Adiabatic Quantum Simulation:

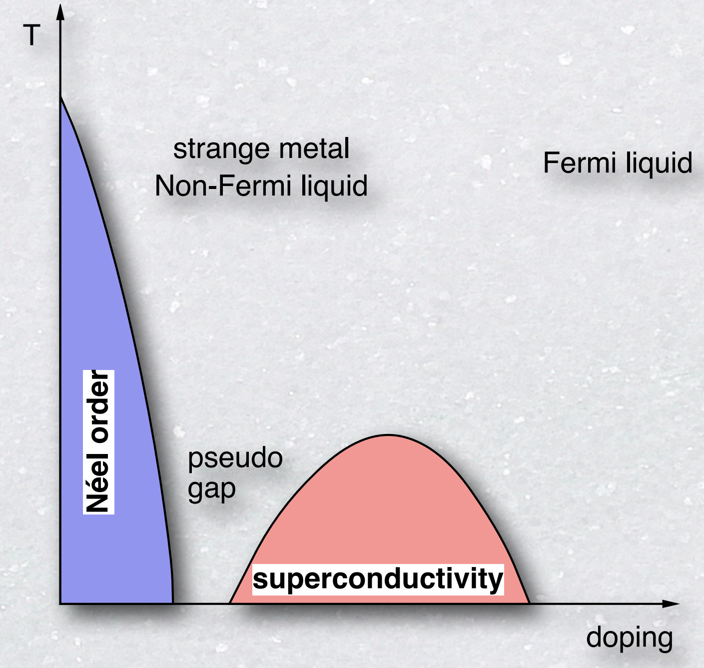
d-wave RVB States and the Phase Diagram of the Fermionic Hubbard Model

Matthias Troyer (ETH Zürich)

Simon Trebst (Microsoft Station Q, Santa Barbara)
Uli Schollwöck (RWTH Aachen)
Peter Zoller (Innsbruck)

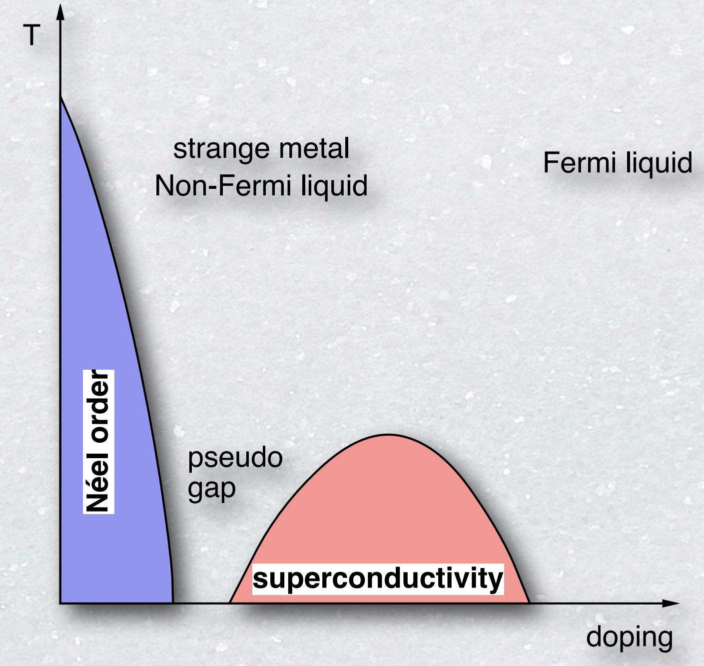
S. Trebst, U. Schollwöck, M. Troyer, P. Zoller, PRL **96**, 250402 (2006)

High temperature superconductivity



High temperature superconductivity

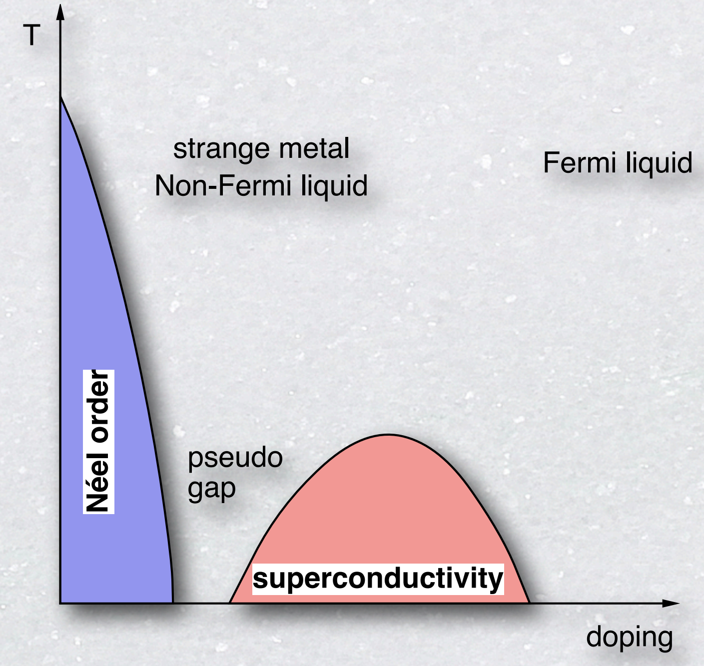
- 1986: Experimental discovery by Bednorz and Müller
  J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986).



High temperature superconductivity

- 1986: Experimental discovery by Bednorz and Müller
  J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986).

- 1987: RVB theory by Anderson
  P. W. Anderson, Science **235**, 1196 (1987).

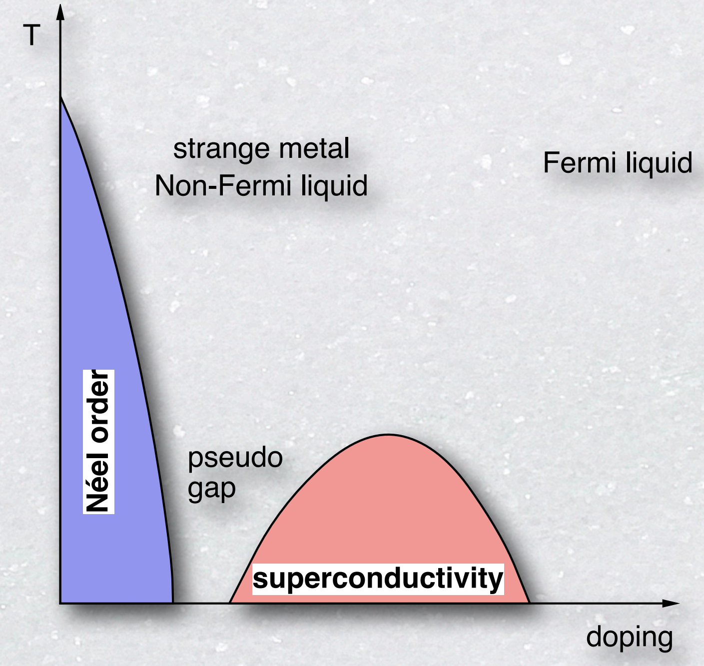


High temperature superconductivity

- 1986: Experimental discovery by Bednorz and Müller
  J. G. Bednorz and K. A. Müller, Z. Phys. B **64**, 189 (1986).

- 1987: RVB theory by Anderson
  P. W. Anderson, Science **235**, 1196 (1987).

- But is it not over yet
  - hard to get clean sample
  - hard to do good experiments
  - hard to solve the theoretical models
  - hard to simulate the theoretical models



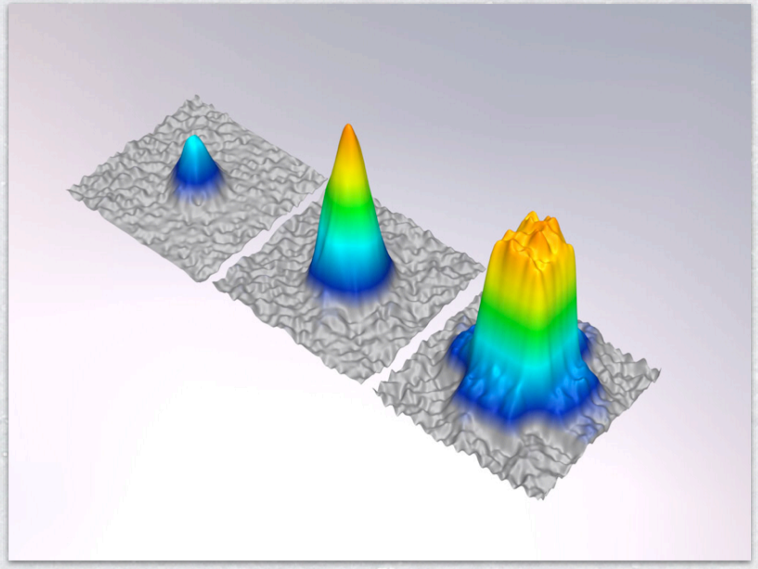
Quantum simulations with lattice fermions

Quantum simulations with lattice fermions

- Ultracold atomic gases in optical lattices allow quantum simulation of the fermionic Hubbard model
  - Attractive case: high-temperature superfluidity
    - W. Hofstetter *et al*, PRL **89**, 220407 (2002)
  - Repulsive case: hard to simulate on classical computers
    - is the ground state superconducting?
    - is the ground state an RVB state?
    - can it explain high-T_c superconductivity?

Quantum simulations with lattice fermions

- Ultracold atomic gases in optical lattices allow quantum simulation of the fermionic Hubbard model
  - Attractive case: high-temperature superfluidity
    - W. Hofstetter *et al*, PRL **89**, 220407 (2002)
  - Repulsive case: hard to simulate on classical computers
    - is the ground state superconducting?
    - is the ground state an RVB state?
    - can it explain high-T_c superconductivity?
- Detection of Fermi surface in ^{40}K
  - M. Köhl *et al*, PRL **94**, 080403 (2005)

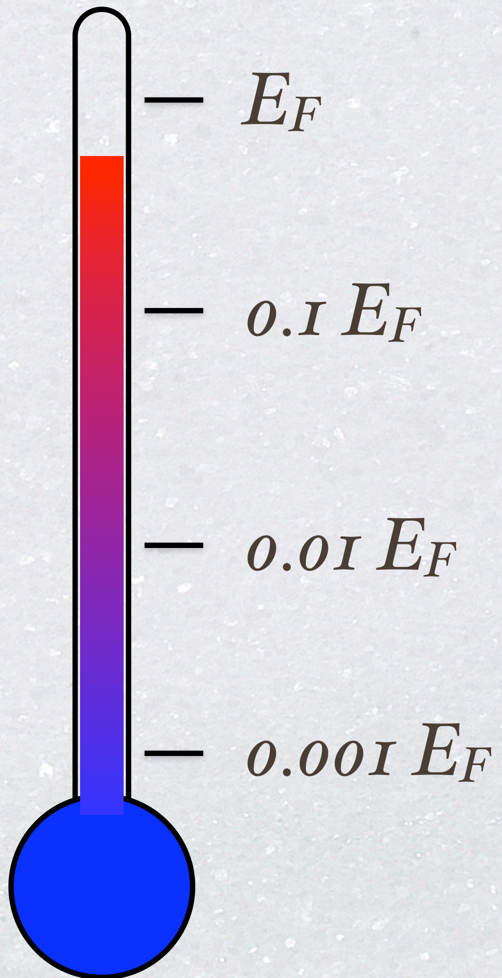


What are the temperature scales?

- Let us take guidance from
  - experiments on high-T_c cuprates
  - simulations of one-dimensional systems

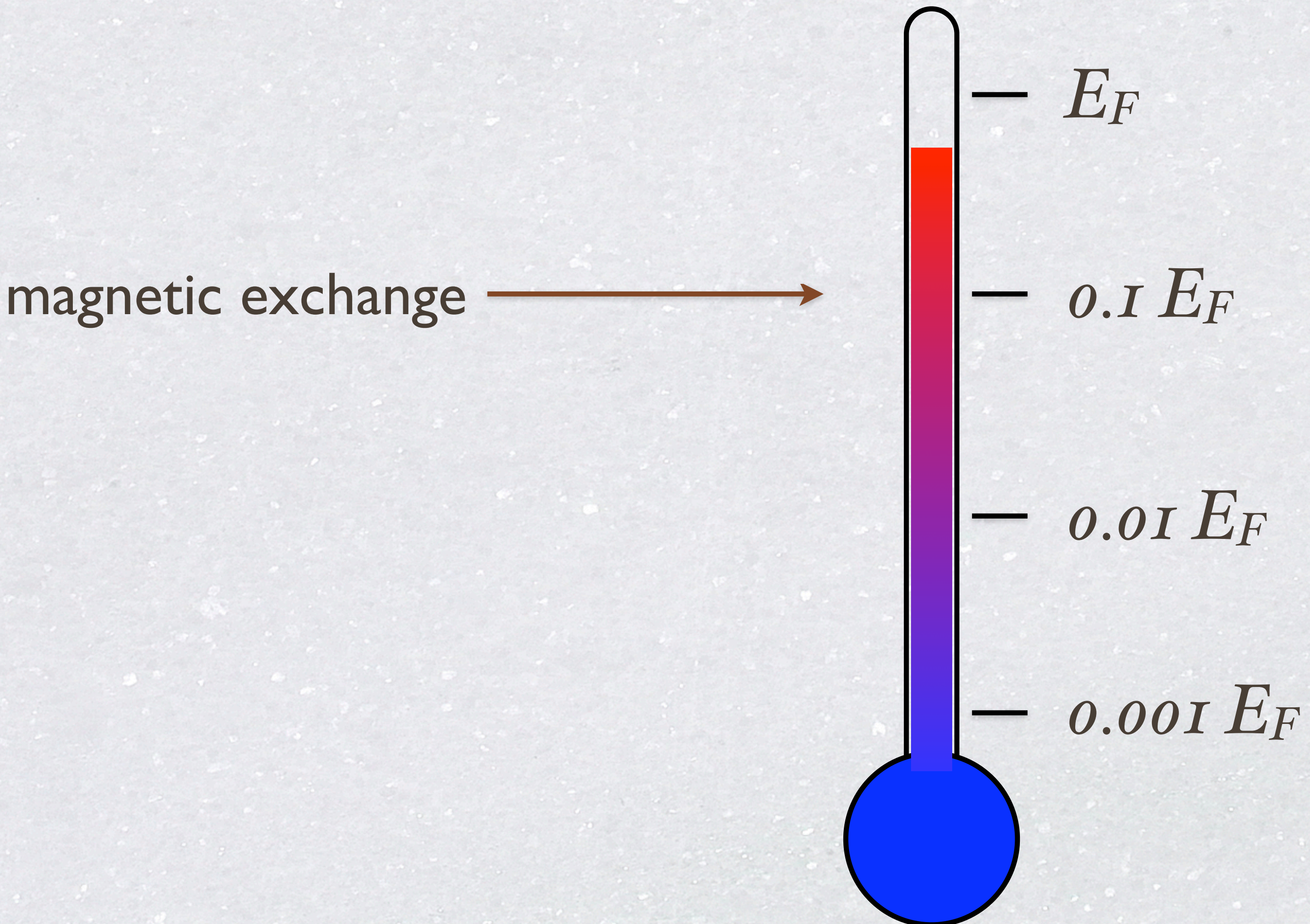
What are the temperature scales?

- Let us take guidance from
  - experiments on high-*Tc* cuprates
  - simulations of one-dimensional systems



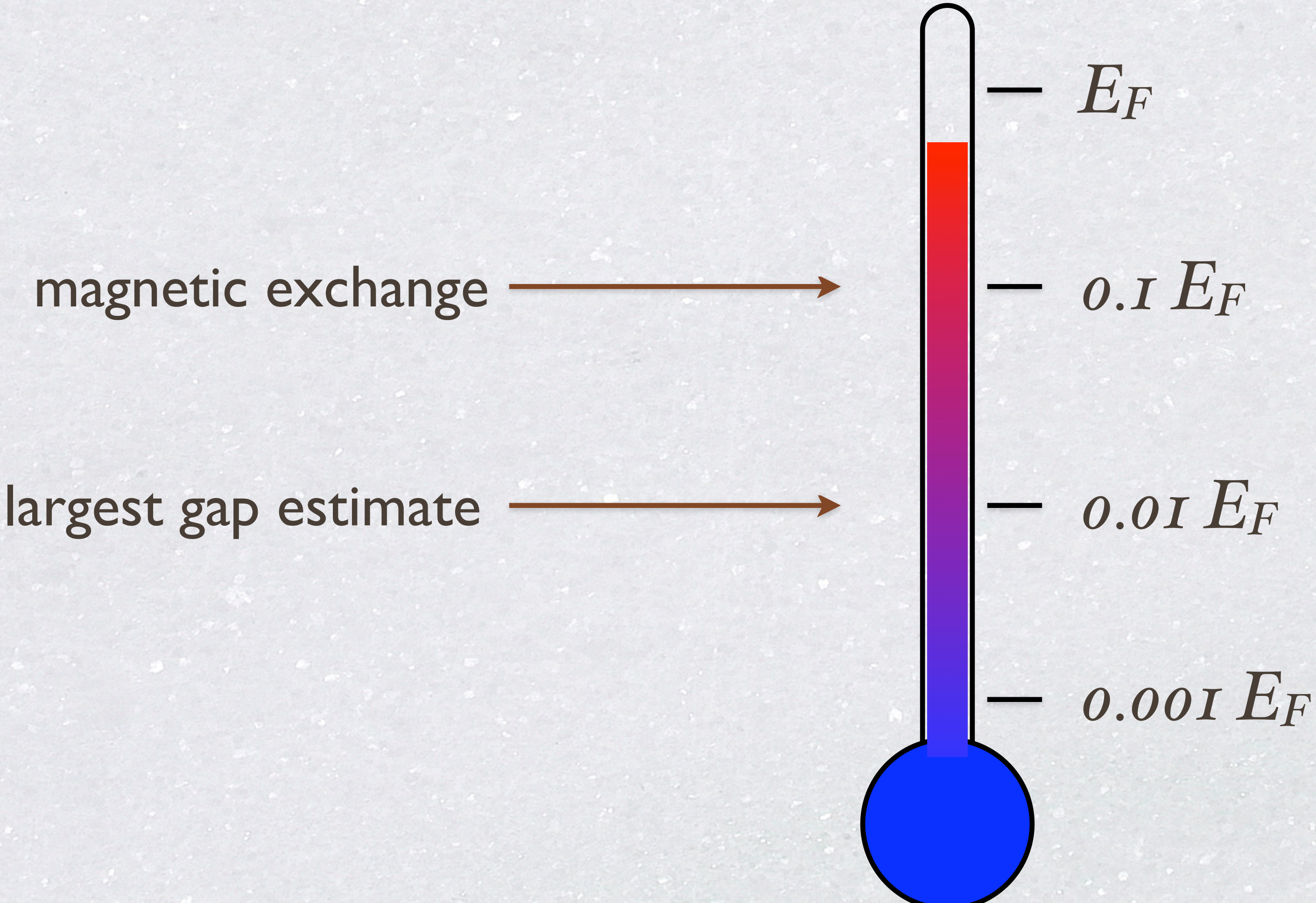
What are the temperature scales?

- Let us take guidance from
  - experiments on high-*Tc* cuprates
  - simulations of one-dimensional systems



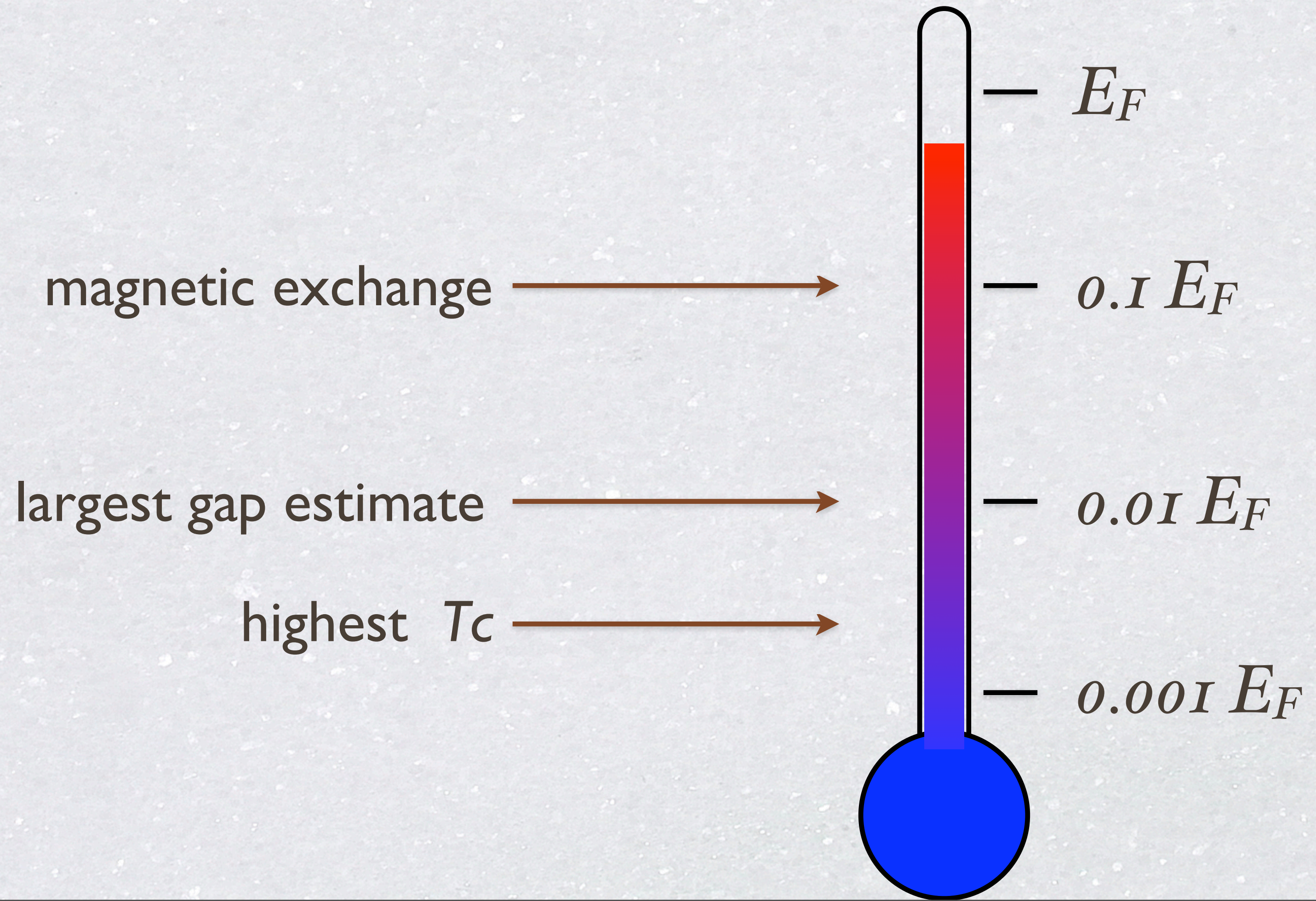
What are the temperature scales?

- Let us take guidance from
  - experiments on high-*Tc* cuprates
  - simulations of one-dimensional systems



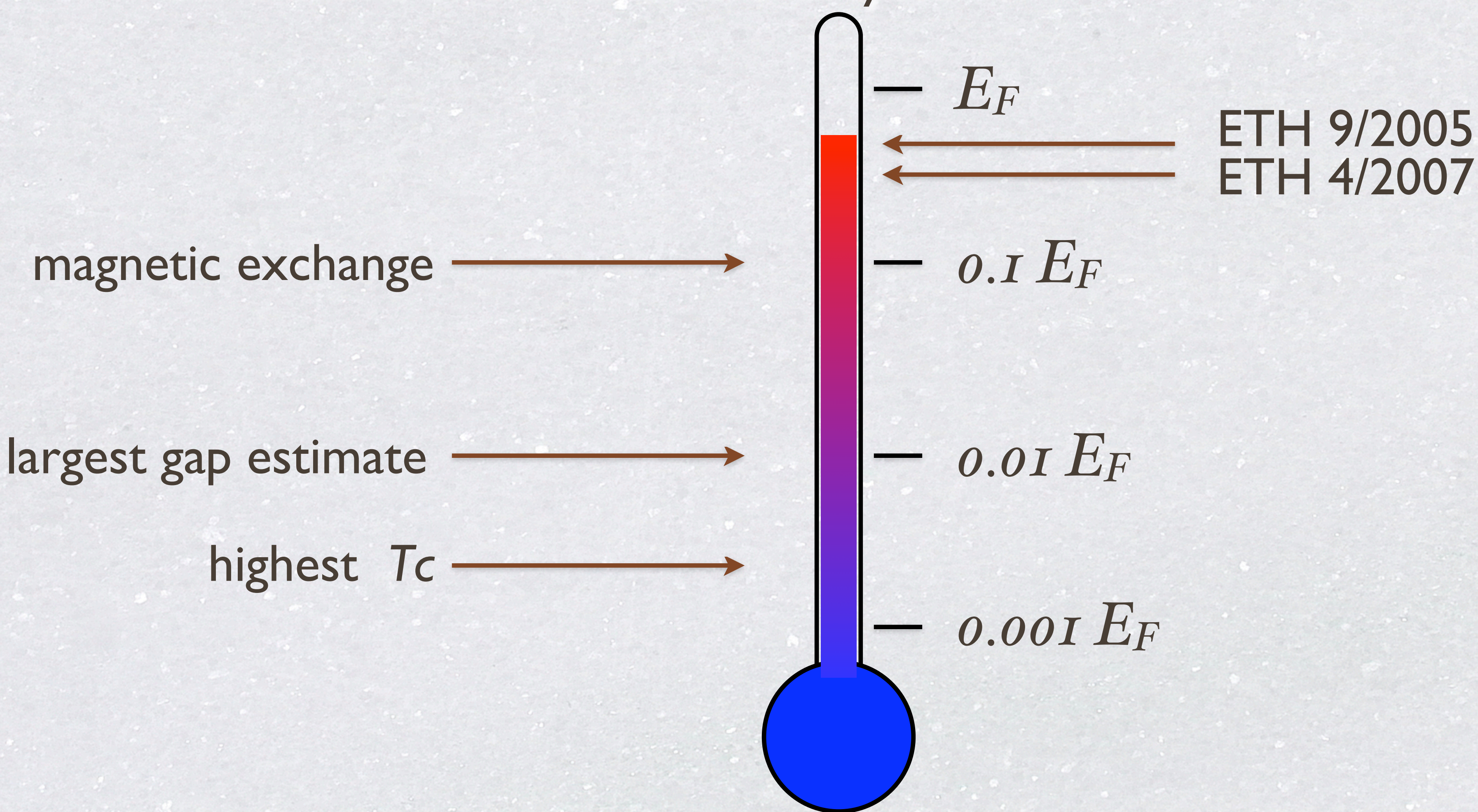
What are the temperature scales?

- Let us take guidance from
  - experiments on high-*Tc* cuprates
  - simulations of one-dimensional systems



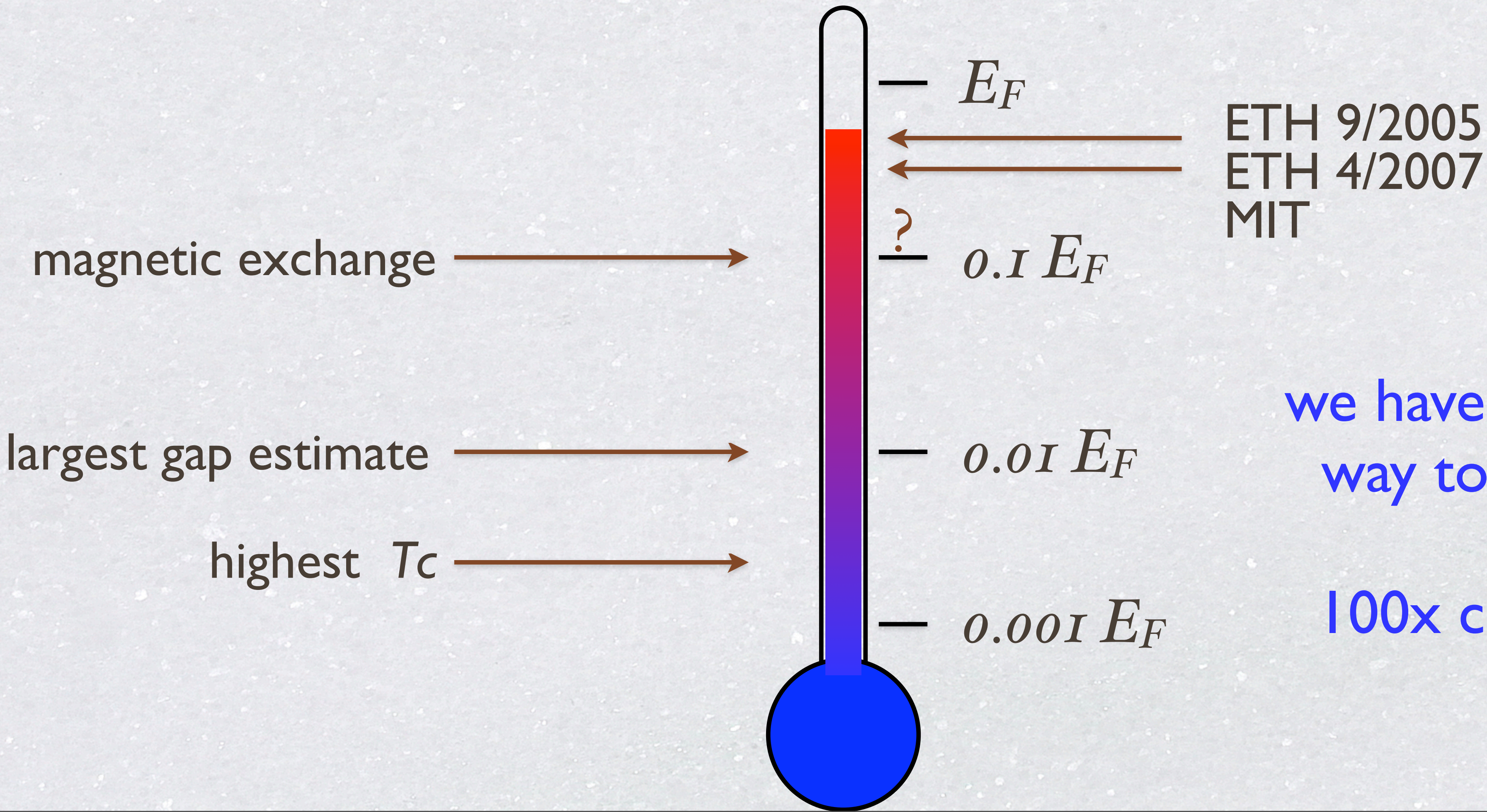
What are the temperature scales?

- Let us take guidance from
  - experiments on high-*Tc* cuprates
  - simulations of one-dimensional systems



What are the temperature scales?

- Let us take guidance from
  - experiments on high-*Tc* cuprates
  - simulations of one-dimensional systems



we have a long way to cool

100x colder

Adiabatic quantum simulation

Adiabatic quantum simulation

- Adiabatic quantum computing
  - Adiabatically transform initial state into the result of a hard computation
    E. Farhi *et al*, Science **292**, 472 (2001)

Adiabatic quantum simulation

- Adiabatic quantum computing
  - Adiabatically transform initial state into the result of a hard computation
    E. Farhi *et al*, Science **292**, 472 (2001)

- Adiabatic quantum simulation
  - Start from a pure initial state of a noninteracting model
  - Adiabatically transform it into the unknown ground state of an interacting model
  - Need to find a path with large gaps so that we can move fast

Adiabatic quantum simulation

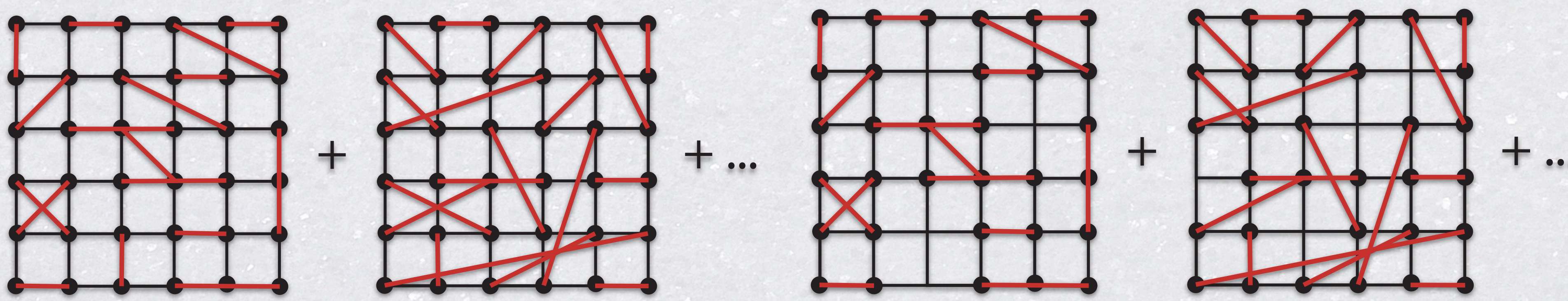
- Adiabatic quantum computing
  - Adiabatically transform initial state into the result of a hard computation
    E. Farhi *et al*, Science **292**, 472 (2001)
- Adiabatic quantum simulation
  - Start from a pure initial state of a noninteracting model
  - Adiabatically transform it into the unknown ground state of an interacting model
  - Need to find a path with large gaps so that we can move fast
- Example: RVB states in Hubbard models

RVB states

- Anderson conjectured that high temperature superconductors might be doped resonating valence bond (RVB) states

half-filling (parent compounds): superposition of singlet coverings

hole-doping: pairs are mobile and condense (BCS)



Gutzwiller-projected BCS wave function: eliminates double occupancies

$$|\Phi\rangle = P_G \prod_k \left(u_k + v_k c^\dagger_{k,\uparrow} c^\dagger_{-k,\downarrow} \right) |0\rangle \rightarrow |\Phi\rangle = P_G \left(\sum_{ij} a(i-j) c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} \right)^{N/2} |0\rangle$$

d-wave symmetry

d-wave symmetry

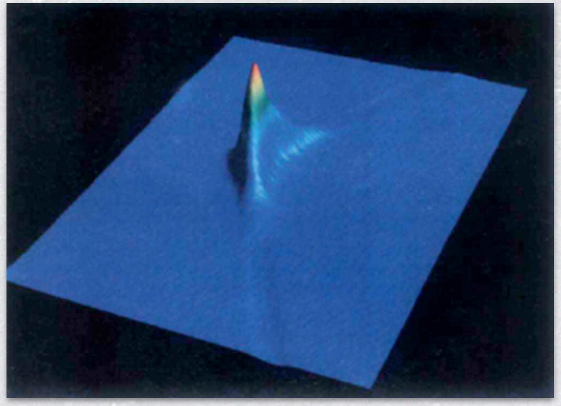
- Anderson originally conjectured s-wave symmetry

d-wave symmetry

- Anderson originally conjectured s-wave symmetry
- *d*-wave symmetry proposed soon thereafter
  - C. Gros, Phys. Rev. B **38**, 931 (1988)
  - G. Kotliar and J. Liu, Phys. Rev. B **38**, 5142 (1988)
  - ...

d-wave symmetry

- Anderson originally conjectured s-wave symmetry
- *d*-wave symmetry proposed soon thereafter
  - C. Gros, Phys. Rev. B **38**, 931 (1988)
  - G. Kotliar and J. Liu, Phys. Rev. B **38**, 5142 (1988)
  - ...
- Experimental tests for *d*-wave symmetry
  - Proposal: M. Sigrist and T.M. Rice, J. Phys. Soc. Jpn. **61**, 4283 (1992)
  - Experiments:
    - C.C. Tsuei *et al*, Nature **373**, 225 (1995)
    - C.C. Tsuei *et al*, Nature **387**, 481 (1997)
    - ...



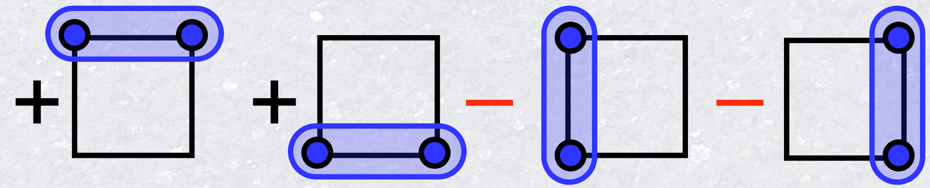
$$\Delta(k_x,k_y) \propto \langle c_{\vec{k}\uparrow} c_{-\vec{k}\downarrow} \rangle \propto \Delta \cdot (\cos k_x - \cos k_y)$$

RVB state on 4-site plaquettes

- *d*-wave RVB pairs

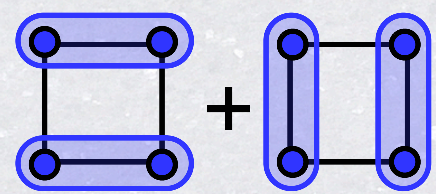
$$s_{i,j} = \frac{1}{\sqrt{2}} \left(c_{i,\uparrow} c_{j,\downarrow} - c_{i,\downarrow} c_{j,\uparrow} \right)$$

$$\Delta_d \approx \frac{1}{2} \left(s_{1,2} + s_{3,4} - s_{1,3} - s_{2,4} \right)$$



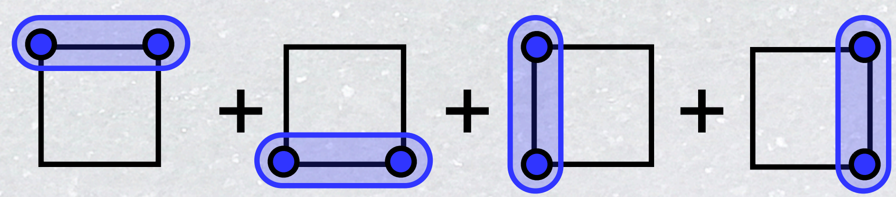
- 4 fermions on a plaquette: *d*-wave RVB state

$$|4\rangle \approx s^\dagger_{1,2} s^\dagger_{3,4} + s^\dagger_{1,3} s^\dagger_{2,4}$$



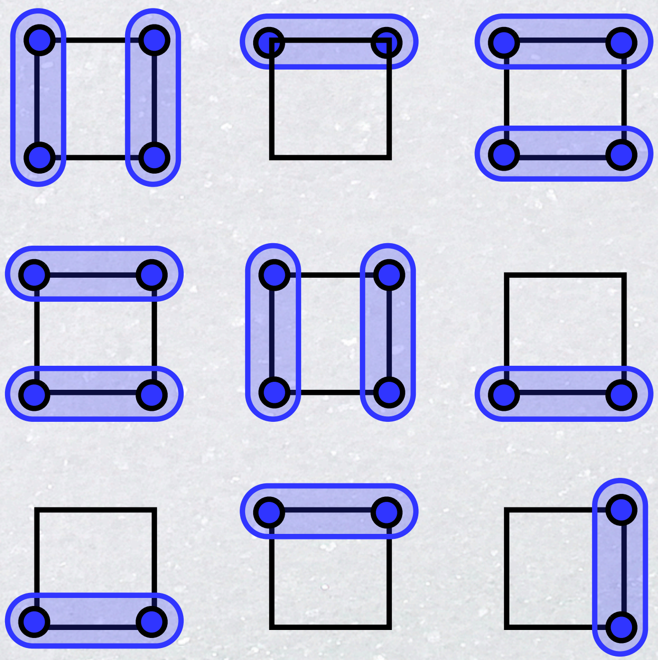
- removing a d-wave pair gives ground state of 2 fermions

$$|2\rangle \approx \Delta_d |4\rangle$$



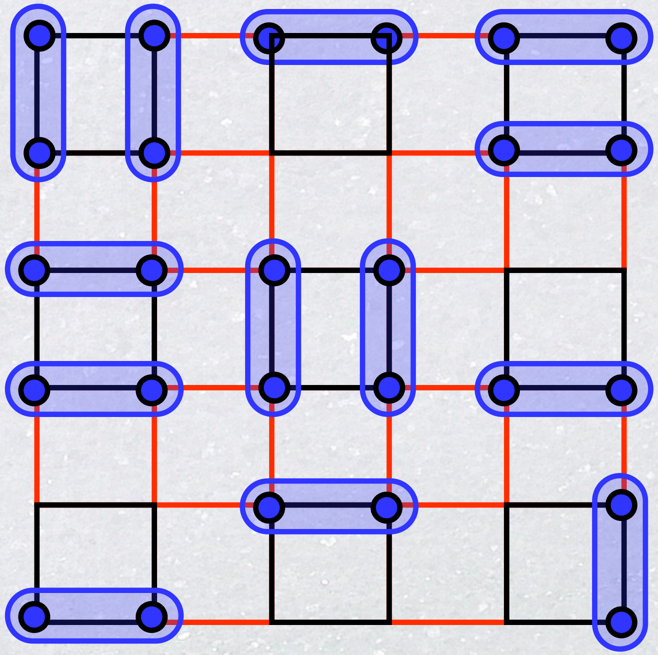
Coupling plaquettes

- Will the *d*-wave RVB state survive the coupling of plaquettes to a square lattice?
  - R.M. Fye, D.J. Scalapino and R.T. Scalettar, Phys. Rev. B **46**, 8667 (1992).
  - E. Altmann and A. Auerbach, Phys. Rev. B **65** 104508 (2002)
  - and many others ...



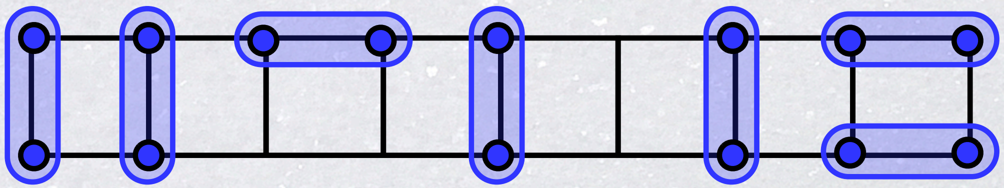
Coupling plaquettes

- Will the *d*-wave RVB state survive the coupling of plaquettes to a square lattice?
  - R.M. Fye, D.J. Scalapino and R.T. Scalettar, Phys. Rev. B **46**, 8667 (1992).
  - E. Altmann and A. Auerbach, Phys. Rev. B **65** 104508 (2002)
  - and many others ...



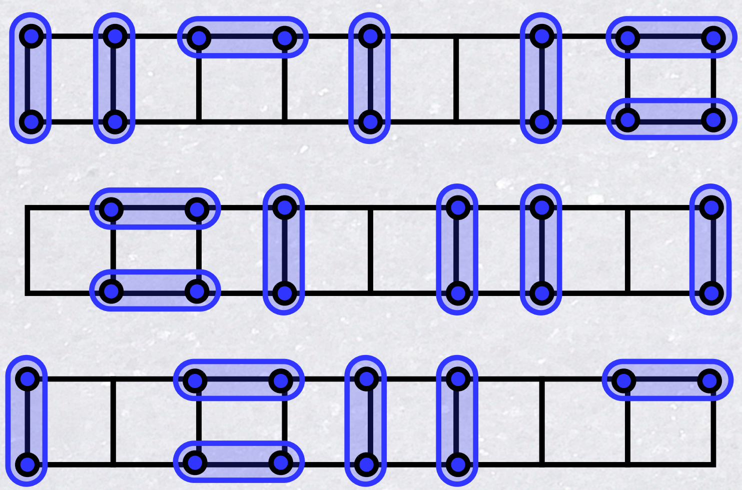
d-wave RVB States on Ladders

- "d-wave" like RVB pairs with quasi-long range order
  - E. Dagotto *et al*, Phys. Rev. B **45**, 5744 (1992)
  - H. Tsunetsugu, M. Troyer, T.M. Rice, Phys. Rev. B **49**, 16078 (1994)
  - R. M. Noack, S. R. White, and D.J. Scalapino, PRL **73**, 882 (1994)
  - C. Hayward *et al*, Phys Rev. Lett. **75**, 926 (1995)
  - M. Troyer, H. Tsunetsugu, T.M. Rice, Phys. Rev. B **53**, 251 (1996)
  - and many others ....



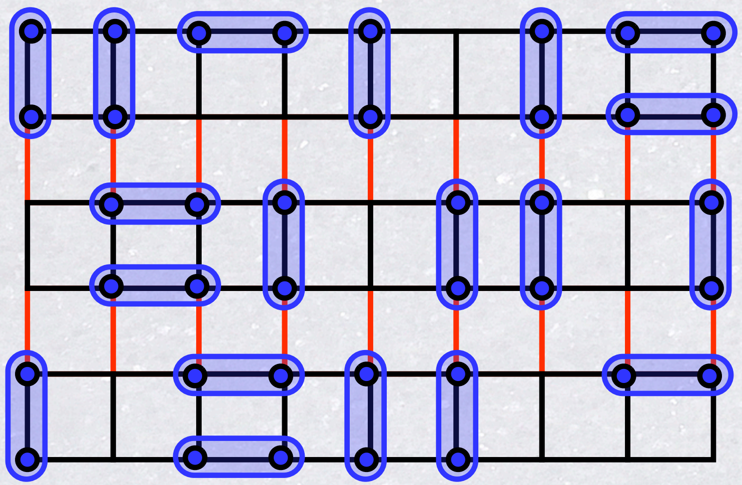
Coupling ladders

- Does the RVB state survive the coupling of ladders?
  - yes for weak coupling, unclear for strong coupling
  - H. Tsunetsugu, M. Troyer, T.M. Rice, Phys. Rev. B **51**, 16456 (1995)
  - E. Arrigoni, E. Fradkin, S.A. Kivelson, Phys. Rev. B **69**, 214519 (2004)
  - ...



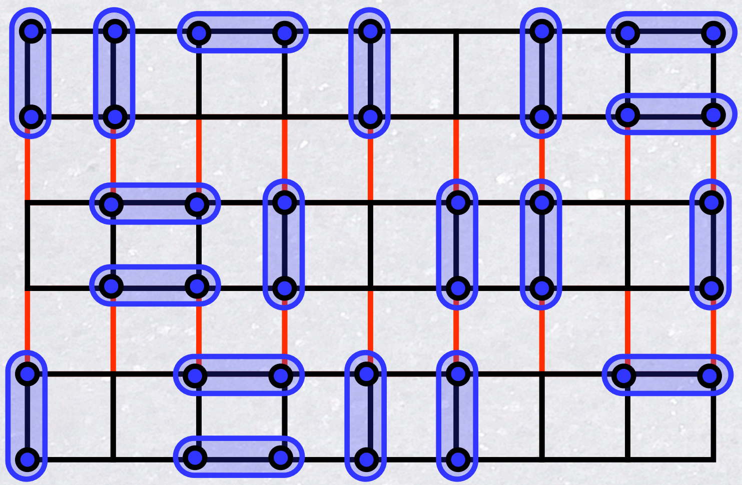
Coupling ladders

- Does the RVB state survive the coupling of ladders?
  - yes for weak coupling, unclear for strong coupling
  - H. Tsunetsugu, M. Troyer, T.M. Rice, Phys. Rev. B **51**, 16456 (1995)
  - E. Arrigoni, E. Fradkin, S.A. Kivelson, Phys. Rev. B **69**, 214519 (2004)
  - ...



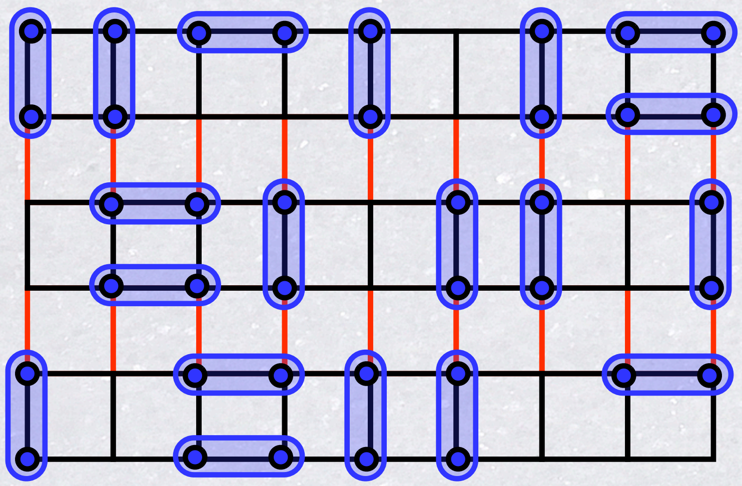
Coupling ladders

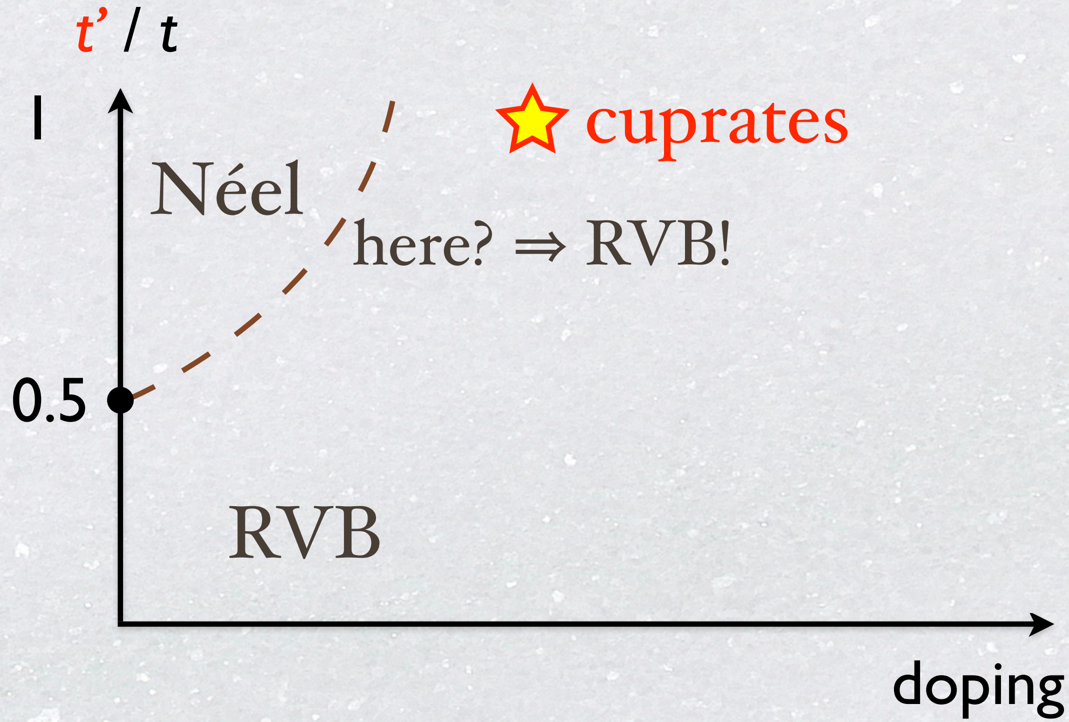
- Does the RVB state survive the coupling of ladders?
  - yes for weak coupling, unclear for strong coupling
  - H. Tsunetsugu, M. Troyer, T.M. Rice, Phys. Rev. B **51**, 16456 (1995)
  - E. Arrigoni, E. Fradkin, S.A. Kivelson, Phys. Rev. B **69**, 214519 (2004)
  - ...



Coupling ladders

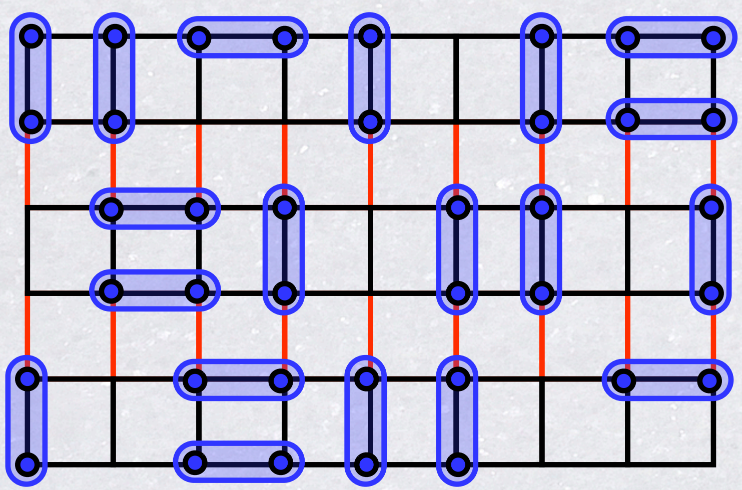
- Does the RVB state survive the coupling of ladders?
  - yes for weak coupling, unclear for strong coupling
  - H. Tsunetsugu, M. Troyer, T.M. Rice, Phys. Rev. B **51**, 16456 (1995)
  - E. Arrigoni, E. Fradkin, S.A. Kivelson, Phys. Rev. B **69**, 214519 (2004)
  - ...

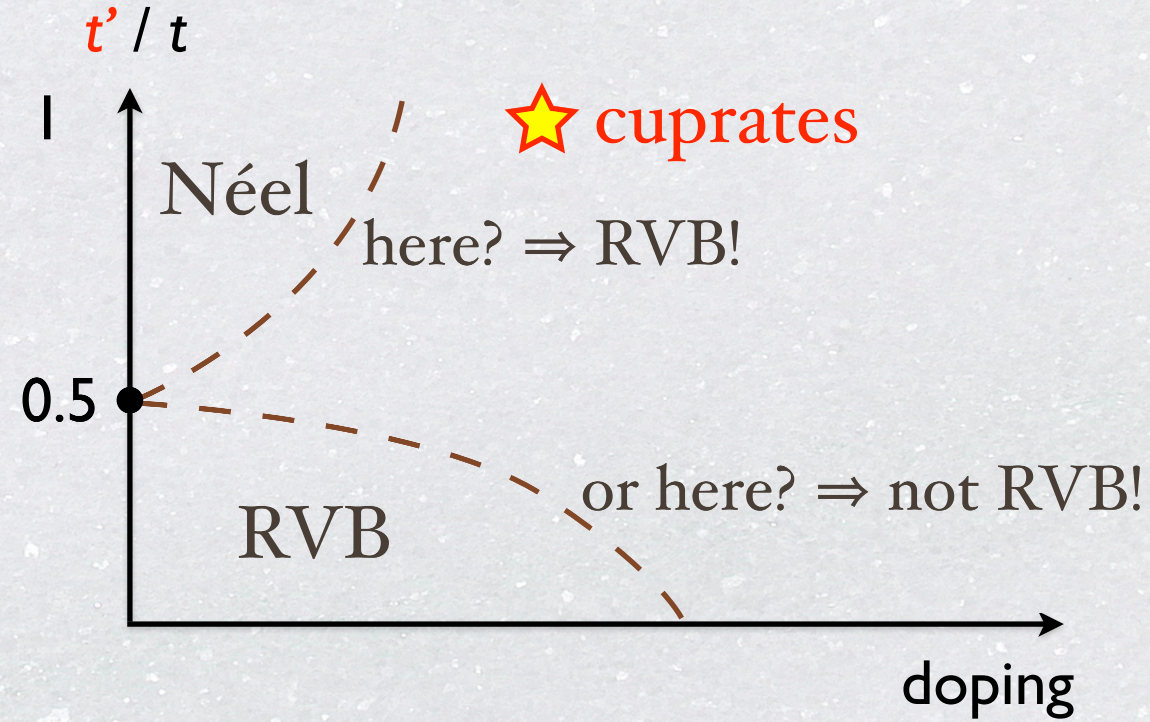




Coupling ladders

- Does the RVB state survive the coupling of ladders?
  - yes for weak coupling, unclear for strong coupling
  - H. Tsunetsugu, M. Troyer, T.M. Rice, Phys. Rev. B **51**, 16456 (1995)
  - E. Arrigoni, E. Fradkin, S.A. Kivelson, Phys. Rev. B **69**, 214519 (2004)
  - ...





The adiabatic quantum simulation

The adiabatic quantum simulation

- Outline
  - cool Fermi gas as far as possible
  - load a **pure initial ground state** into an optical lattice
  - **adiabatically tune** the model to desired interaction parameters
  - test the progress at (several) solvable intermediate points

The adiabatic quantum simulation

- Outline
  - cool Fermi gas as far as possible
  - load a **pure initial ground state** into an optical lattice
  - **adiabatically tune** the model to desired interaction parameters
  - test the progress at (several) solvable intermediate points
- Watch out:
  - try to keep a large gap to excited states
  - avoid level crossings
  - avoid mixing in states from wrong symmetry sectors

AMO Toolbox I: pattern loading

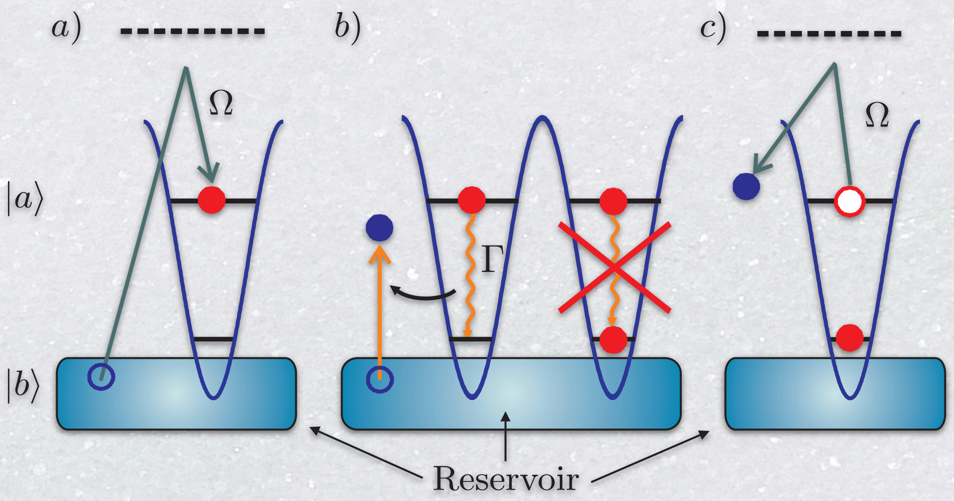
AMO Toolbox I: pattern loading

- Evaporatively cooled Fermi gas in an optical lattice:
  - will have too much entropy ⇒ too high temperature

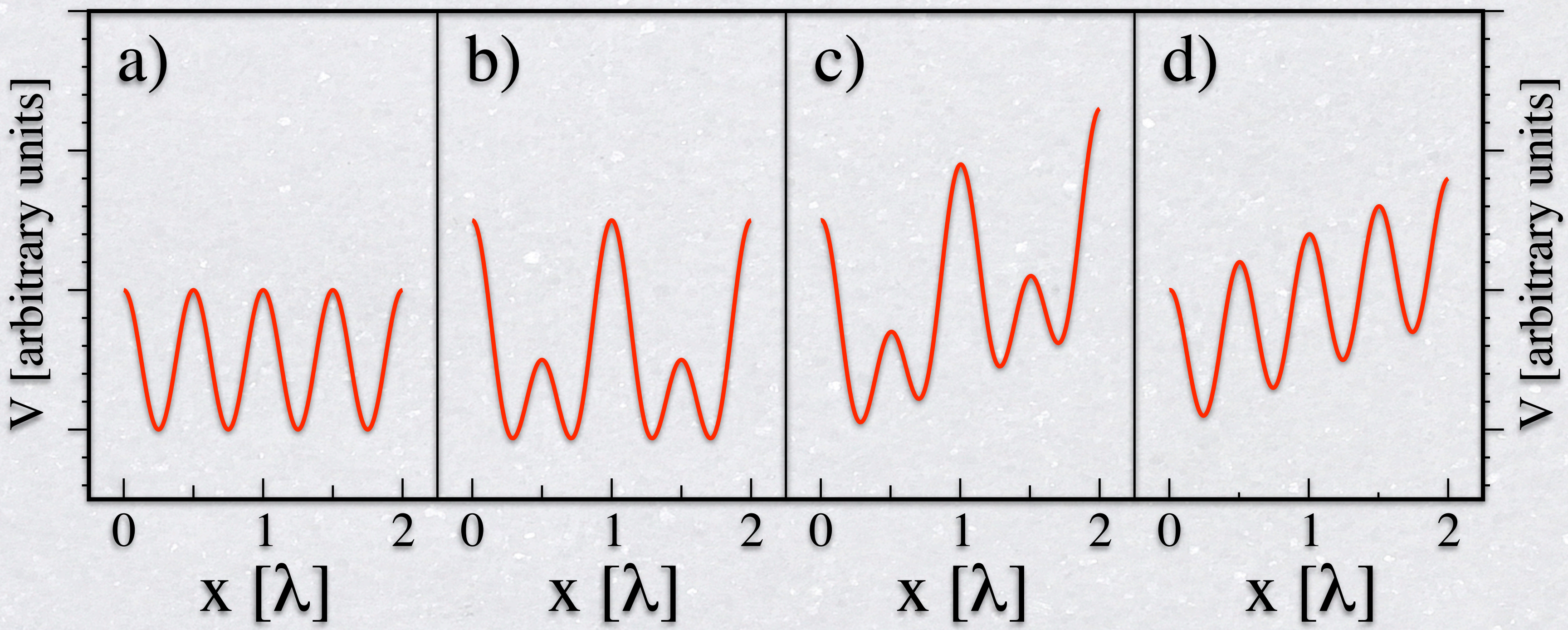
AMO Toolbox I: pattern loading

- Evaporatively cooled Fermi gas in an optical lattice:
  - will have too much entropy ⇒ too high temperature

- Pattern loading:
  - pump into exited state of a lattice
  - atoms relax to ground state in lattice well
  - pump more atoms
  - then get rid of excited atoms
  - Rabl *et al*, PRL **91**, 110403 (2003)
    Griessner *et al*, PRA **72**, 032332 (2005)



AMO Toolbox II: superlattice and ramps

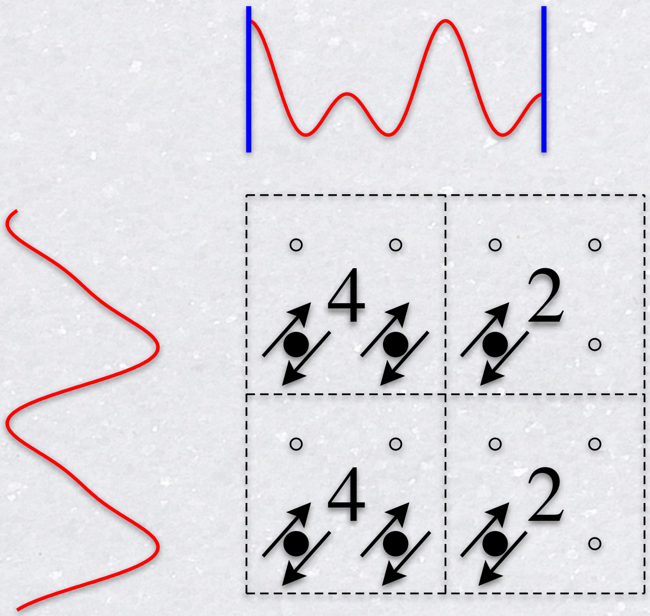


a. One-dimensional optical lattice

b. Superlattice

c. + d. Linear ramp

Adiabatically preparing plaquette RVB states

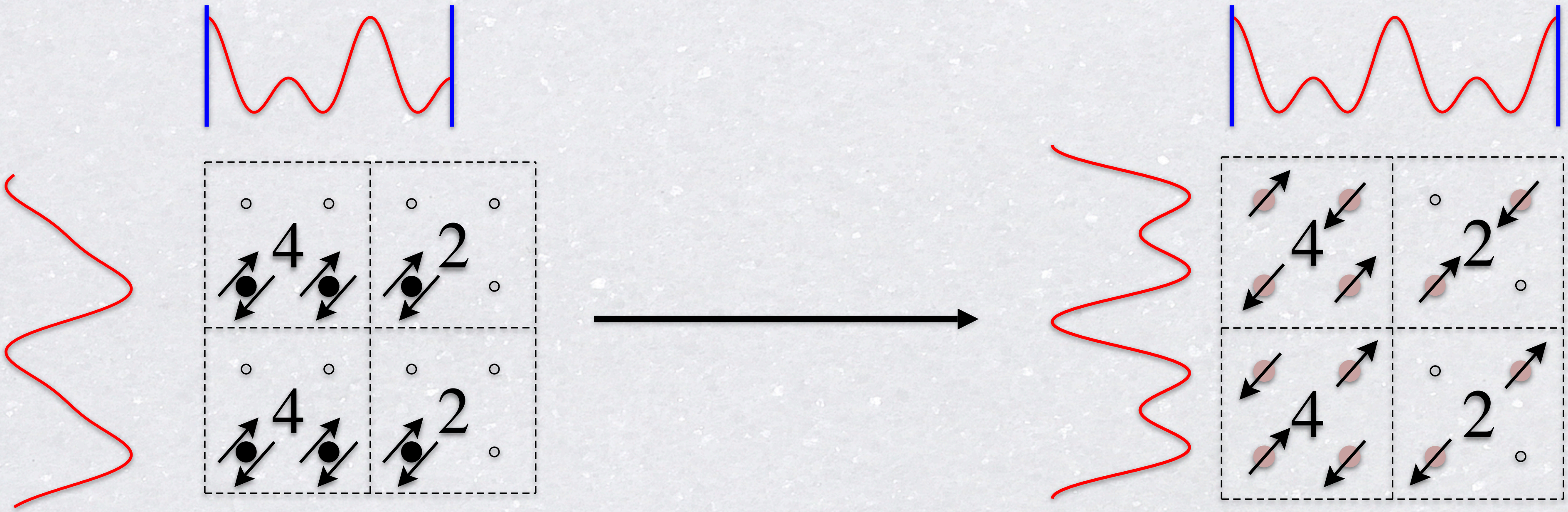


Pattern loaded isolated plaquettes

- every other chain empty: $\mu_\perp >> t_\perp$

- zero horizontal hopping: t = 0

Adiabatically preparing plaquette RVB states



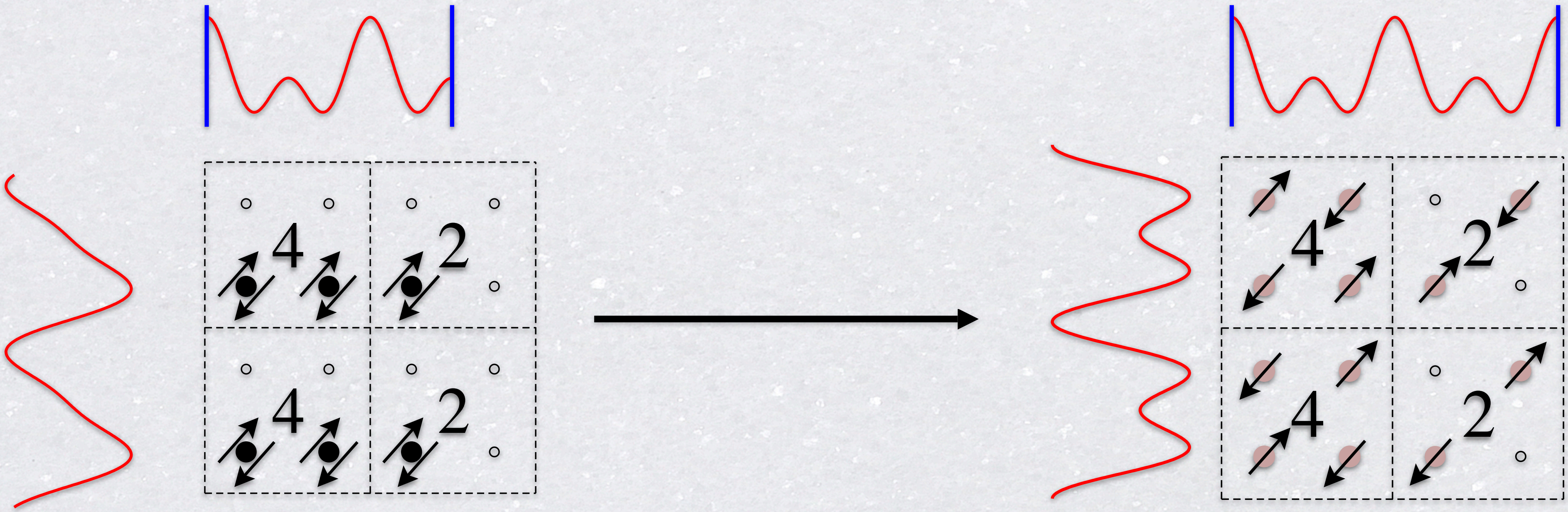
Pattern loaded isolated plaquettes

- every other chain empty: $\mu_\perp >> t_\perp$
- zero horizontal hopping: $t = 0$

true plaquettes

- full interactions
-ground states for 4, 2 atoms

Adiabatically preparing plaquette RVB states



Pattern loaded isolated plaquettes

- every other chain empty: $\mu_\perp >> t_\perp$

- zero horizontal hopping: $t = 0$

true plaquettes

- full interactions

-ground states for 4, 2 atoms

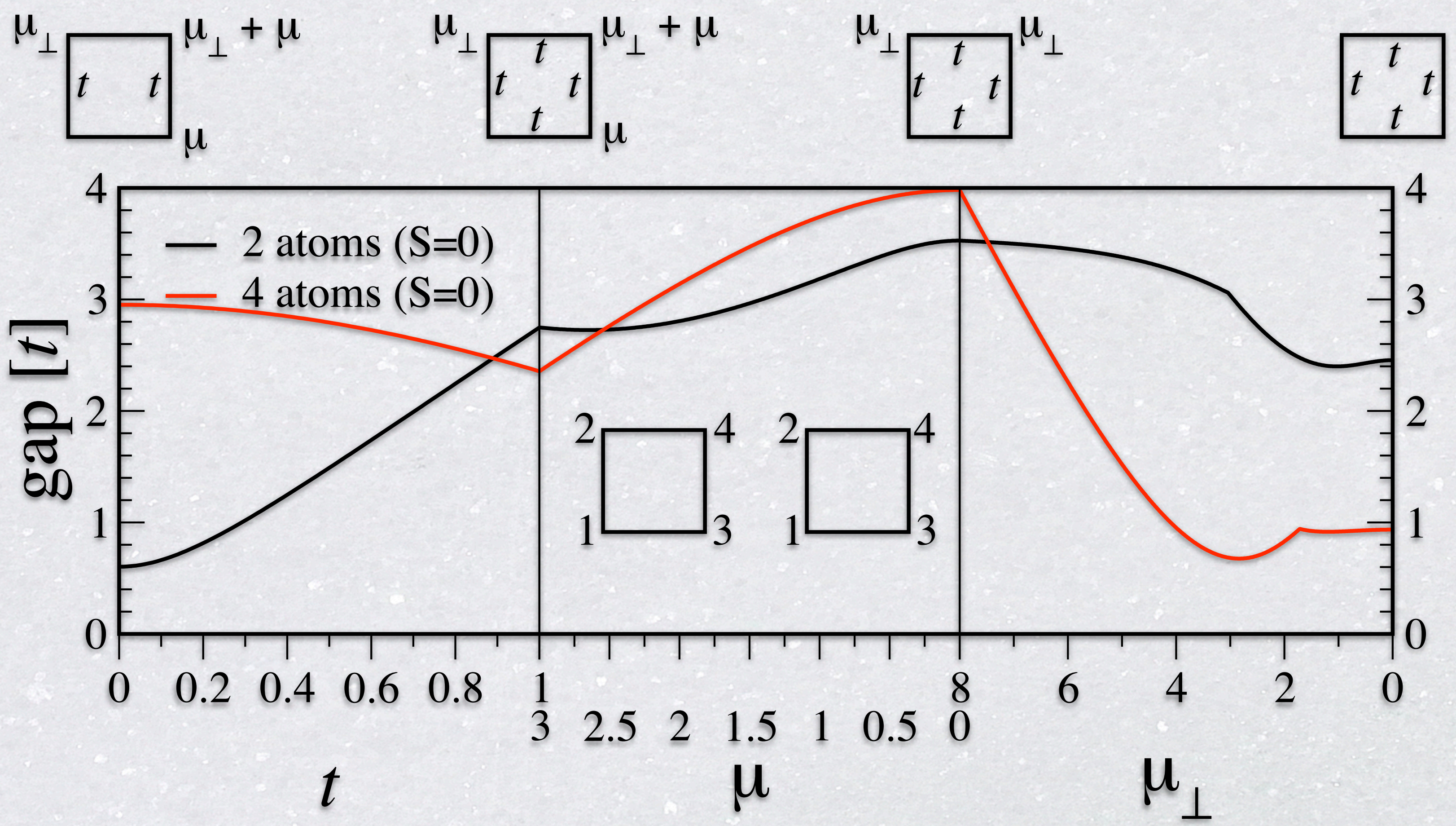
Which path to use to tune μ, $\mu_\perp$, $t_\perp$?

Preparing *d*-wave RVB states

1. ramp up hoppings t

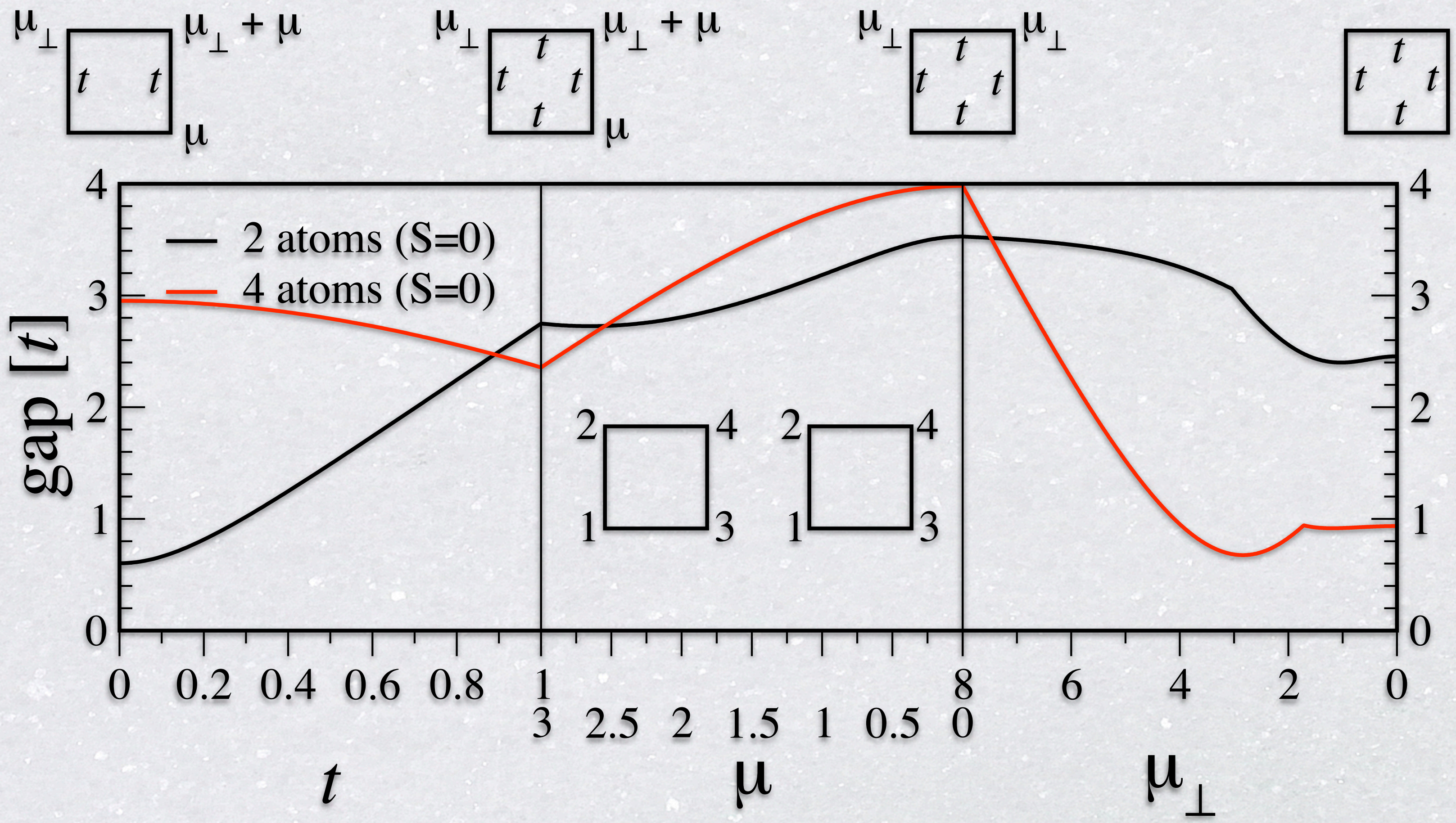
2. ramp down in-chain μ

3. ramp down intra-chain $\mu_\perp$



Preparing *d*-wave RVB states

1. ramp up hoppings t
2. ramp down in-chain μ
3. ramp down intra-chain $\mu_\perp$



Protected by gaps: fidelity > 99% for times ~ 50/t

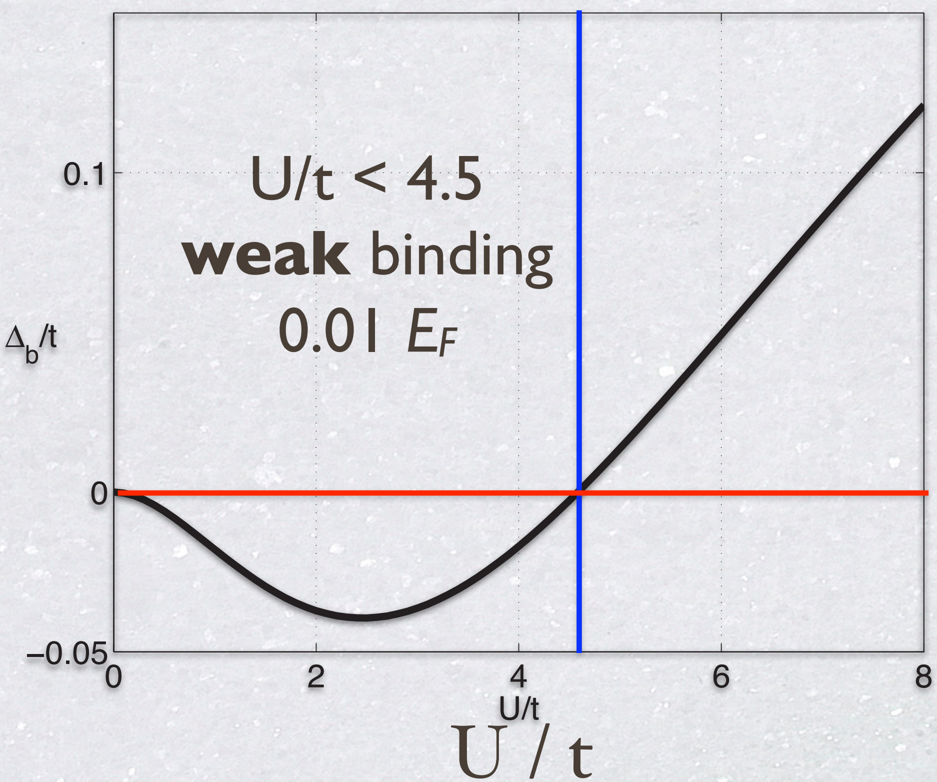
Watch out: other routes can give s-wave states

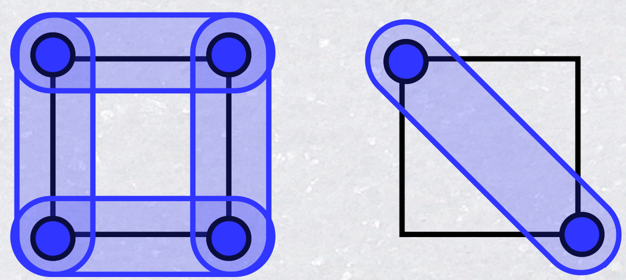
Binding energy of two holes

- Will two holes remain bound when we couple and decouple plaquettes?

$$\Delta_{\text{bind}} = E(N) + E(N-2) - 2E(N-1)$$

Altmann & Auerbach, PRB 65 104508 (2002)



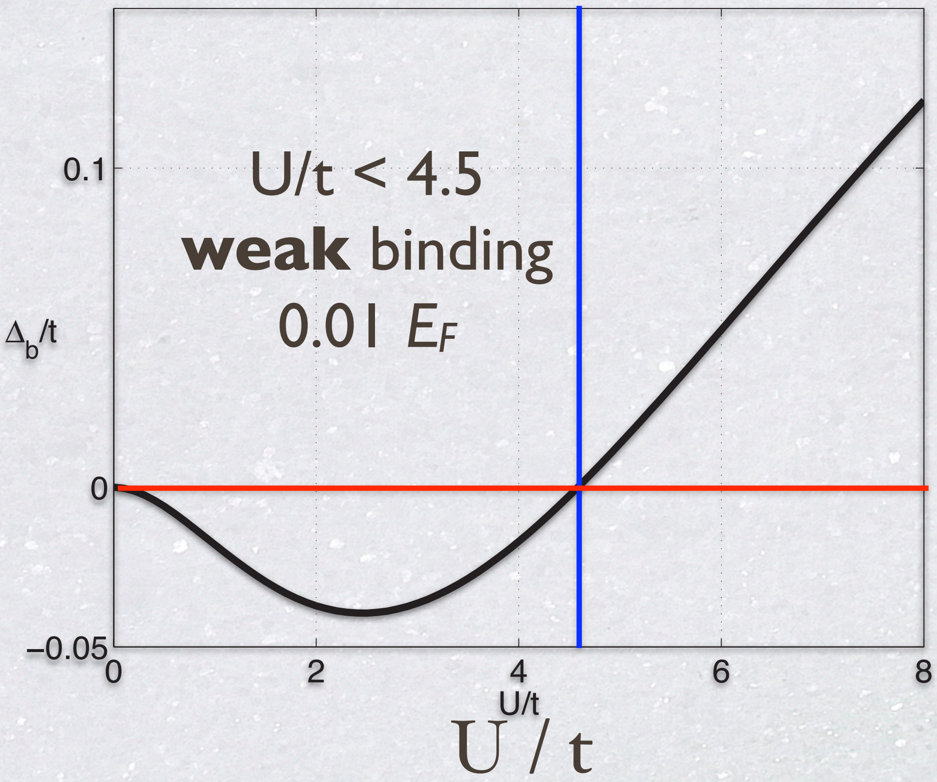


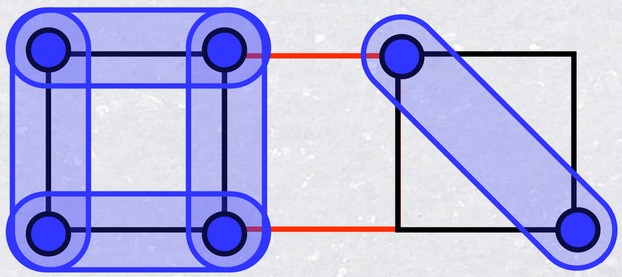
Binding energy of two holes

- Will two holes remain bound when we couple and decouple plaquettes?

$$\Delta_{\text{bind}} = E(N) + E(N-2) - 2E(N-1)$$

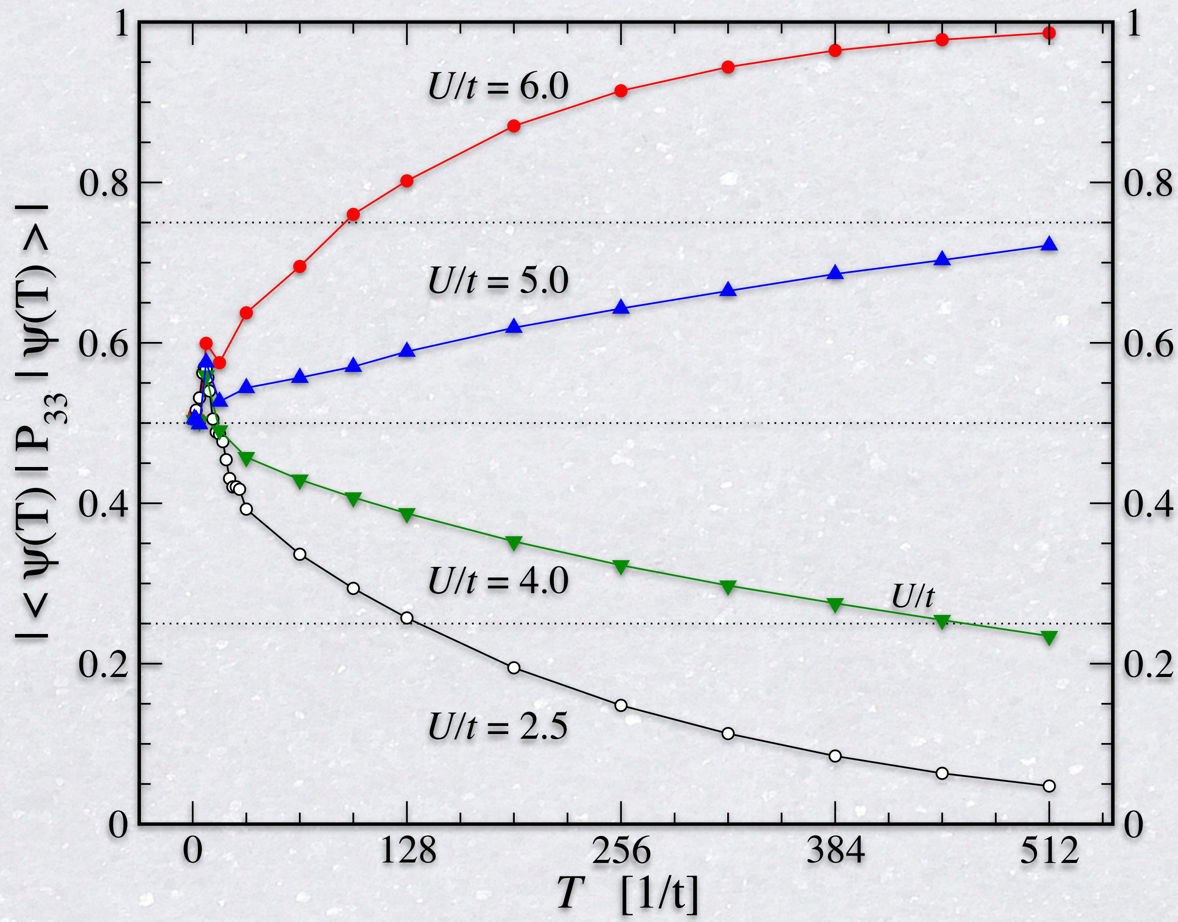
Altmann & Auerbach, PRB 65 104508 (2002)





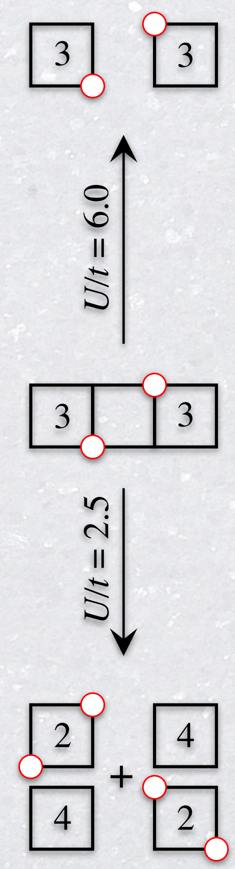
Decoupling two plaquettes

Pair breaking probability



can form 2 molecules

pairs unbind for U>4.5



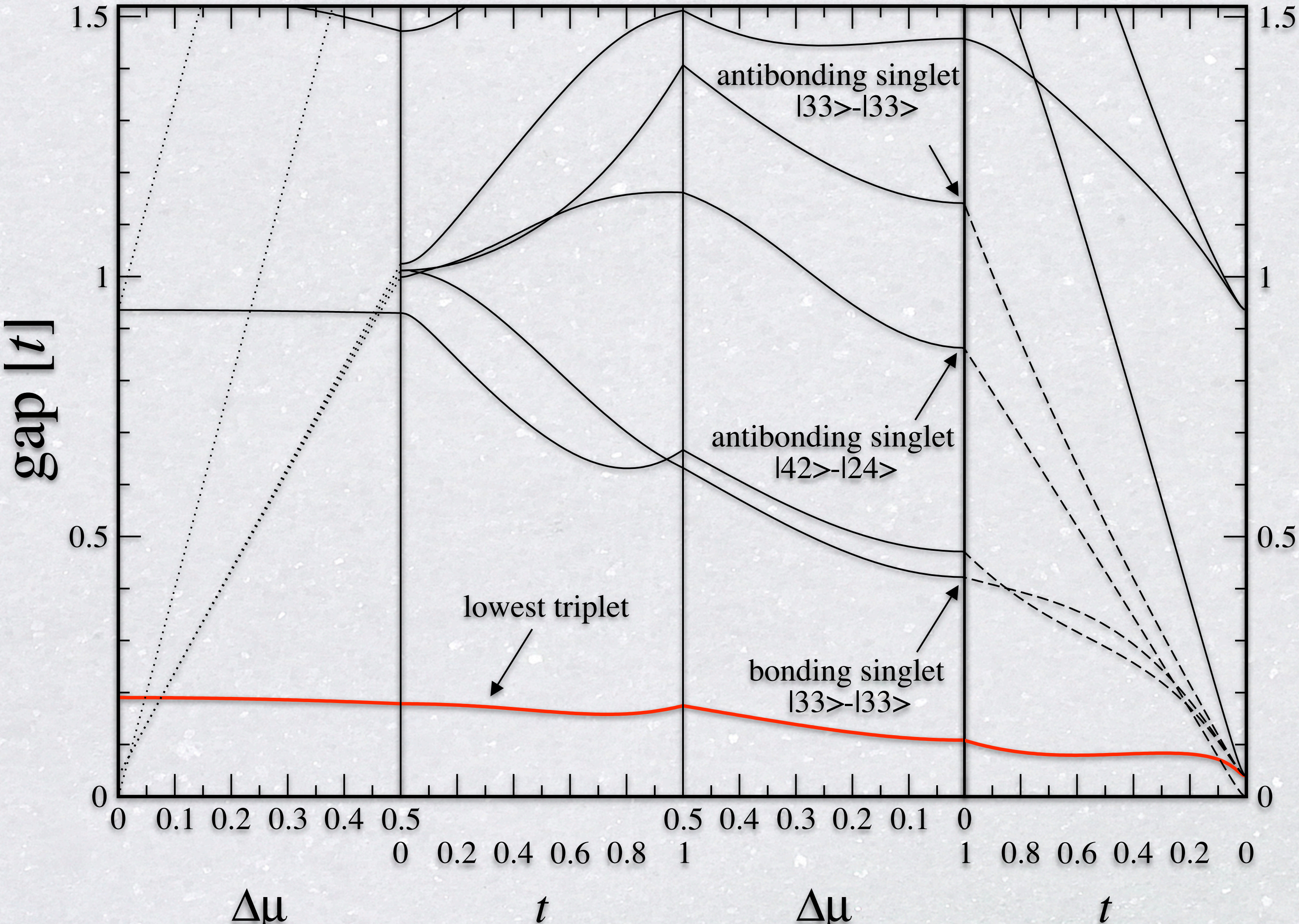
pairs bind for U<4.5

Decoupling time (non-linear ramping)

~500 1/t (about 500 ms)

can form 3 molecules

All details can be calculated



binding energy:

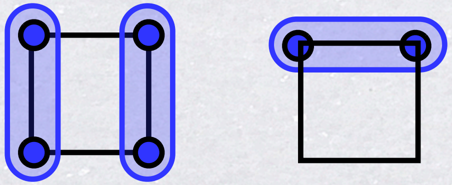
tiny gap!

requires long time scales for decoupling

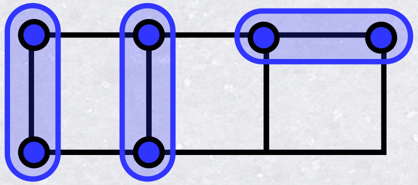
From plaquettes to ladders

Assuming hopping of 1 kHz

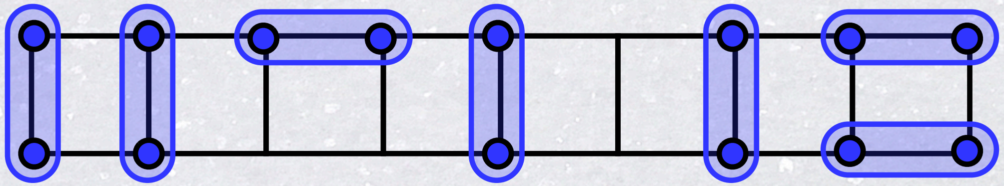
- **Creating isolated RVB plaquettes: 50 ms**



- **Coupling plaquettes: 100 ms**



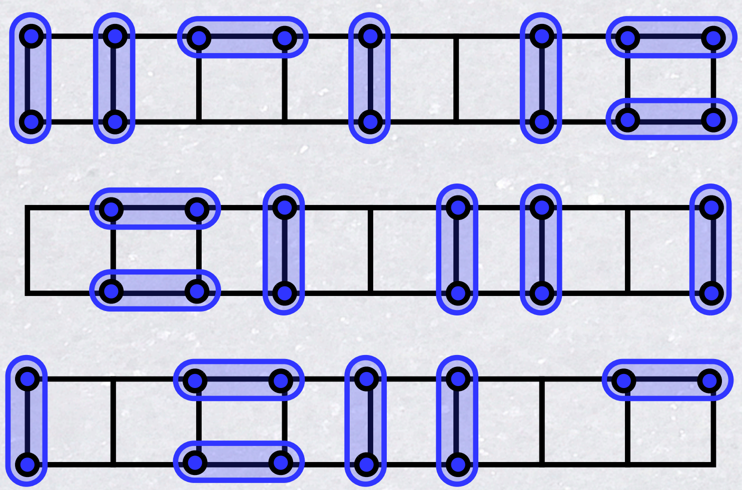
- Pairing on plaquettes can be measured in 500 ms
- **Creating ladders: 250 ms**

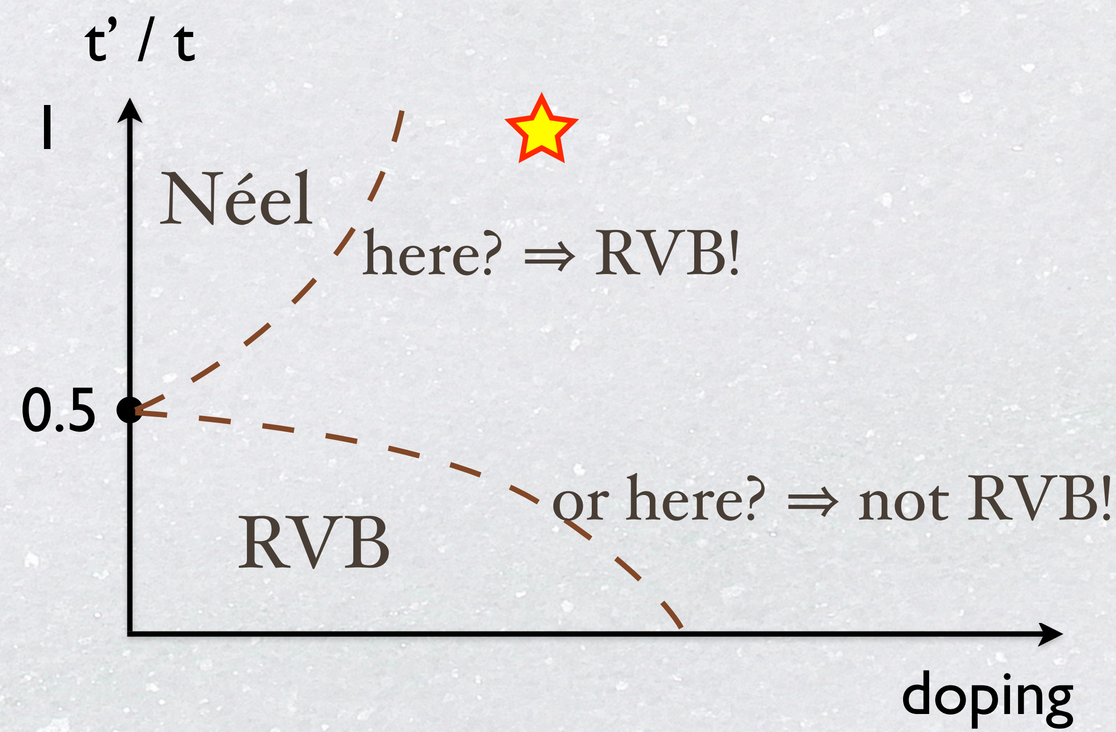


- All time scales are smaller than decoherence time

Quantum simulation of RVB states

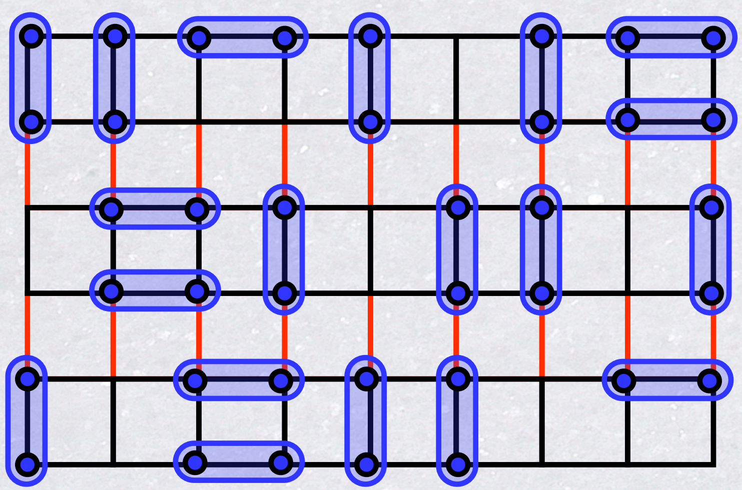
- Experiment can go further than we could and test whether
  - the RVB states survives when going to the uniform square lattice?
  - or is there a phase transition to a new phase?
- Either answer would be very important

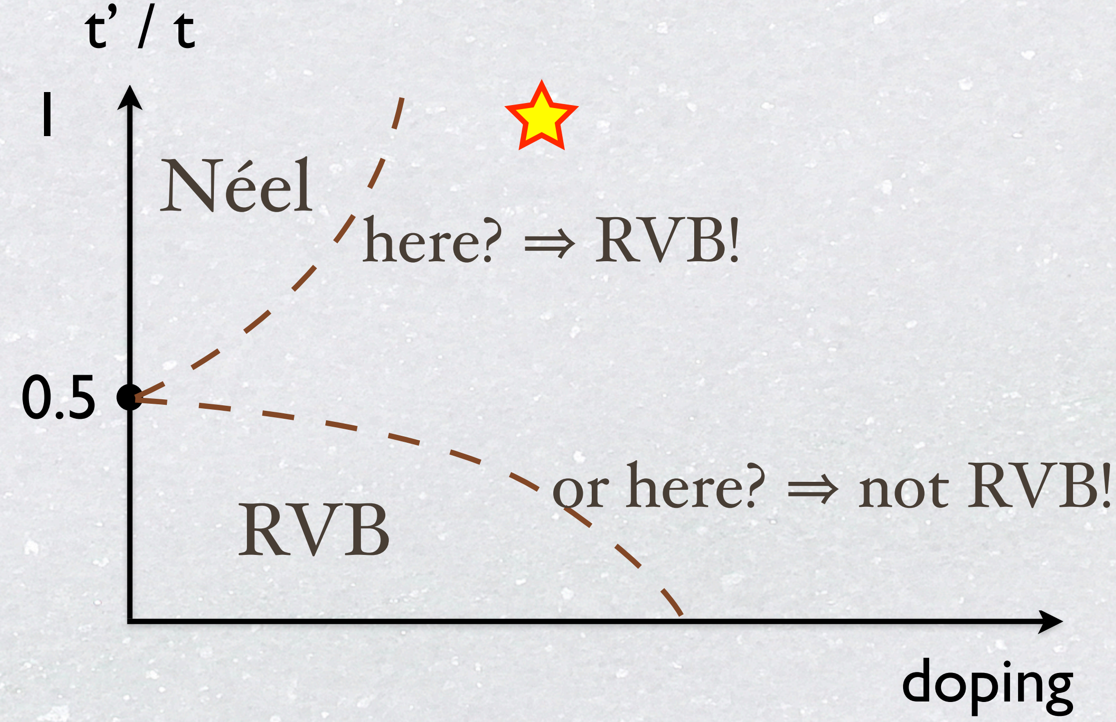




Quantum simulation of RVB states

- Experiment can go further than we could and test whether
  - the RVB states survives when going to the uniform square lattice?
  - or is there a phase transition to a new phase?
- Either answer would be very important



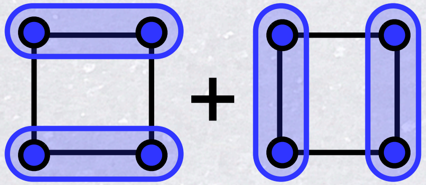


Measuring d-wave pairing

- How can we measure d-wave pairing?
  - convert *d*-wave pair on a plaquette into a molecule in the center of the plaquette $m_p^\dagger \Delta_d(p)$
  - state-selective molecule formation by laser-induced Raman transition
  - then measure phase coherence of the bosonic molecules

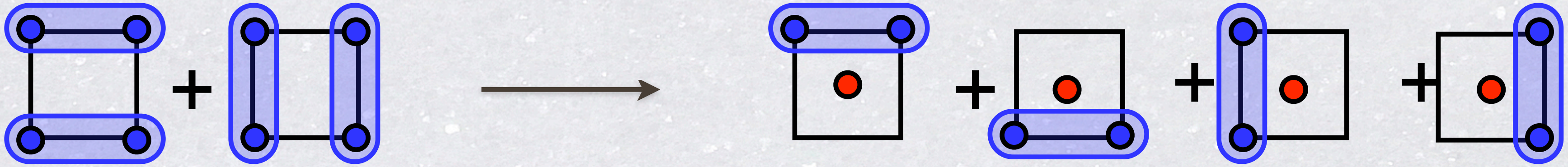
Measuring d-wave pairing

- How can we measure d-wave pairing?
  - convert *d*-wave pair on a plaquette into a molecule in the center of the plaquette $m_p^\dagger \Delta_d(p)$
  - state-selective molecule formation by laser-induced Raman transition
  - then measure phase coherence of the bosonic molecules



Measuring d-wave pairing

- How can we measure d-wave pairing?
  - convert *d*-wave pair on a plaquette into a molecule in the center of the plaquette $m_p^\dagger \Delta_d(p)$
  - state-selective molecule formation by laser-induced Raman transition
  - then measure phase coherence of the bosonic molecules



Summary

- Adiabatic quantum simulation
  - Start from a pure initial state of a noninteracting model
  - Adiabatically transform it into the unknown ground state of an interacting model
  - Can reach ground states of interacting quantum systems in short times

- Example: RVB states in Hubbard models
  - Weakly coupled plaquettes and ladders have *d*-wave RVB ground states
  - Energy scales are very low (gap less than $0.01 E_F$)
  - Seems impossible to reach these states by simple cooling
  - But can be prepared adiabatically in very short times from filled bands!
  - Ground state of 2D fermionic Hubbard model can be tested

S. Trebst, U. Schollwöck, M. Troyer, P. Zoller, PRL **96**, 250402 (2006)