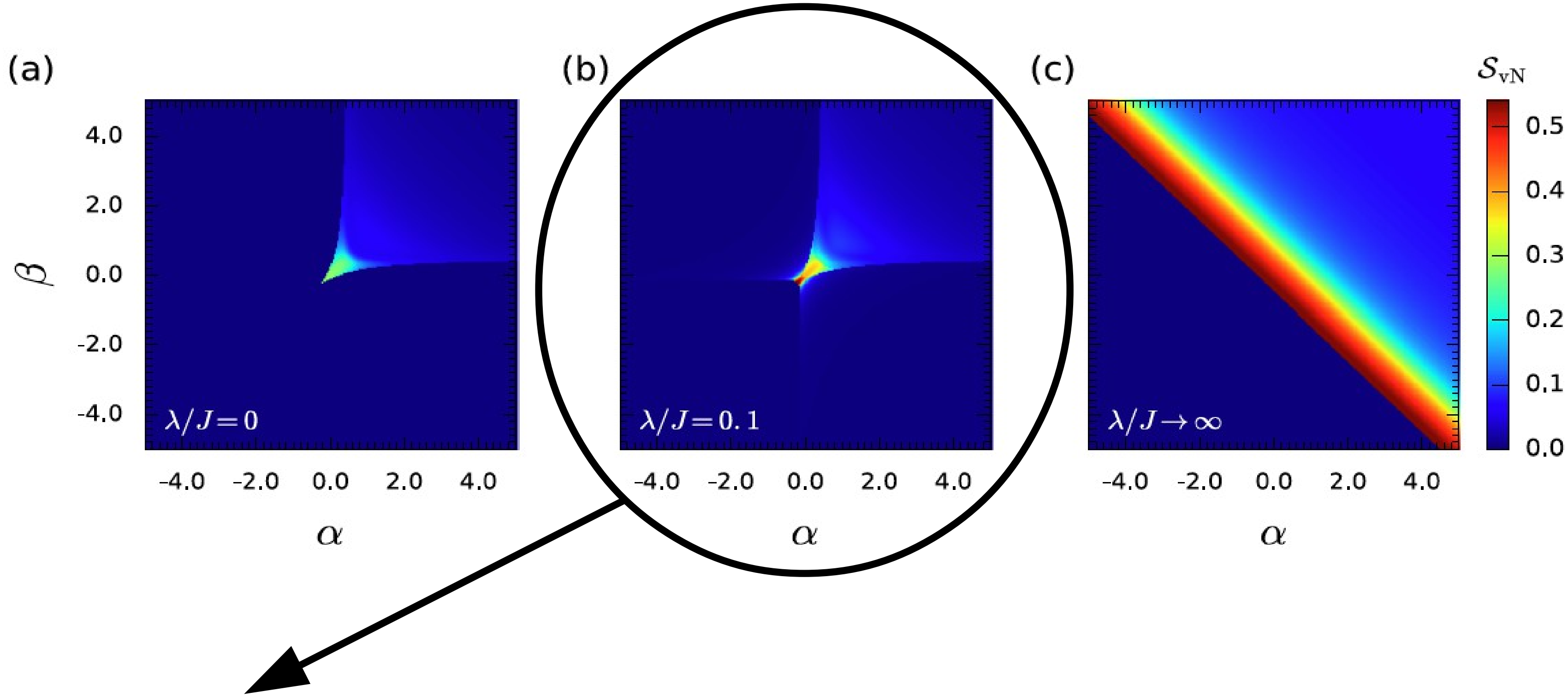
Central result = von-Neumann spin-orbital entanglement entropy



- Relatively small area of nonzero entanglement
- Why the entanglement largely vanishes? Does it agree with existing results?
- **Question #1:** Does the λ=0 result make sense?

Results

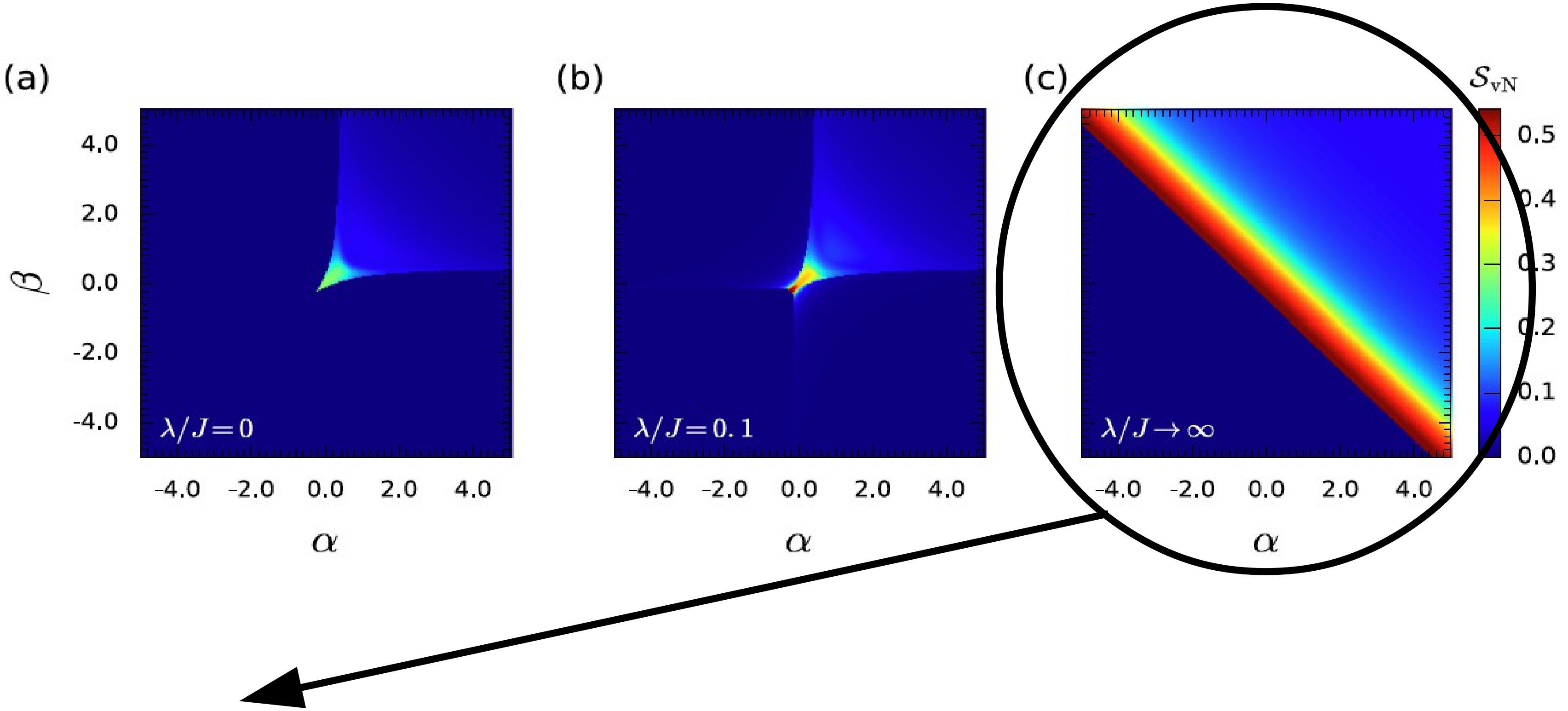
Central result = von-Neumann spin-orbital entanglement entropy



- Still relatively small area of nonzero entanglement
- **Question #2**: Is the "small" λ qualitatively similar to the λ=0 case?

Results

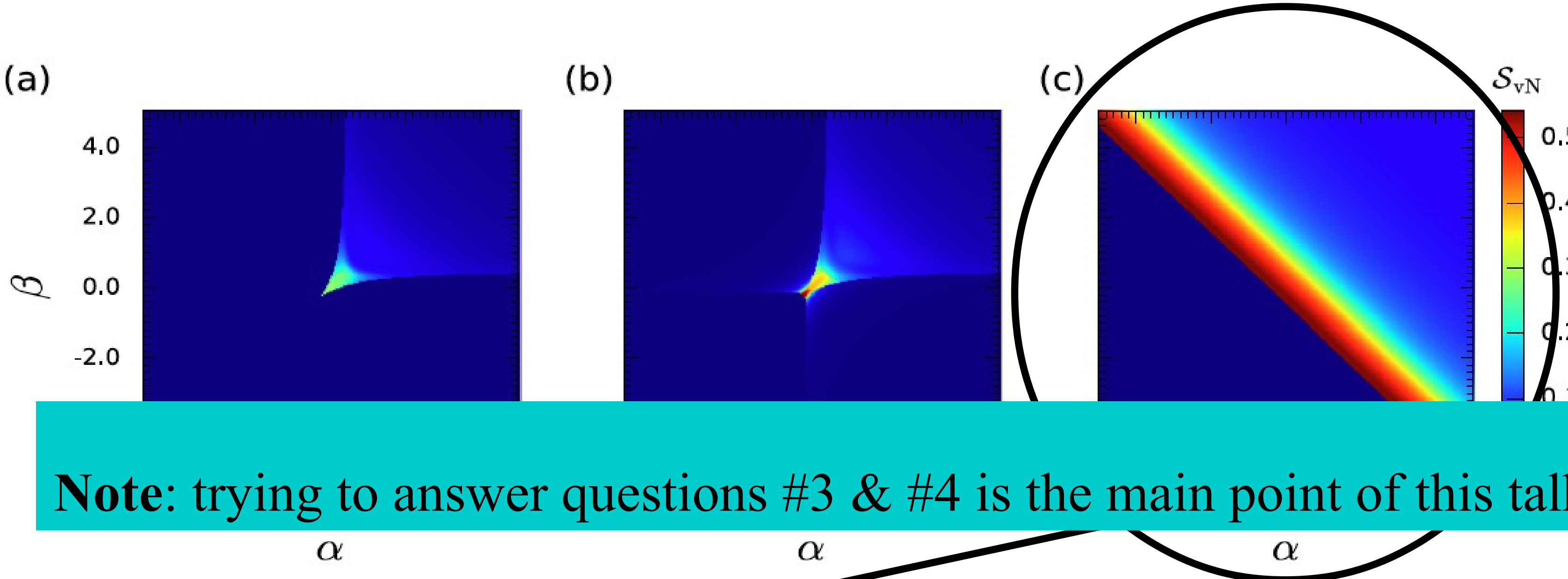
Central result = von-Neumann spin-orbital entanglement entropy



- Drastic increase of entanglement in the model parameter space
- **Question #3**: Why there is such an increase of entanglement for “large” λ?
- **Question #4**: Why for “large” λ the spin-orbital entanglement *can* vanish?

Results

Central result = von-Neumann spin-orbital entanglement entropy

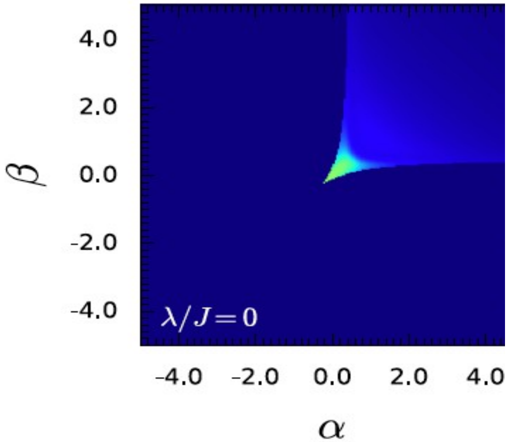


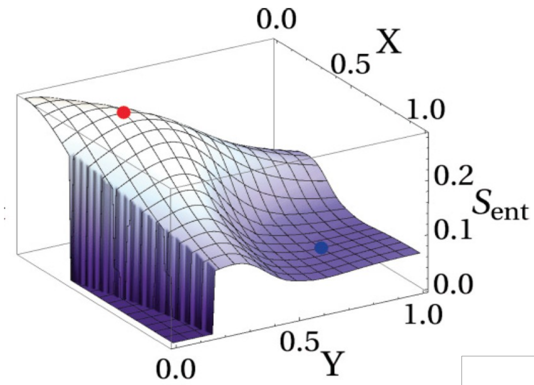
Note: trying to answer questions #3 & #4 is the main point of this talk...

- Drastic increase of entanglement in the model parameter space
- **Question #3**: Why there is such an increase of entanglement for “large” λ?
- **Question #4**: Why for “large” λ the spin-orbital entanglement *can* vanish?

Q1: Does the λ=0 result make sense?

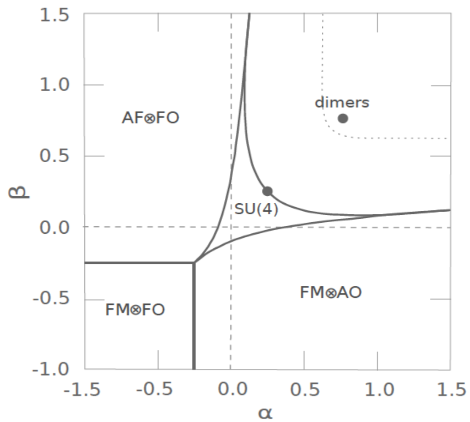
1) Benchmarking against existing results:





R. Lundgren *et al.*, PRB **86**, 22442 (2012)

2) Understanding this result → phase diagram of the SU(2)xSU(2) model:



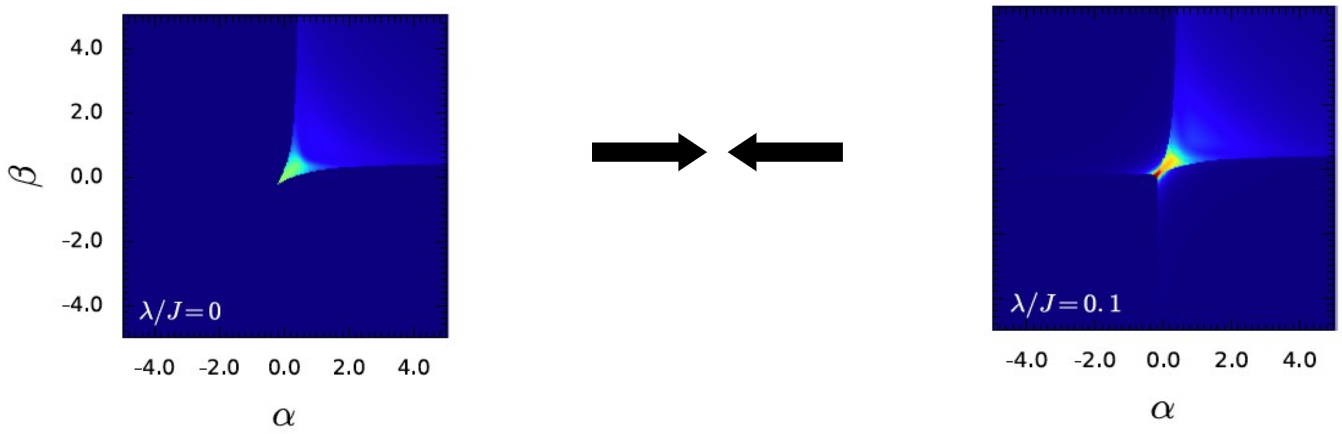
- 3 product phases
- 2 entangled phases:
  - – AF gapless "SU(4) singlet"
  - – AF gapped dimerised

Y. Q. Li et al., PRL **81**, 3527 (1998);

S. K. Pati *et al.*, PRL **81**, 5406 (1998);

R. Lundgren *et al.*, PRB **86**, 224422 (2012)

Q2: Is the "small" λ qualitatively similar to the λ=0 case?



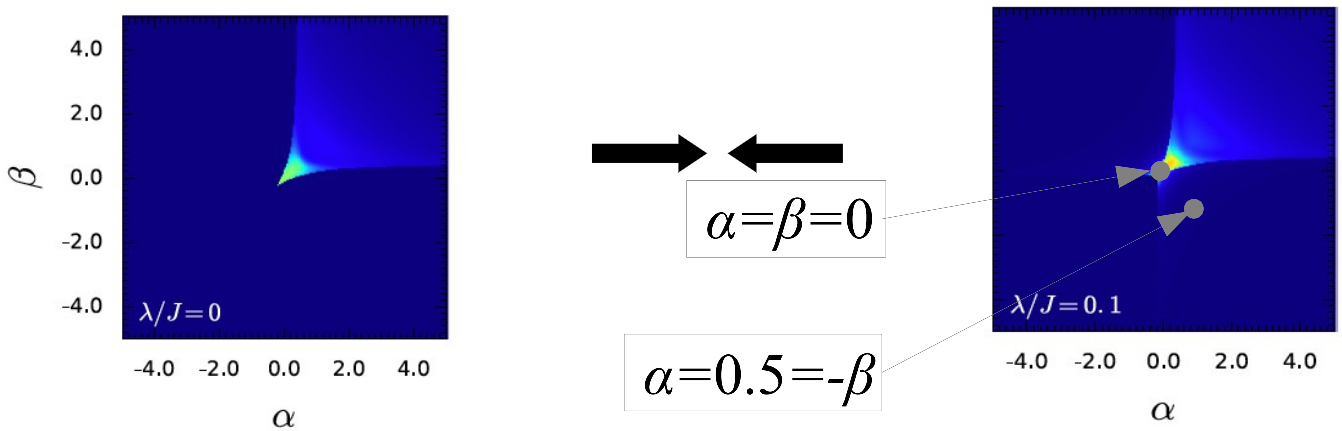
To verify the nature of the ground state at λ=0.1J *versus* at λ=0

$\rightarrow$

we look at 2 specific values of (α, β)

& study the evolution of the ground state properties with λ

Q2: Is the “small” λ qualitatively similar to the λ=0 case?



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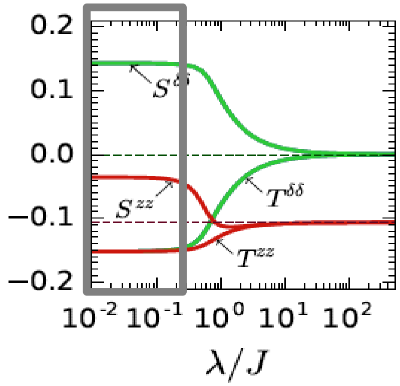
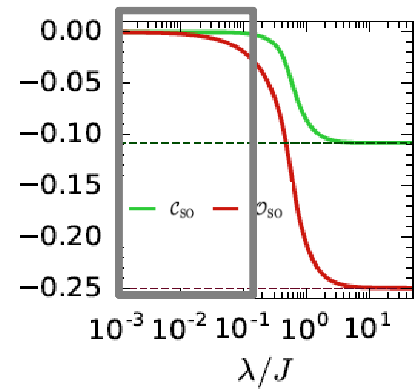
1) α=0.5=-β: overall still dominant FM/AO, still disentangled





but spatial anisotropy in spins induced → ***perturbed* FMxAO**

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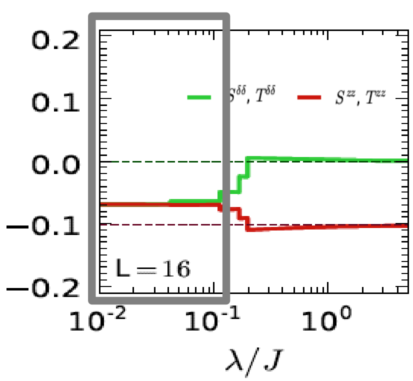
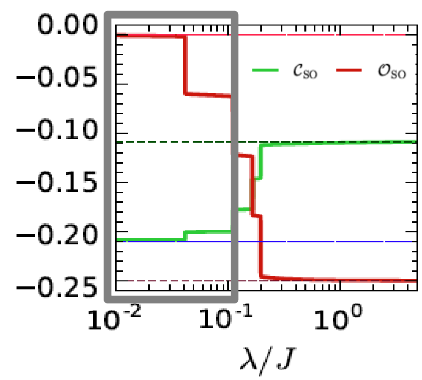
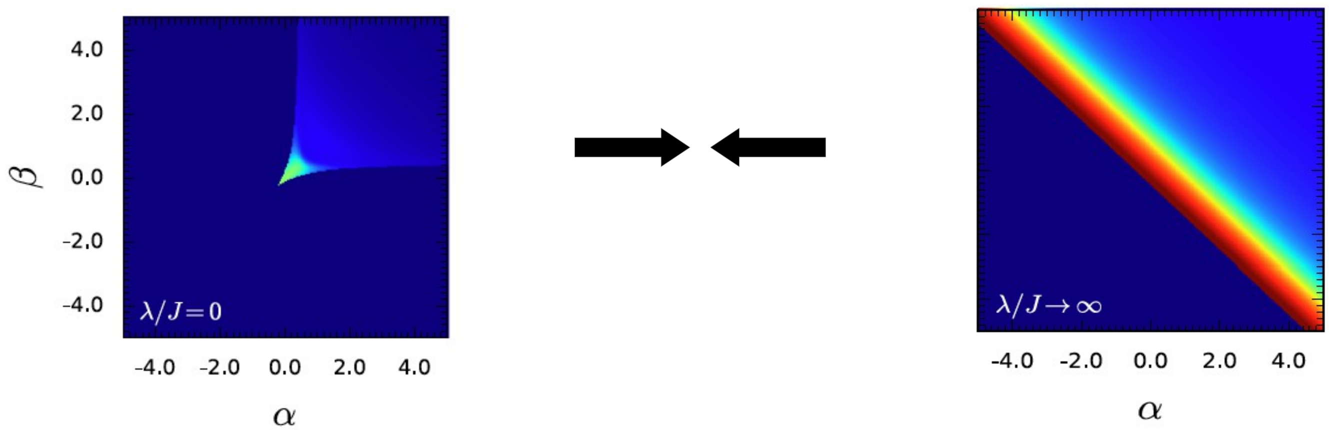
2) α=β=0: still no difference between spins and orbitals, still entangled





but spatial anisotropy induced & changes in $\mathcal{C}_{SO}$ → **distinct entangled phase**

Q3: Why there is such an increase of entanglement for “large” λ?



- Rewrite the Hamiltonian, highlighting terms responsible for entanglement

$$\mathcal{H}/J = \sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} \mathbf{T}_i \cdot \mathbf{T}_{i+1} + \alpha \mathbf{T}_i \cdot \mathbf{T}_{i+1} + \beta \mathbf{S}_i \cdot \mathbf{S}_{i+1} + 2\frac{\lambda}{J} S_i^z T_i^z \right)$$

- Once $\alpha \sim \beta \sim 0$ → finite spin-orbital entanglement expected for any λ

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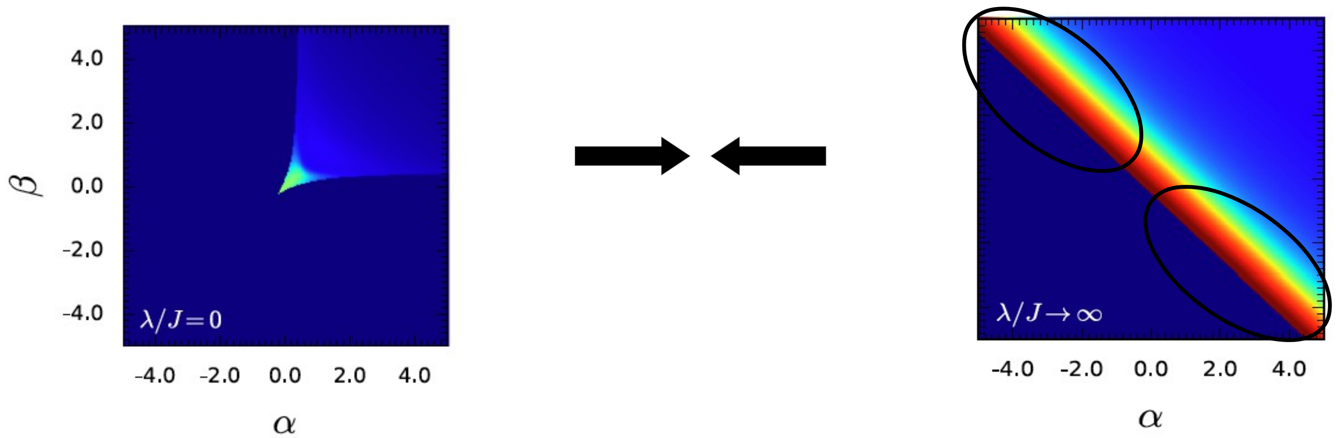

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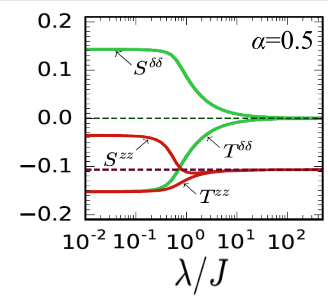
- What about α~-$\beta \neq 0$? Why such an increase in entanglement for "large" λ?

  – "Large" λ supports $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle \simeq \langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$

It wants spins and orbitals on "equal footing"

Indeed:



– Once α~-β & **since** $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle \simeq \langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$

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i.e. the intersite terms fully entangled

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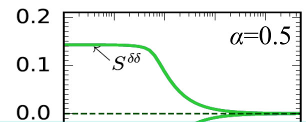

"Cooperation" between superexchange & spin-orbit coupling

→ huge increase in spin-orbital entanglement

- Once $\alpha \sim -\beta$ & **since** $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle \simeq \langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$

→

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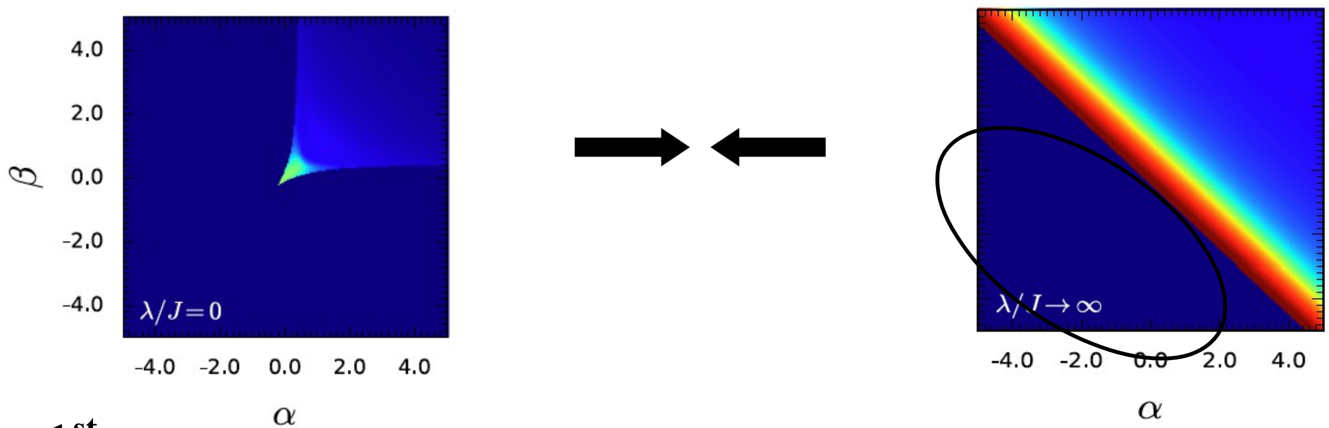
Q4: Why for “large” λ the spin-orbital entanglement *can* vanish?



Trying the 1st way…:

- Rewrite the Hamiltonian, highlighting terms responsible for entanglement

$$\mathcal{H}/J = \sum_i \left(\mathbf{S}_i \cdot \mathbf{S}_{i+1} \mathbf{T}_i \cdot \mathbf{T}_{i+1} + \alpha \mathbf{T}_i \cdot \mathbf{T}_{i+1} + \beta \mathbf{S}_i \cdot \mathbf{S}_{i+1} + 2\frac{\lambda}{J} S_i^z T_i^z \right)$$

- Once $\alpha \sim \beta$ & **<u>if</u>** $\langle \mathbf{S}_i \cdot \mathbf{S}_{i+1} \rangle \simeq \langle \mathbf{T}_i \cdot \mathbf{T}_{i+1} \rangle$ due to “large” λ

  $\rightarrow$ then perhaps indeed small entanglement for large enough $|\alpha| \sim |\beta|$

- But this does *not* nicely explain vanishing entanglement for $\alpha + \beta < -1/2$

Q4: Why for "large" λ the spin-orbital entanglement *can* vanish?

2nd way to understand it:

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2nd way to understand it:

- **Derive an effective model assuming "large" λ**

$$\mathcal{H}_{\rm eff} = \frac{J}{2} \sum_i \left(\tilde{J}_i^x \tilde{J}_{i+1}^x + \tilde{J}_i^y \tilde{J}_{i+1}^y + 2(\alpha+\beta) \tilde{J}_i^z \tilde{J}_{i+1}^z \right)$$

where $\tilde{J}$=1/2 is isospin operator with e.g.

$$\tilde{J}_i^z = \frac{1}{2} \left(n_{i,|\uparrow a\rangle} + n_{i,|\downarrow b\rangle} \right)$$

[Similar procedure as for the t_{2g} spin-orbital model of the iridium oxides, cf. G. Jackeli & G. Khaliullin, PRL **102**, 017205 (2009)]

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- Next, rewrite a *good proxy* for spin-orbital entanglement in this basis:

$$\tilde{\mathcal{C}}_{\text{SO}} = \frac{1}{2L}\sum_{i=1}^{L}\left[\langle \tilde{J}_i^x \tilde{J}_{i+1}^x + \tilde{J}_i^y \tilde{J}_{i+1}^y\rangle - 2\langle \tilde{J}_i^z \tilde{J}_{i+1}^z\rangle^2 + \frac{1}{8}\right]$$

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- Derive an effective model assuming "large" λ

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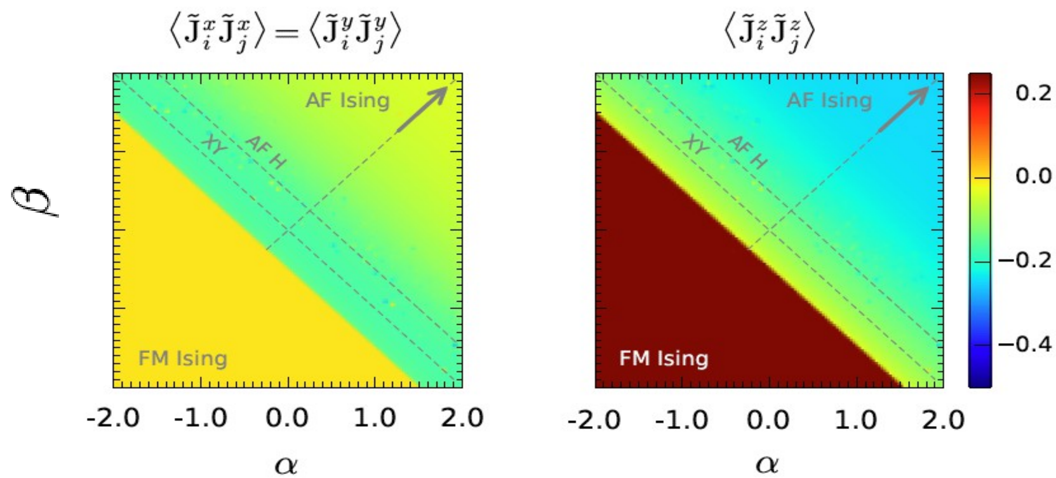
- **Altogether**:

Go to effective Hamiltonian assuming "large" λ and calculate correlators

Q4: Why for "large" λ the spin-orbital entanglement *can* vanish?

2nd way to understand the problem is easier...:

- Go to effective Hamiltonian, valid for "large" λ, and calculate correlators



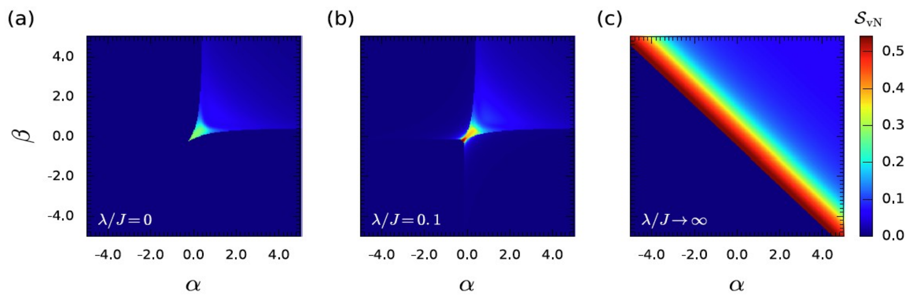
- This shows that the **proxy for spin-orbital entanglement**:

$$\tilde{C}_{SO} = \frac{1}{2L} \sum_{i=1}^{L} \left[\langle \tilde{J}_i^x \tilde{J}_{i+1}^x + \tilde{J}_i^y \tilde{J}_{i+1}^y \rangle - 2 \langle \tilde{J}_i^z \tilde{J}_{i+1}^z \rangle^2 + \frac{1}{8} \right]$$

vanishes for $\alpha + \beta < -1/2$ due to the onset of Ising FM (in $\tilde{J}$ isospins)

Summary

Spin-orbital entanglement entropy for 3 values of spin-orbit coupling λ



- For "small" λ:
  - – spin-orbit coupling rather does *not* induce extra entanglement
  - – phases *can* be distinct w.r.t. $\lambda=0$
- For "large" λ:
  - – a novel spin-orbitally entangled phase, even if no entanglement at $\lambda=0$
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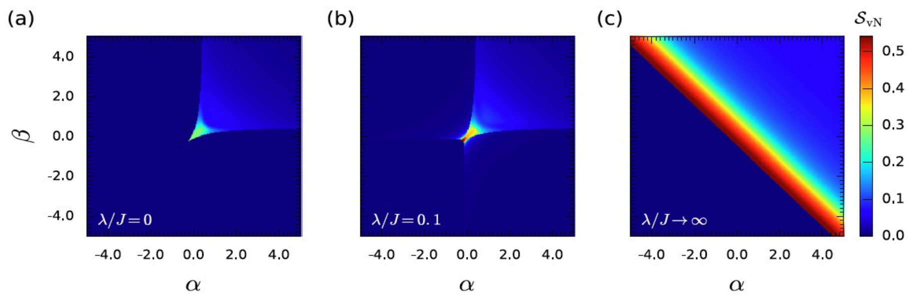

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Conclusions

[MAIN RESULT]

For "large" λ:

– a novel spin-orbitally entangled phase, even if no entanglement at $\lambda=0$

– a novel phase, though with *vanishing* entanglement

⬇

[TAKE-HOME MESSAGE]

1) Entanglement *can* be triggered by a joint action of:

on-site spin-orbit coupling and superexchange

2) But entanglement *can* also vanish, even if spin-orbit coupling is large

Conclusions

[MAIN RESULT]

For "large" λ:

– a novel spin-orbitally entangled phase, even if no entanglement at λ=0

– a nove

Ad. 1) → *Supposedly* the case of iridates

Ad. 2) → Maybe a bit academic but should not be forgotten

[TAKE-HOME MESSAGE]

1) Entanglement *can* be triggered by a joint action of:

on-site spin-orbit coupling and superexchange

2) But entanglement *can* also vanish, even if spin-orbit coupling is large

PS: RVB mean-field theory

Schwinger bosons:

$$S_i^+ = f_{i\uparrow}^\dagger f_{i\downarrow} \quad S_i^- = f_{i\downarrow}^\dagger f_{i\uparrow},$$
$$T_i^+ = f_{ia}^\dagger f_{ib} \quad T_i^- = f_{ib}^\dagger f_{ia},$$

$$\sum_\alpha f_{i\alpha}^\dagger f_{i\alpha} + h_i^\dagger h_i = 1$$

$$\sum_\sigma f_{i\sigma}^\dagger f_{i\sigma} + h_i^\dagger h_i = 1$$

Constrained fermions:

$$f_{i\alpha\sigma}^\dagger = f_{i\sigma}^\dagger f_{i\alpha}^\dagger h_i \qquad \sum_{\alpha\sigma} f_{i,\alpha\sigma}^\dagger f_{i,\alpha\sigma} = 1$$

⬇

$$\mathcal{H} = -J \sum_{\langle ij\rangle,\alpha,\sigma,\alpha',\sigma'} (f_{i\alpha\sigma}^\dagger f_{j\alpha\sigma} + h.c.)(f_{j\alpha'\sigma'}^\dagger f_{i\alpha'\sigma'} + h.c.)$$
$$+ \frac{1}{2} E_z \sum_{i\sigma} (f_{ia\sigma}^\dagger f_{ia\sigma} - f_{ib\sigma}^\dagger f_{ib\sigma}).$$

Mean-field for constrained fermions:

$$\mathcal{H}_{\mathrm{MF}} = \sum_{k,\sigma} (\varepsilon_{ka} f_{ka\sigma}^\dagger f_{ka\sigma} + \varepsilon_{kb} f_{kb\sigma}^\dagger f_{kb\sigma})$$

$$\varepsilon_{ka/b} = -\langle\chi_{ij}\rangle 2J\cos k \mp E_z/2; \ \langle\chi_{ij}\rangle = 2\sqrt{2}\cos(\delta_k)/\pi$$

$$\delta_k = \arcsin[E_z\pi/(4J)]/2 \text{ when } E_z < 4J/\pi \qquad \delta_k = \pi/4 \text{ when } E_z \geq 4J/\pi$$

PS: RVB mean-field theory

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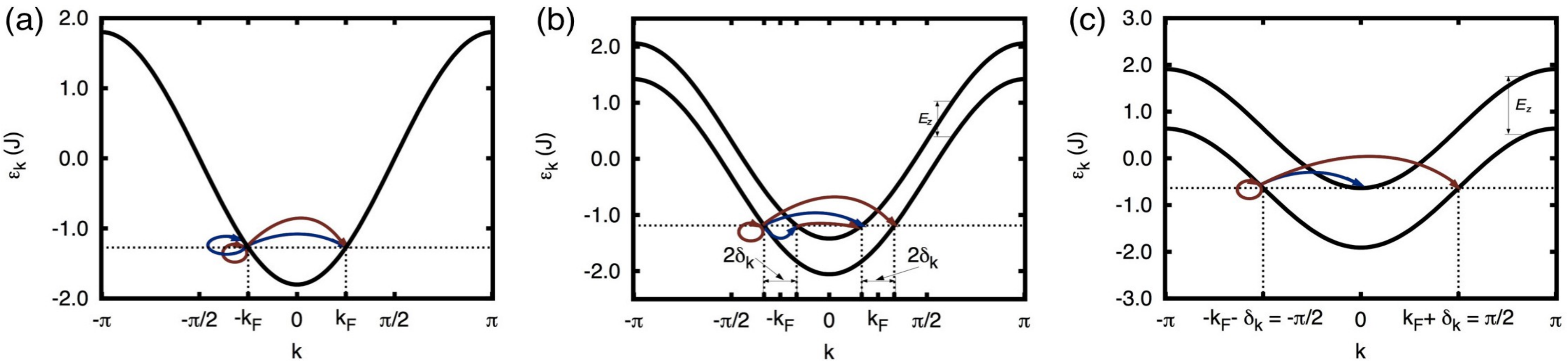


$E_z = 0$ $\quad E_z = E_z^{cr}/2$ $\quad E_z = E_z^{cr}$

Distinct 'topology' of the Fermi 'surface' (E_z)

→ distinct orbital and spin spectra (E_z)

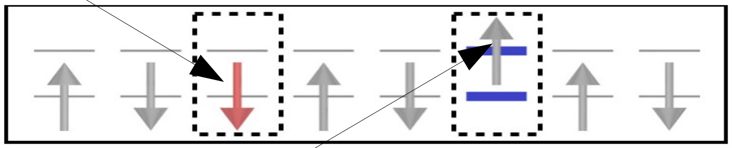
PS: Entanglement vs. separation

Note: “analytics” (RVB mean-field) → **always** **entanglement**

So why **separation** **suggested in another approach** to the '**realistic**' chain?

→ freedom of choosing the basis in the 'realistic' case:

orbital q. number for all electrons in lower orbital (incl. spinon) can be neglected



spin q. number for all electrons in upper orbital (→ orbiton) can be neglected