Do the single band Hubbard models describe superconductivity in the cuprates?

- My title is really two questions
- Downfolding from a three band model
  - ➡ Mapping to a 1 band model is precise and easy
  - ➡ It gives you more than you thought
- Understanding the key new density-dependent hopping term

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Does the single band Hubbard model describe superconductivity in the cuprates?

We should split this question into two parts:

1. *Do the properties of the Hubbard model accurately match those of the cuprates?*
   - ➡ An enormous amount of work. Now there is increasing acceptances that simulations are key; many new algorithms!
   - ➡ Using a number of methods, including multi-messenger studies, we are getting answers to this question!
   - ➡ But: the models are extremely sensitive to small parameters, e.g. the t-J model seems not to have hole-doped SC but the Hubbard model does

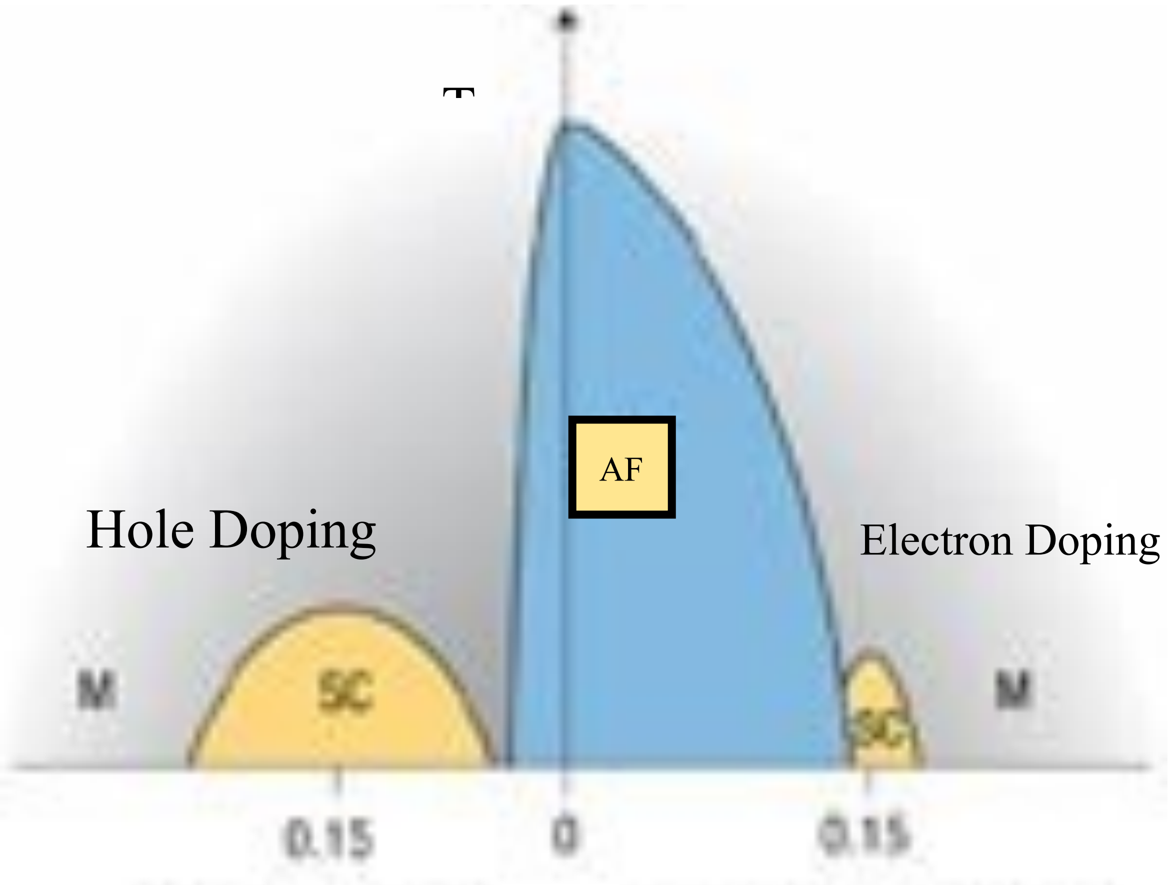
2. *Can we renormalize down to the Hubbard model reliably and controllably from a more precise higher-energy model?*
   - ➡ Surprisingly little work, most from the 1980's & 90's
   - ➡ Ideally we would go all the way back to the continuum all electron Hamiltonian. We are not there yet, but we can do very well going from a three band model.

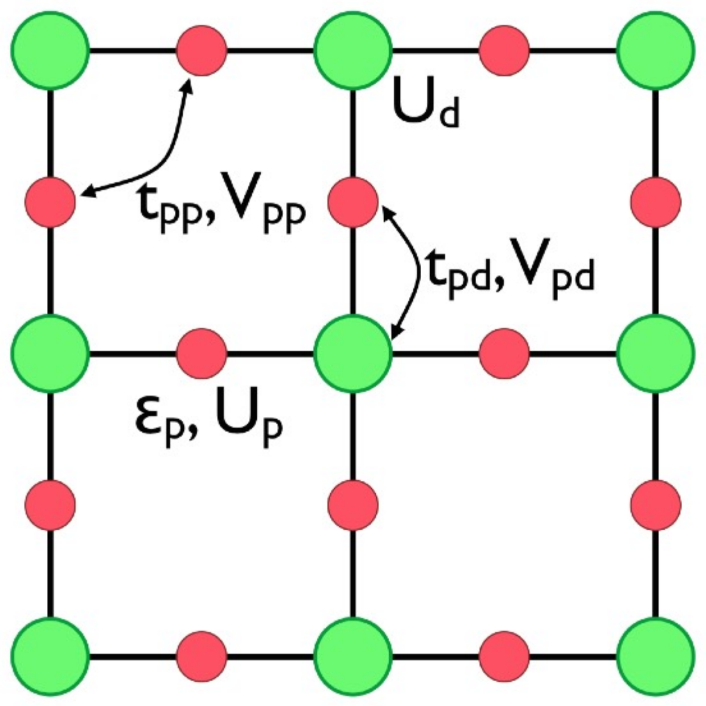
Answering either question perfectly indirectly answers the other

The 2D Hubbard model

<u>We are interested in a family of models:</u>

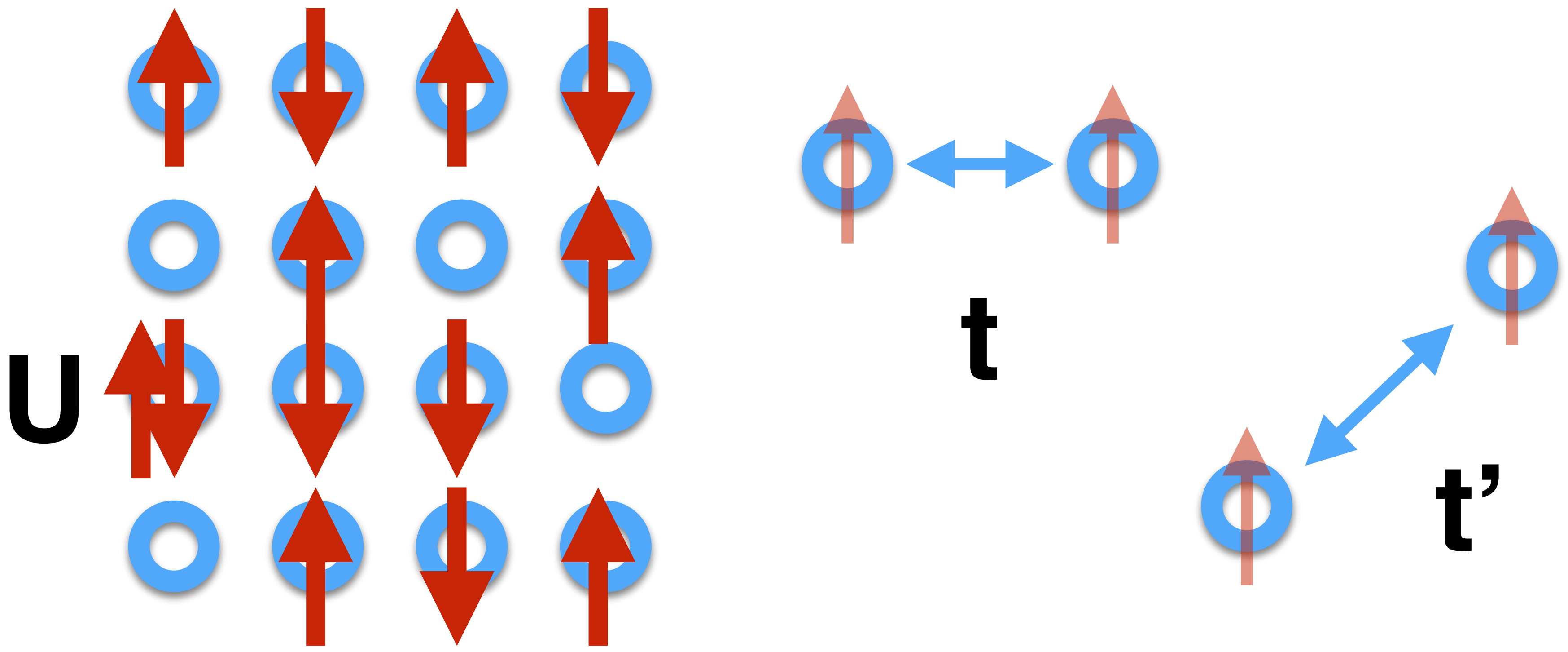
The **three band Hubbard model** has the most realistic description of the cuprates





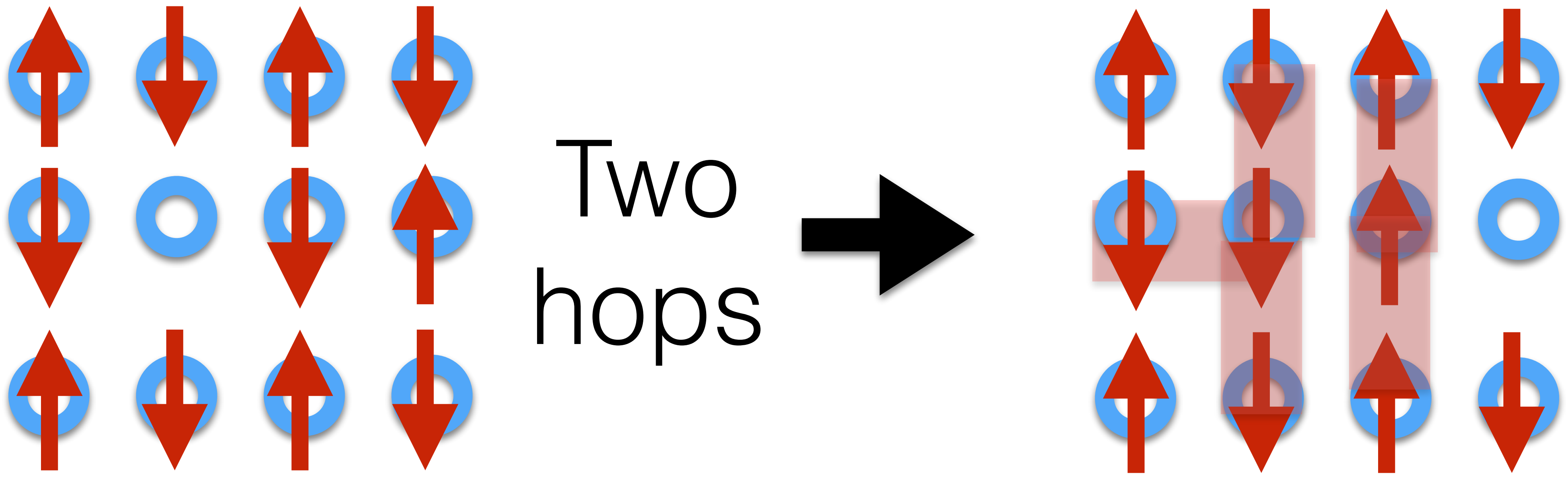
The **one band Hubbard model** is simpler and more general, and has both weak and strong coupling regimes. This is the "Ising model" of interacting electrons: all the entanglement, omitting orbital details, but unlike the 2D Ising model, analytic treatments are very limited.

The **t-J model** is simpler still, applying to the strong coupling regime only. Double occupancy is integrated out, generating an AF exchange term



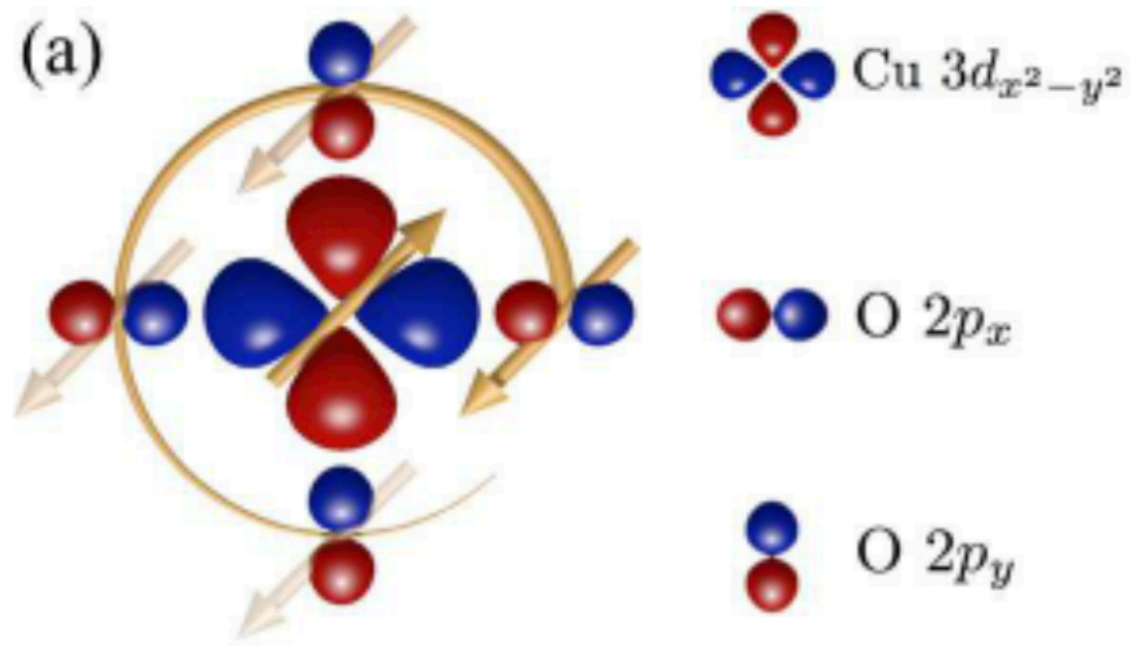
$$H = -\sum_{\langle ij\rangle,\sigma} t_{ij}(c_{i\sigma}^{\dagger}c_{j\sigma} + c_{j\sigma}^{\dagger}c_{i\sigma}) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}.$$

Frustrated hole hopping is key to the physics



Zhang Rice singlets: mapping from three bands to one

- Zhang-Rice (1988) treatment of the three band model: exact diagonalization of 5-site cluster (1 Cu, 4 surrounding O's) in the two-hole sector found a low energy (Zhang-Rice) singlet between a hole on a Cu and a hole on the symmetric 4-site O state.
- The large gap found was argued to allow discarding other states and is the basis for a single band model.
- In the early days people like Eskes & Sawatzky (1991) improved on the arguments (e.g. adding t_{pp}). One constructs Wannier functions from the singlet O band.
- A number of experiments have helped validate the basic idea of the ZR singlet



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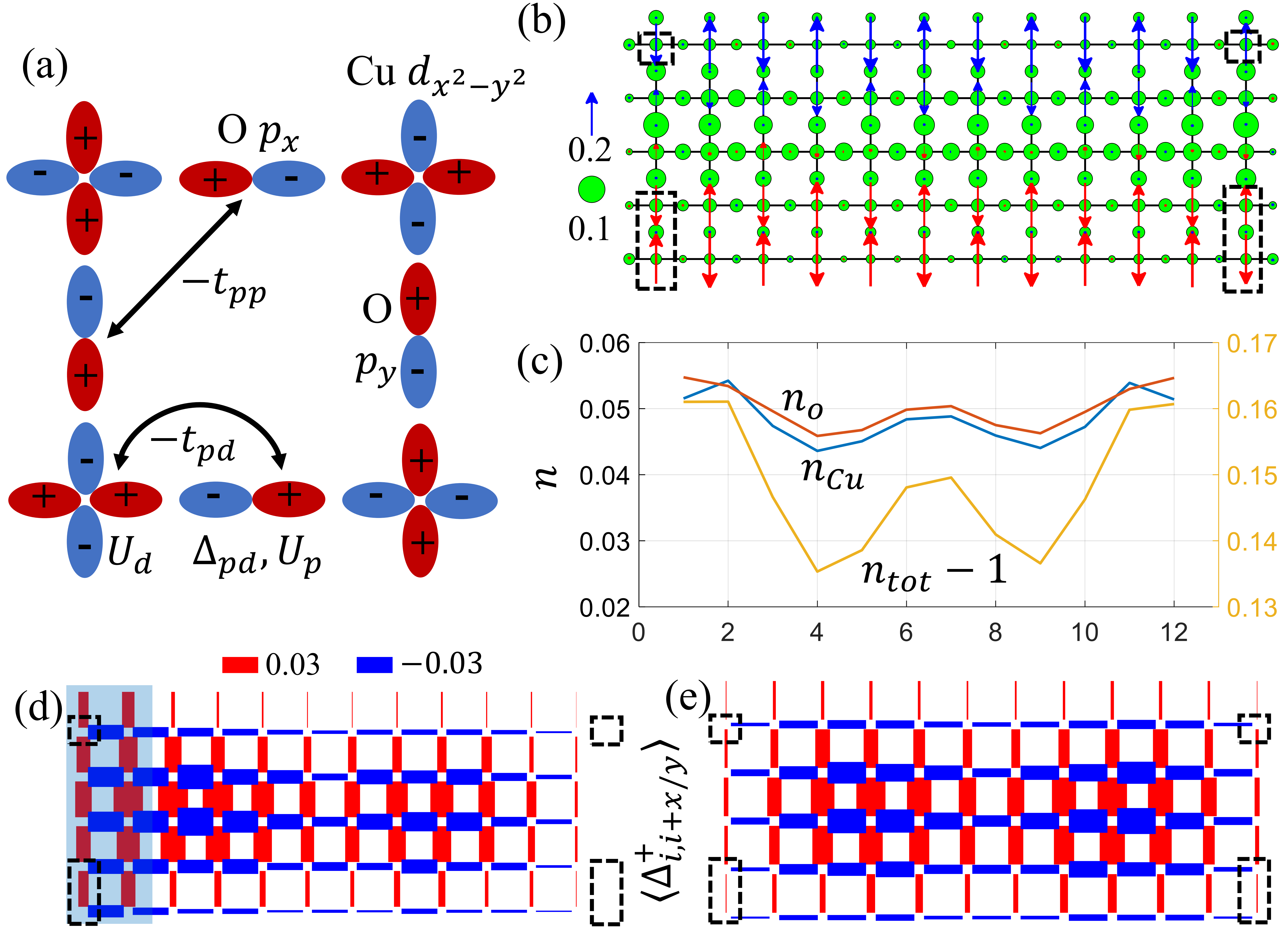
Questions

1. Can we justify the reduction to one band via modern simulations of the three-band model?
2. Can we make the downfolding systematic and quantitative?
3. Do we have all the important terms in the one band model?

Three band Hubbard DMRG simulations



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See arXiv:2303.00756

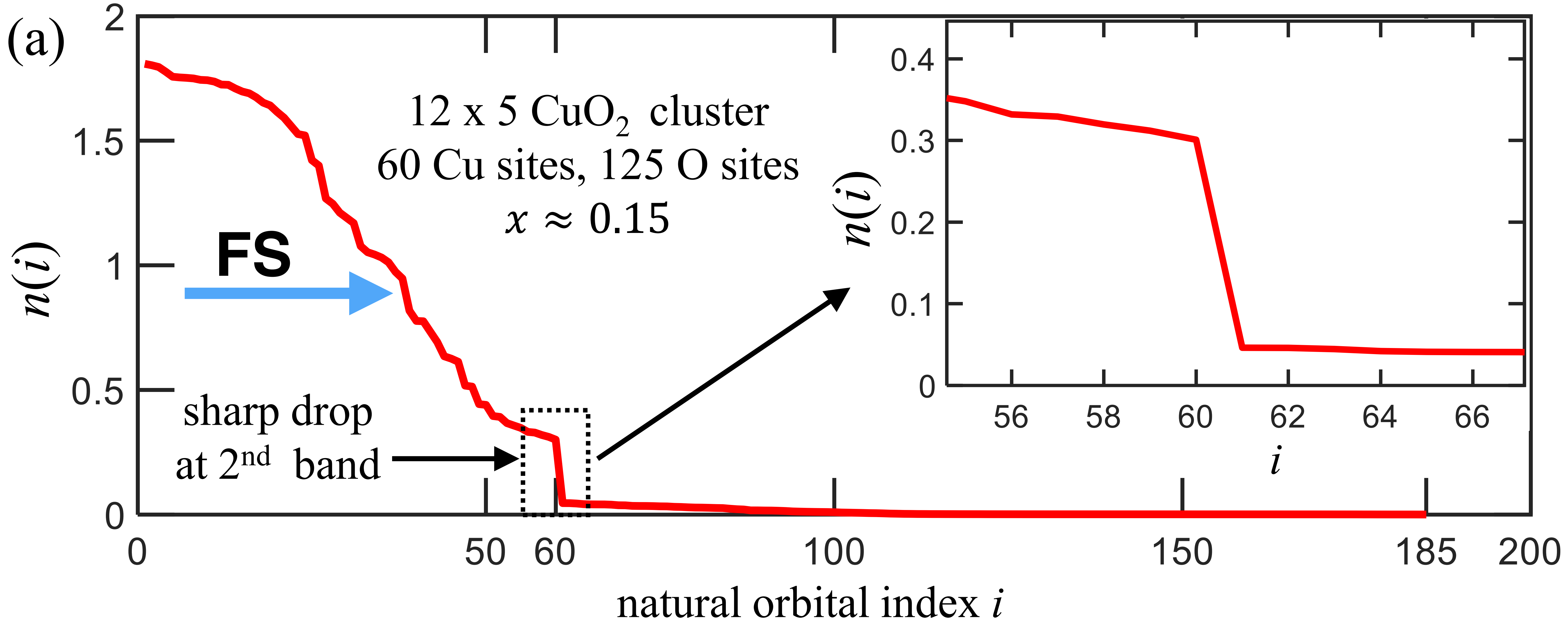
Width-5 is the best we can do currently with DMRG

Arrange with 1 stripe down the middle so not frustrated (likes stripes anyway)

Good pairing response from pair field at one edge, but we make no claims about infinite 2D limit!

Natural Orbitals

- Natural orbitals: diagonalize the equal-time Green's function $\langle c_i^\dagger c_j \rangle$; eigenvalues are the occupancies, eigenvectors are the NOs. Super-basic tool of quantum chemistry, fastest CI expansions
- For a uniform el. gas, NOs are plane waves, occupancies are n_k
- For mean field/HF or DFT, get the usual Fermi step function, but interactions smear out Fermi surface



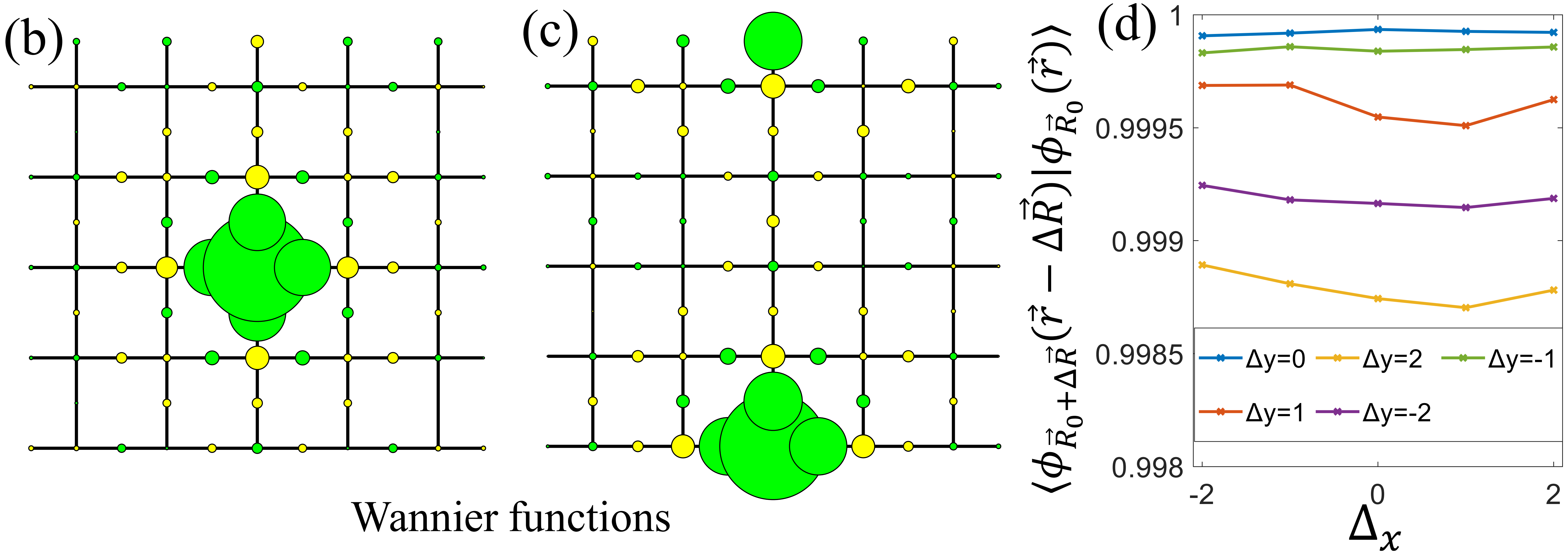
- No sharp drop a FS: very strong interactions
- Very sharp drop at end of first band, down to negligible occupancies for higher bands: very strong justification of the mapping to a single band! Zero occupancy means zero error in truncation.
- Very little finite size effects in this dropoff: narrower, shorter cylinders, not shown. Drop is a local property, we don't need to worry about thermodynamic limit.

- We might have had to perform Schrieffer-Wolf type many-particle rotations to get near-zero occupancies, e.g. $c_i \to \sum_j A_{ij} c_j + \sum_{jkl} A_{jkl} c_j^\dagger c_k c_l$

Very easy downfolding!

Form Natural Orbital Wannier functions for the first band

<u>Recipe</u>:
1. project delta function on each Cu site onto 1st band of NOs
2. Symmetrically orthonormalize these functions



Wannier functions

Resulting Wannier functions are nearly translationally invariant. Now rotate/project the three band H into a single band model Wannier model

Now truncate the Wannier Hamiltonian by size of coefficients

- Results depend on 3 band parameters and doping, but the dependence is not too big near "standard" parameters
- H has expected U, t, t', t'' but U/t is unexpectedly large: $U/t \approx 13$ (12.6 hole doping, 13.7 electron doping)
- But the biggest surprise is **large** density dependent hopping terms:

$$\sum_{i,\delta_i,\sigma} - t_n^\delta (c^\dagger_{i+\delta,\sigma} c_{i,\sigma} + c^\dagger_{i,\sigma} c_{i+\delta,\sigma}) n_{\bar{\sigma} i}$$

All ops on just two sites

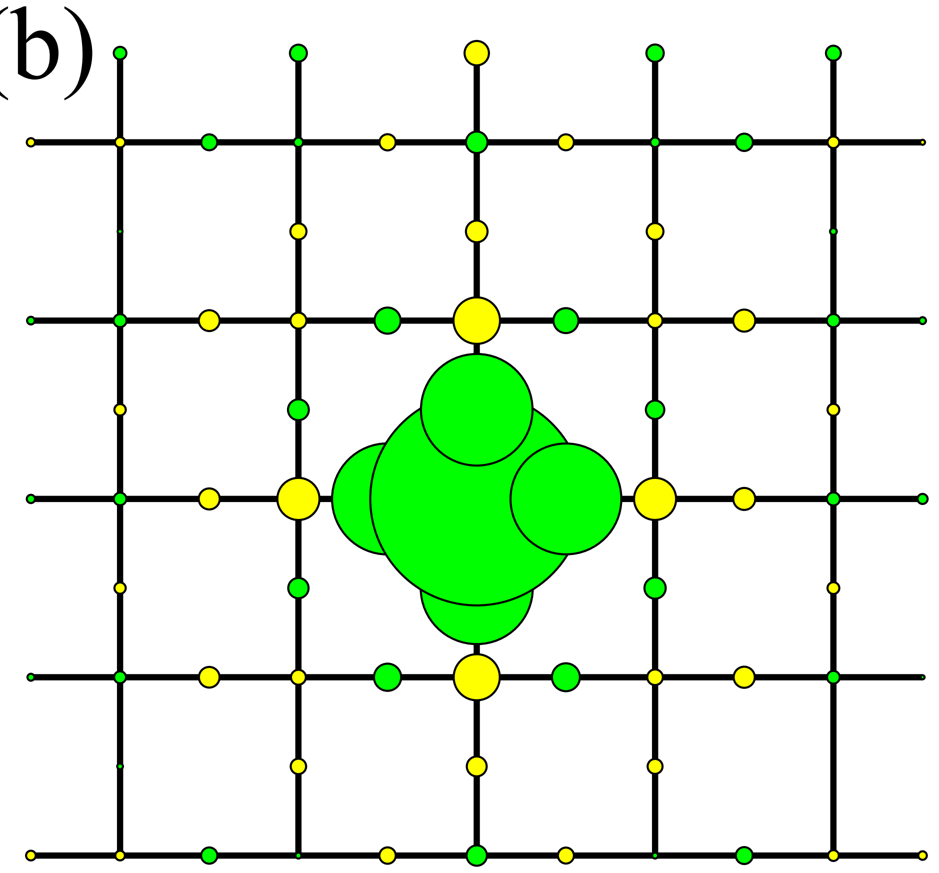
	case $(U_d,\ \Delta_{pd},\ n)$	t_n	t'	t'_n	t''	t''_n	U
$t \equiv 1$	**h1*** (6.0, 3.5, 1.15)	0.60	0.07	0.05	-0.04	-0.09	12.6
	e1 (6.0, 3.5, 0.85)	0.52	0.08	0.08	-0.05	-0.04	13.7

The nn t_n parameter is **large**! almost twice a typical J

This type of term has been mentioned a few times, but sometimes dismissed without further study (Laughlin). But Werner, Parcollet, Georges, Hassan (PRL 2005) pointed out is importance for deriving Hubbard for cold atoms!
Hirsch took it in his own direction… perhaps suppressing other studies…

The origin of t_n is extremely simple and robust!

The Wannier function is very local; we can consider only three amplitudes, α, β, γ for onsite Cu, nn O, and nn Cu sites. β is directly tied to the undoped O occupancy, say ~0.15, and we find $\beta \sim 0.2 - 0.25$: this is almost model independent. Orthogonality of the nn Wanniers means $2\alpha\gamma + \beta^2 \approx 0$, or with $\alpha \sim 0.9$, then $\gamma \sim -\beta^2/2 \sim -0.03$



t_n comes from transforming $U n_\uparrow n_\downarrow$, where only one operator is moved, so $t_n \sim U_{dd}\alpha^3\gamma \sim 0.2$ in units of t_{pd}

t itself is ~0.3, so the ratio ~~2/3 in agreement with the precise transformation

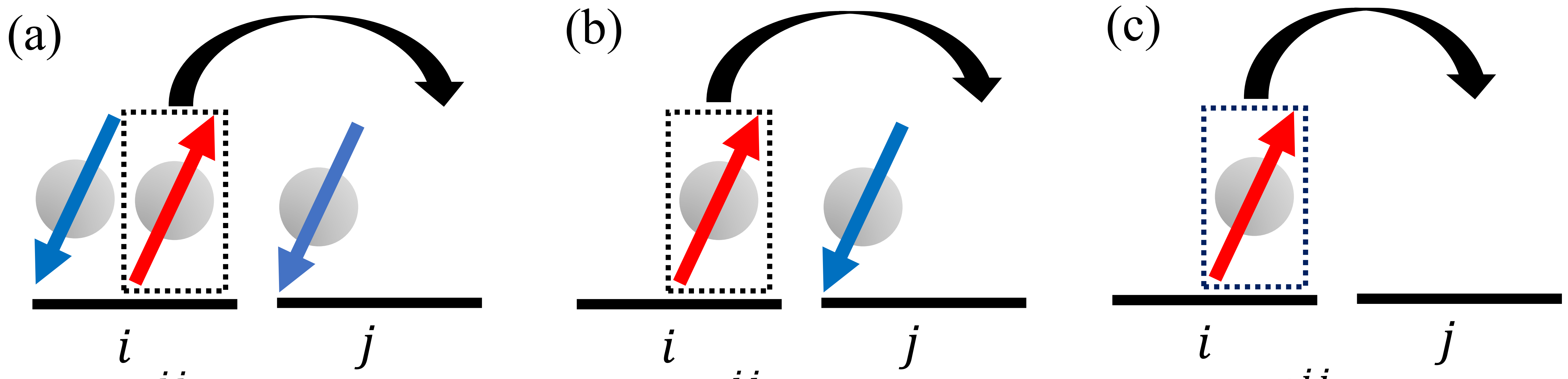
Effect of t_n

The first thing you can do is reduce it to an ordinary hopping using mean field, putting brackets $\langle n \rangle$. This then adds directly to the ordinary hopping, increasing it by ~50% ! This fixes our U/t ratio that seemed too big: $U/t_{\text{eff}} \sim 7.5$

But simulations show the Hubbard model is very sensitive to even parameters ~0.1, so how can we trust mean field??

This term is very sensitive to other holes nearby:

$$\hat{t}_{n\uparrow}^{ij} = t_n C_{j\uparrow}^{+} C_{i\uparrow} (n_{i\downarrow} + n_{j\downarrow}) + \text{h.c.}$$

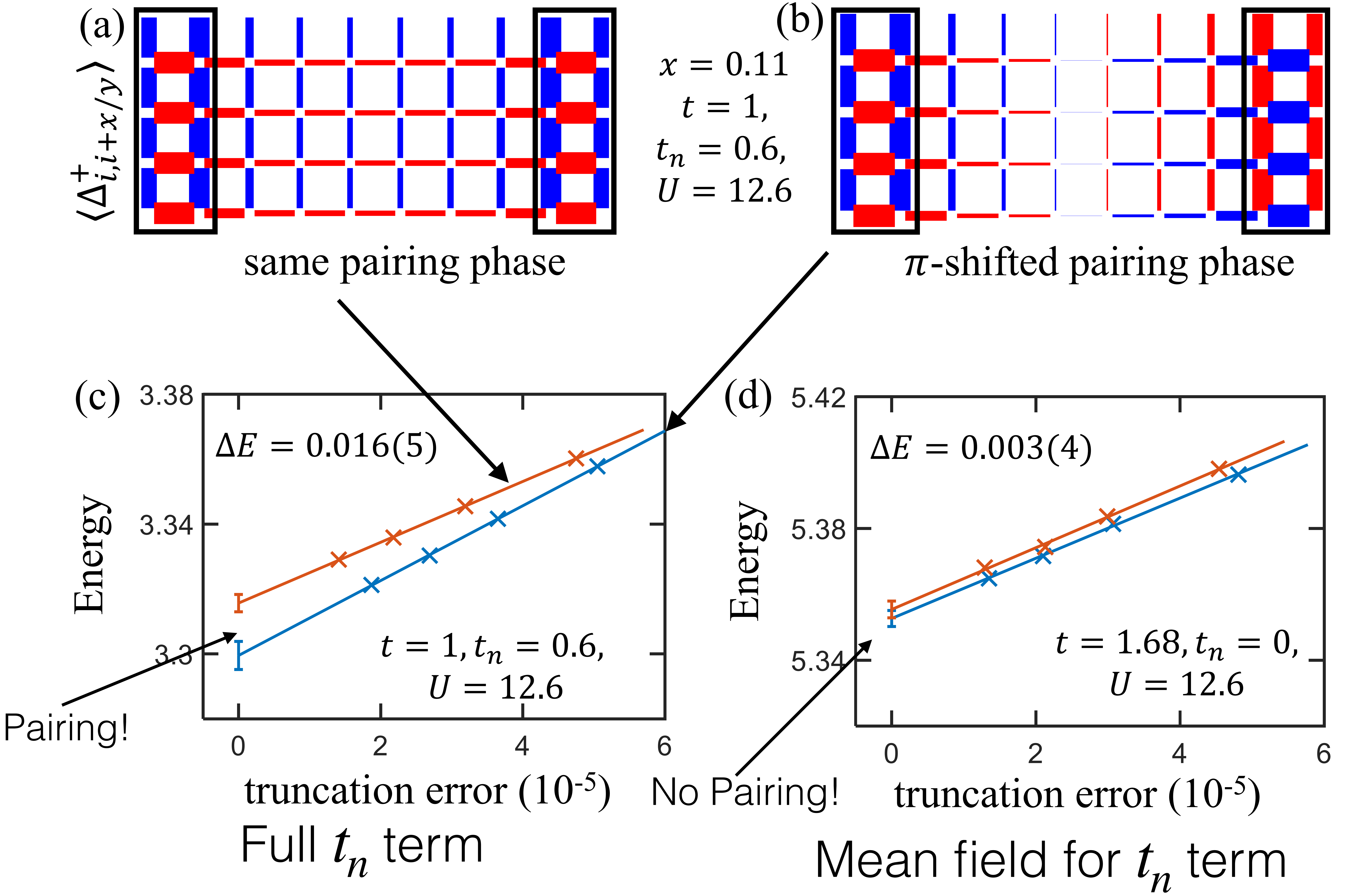


$\hat{t}_n^{ij} \sim 2 t_n C_{j\uparrow}^{+} C_{i\uparrow}$ $\hat{t}_n^{ij} \sim t_n C_{j\uparrow}^{+} C_{i\uparrow}$ $\hat{t}_n^{ij} \sim 0$

Thus this term might affect pairing beyond mean field.

Pairing enhanced due to the t_n term

Pair field applied at edges, with and w/o twist



This measurement is not meant to test 2D pairing order—only as a quantitative test for local relative differences in pairing tendencies.

t_n brings up pairing significantly on the hole doped system, (and supresses it on the electron doped side—not shown)

Conclusions: Does the single band Hubbard model describe superconductivity in the cuprates?

2. *Can we renormalize down to the Hubbard model reliably and controllably from a more precise higher-energy model?*

- ➡ Examining the natural orbital occupancies from DMRG simulations of a 3 band model strongly supports a mapping to a single band model
- ➡ A straightforward, robust Wannier downfolding produces large density-assisted hopping terms which are key to getting the right U/t in mean field. We argue that they are too big to rely on mean field. Preliminary DMRG simulations indicate these terms enhance pairing on the hole-doped side, and not on the electron doped side.

Answering either question perfectly indirectly answers the other

How does this square with progress in question 1?

1. *Do the properties of the Hubbard model accurately match those of the cuprates?*

Superconductivity in the models is very sensitive, certainly to t’ or Hubbard versus t-J, but also to boundary conditions, cylinder sizes, etc.

Maybe the models would be less sensitive, and give more robust SC with t_n turned on.