An effecient numerical approach to model 2D S=1/2 antiferromagnet and doped CuO2 planes.

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Outline

1) Introduction

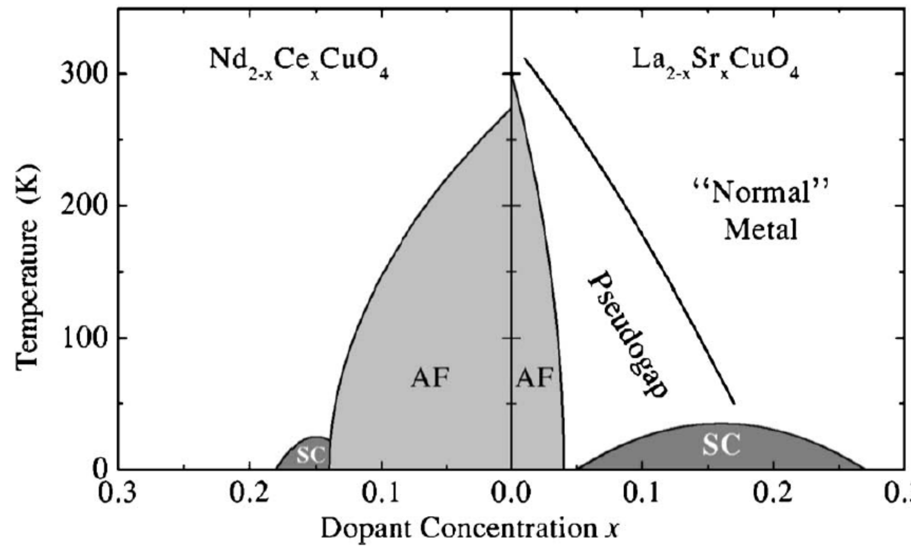
2) Numerical Approach

3) Application to Doped Scenarios

4) Summary

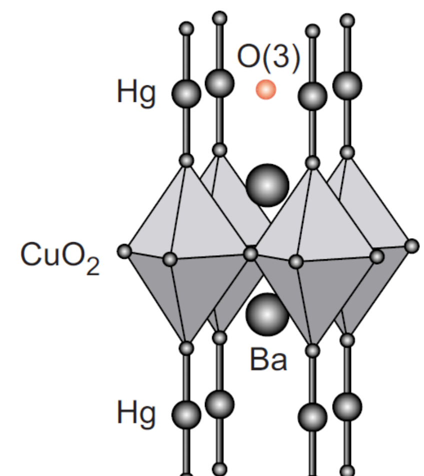
Motivations

- A full understanding of cuprates should elucidate the role of a doped AFM.



Rev. Mod. Phys. 75 473 (2003)

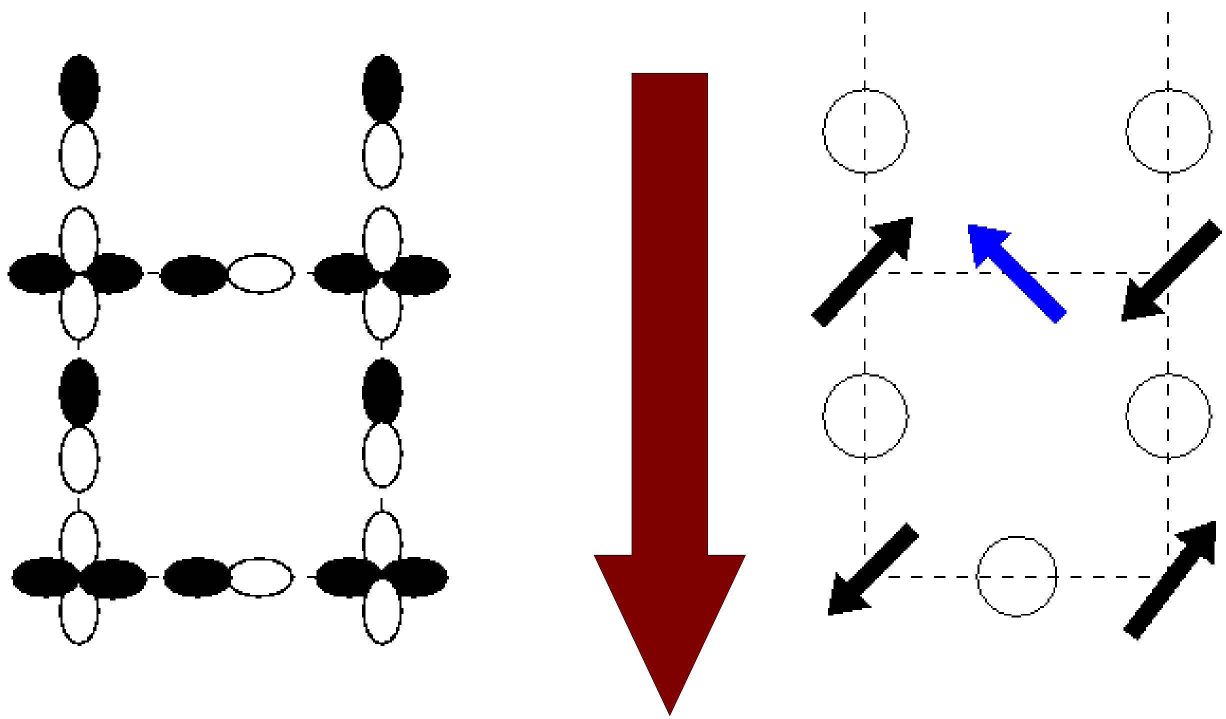
- Can we make more direct comparisons between models with increasing level of microscopic details?



Phys. Rev. B 78 054578 (2008)

3-band → 2+1 band

$$
\begin{aligned}
H_{3B} =& t_{pd}\sum[(p^\dagger_{l+\epsilon,\sigma} - p^\dagger_{l-\epsilon,\sigma})d_{l,\sigma} + h.c.] + t_{pp}\sum(-1)^{n_\delta} p^\dagger_{l+\epsilon+\delta,\sigma}p_{l+\epsilon,\sigma} - t'_{pp}\sum(p^\dagger_{l-\epsilon,\sigma} + p^\dagger_{l+3\epsilon,\sigma})p_{l+\epsilon,\sigma} \\
&+\Delta_{pd}\sum p^\dagger_{l+\epsilon,\sigma}p_{l+\epsilon,\sigma} + U_{pp}\sum p^\dagger_{l+\epsilon,\uparrow}p_{l+\epsilon,\uparrow}p^\dagger_{l+\epsilon,\downarrow}p_{l+\epsilon,\downarrow} + U_{dd}\sum d^\dagger_{l,\uparrow}d_{l,\uparrow}d^\dagger_{l,\downarrow}d_{l,\downarrow}.
\end{aligned}
$$



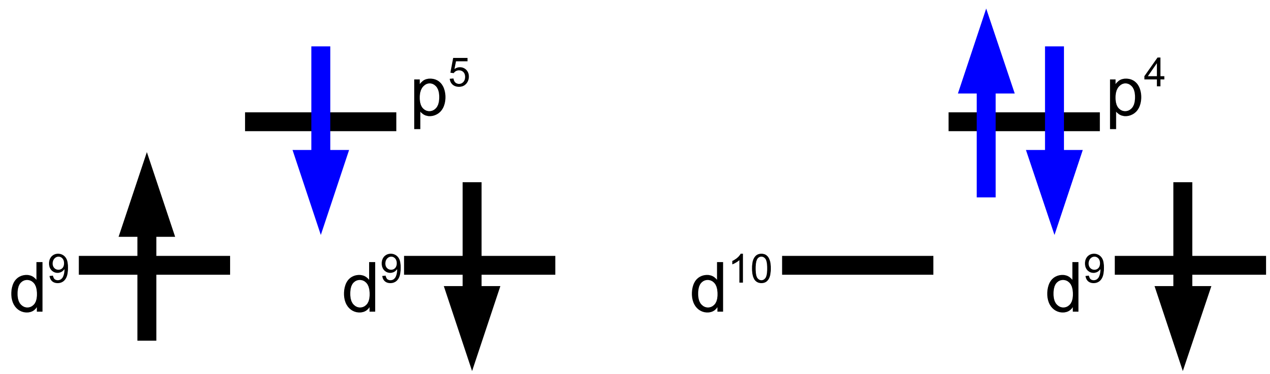
$$p^\dagger_{l+\epsilon,\sigma}\prod|\sigma_l\rangle$$

$$H_{\text{eff}} = T_0 + T_{\text{swap}} + H_{J_{pd}} + H_{J_{dd}}$$

B. Lau, M. Berciu, and G. A. Sawatzky, Phys. Rev. Lett. 106 036401 (2011)

Exchange terms

- $H_{J_{dd}} = J_{dd} \sum \overline{S}_{l \pm 2\epsilon} \cdot \overline{S}_l \Pi_\sigma (1 - p^\dagger_{l \pm \epsilon, \sigma} p_{l \pm \epsilon, \sigma})$



- $H_{J_{pd}} = J_{pd} \sum \overline{S}_l \cdot \overline{S}_{l \pm \epsilon}$

- $\sqrt{\frac{1}{6}} (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) |\boldsymbol{\sigma}\rangle_h - \sqrt{\frac{2}{3}} |\boldsymbol{\sigma}\boldsymbol{\sigma}\rangle | -\boldsymbol{\sigma}\rangle_h$

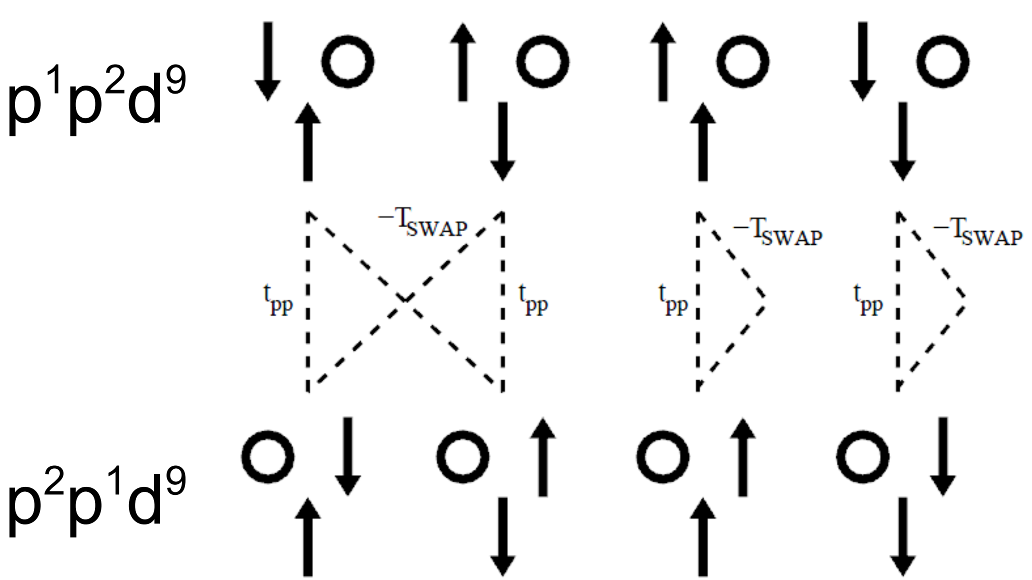
Emery and Reiter, PRB 38 4547 (1988)

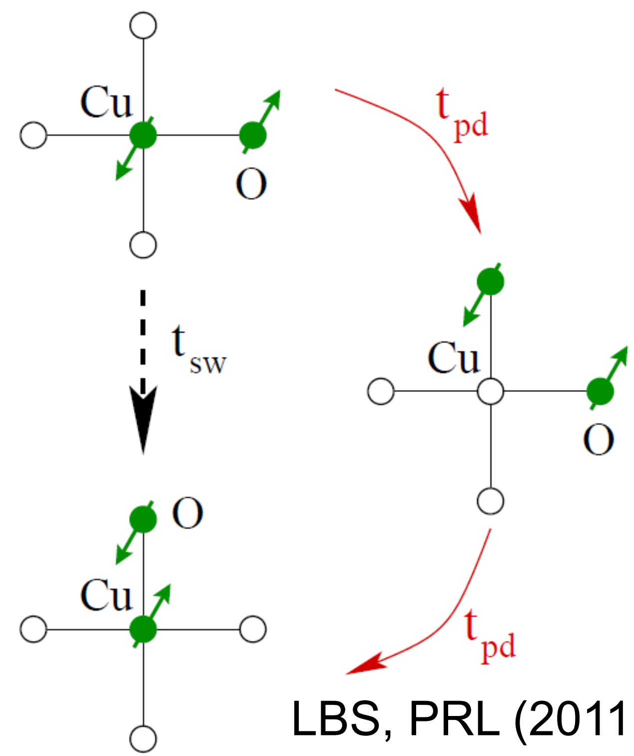
LBS, PRL (2011)

Kinetic Terms

$$T_0 = t_{pp} \sum (-1)^{n_\delta} p^\dagger_{l+\epsilon+\delta,\sigma} p_{l+\epsilon,\sigma}$$
$$\qquad - t'_{pp} \sum (p^\dagger_{l-\epsilon,\sigma} + p^\dagger_{l+3\epsilon,\sigma}) p_{l+\epsilon,\sigma}$$

$$T_{swap} = -t_{sw} \sum (-1)^{n_\eta} p^\dagger_{l+\epsilon+\eta,\sigma} p_{l+\epsilon,\sigma'} |\sigma'_{l_{\epsilon,\eta}}\rangle\langle\sigma_{l_{\epsilon,\eta}}|$$





LBS, PRL (2011)

Benefits

- charge-transfer physics, AFM physics, and a more faithful 2D lattice structure.
- has the same form (Heisenberg) as the t-J model at zero-doping limit.
- direct comparison with the t-J model can single out the implications of oxygen-specific physics.

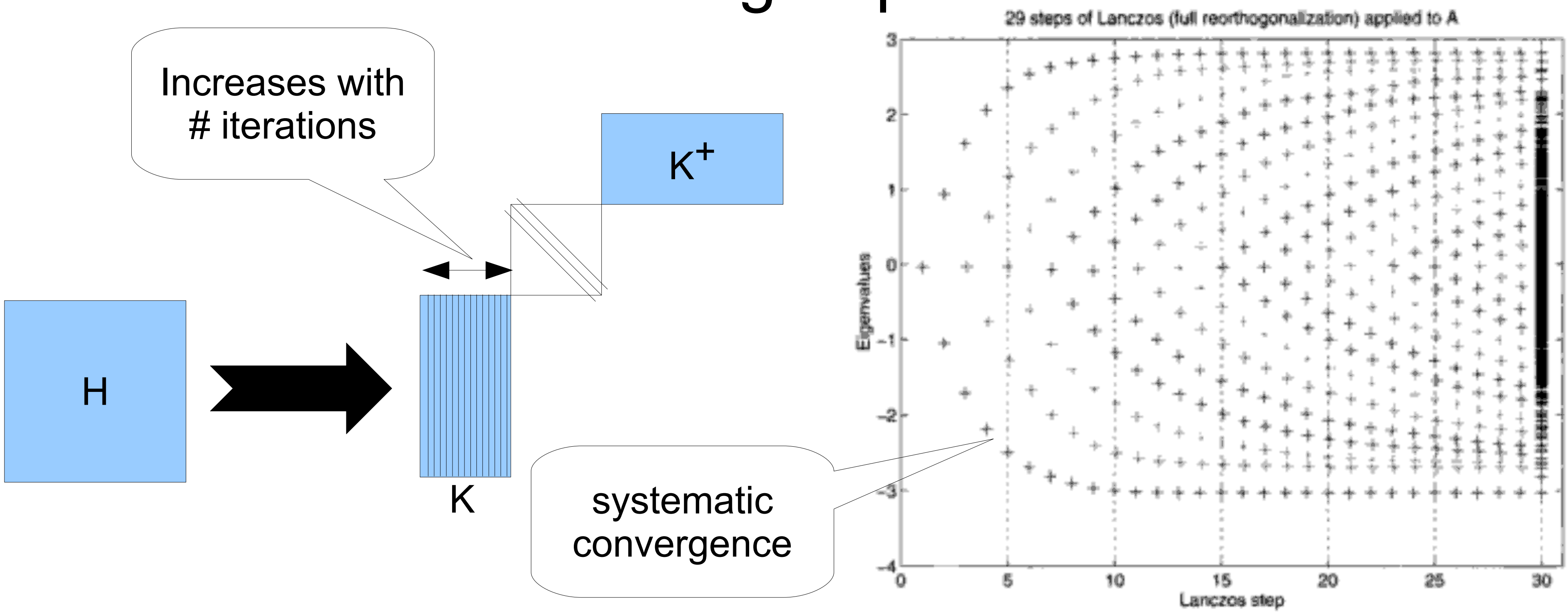
Direct Comparison

- Matrix diagonalization is a good starting point.
- t-J model: N=40 for 0 hole; N=32 for 1, 2, 4 holes; doping removes spin degrees of freedom.
- previous multiband attempts: 2 holes for N=16
- New numerical formulation: N=64 for 0 hole, N=32 for 1 and 2 holes.

Numerical Approach

Lanczos Tridiagonalization

- Repeated application of H to a random vector will yield an extremal eigen-pair eventually.
- Lanczos: a much smaller basis is constructed by selection of dominent eigen-pairs.

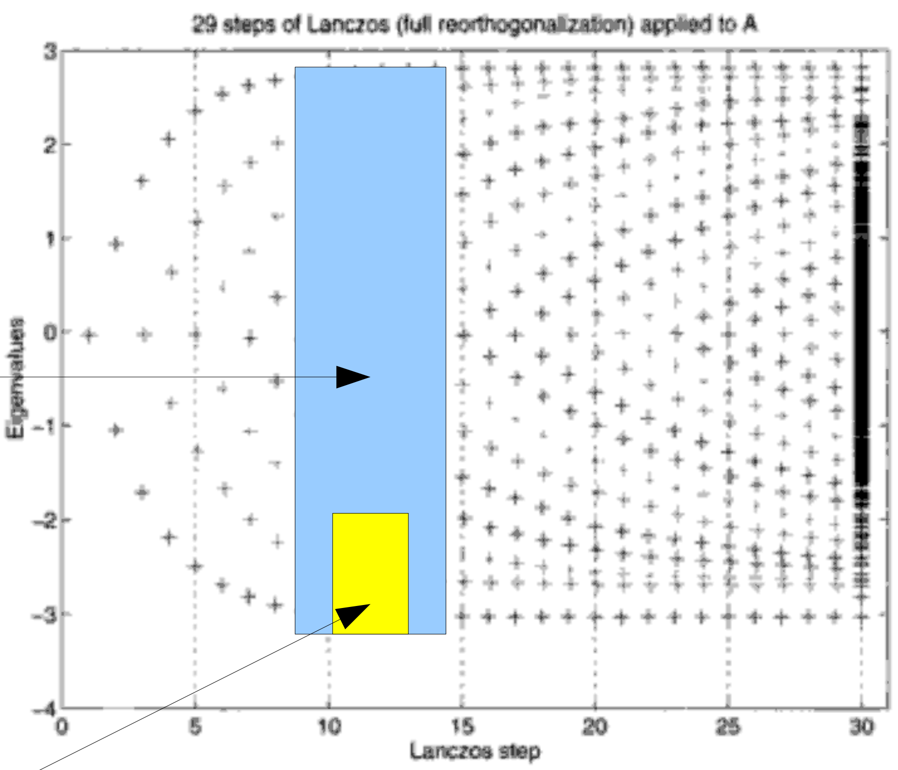


J. Demmel, Applied numerical linear algebra (1997)

Basic Idea

- In practice, Lanczos is limited by the exponentially scaling matrix size.

- The standard procedure is block-diagonalization using quantum numbers.

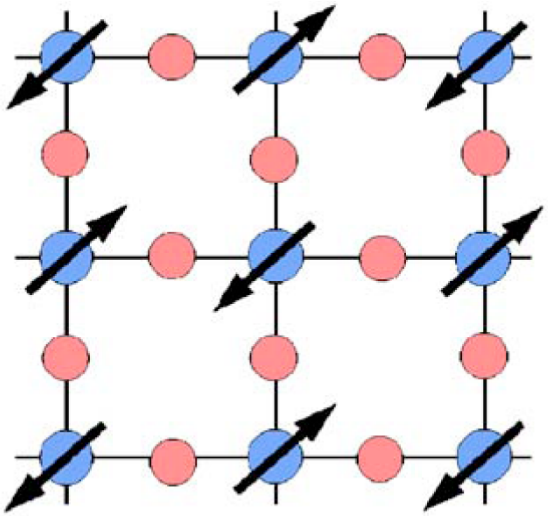


- We know additional attributes.

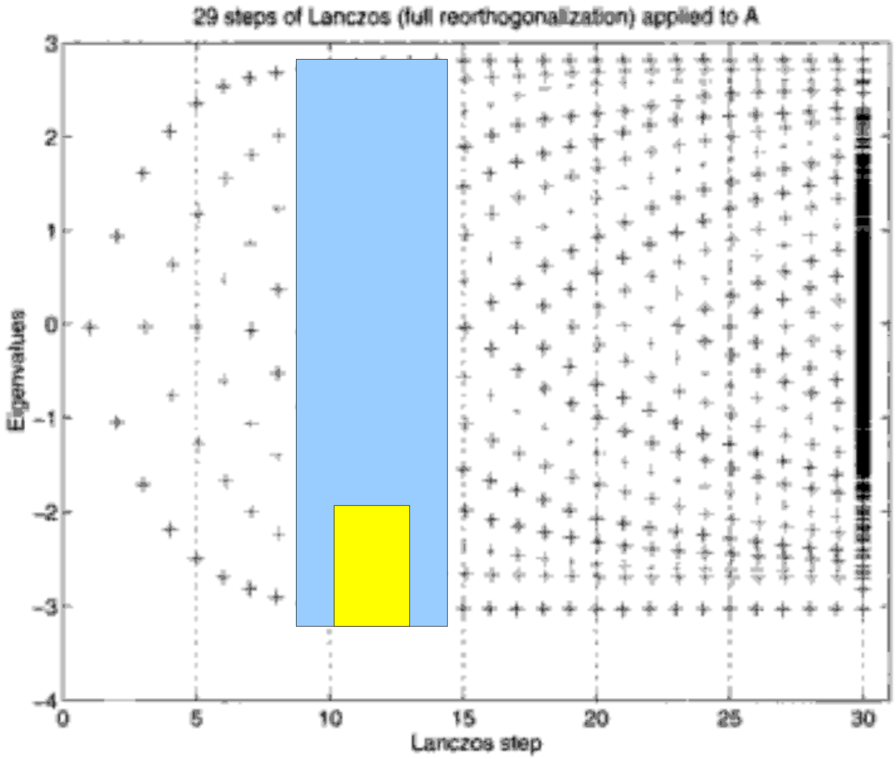
Recall...

- S=1/2 Heisenberg AFM at zero-doping

$$H_{J_{dd}} = J_{dd} \sum \overline{S}_{l\pm 2\epsilon} \cdot \overline{S}_l \Pi_\sigma (1 - p^\dagger_{l\pm\epsilon,\sigma} p_{l\pm\epsilon,\sigma})$$



Rev. Mod. Phys. 78 17 (2006)



Staggered Magnetization

- consider a spin-rotational invariant bi-partite description, e.g.

$$|S=0, S^z=0\rangle = \sum \frac{(-1)^{S_A - m_A}}{\sqrt{2S_A+1}} \delta_{S_A, S_B} \delta_{m_A, -m_B} |S_A, m_A\rangle |S_B, m_B\rangle$$

- GS's staggered magnetization is known

$$\hat{m^2} = \frac{1}{N^2} \left(\sum_r (-1)^{|r|} \hat{S}_r \right)^2 = \frac{(\hat{S}_A - \hat{S}_B)^2}{N^2} = \frac{1}{N^2} (2\hat{S}_A^2 + 2\hat{S}_B^2 - \hat{S}^2)$$

- m^2 and other numerical signtures suggest within each sublattice, N/8 spins add to zero while the rest adds to maximal value.

B. Lau, M. Berciu, and G. A. Sawatzky, Phys. Rev. B 81 172401 (2010)

Requirements

- Select basis states according to sub-lattice spin.
- Systematic convergence.
- Basis transformation + Lanczos must cost less than Lanczos on original basis.
- Extendable to doped scenario.

Basis Formulation

- octa-partition of spins, e.g. a singlet Clebsch-Gordan series

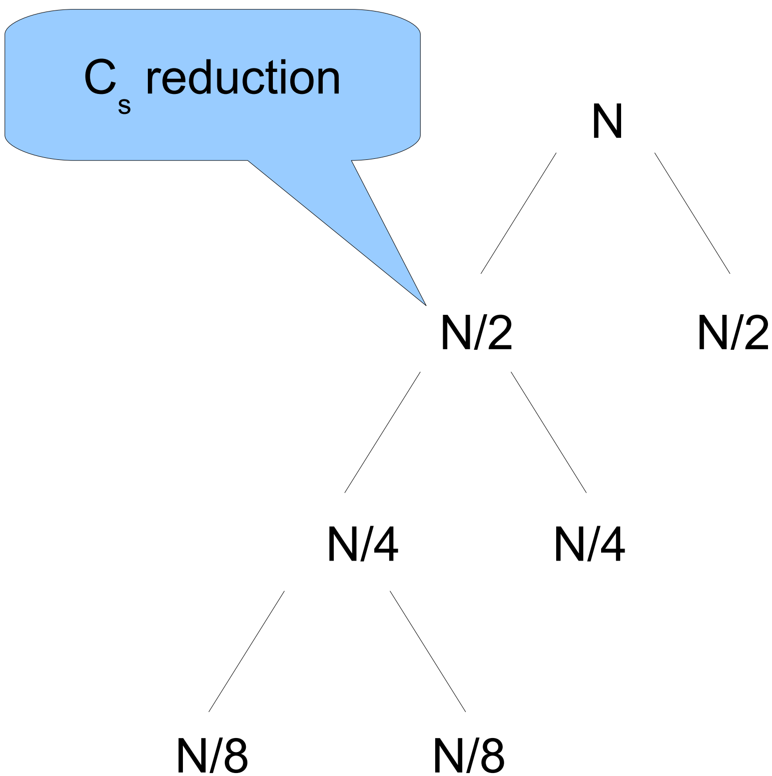
$$|0,0,f(\{S_i\})\rangle = \sum c_{\{S_i,m_i\}} \prod_{i=0}^{7} |S_i, m_i\rangle$$

- Easy bookkeeping of hopping matrix elements for doped wavefunction of the form

$$\frac{1}{\sqrt{N}} \sum e^{iKl} p^{\dagger}_{l,\sigma_l} \left(\prod_{\Delta l} p^{\dagger}_{l+\Delta l,\sigma_{\Delta l}} \right) |\overline{\sigma}\rangle_l$$

LBS PRB (2010)

Recursive Enumeration



- Define completeness $C_s \in [0, 1]$.
- Include N/2-basis states with sub-lattice spin of N/4 down to $S_{A/B} \geq N/4(1-C_s)$.

LBS PRB (2010)

Postulation

- ¼ is the lowest C_s which allows N/8 sub-lattice spins adding to zero. The corresponding basis should capture low-energy states.

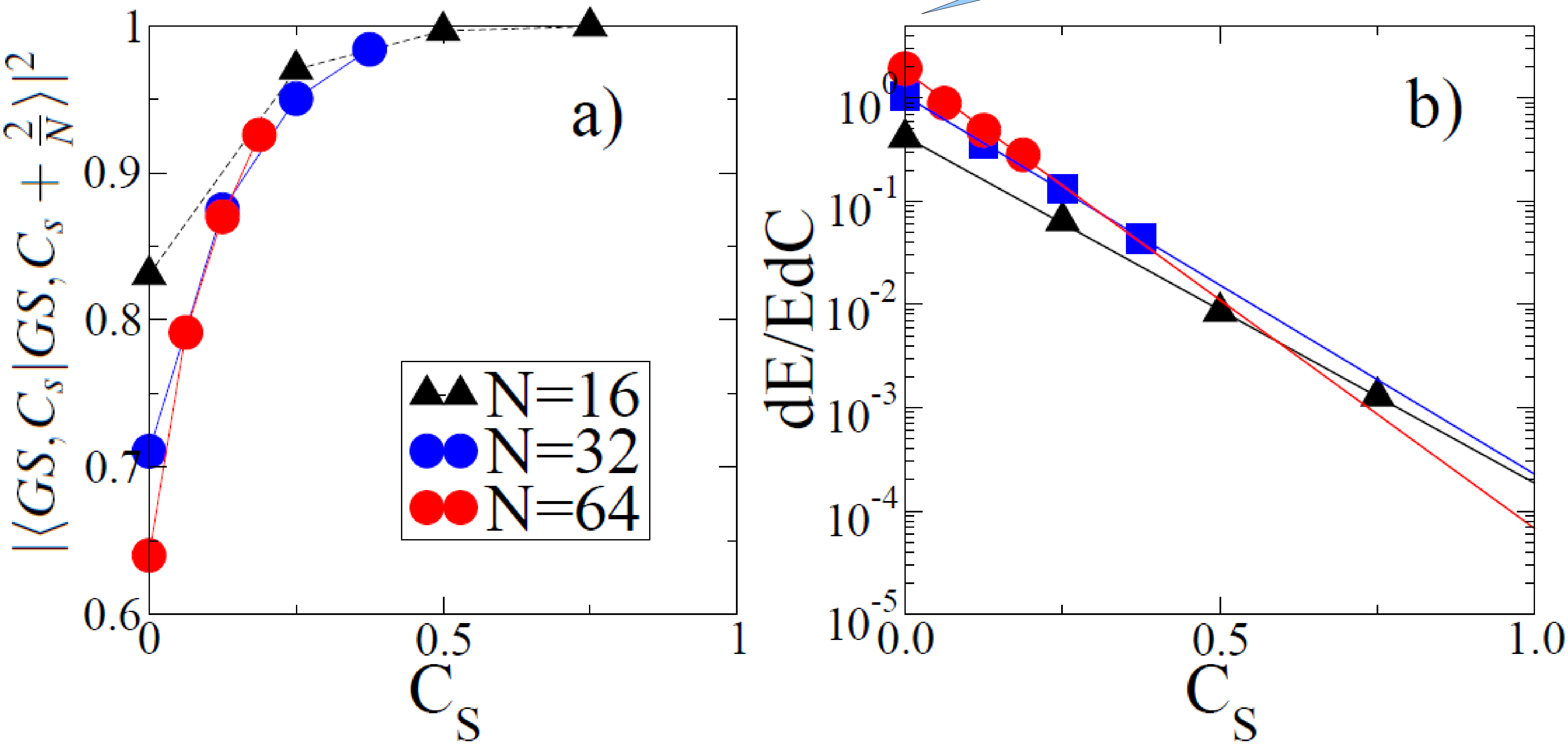
- can extract explicit wavefunctions for undoped case with up to 64 spins.

N	$C_s = \frac{1}{4}$	$S = 0$	$S_z = 0$	Full
16	50	1430	12870	2^{16}
32	11042	35357670	601080390	2^{32}
64	9.8×10^8	5.55×10^{16}	1.83×10^{18}	2^{64}

LBS PRB (2010)

Convergence (undoped)

Fractional error
in log-scale



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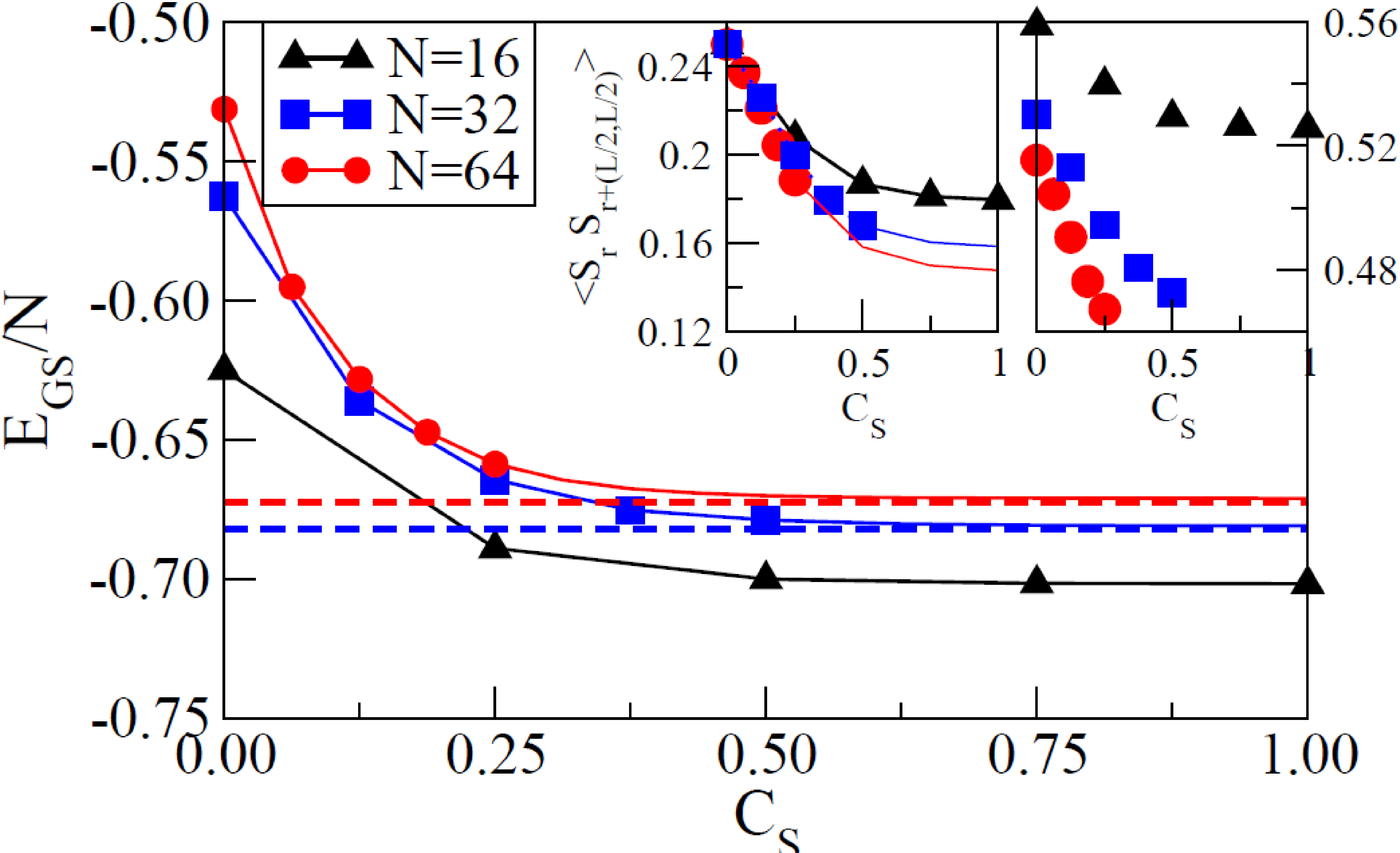
Observables (undoped)

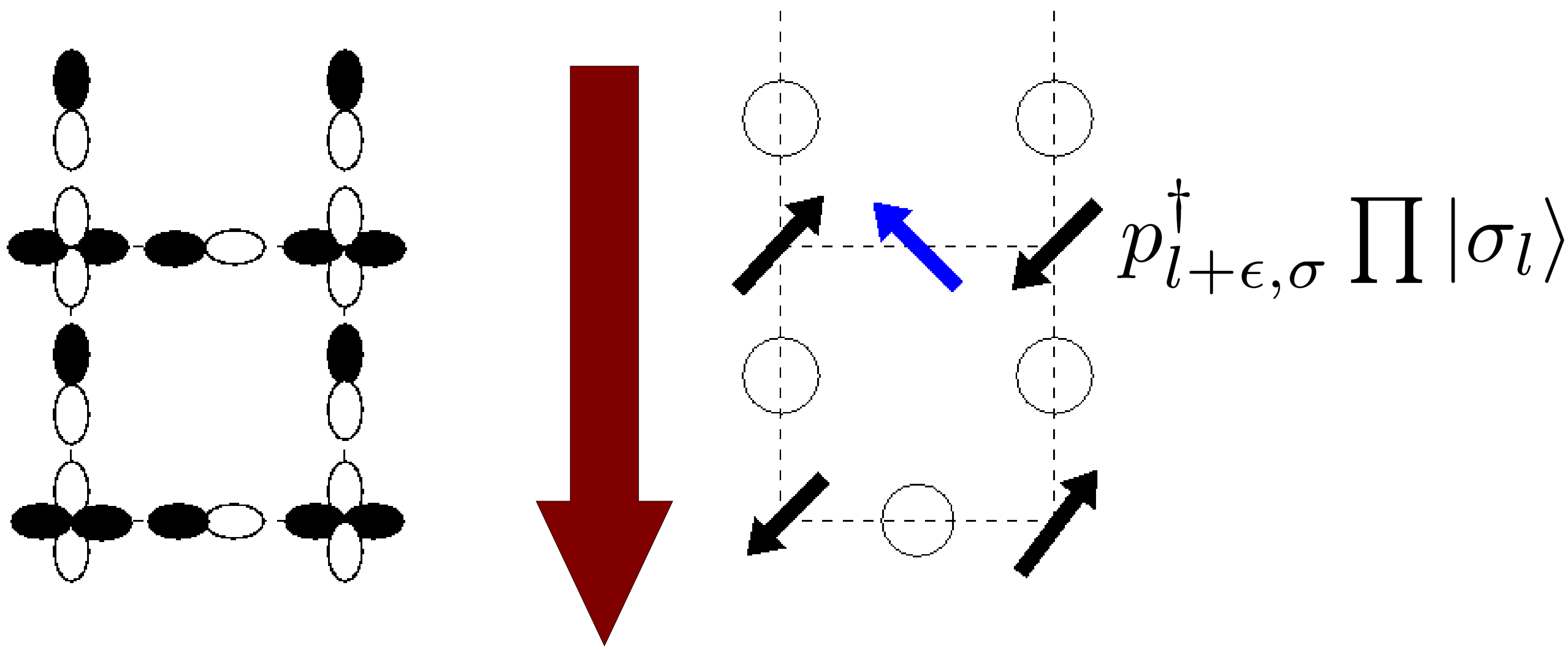


LBS PRB (2010)

Application to doped AFM

Recall...

$$H_{3B} = t_{pd}\sum[(p^\dagger_{l+\epsilon,\sigma} - p^\dagger_{l-\epsilon,\sigma})d_{l,\sigma} + h.c.] + t_{pp}\sum(-1)^{n_\delta} p^\dagger_{l+\epsilon+\delta,\sigma}p_{l+\epsilon,\sigma} - t'_{pp}\sum(p^\dagger_{l-\epsilon,\sigma} + p^\dagger_{l+3\epsilon,\sigma})p_{l+\epsilon,\sigma}$$
$$+\Delta_{pd}\sum p^\dagger_{l+\epsilon,\sigma}p_{l+\epsilon,\sigma} + U_{pp}\sum p^\dagger_{l+\epsilon,\uparrow}p_{l+\epsilon,\uparrow}p^\dagger_{l+\epsilon,\downarrow}p_{l+\epsilon,\downarrow} + U_{dd}\sum d^\dagger_{l,\uparrow}d_{l,\uparrow}d^\dagger_{l,\downarrow}d_{l,\downarrow}.$$

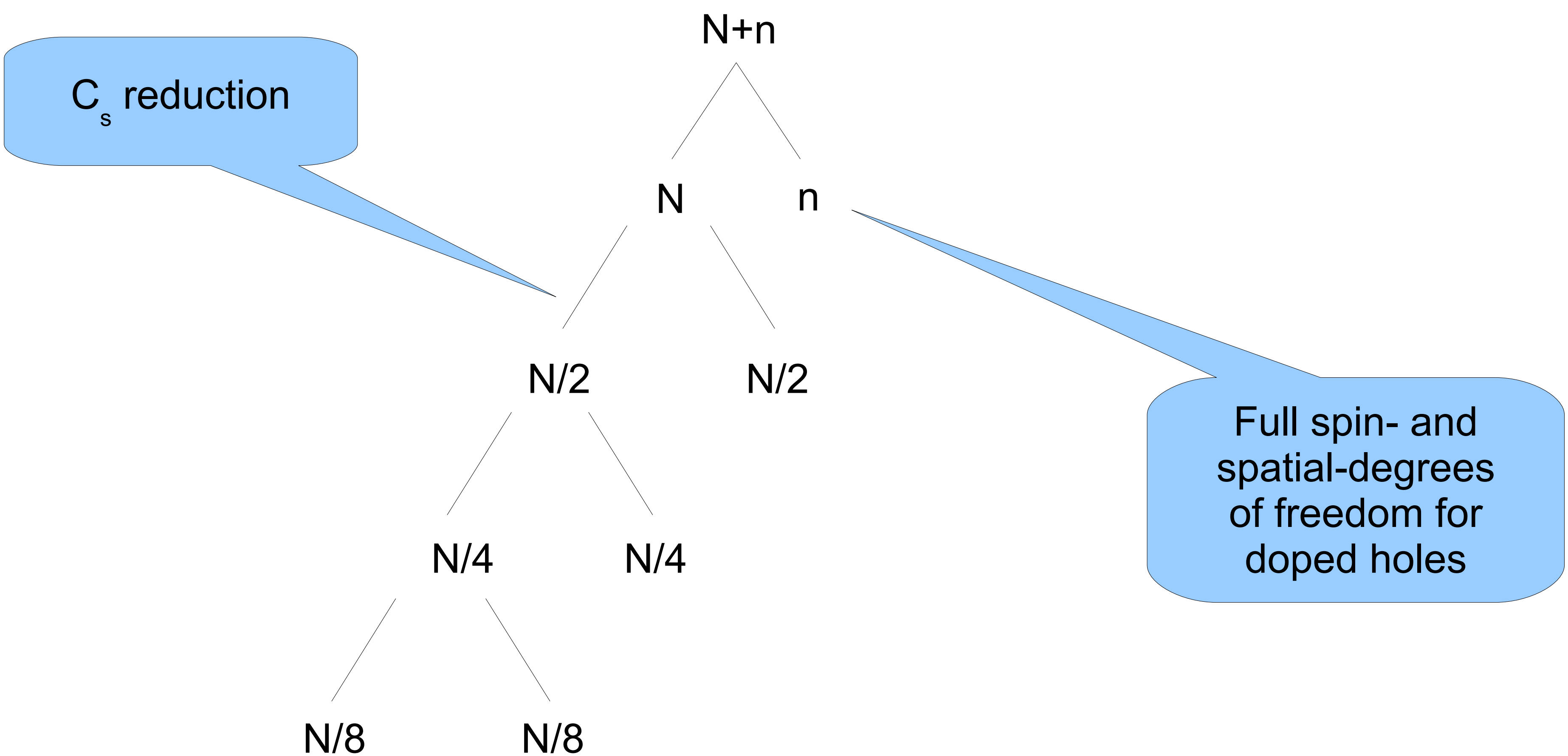


$$H_{\text{eff}} = T_0 + T_{\text{swap}} + H_{J_{pd}} + H_{J_{dd}}$$

B. Lau, M. Berciu, and G. A. Sawatzky, Phys. Rev. Lett. 106 036401 (2011)

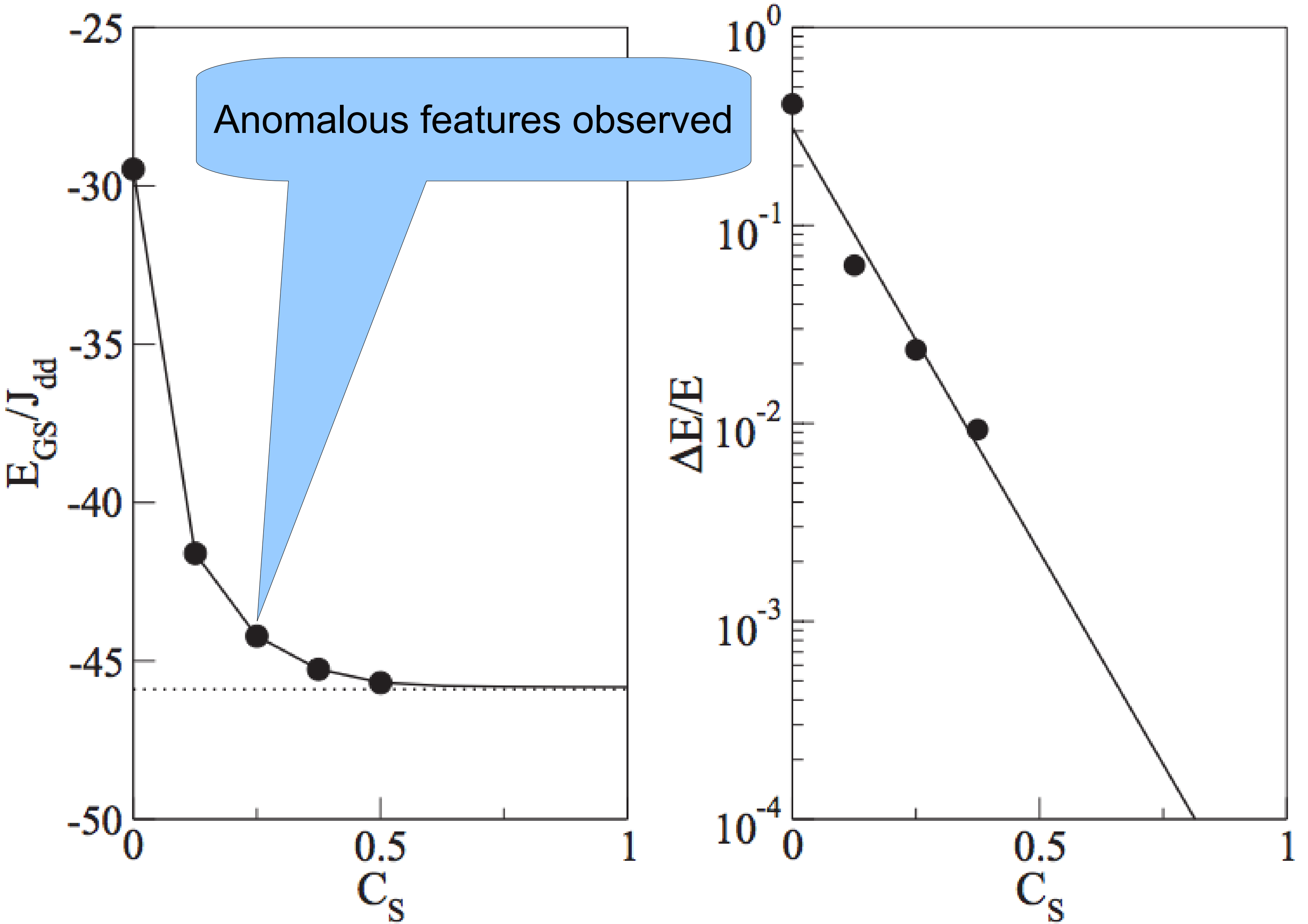
Generalization

- (N+n)-hole basis of the form $\frac{1}{\sqrt{N}}\sum e^{iKl} p^{\dagger}_{l,\sigma_l}\left(\prod_{\Delta l} p^{\dagger}_{l+\Delta l,\sigma_{\Delta l}}\right)|\overline{\sigma}\rangle_l$

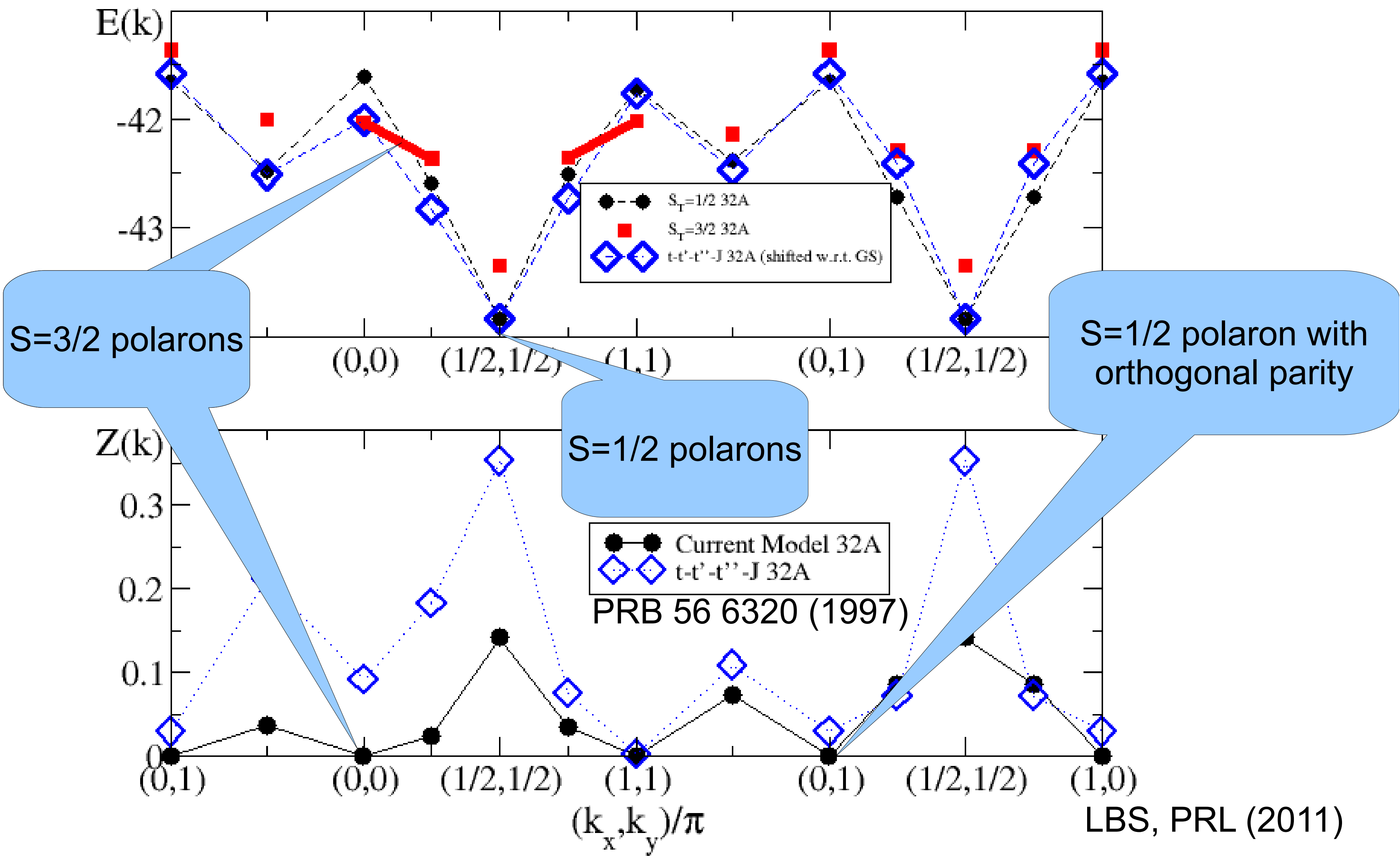


B. Lau, M. Berciu, and G. A. Sawatzky, Phys. Rev. B 84 165102 (2011)

Convergence (1 hole, N=32)



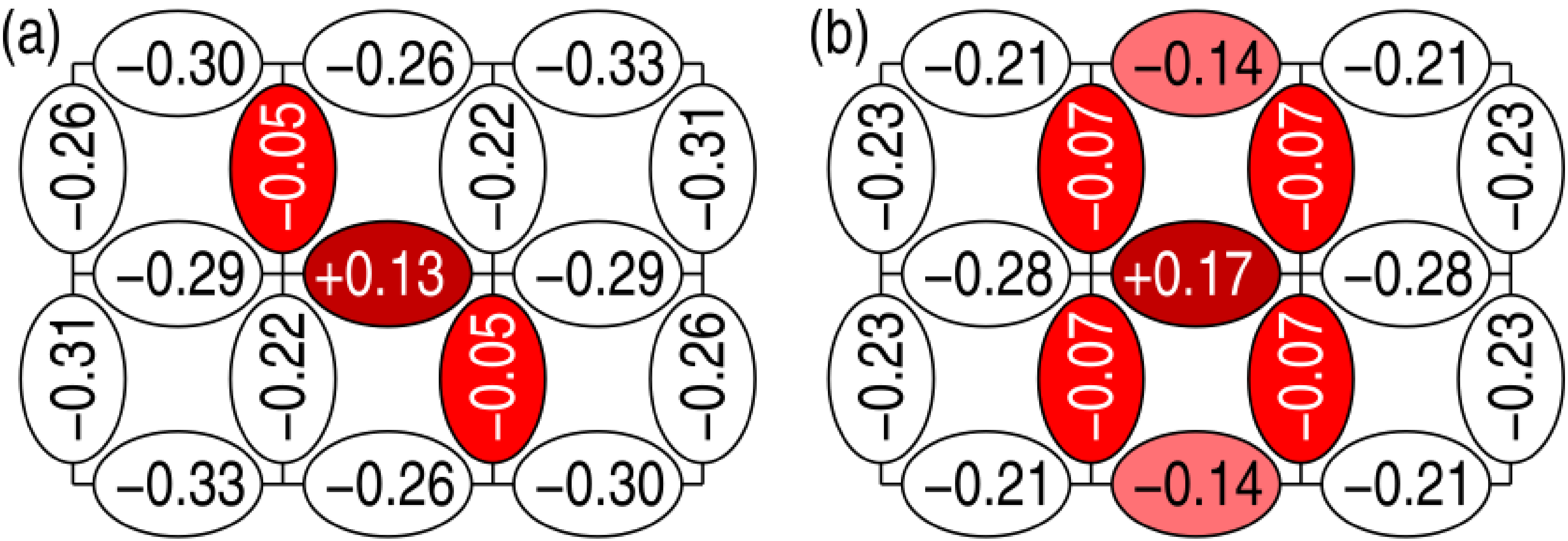
Solution (C_s=1 1-hole N=32)



Polaronic structure (1-hole, N=32)

- A local spin degree of freedom around the S=1/2 three-spin-polaron core.

S=1/2 S=3/2



Further numerical support of C_s

- Tabulate exact one-hole GS's probability in terms of sub-lattice spin.

C_s

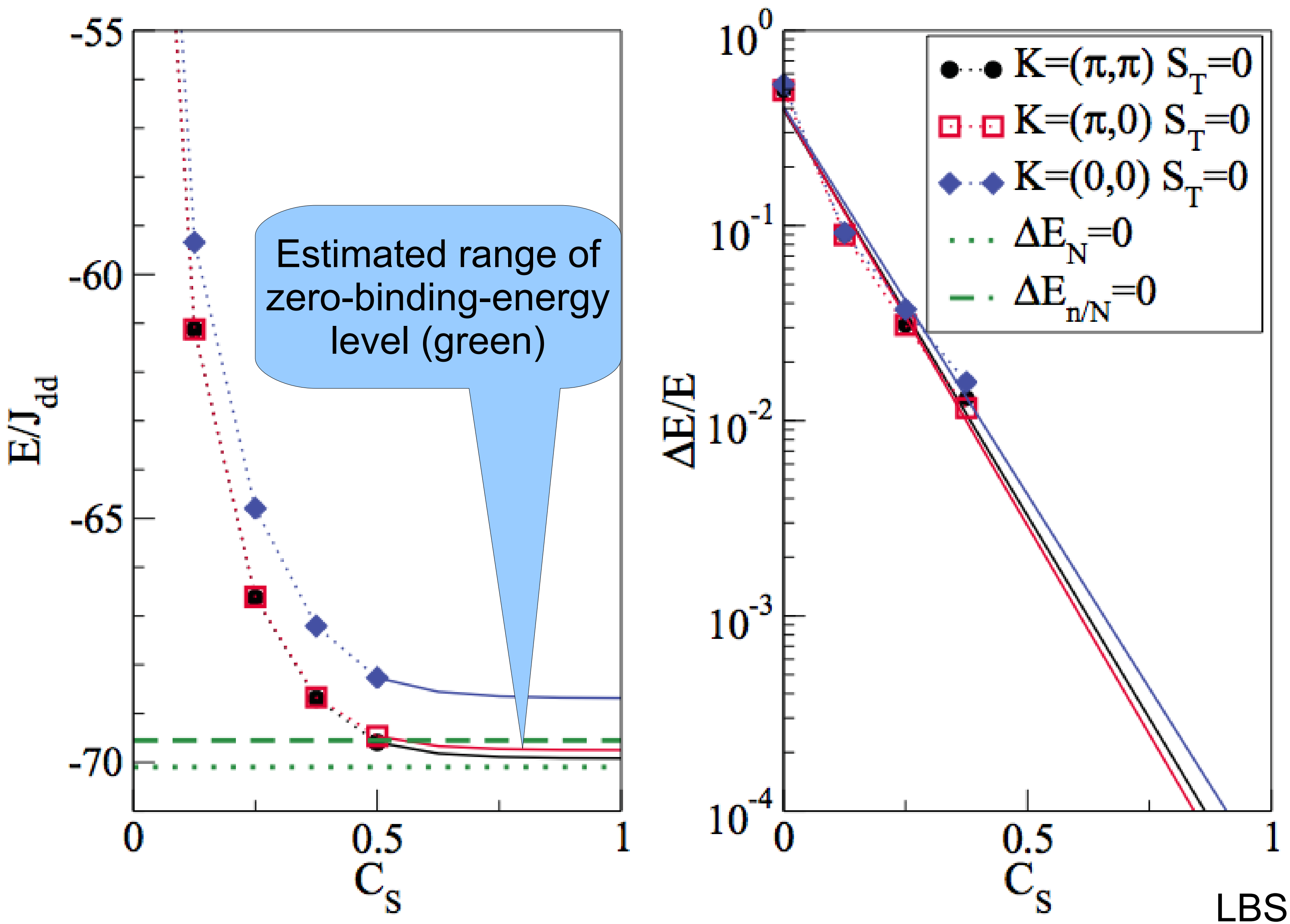
$s_A \backslash s_B$	0	1	2	3	4	5	6	7	8
0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
1	0.00	0.02	0.03	0.00	0.00	0.00	0.00	0.00	0.00
2	0.00	0.03	0.14	0.16	0.00	0.00	0.00	0.00	0.00
3	0.00	0.00	0.16	0.69	0.68	0.00	0.00	0.00	0.00
4	0.00	0.00	0.00	0.68	2.52	2.21	0.00	0.00	0.00
5	0.00	0.00	0.00	0.00	2.21	7.06	5.28	0.00	0.00
6	0.00	0.00	0.00	0.00	0.00	5.28	14.24	8.44	0.00
7	0.00	0.00	0.00	0.00	0.00	0.00	8.44	18.06	6.85
8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	6.85	9.97

$C_s=1/4$

- $C_s \sim 1/4 + O(1/N)$ required.

LBS, PRB (2011)

Convergence (2 holes, N=32)



LBS, PRB (2011)

Some N=32 two-hole Results

- Charges form S=1/2 cores, but their spin entities are carried outside of the cores.
- Band-structure distinctly different from N=16 three-band. Similar to N=32 t-t'-t''-J model, but...
- Exception: the lowest S=0 state is a d_{x2-y2} local pair. Located $\sim W_{1h}$ above GS, it is a direct signature of competition between kinetic energy and d_{x2-y2} local attraction at low-doping.

LBS, PRB (2011)

Summary

- A stable, systematic, and efficient approach for doped and undoped AFM.
- 1- and 2-hole N=32 comparison quantified several oxygen-specific characters.