The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

1859-35

Summer School on Novel Quantum Phases and Non-Equilibrium Phenomena in Cold Atomic Gases

27 August - 7 September, 2007

Tutorial on DMRG and applications to cold atoms out-of-equilibrium

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Tutorial on DMRG & applications to cold atoms out-of-equilibrium

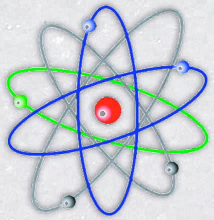
Ulrich Schollwöck
RWTH Aachen

on new common grounds

many-body theory

$$Z = \mathrm{Tr}\exp(-\beta\hat{H})$$

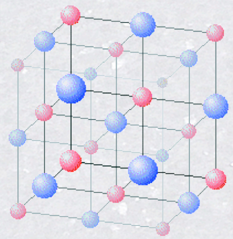
atomic optics



ultracold atom gases ...

physical challenges

condensed matter



... a new toolbox

progress in methods

quantum information

$$|qubit\rangle = \alpha|0\rangle + \beta|1\rangle$$

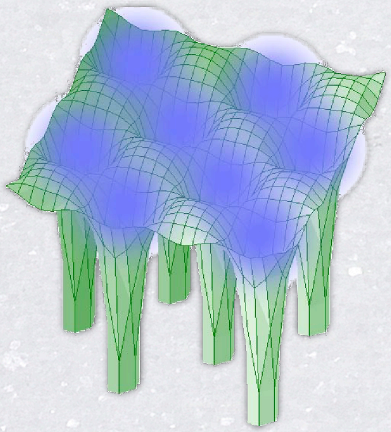
the physics:
condensed matter meets atomic optics

approximations in solids

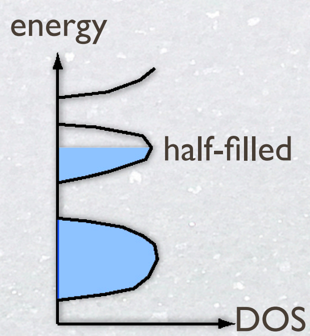
- fundamental electronic Hamiltonian

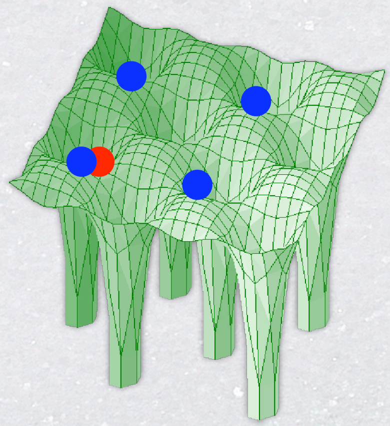
$$H=\sum_{j=1}^{e^-}\frac{\vec{p}_j^{\,2}}{2m_e}+\frac{1}{2}\sum_{i\neq j}^{e^-}\frac{e^2}{\left|\vec{r}_i-\vec{r}_j\right|}+\sum_{j}^{e^-}V_{eff}(\vec{r}_j)$$

- problem: electron-electron interactions



effective potential
one-electron picture
band conductor

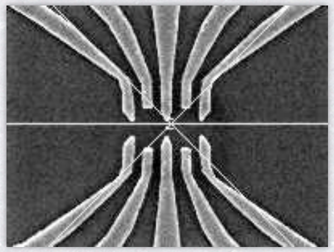




strong correlation
many-particle picture
Mott insulator

why strong correlations?

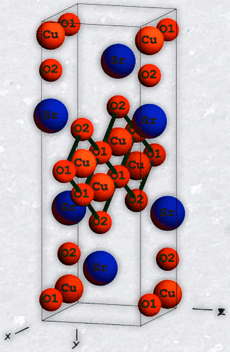
0 dimensions



magnetic
impurity physics

quantum dots

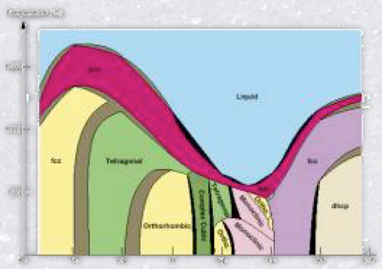
1 dimension



spin chains & ladders

Luttinger liquid

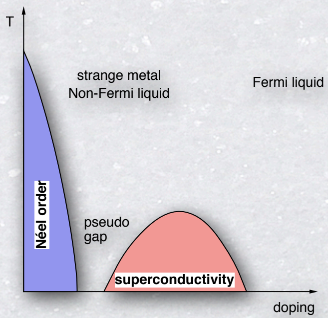
3 dimensions



realistic modelling:

transition metal,
rare earth compounds

2 dimensions

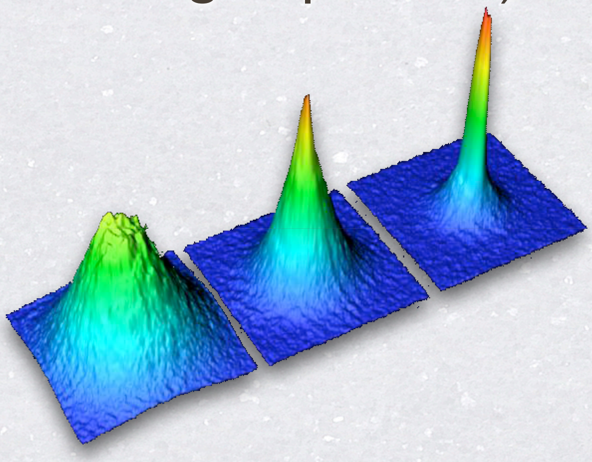


frustrated magnets

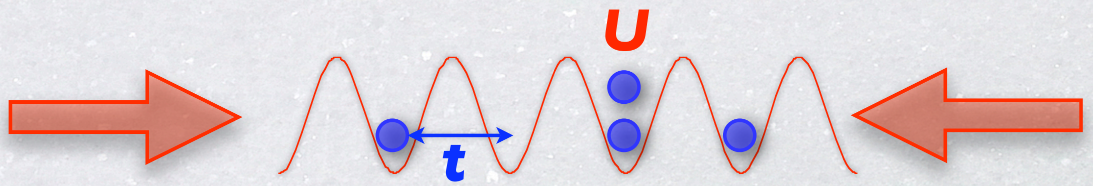
high-T_c superconductors

cold atomic gases in optical lattices

- ultra-cold bosonic atoms form Bose-Einstein condensate (Boulder & MIT groups, 1995)



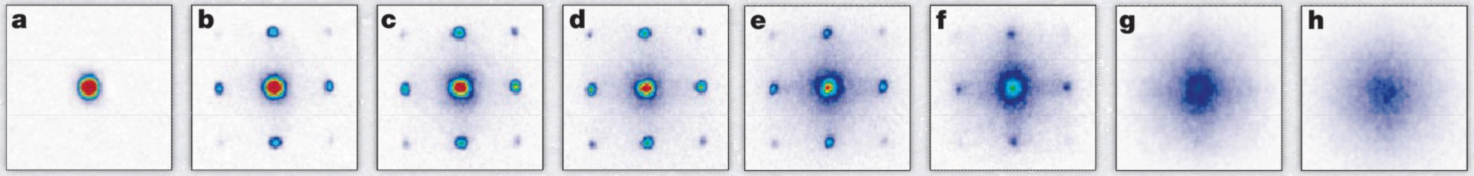
- standing waves from laser superimpose an optical lattice
  - Greiner et al (Munich group), Nature '02



- very well described by bosonic Hubbard model

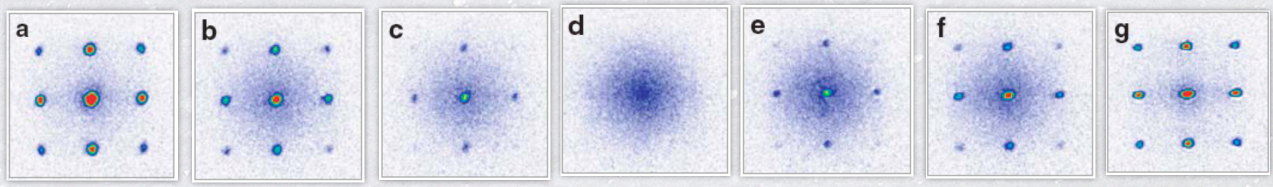
lattice bosons: control & tunability

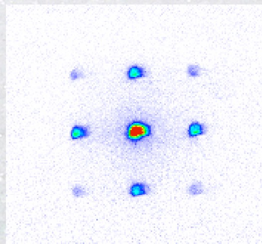
- controlled tuning of interaction *U*/*t* in time via lattice depth
- adiabatic change of *U*/*t*: quantum phase transition
  superfluid condensate to Mott-insulator
  - momentum distribution function



superfluid → adiabatic increase of interaction *U* → Mott insulator

- sudden change of *U*/*t* to Mott insulator: collapse and revival



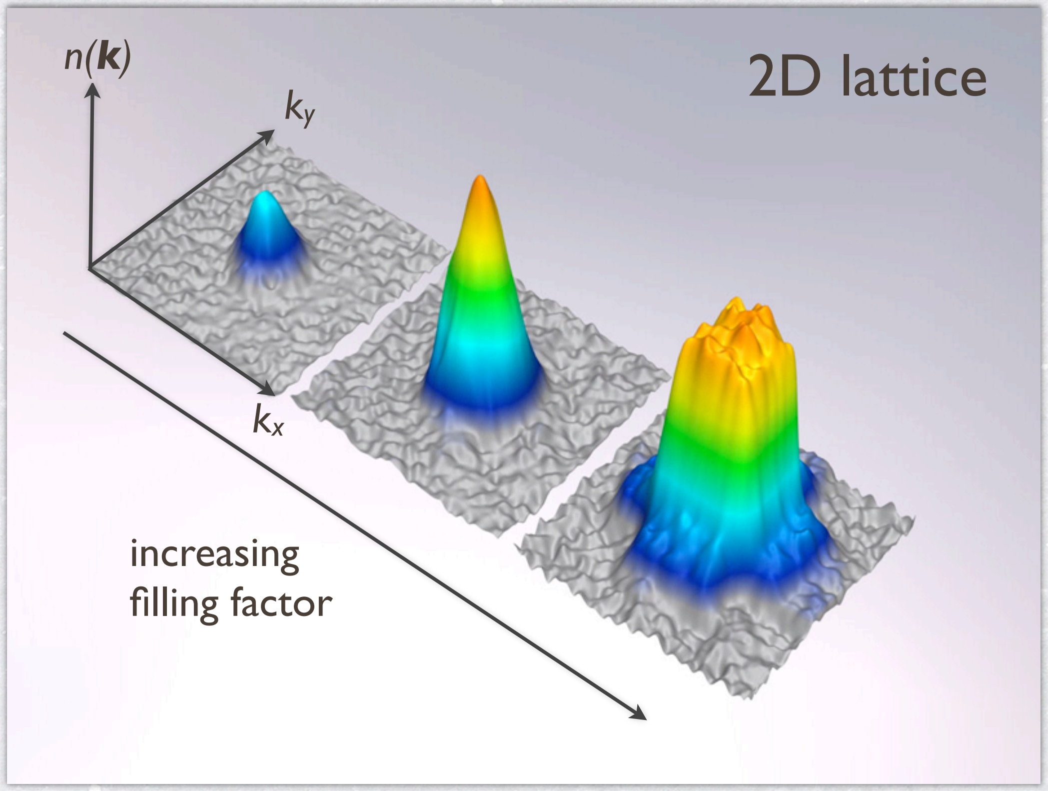


→ time →

- quantum optics meets strong correlations: quantum simulator

experiments on lattice fermions

- detection of Fermi surface for ^{40}K in an optical lattice
- momentum distribution
- hyperfine levels = spin levels



M. Köhl *et al* (Esslinger group), PRL ‘05

the methods:
classical simulations of quantum systems

compression of information

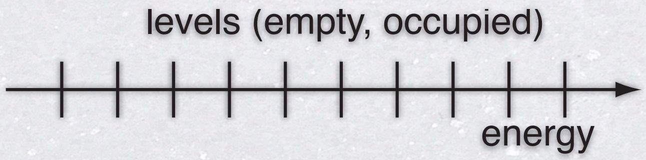
- compression of information necessary and desirable
  - diverging number of degrees of freedom
  - emergent macroscopic quantities: temperature, pressure, ...
- classical spins
  - thermodynamic limit: $N \to \infty$ $2N$ degrees of freedom (linear)
- quantum spins
  - superposition of states
  - thermodynamic limit: $N \to \infty$ 2^N degrees of freedom (exponential)

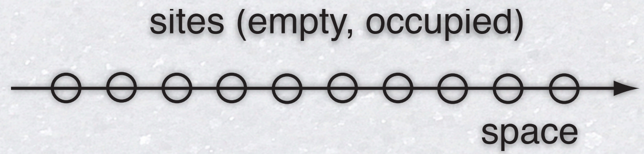
classical computers and simulators

- large-scale quantum computers and simulators far away
- what can we do with classical computers?
  - exact diagonalizations
    - limited to small lattice sizes: 40 (spins), 20 (electrons)
  - stochastic sampling of state space
    - quantum Monte Carlo techniques
    - negative sign problem for fermionic and frustrated spin systems
  - physically driven selection of subspace: decimation
    - variational methods
    - renormalization group methods
    - **how do we find the good selection?**

“one-dimensional” decimation

- arrange degrees of freedom on one axis





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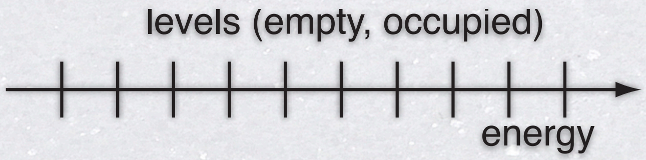
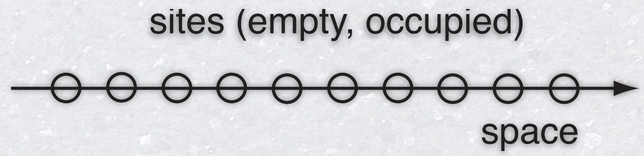
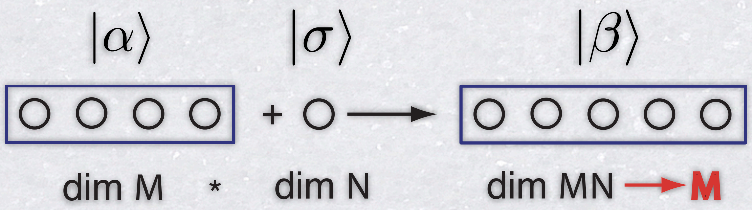




- enlarge Hilbert space by adding site after site



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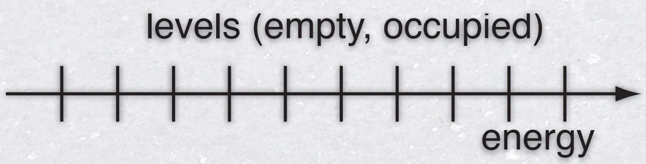

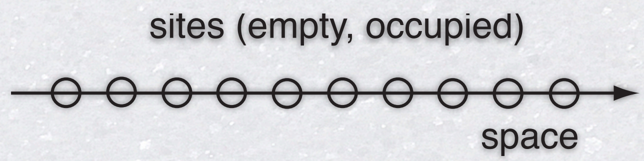

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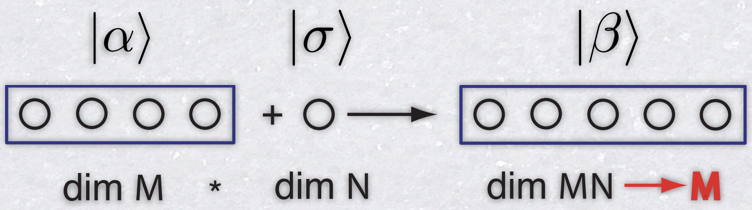


- decimate Hilbert space: reduced basis, method-dependent

$$|\beta\rangle = \sum_\alpha \sum_\sigma \boxed{\langle\alpha\sigma|\beta\rangle} |\alpha\rangle|\sigma\rangle \quad \text{or} \quad |\beta\rangle = \sum_\alpha \sum_\sigma \boxed{A_{\alpha\beta}[\sigma]} |\alpha\rangle|\sigma\rangle$$

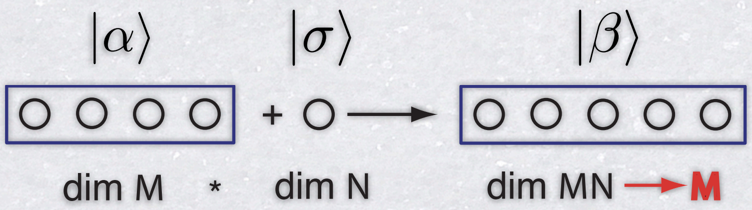
M x M matrices

“one-dimensional” decimation

Schollwöck, J.Magn.Mag.Mat., in press (2006)

- arrange degrees of freedom on one axis

- enlarge Hilbert space by adding site after site



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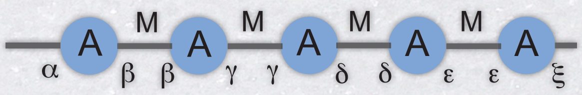
M x *M* matrices

- is there an optimal decimation prescription?

matrix product states

- recursion through all system sizes

see e.g. Schollwöck, J.Magn.Mag.Mat., in press (2006)



- total system wave functions

$$|\psi\rangle = \sum_{\sigma_1 \ldots \sigma_L} \boxed{(A_1[\sigma_1]\ldots A_L[\sigma_L])}\, |\sigma_1 \ldots \sigma_L\rangle$$

scalar coefficient:
~ matrix product

- matrix product state (MPS): generic structure for decimation
  - control parameter: matrix dimension *M*
  - *A*-matrices determined by decimation prescription

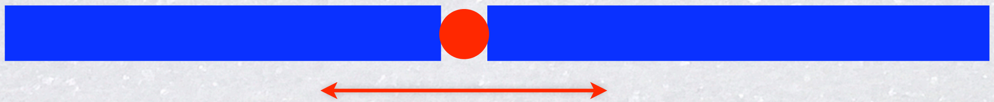
ground states: DMRG

- optimal: find (M x M) A-matrices minimizing $\langle\psi|\hat{H}|\psi\rangle$

  highly non-linear

- density-matrix renormalization group (DMRG) does the job linearly (White, PRL '92)
  - start from some set of A-matrices ("warm-up")
  - sequentially choose one A to minimize $\langle\psi|\hat{H}|\psi\rangle$ constraining all others

AAAAAAAAAAAAAAAAAAAAAAAAAAA

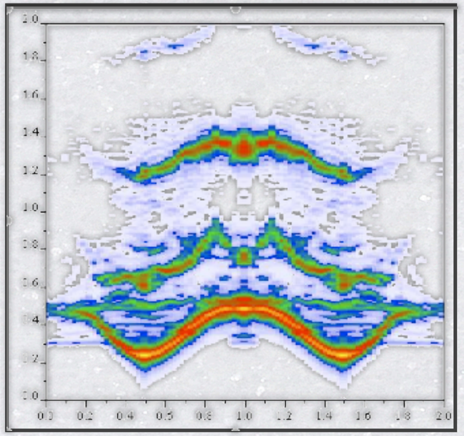


- variational method, typically reaches energy minimum: optimal!

Takasaki, Hikihara, Nishino, J. Phys. Soc. Jpn. 68, 1537 (99); Verstraete, Porras, Cirac, PRL (04)

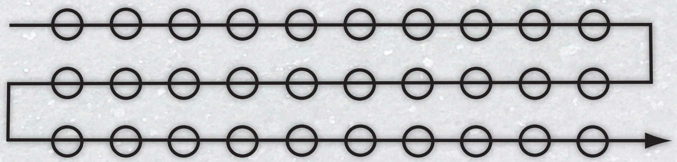
how good is optimal?

- is the optimal M x M MPS close to the true ground state?
- empirical evidence:
  one-dimensional ground state physics & thermodynamics at unprecedented precision (US, RMP **77,** 259 (2005))
  - up to O(1000) lattice sites
  - no sign problem: fermions!
  - extrapolations in M (up to 10,000)
  - almost machine precision: chains of spins M 200-500, fermions 500-1000



structure function of a spin chain (US)

- modest results in 2D
- QIT: entanglement scaling!



entanglement

- quantum states: superpositions

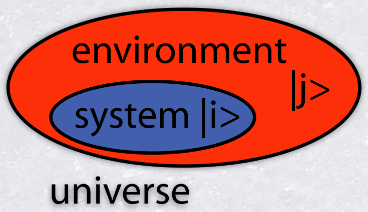
$$|\psi\rangle = \sum \alpha_i |\psi_i\rangle$$

- many-body quantum states: (bipartite) entanglement

classical $|\psi\rangle = |\uparrow\rangle|\downarrow\rangle$ product

quantum $|\psi\rangle \sim |\uparrow\rangle|\uparrow\rangle + |\downarrow\rangle|\downarrow\rangle$ entangled

- measuring bipartite entanglement *S*: reduced density matrix



$$|\psi\rangle = \sum \psi_{ij}|i\rangle|j\rangle \quad \hat{\rho} = |\psi\rangle\langle\psi| \to \hat{\rho}_S = \mathrm{Tr}_E \hat{\rho}$$

$$S = -\mathrm{Tr}[\hat{\rho_S} \log_2 \hat{\rho_S}] = -\sum w_\alpha \log_2 w_\alpha$$

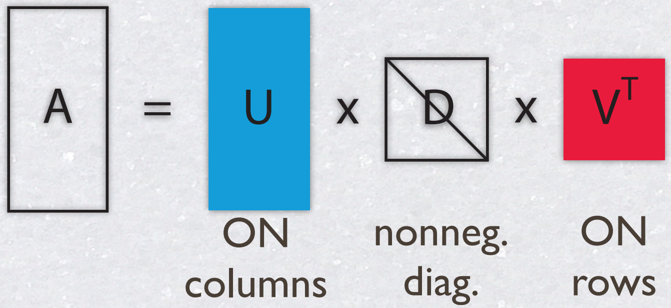
Schmidt decomposition

- calculating entanglement in a general quantum state $|\psi\rangle = \sum \psi_{ij} |i\rangle |j\rangle$

  $N^S N^E$ coefficients

- singular value decomposition of matrix $A_{ij} = \psi_{ij}$

$$A = UDV^T$$



- Schmidt decomposition

$$|\psi\rangle = \sum_{\alpha=1}^{N_{\text{Schmidt}}} \sqrt{w_\alpha} |w_\alpha^S\rangle |w_\alpha^E\rangle \qquad N_{\text{Schmidt}} \leq \min(N^S, N^E) \text{ coeffs.}$$

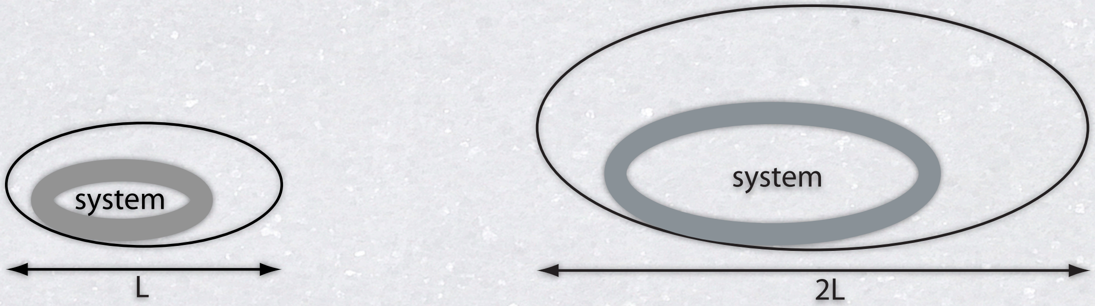
- reduced density matrices

$$\hat{\rho}_S = \sum_{\alpha}^{N_{\text{Schmidt}}} w_\alpha |w_\alpha^S\rangle\langle w_\alpha^S| \quad \hat{\rho}_E = \sum_{\alpha}^{N_{\text{Schmidt}}} w_\alpha |w_\alpha^E\rangle\langle w_\alpha^E| \quad \text{identical spectra}$$

- system and environment share bipartite entanglement

area law

- bipartite entanglement shared property of system and environment
- (hyper)surface property



effective surface width (grey): correlation length

- scaling obeys area law in *d* dimensions

$$S \sim L^{d-1} (\times \xi)$$

- keep in mind: what happens at criticality?

Bekenstein,
PRD 7, 2333 (73)
Callan, Wilczek,
Phys. Lett. B, 333 (95)

bipartite entanglement in DMRG

- arbitrary bipartition

AAAAAAAA AAAAAAAAAAAAAAA

$$|\psi\rangle = \sum_{\alpha}^{M} \sqrt{w_\alpha} |\alpha_S\rangle |\alpha_E\rangle$$

Schmidt decomposition

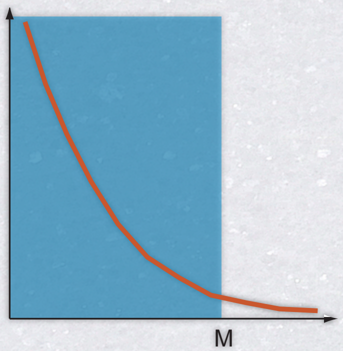
- reduced density matrix and bipartite entanglement

$$\hat{\rho_S} = \sum_{\alpha} w_\alpha |\alpha_S\rangle\langle\alpha_S|$$

$$S = -\sum_{\alpha} w_\alpha \log_2 w_\alpha \leq \log_2 M$$

codable maximum

- typical decay of density matrix spectrum

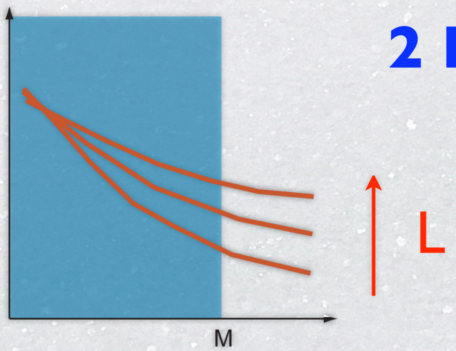


1 D

fast decay

small loss

good



2 D

decay slows down

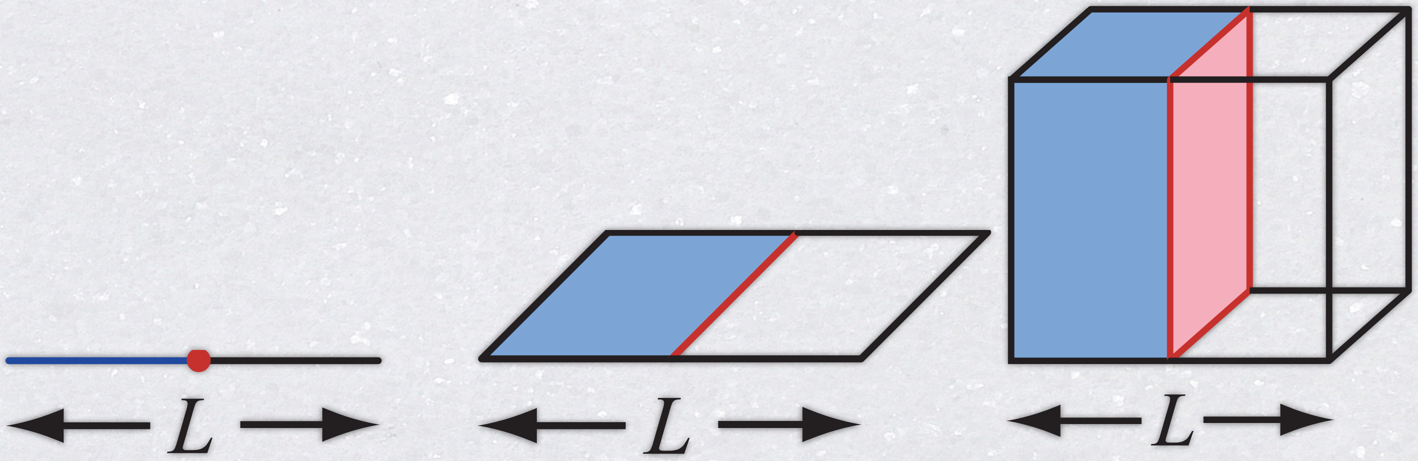
big loss

bad

entanglement scaling: gapped systems

Latorre, Rico, Vidal, Kitaev (03)

- entanglement grows with system surface: area law



gapped $S(L) \sim \text{cst.}$ $S(L) \sim L$ $S(L) \sim L^2$ black hole

$$\boxed{S \leq \log_2 M \Rightarrow M \geq 2^S}$$

states $M > 2^{cst.}$ $M > 2^L$ $M > 2^{L^2}$

entanglement scaling: critical systems

- 1D: logarithmic correction

  $$S_L = \frac{c+\bar{c}}{6} \log_2 L$$ central charges

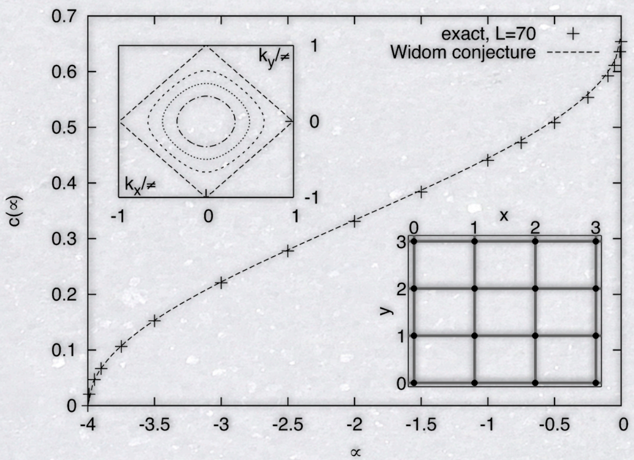
  Latorre, Rico, Vidal, Quant. Inf. Comp. 4, 48 (2004)

  $M > L^k$ $\quad k = (c+\bar{c})/6 \quad$ *k* is small: DMRG works quite well

- 2D: rich scaling behaviour, DMRG still fails

  Barthel, Chung, US, PRA 74, 022329 (2006)

  - fermionic systems



1D Fermi surface:
logarithmic correction
c = surface length

$$S \sim c(\mu) L \log_2 L$$

0D Fermi surface (not shown):
sub-log diverging correction

  - bosonic systems: no logarithmic correction tunability:

can we go beyond 1D statics?

time-dependence in

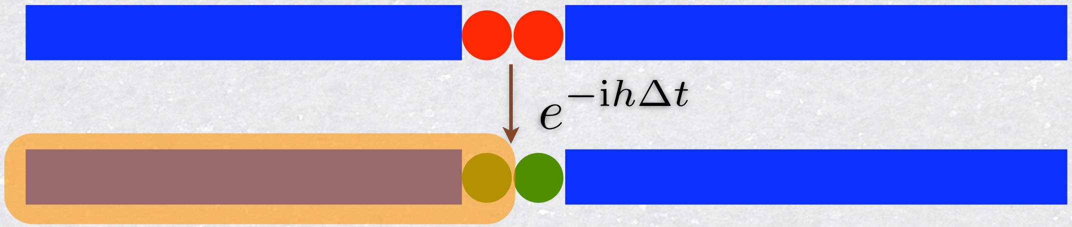
strongly correlated systems

time-dependent DMRG

Daley, Kollath, US, Vidal, J. Stat. Mech (2004) P04005; White, Feiguin PRL '04

$$|\psi(t+\Delta t)\rangle = \exp(-\mathrm{i}\hat{H}\Delta t)|\psi(t)\rangle$$

- Trotter decomposition: $\exp(-\mathrm{i}\hat{H}\Delta t) = \ldots e^{-ih_i\Delta t}e^{-ih_{i+1}\Delta t}\ldots \boxed{+\,O(\Delta t^2)}$
- local infinitesimal time step



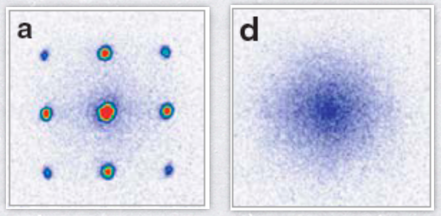
$|\psi\rangle \rightarrow$ AA

$e^{-ih\Delta t}|\psi\rangle \rightarrow$ A'A'

  - exact bond evolution
  - optimal state selection: M highest-weight eigenstates of density matrix
  - approximate DMRG description follows time-evolving state
- global infinitesimal time step

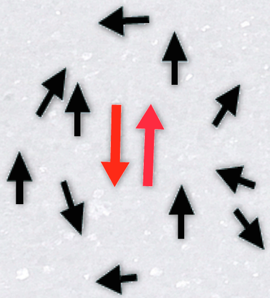
time-dependent DMRG

driven QPT



Daley, Kollath, US, Vidal, JSTAT ‘04
Clark, Jaksch, PRA ‘05
Trebst, US, Troyer, Zoller, PRL ‘05

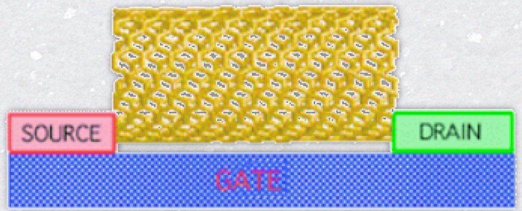
decoherence



Friedrich, US, Khaetskii (in prep.)

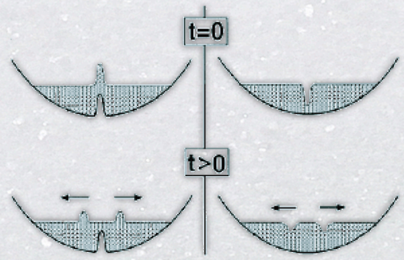
- strong correlation out of equilibrium
- large system sizes
- long times
- controlled error
- 1D systems

transport



Gobert, Kollath, US, Schütz, PRE ‘05
Al-Hassanieh et al (OakRidge), ‘06

response

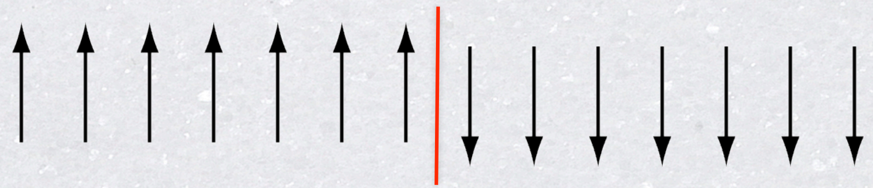


Kollath, ..., US, Giamarchi, PRL ‘06
Kollath, US, v Delft, Zwerger, PRA ‘05
Kollath, US, Zwerger, PRL ‘05
White, Feiguin, PRL ‘04

quantum dynamics far from equilibrium

dynamics far from equilibrium

- prepare ferromagnetic domains in an S=1/2 antiferromagnet
  far from equilibrium state



- antiferromagnetic dynamics dissolves domain wall
  - XY chain
  - Heisenberg chain
- shock fronts, magnetization carriers?
- ballistic or non-ballistic (diffusive) magnetization transport?

Gobert, Kollath, US, Schütz, PRE 71, 036102 (‘05)

XY model dynamics

QuickTime™ and a
3ivx D4 4.5.1 decompressor
are needed to see this picture.

- solution quasiexact on timescales shown
- ballistic transport, quantized magnetization carriers

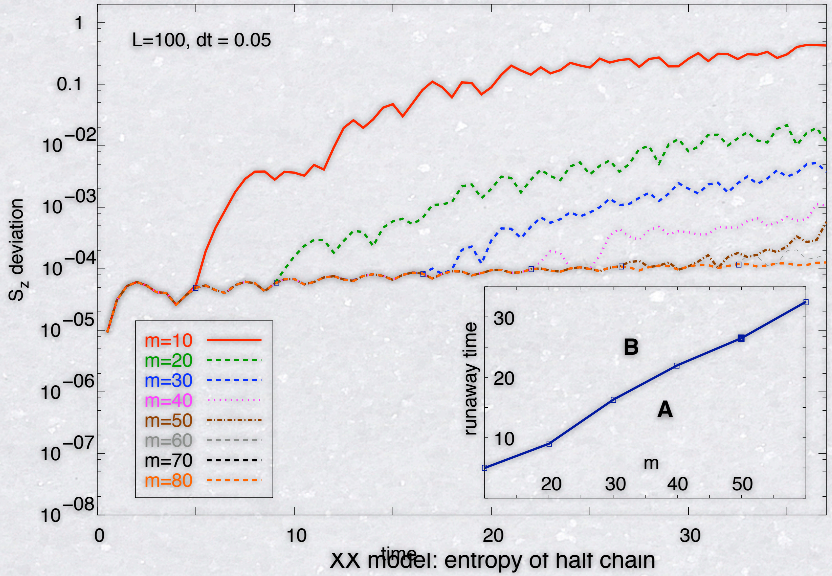
Heisenberg model dynamics

QuickTime™ and a
3ivx D4 4.5.1 decompressor
are needed to see this picture.

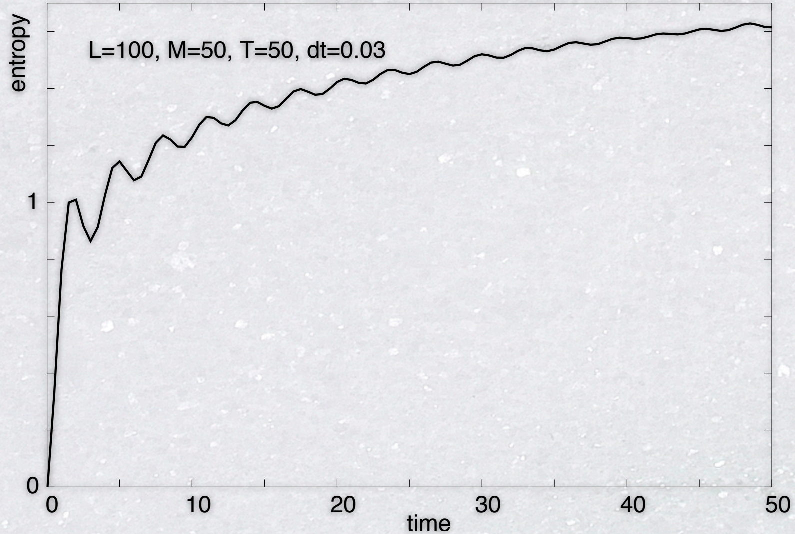
- non-ballistic transport on timescales shown
- precursor structures at carrier velocity

need more analytics!

error analysis



XX model: entropy of half chain



- Trotter decomposition error:

$$(\Delta t)^n \times (T/\Delta t) \propto T$$

ultimately irrelevant

- Lieb-Robinson propagation error:

exponential in T

Hastings, Osborne (04)

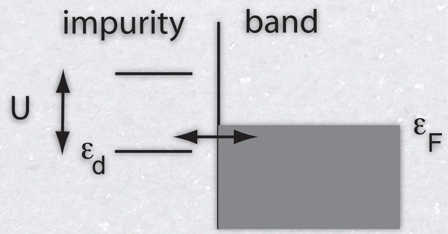
numbers of states increases exponentially in time: will we hit the wall before the physics happens?

can we go beyond 1D?

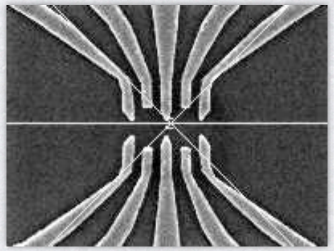
0D, 2D, 3D

quantum impurities and dots

- magnetic impurities in metals



quantum dots

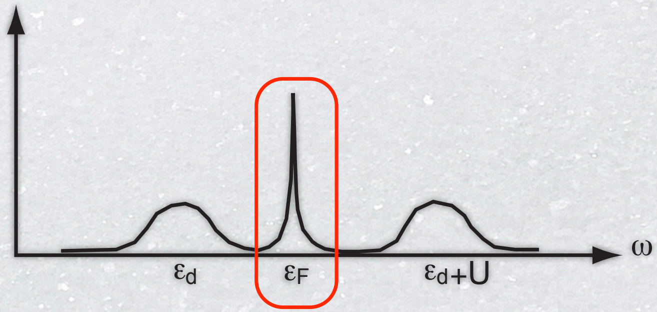


- Anderson model

$$\hat{H}_A = \sum_{\mu} \epsilon_d c^{\dagger}_{d\mu} c_{d\mu} + \frac{U}{2} n_{d\uparrow} n_{d\downarrow} + \int d\epsilon\, \epsilon a^{\dagger}_{\epsilon\mu} a_{\epsilon\mu} + \left(\frac{\Gamma}{\pi}\right)^{1/2} \int d\epsilon \left(a^{\dagger}_{\epsilon\mu} c_{d\mu} + c^{\dagger}_{d\mu} a_{\epsilon\mu}\right)$$

impurity band hybridization

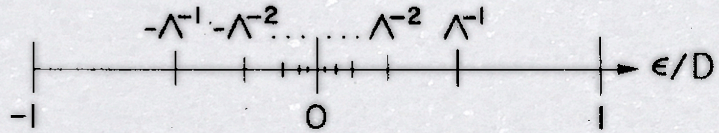
- spectral density at impurity: resonance



Wilson's numerical RG

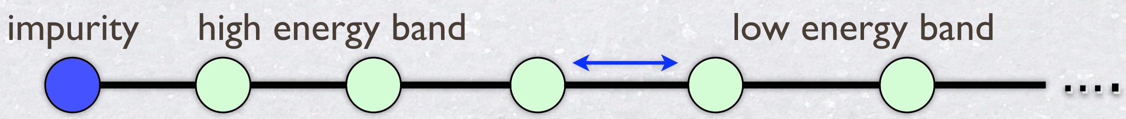
Wilson RMP '75

- focus on conduction band states close to Fermi edge

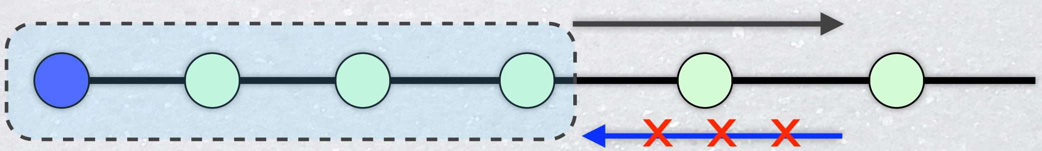


discretization parameter Λ

- problem maps to semi-infinite non-interacting chain with decaying hoppings



- diagonalize high-energy part
- add "sites", diagonalize, retain *M* lowest-energy eigenstates

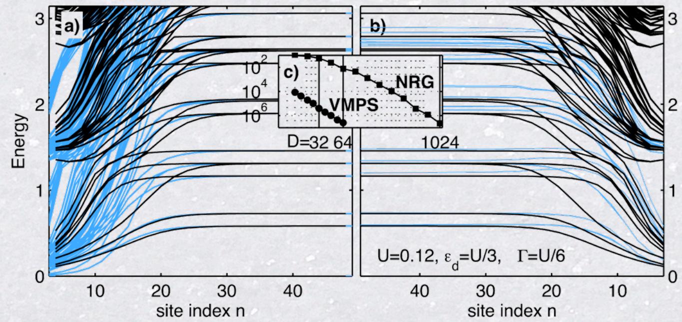


no feedback!

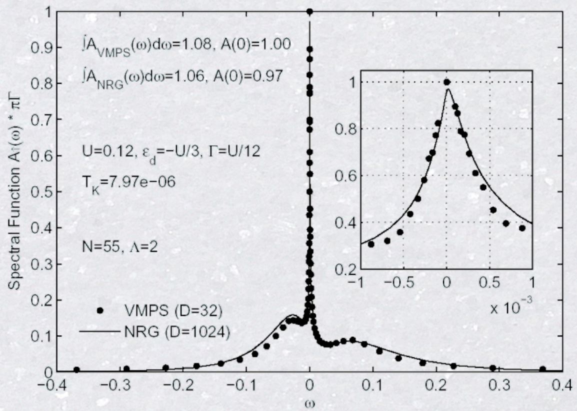
DMRG meets NRG

Verstraete, Weichselbaum, US, Cirac, v Delft '05

- NRG and DMRG: (M x M) matrix product states
- DMRG variationally optimal
- apply DMRG to NRG-type Hamiltonian: improves NRG

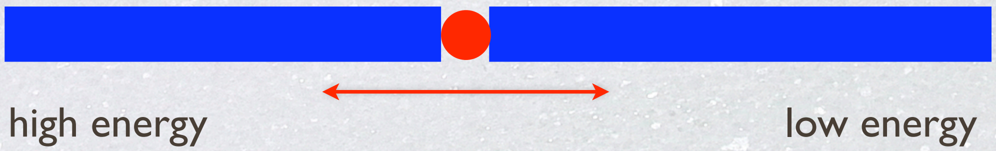


energy flow



impurity spectral function

- bidirectional feedback between all energy scales



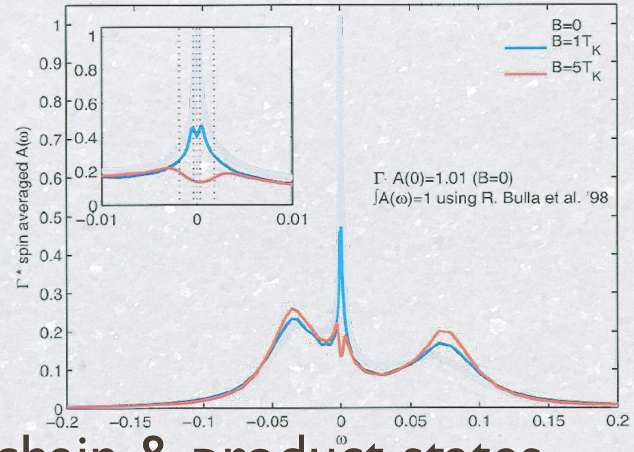
high energy accessible
speed-up > 1,000

feedback: speed & flexibility

- relax/adapt logarithmic discretization

high energies

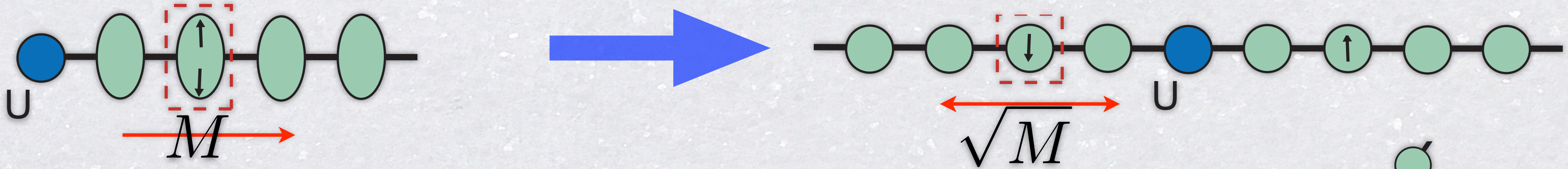
multiple resonances (external fields)



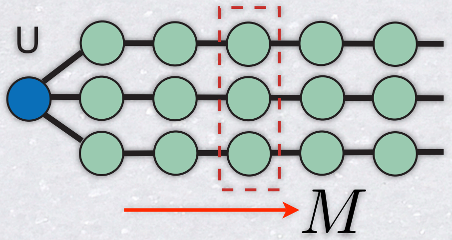
- bath sites non-interacting: unfolding of chain & product states

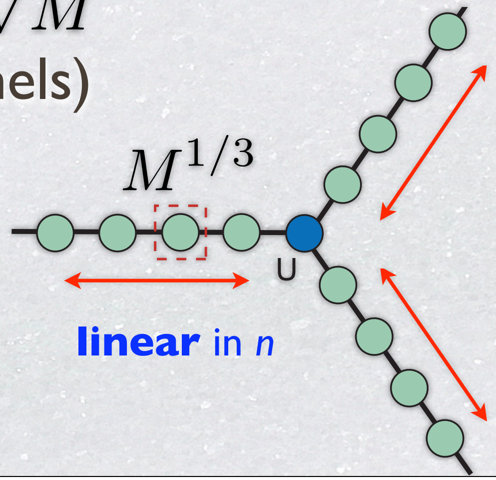
~ product of 2 states

speed up by 1,000



- star geometry for multiple bands (*n* channels)



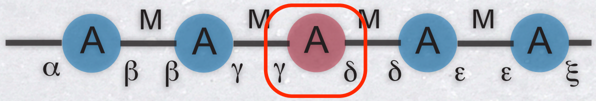


- allows time-evolution

outlook: two dimensions

- **matrix** products in **one** dimension

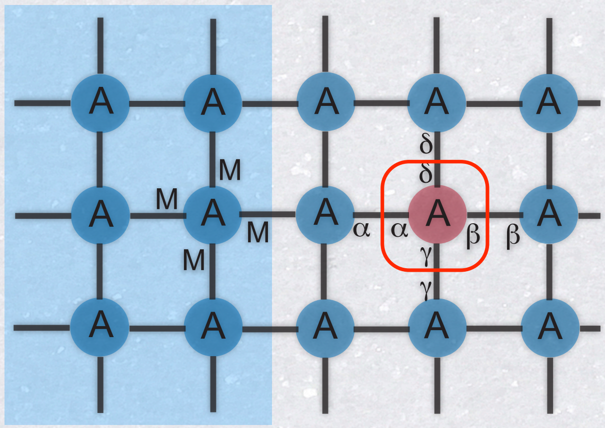
$$|\psi\rangle =$$



rank 2 tensor

- **tensor** contractions in **two** dimensions Nishino '99

$$|\psi\rangle =$$



rank 4 tensor

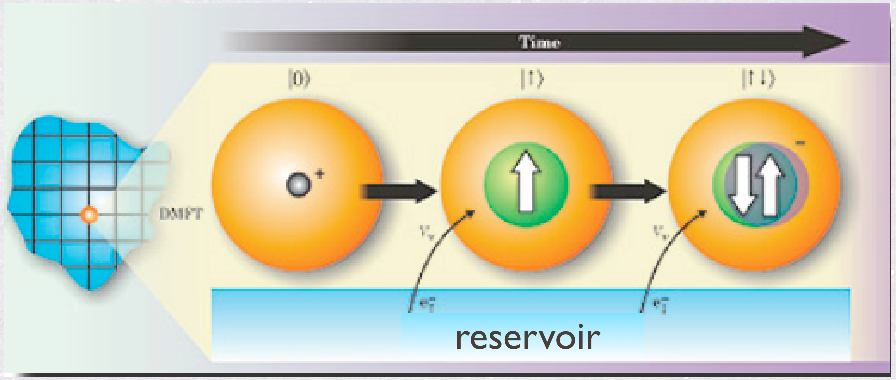
  - correct entanglement scaling properties
  - evaluation feasible, but highly complex; bad scaling with M Verstraete, Cirac '04
- development of efficient implementations (still?) problematic

outlook: towards real materials

McCulloch, US, Parcollet, Georges, in progress

- real materials: band structure + correlation effects
  LDA + DMFT

- dynamical mean-field theory



interacting lattice model

local impurity problem

$$G_{\mathrm{lattice}} = G_{\mathrm{imp}}(\epsilon_i, U, \Gamma(\omega))$$ ← electronic bath

(Kotliar & Vollhardt)

- real materials (*d*,*f*-orbitals): multiple bands, local clusters

- powerful new DMRG-based impurity solver will help

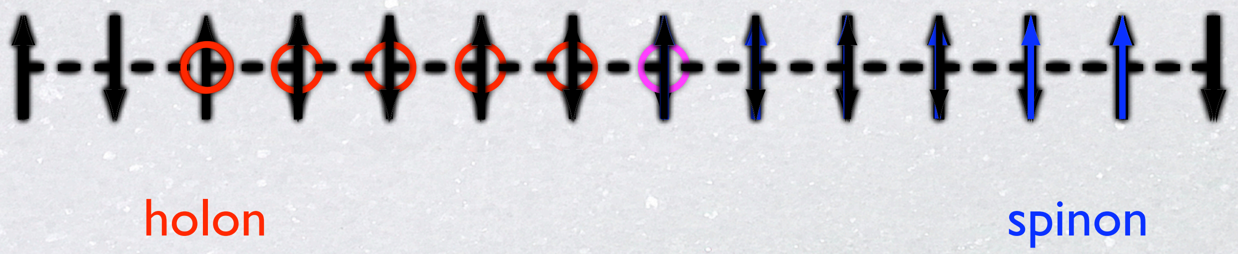
DMRG & applications to cold atoms out-of-equilibrium II

Ulrich Schollwöck
RWTH Aachen

application:
spin-charge separation in ultracold atom gases in an optical lattice

spin-charge separation

- what do repulsive interactions do to an electron gas?
- 3D: Fermi liquid theory
  - fermionic quasi-particles
- 1D: Luttinger liquid theory
  - collective modes of spin and charge
  - spin-charge separation



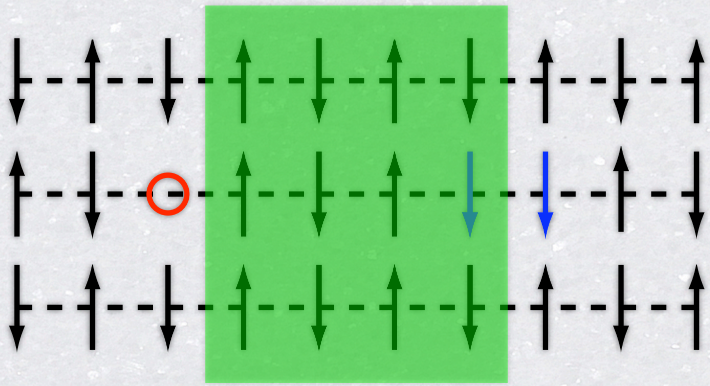
spin-charge separation

one dimension

holon

spinon

two dimensions

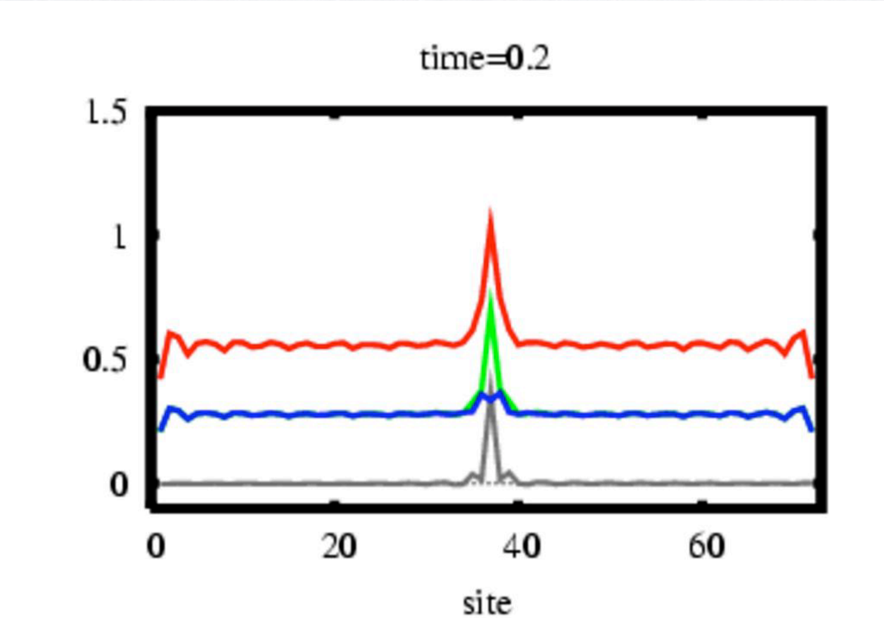


spin mismatch

prevents separation

single-particle excitation

- quarter-filled Hubbard chain: $U/t=4$
- add spin-up electron at chain center at time=0
- measure charge and spin density



time-dependent
DMRG

charge

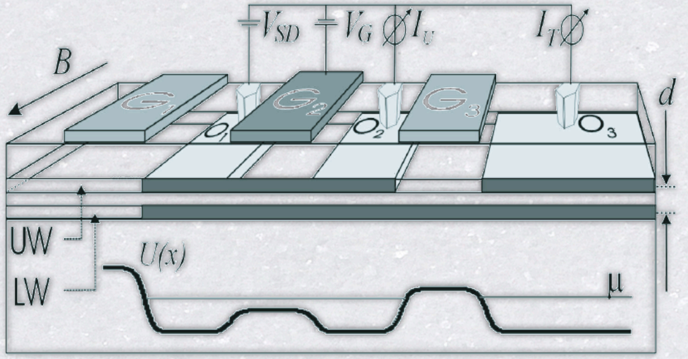
spin

- separation of charge and spin

Kollath, US, Zwerger, PRL 95, 176401 ('05)

experimental verification

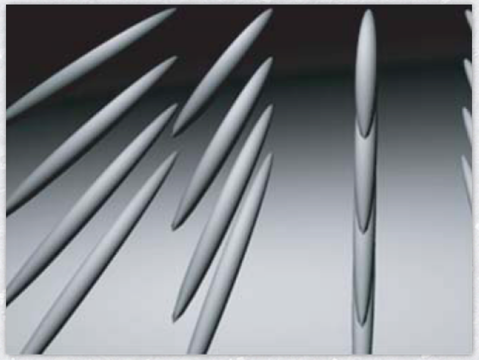
solid state setup



Auslaender *et al*, Science '05

interactions
fixed and unknown

ultracold atom setup



array of 1D atomic wires (Bloch, Esslinger)

interactions
tunable and known

how?

Kollath, US, Zwerger, PRL '05

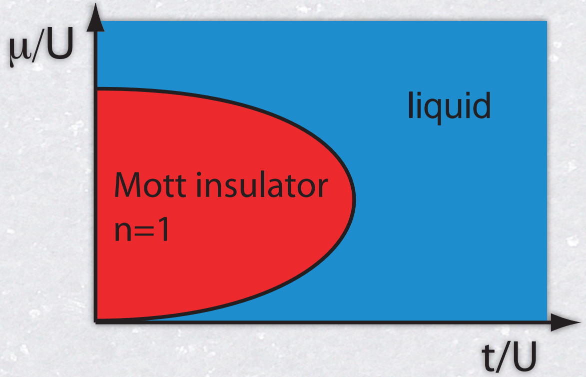
coexistence of insulator and liquid

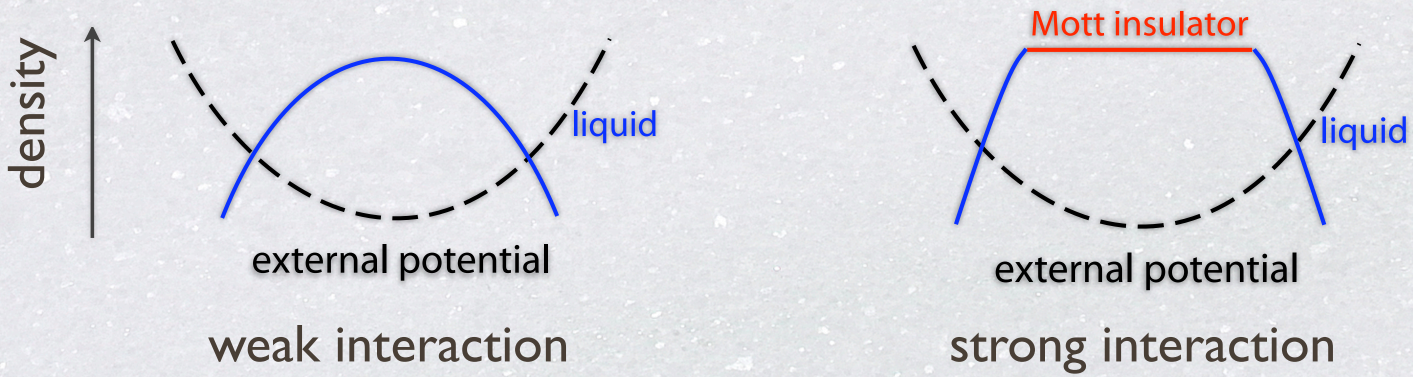
- fermionic Hubbard model

$$\hat{H} = -t\sum_{i\sigma}(c^\dagger_{i\sigma}c_{i+1\sigma} + h.c.) + U\sum_i n_{i\uparrow}n_{i\downarrow} \boxed{-\sum_i \mu_i n_i}$$

nearest-neighbor hopping onsite repulsion chemical potential

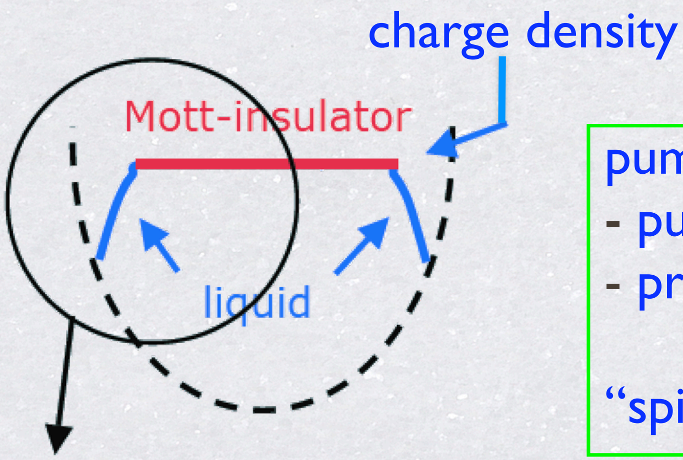
- liquid: charge and spin transport
- Mott insulator: only spin transport
- harmonic trapping potential
  spatially varying density





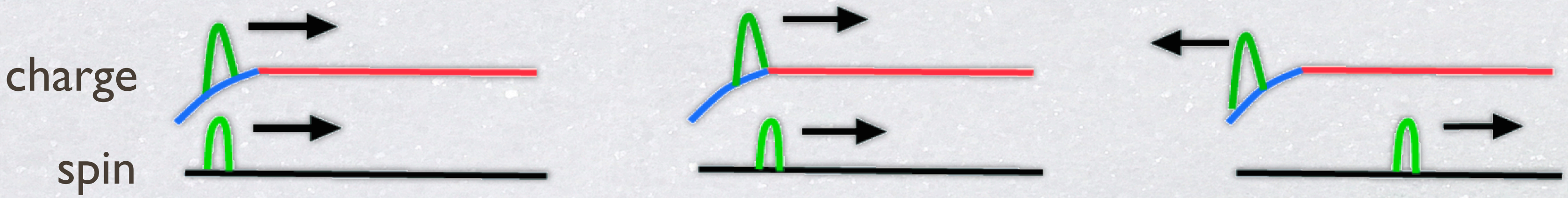
experimental setup: idea

problem: tubes of unequal filling smear signal; need standard



pump & probe:
- pump charge/spin perturbation
- probe elsewhere

"spin" selective laser



perturb system in charge and spin

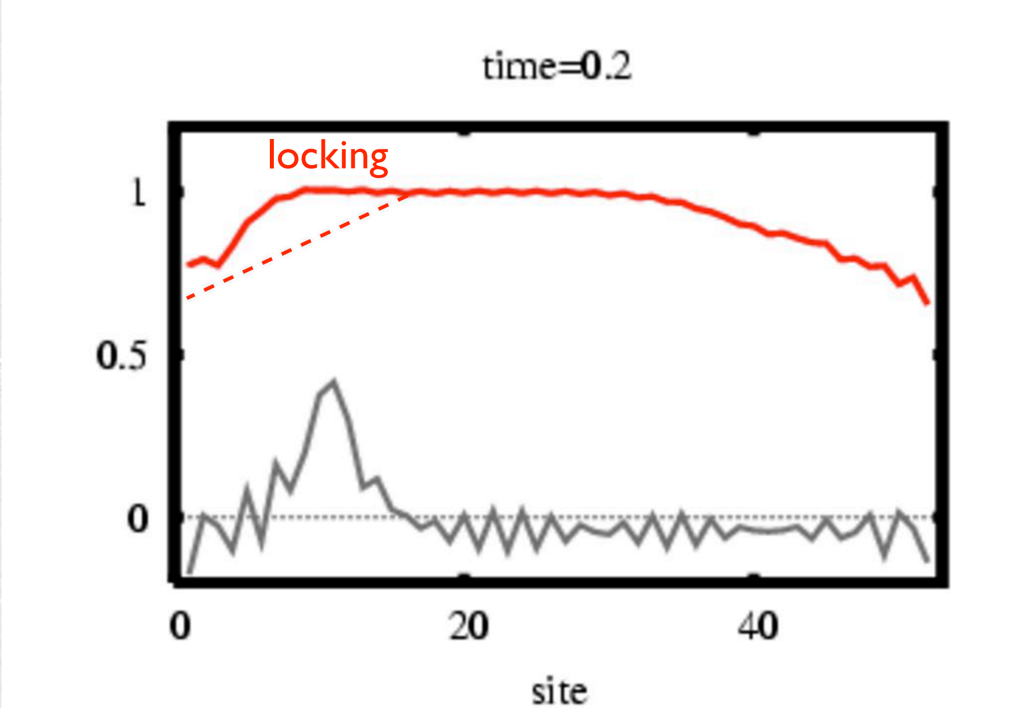
perturbation evolves

charge reflected at MI spin goes through

what happens ...

- charge and spin evolution in time with DMRG
- absolute precision: better than 0.001 in all quantities

U/*t*=4



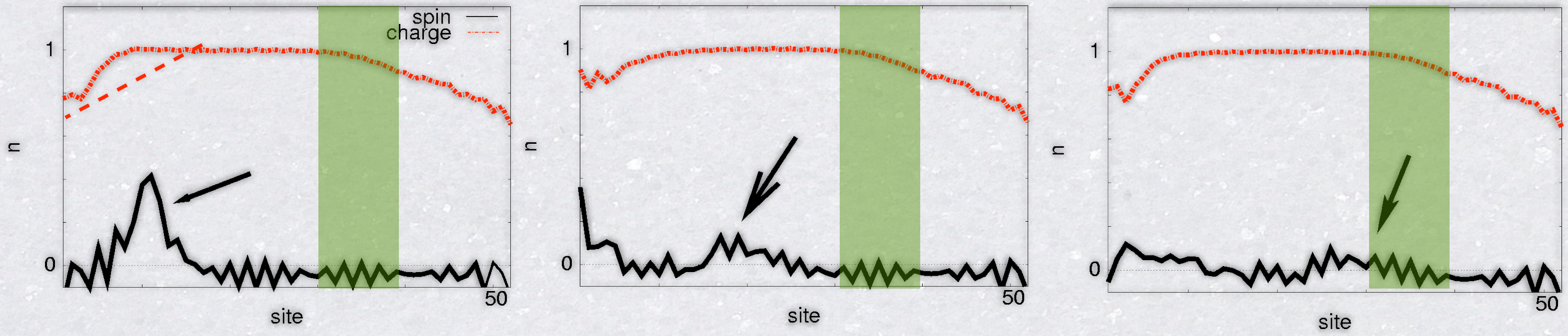
time-dependent DMRG

charge

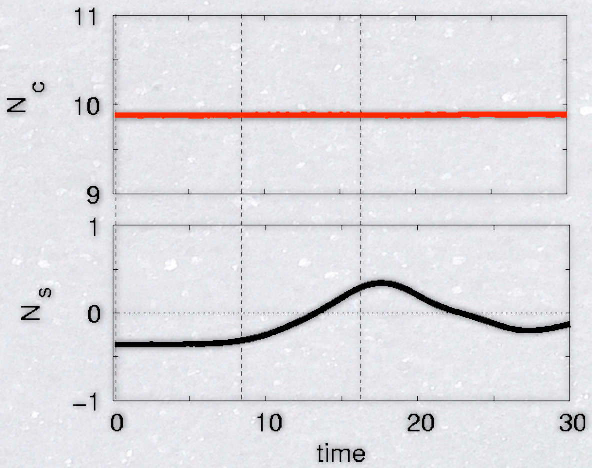
spin

... and how to detect it

- stills from movie: measurable?



- experimentally inevitable averaging helps!



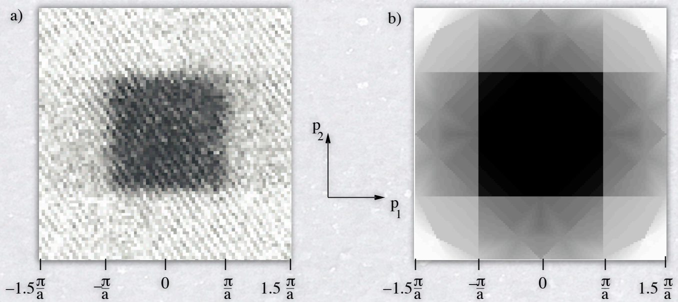
summed charge (10 sites)

summed spin (10 sites)

clear evidence of spin-charge separation

how hot are ultracold fermions?

- full lattice: fermions in higher Brillouin zone



experiment: Stöferle *et al,* '05

simulation: Katzgraber *et al,* '05

$T \approx 0.5\ E_{\mathrm{Fermi}}$

- by far too hot for many strong correlation phenomena

$T \approx 30$ K $\quad T_{\mathrm{Fermi}} \approx 30{,}000$ K $\quad$ ratio: 0.001

- escape routes for "T=0" simulations
  - dramatically enhanced cooling techniques (how?)
  - switch to analogous bosonic problem
  - adiabatic preparation of pure quantum state

Trebst, US, Troyer, Zoller PRL '06

SC separation in two-species bosons

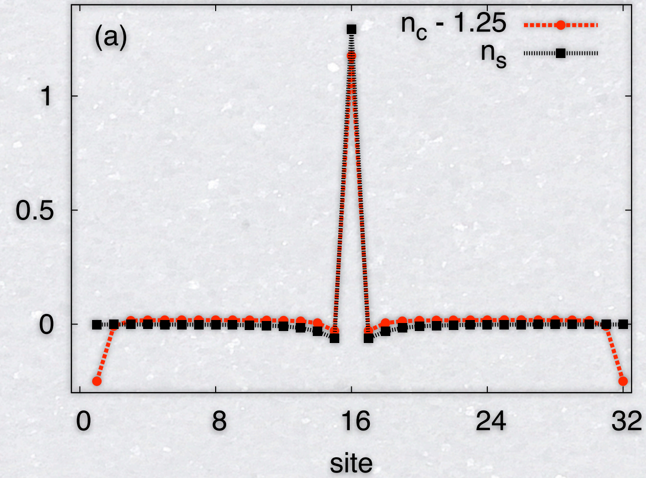
Kleine, Kollath, McCulloch, Giamarchi, US, arXiv:0706.0709

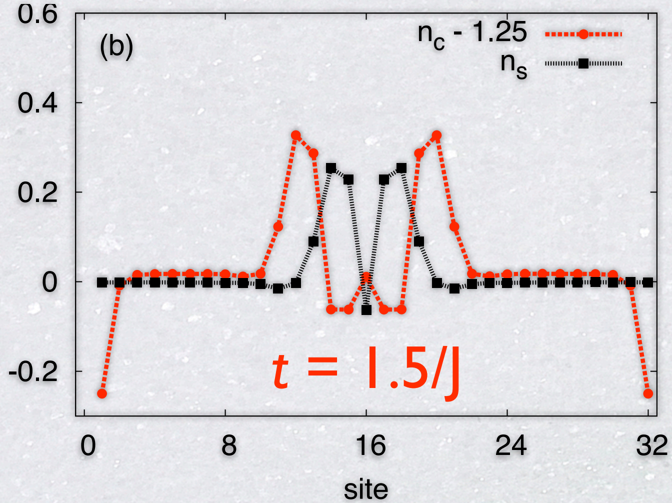
- „spin“-“charge“ separation: low-energy separation of symmetric and antisymmetric combination of two flavours
- SU(2) symmetry not essential!
- two species of bosons:
  - charge is sum of bosonic densities
  - spin is difference of bosonic densities
- competition: interspecies (AB) vs. intraspecies (AA,BB) repulsion
- phase separation must be avoided! $U_{AB} \leq U_{AA}, U_{BB}$

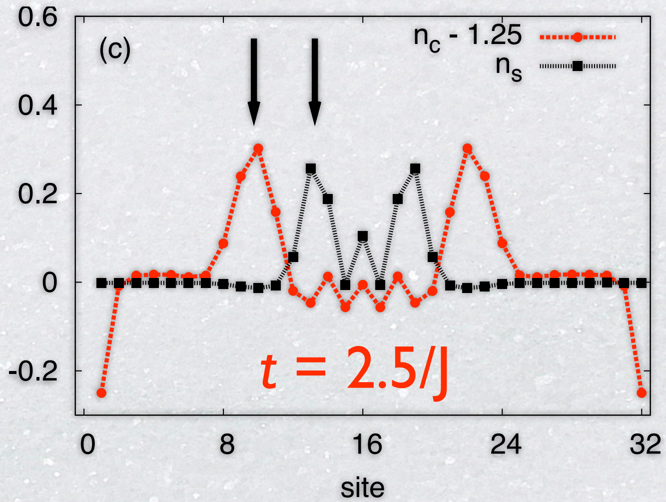
two-species bosons: movie snapshots

Kleine, Kollath, McCulloch, Giamarchi, US, arXiv:0706.0709

- single-particle excitation: insert one boson type A
- density 0.625/species



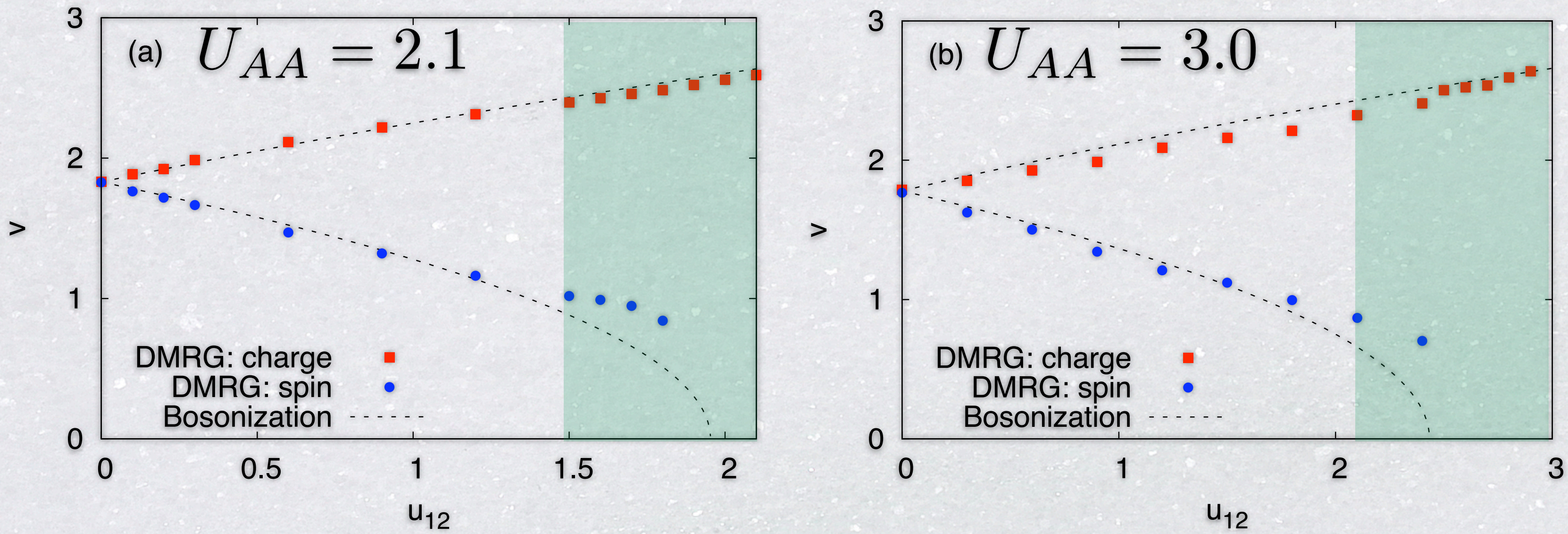




SC separation in two-species bosons

Kleine, Kollath, McCulloch, Giamarchi, US, arXiv:0706.0709

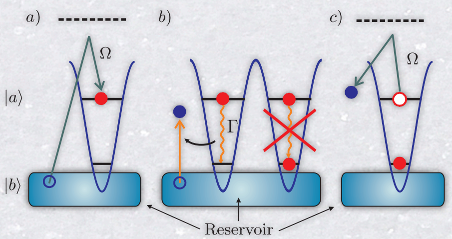
- bosonization analysis: numerics for single-species LL parameters
- bosonization in good agreement with DMRG,
  but fails quantitatively in experimentally relevant regime
  $U_{AB} \approx U_{AA}, U_{BB}$

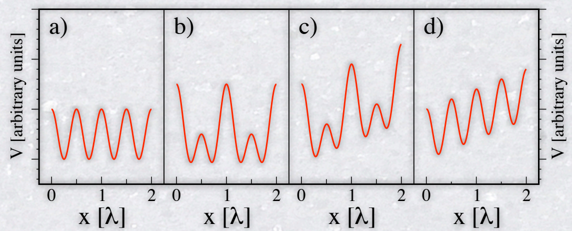


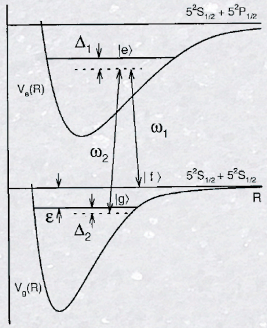
application:
adiabatic construction of *d*-wave RVB states in a 2D square lattice

adiabatic pure state preparation

initial state preparation → adiabatic transformation → state detection







Pauli blocking

tuning (super)lattices

spectroscopy

pattern loading
double occupation
entropy zero

Rabl *et al*, PRL '03

$$\hat{H}_{\text{init}} \longrightarrow \hat{H}_{\text{final}}$$
$$|0_{\text{init}}\rangle \longrightarrow |0_{\text{final}}\rangle$$

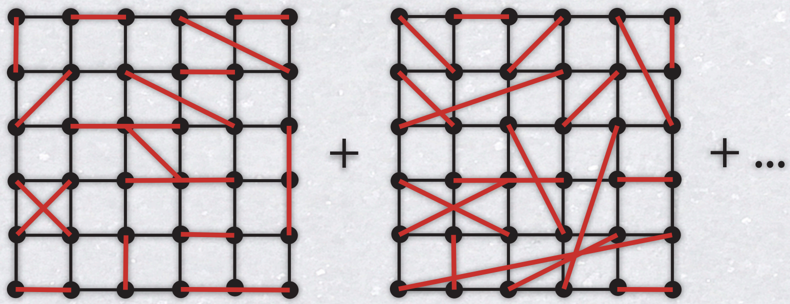
simulation:
- path existence
- path speed: adiabaticity vs stability

found path to *d*-wave RVB ground state (?) of doped 2D Hubbard

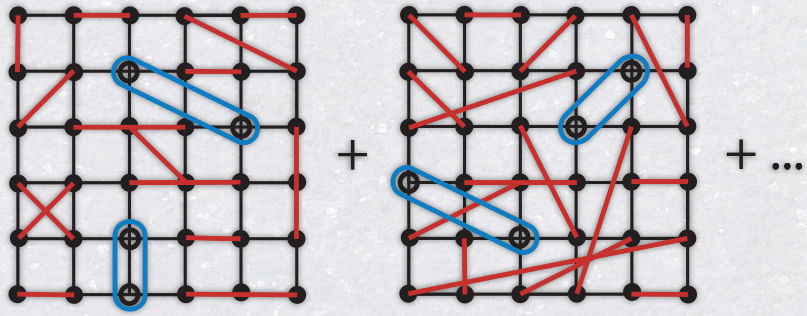
d-wave RVB in the 2D Hubbard model?

- high-T_c superconductors = doped resonating valence bond (RVB) states? (Anderson '87)

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



hole-doping:
hole pairs condense (BCS)

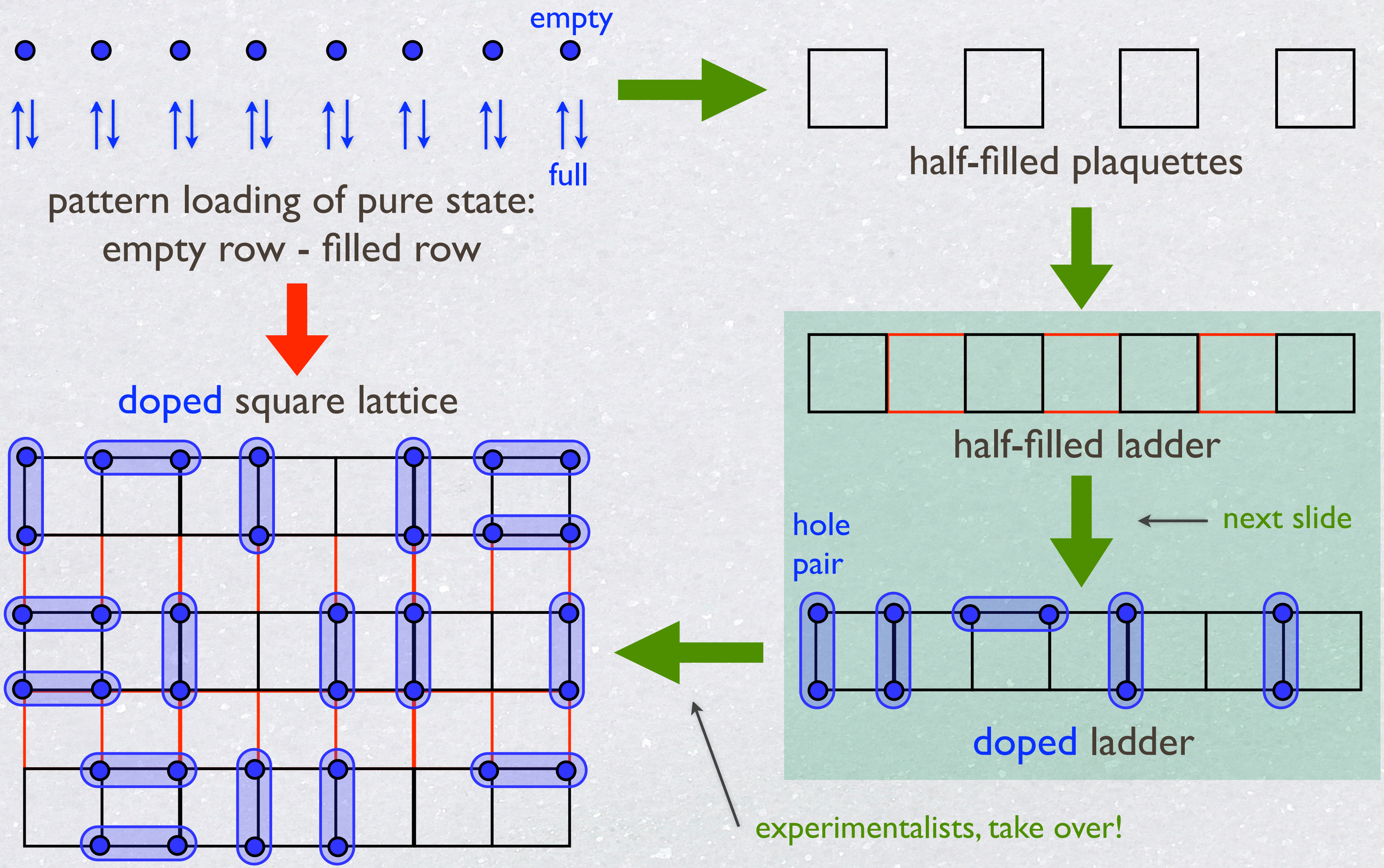


Gutzwiller-projected BCS wave function: eliminates double occupancies

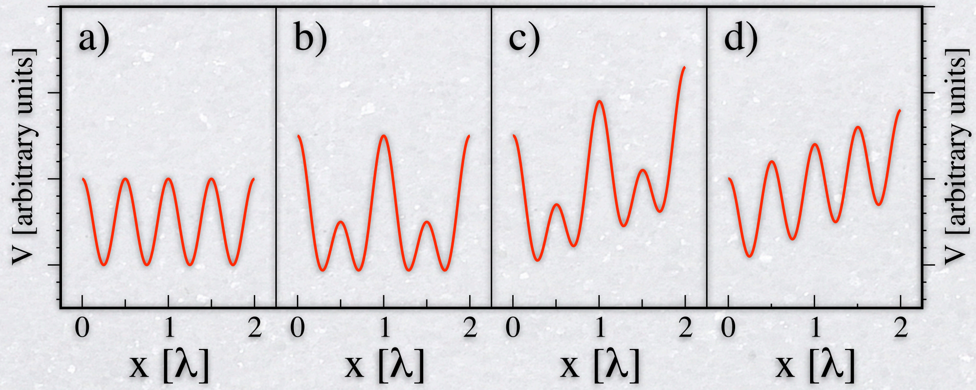
$$|\Phi\rangle = P_G \prod_k \left(u_k + v_k c^\dagger_{k\uparrow} c^\dagger_{-k\downarrow} \right) |0\rangle \rightarrow |\Phi\rangle = P_G \left(\sum_{ij} a(i-j) c^\dagger_{i,\uparrow} c^\dagger_{j,\downarrow} \right)^{N/2} |0\rangle$$

- *d*-wave symmetry

adiabatic path



Toolbox II: superlattice and ramps

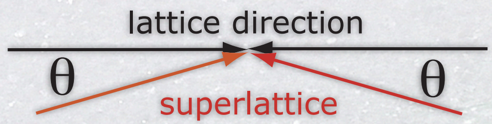


a. One-dimensional optical lattice

b. Superlattice

- interfere laser beams propagating at angles $\pm\theta$
- no additional laser frequency
- modulates hoppings and chemical potential

$$V(x) = V_x' \sin(k'x + \Phi)$$
$$k' = k\cos(\theta)$$



c. + d. Linear ramp

- from wing of laser beam

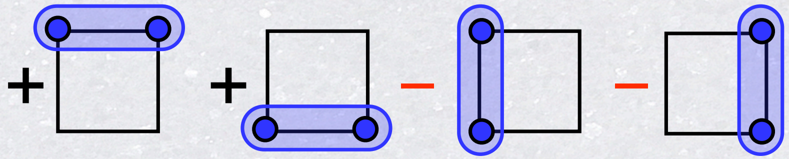
$$V''(x) = V''x$$

4-site Plaquettes

- contain *d*-wave RVB pairs

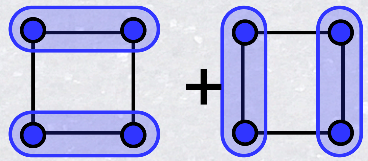
$$s_{i,j} = \frac{1}{\sqrt{2}}\left(c_{i,\uparrow}c_{j,\downarrow} - c_{i,\downarrow}c_{j,\uparrow}\right)$$

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



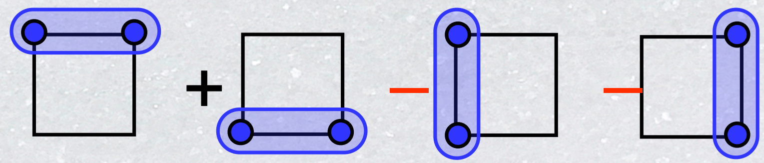
- 4 electrons on a plaquette: 2 *d*-wave RVB pairs

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

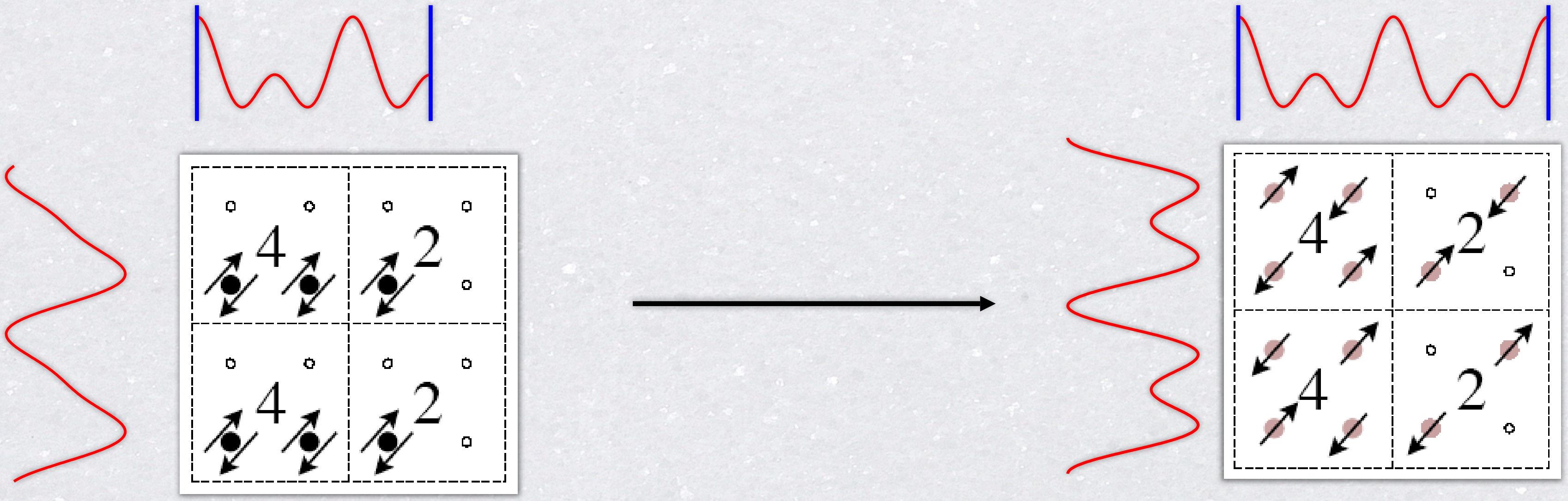


- 2 electrons on a plaquette: 1 *d*-wave RVB pair

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



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

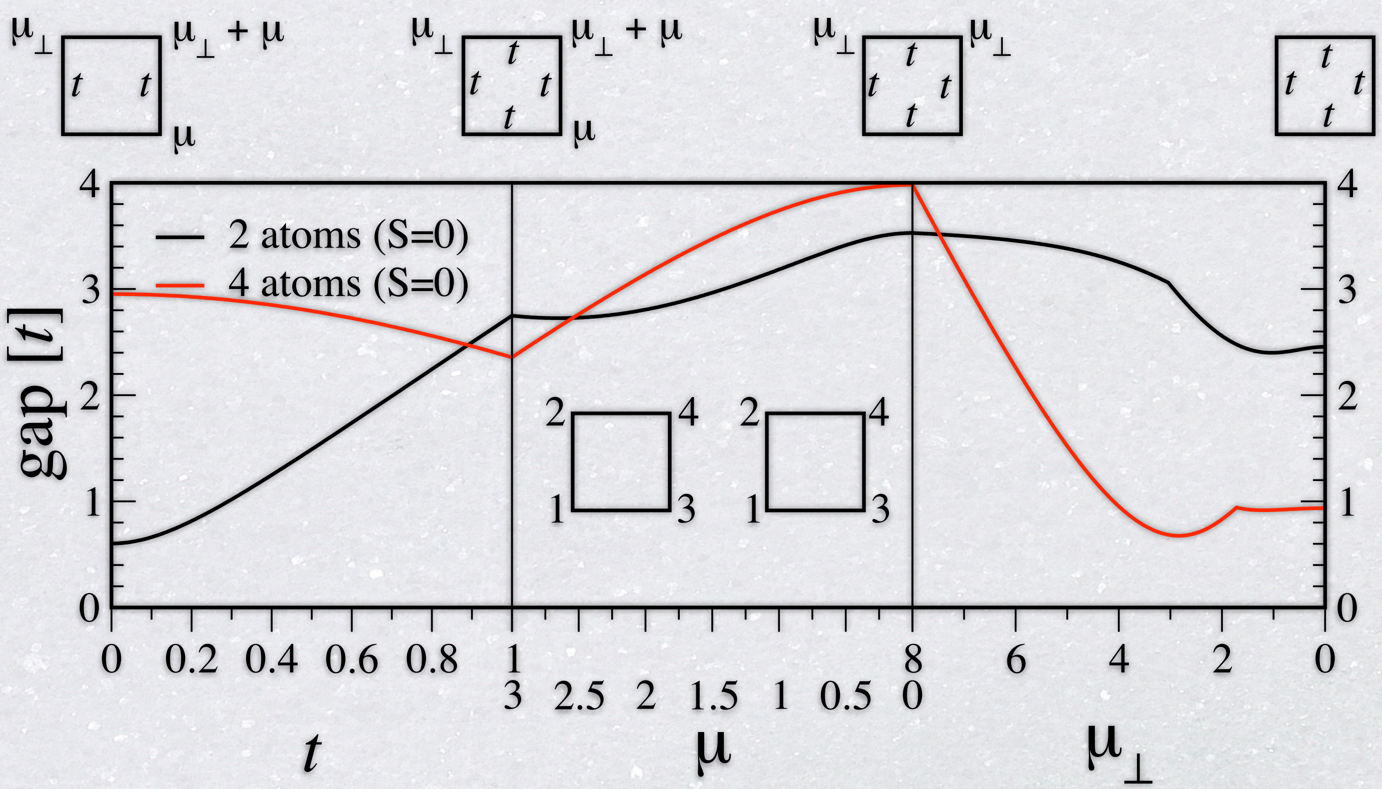
Which path to use to tune μ, $\mu_\perp$, $t_\perp$?

Preparing *d*-wave RVB states

1. ramp up hoppings t

2. ramp down in-chain μ

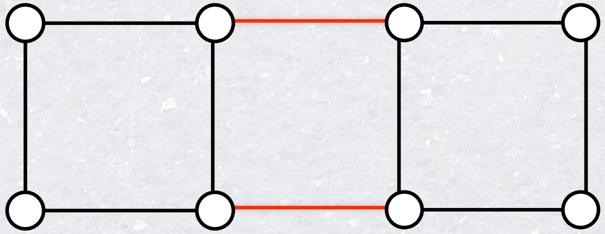
3. ramp down intra-chain $\mu_\perp$



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

Watch out: other routes can give s-wave states

Coupling of two RVB-plaquettes

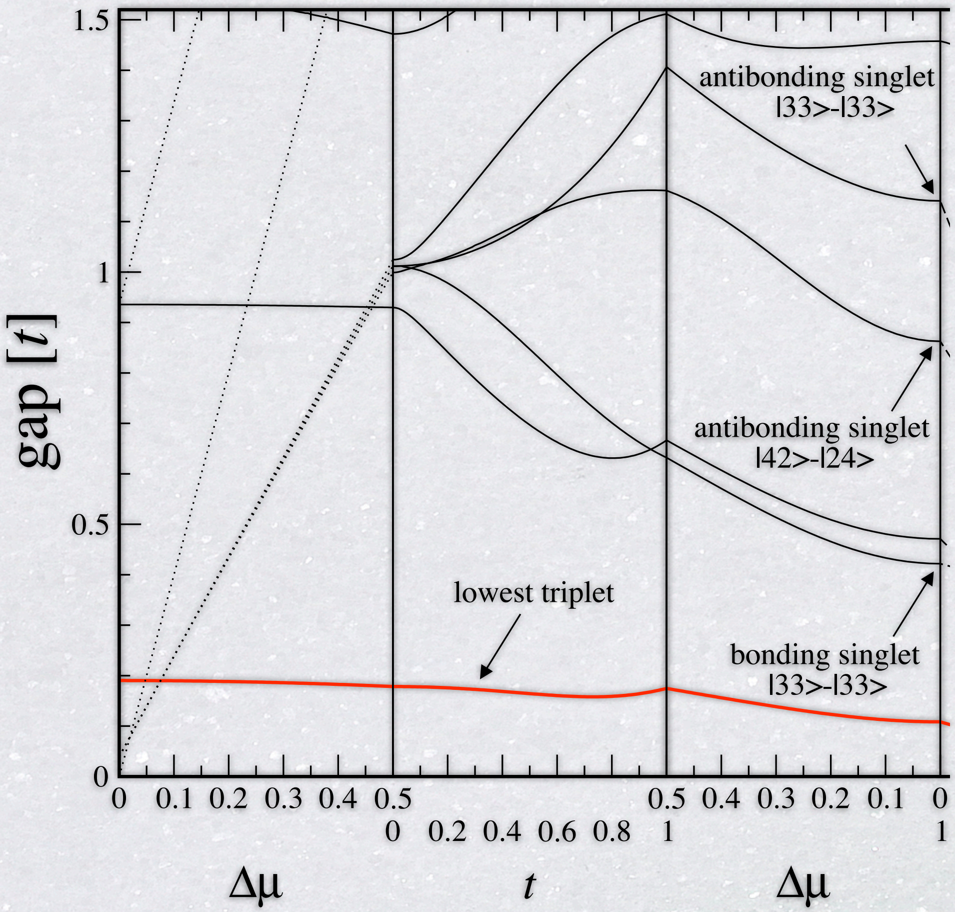


- Switch on inter-plaquette hopping
- Half-filled plaquettes (4+4): large gaps, no problem
- Doped plaquettes (4+2): problem with reflection symmetry
  - Initial state is mixture of even and odd state

$$|4\rangle|2\rangle = \frac{|4\rangle|2\rangle + |2\rangle|4\rangle}{2} + \frac{|4\rangle|2\rangle - |2\rangle|4\rangle}{2}$$

  - Problem: parity mixture remains throughout evolution!
- Solution: break reflection symmetry with potential ramp

Coupling of two plaquettes

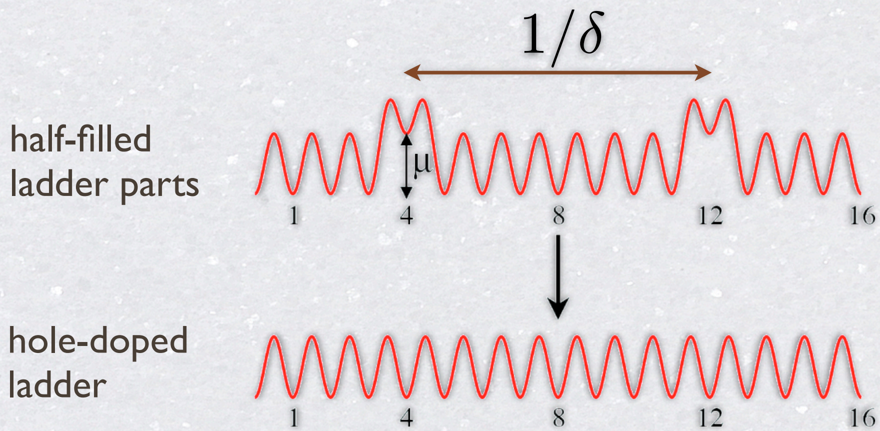


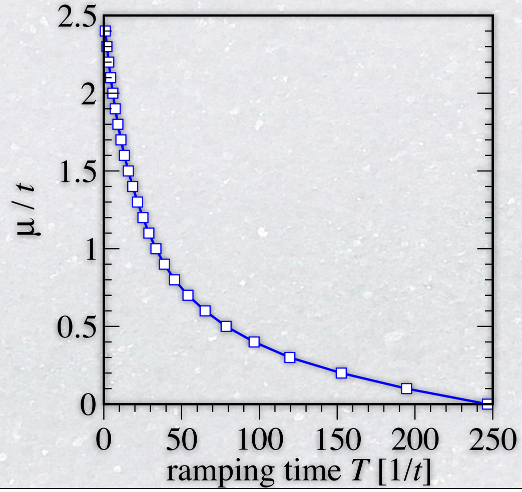
1. turn on potential ramp to break symmetry
2. turn on hopping
3. turn off potential ramp to restore symmetry

Large gaps => short times

doping a half-filled ladder

- doping δ : hole pairs "crystallize" $a_P = 1/\delta$
- prepare ladder segments separated by empty rungs
  - empty rungs at preferential hole locations
- reduce chemical potential
  - holes appear minimal particle motion
  - phase coherence between ladder parts
- DMRG, 2x32 ladder, 56 particles
  - ramping-down speed must decrease
  - 99% fidelity in 1/2 s





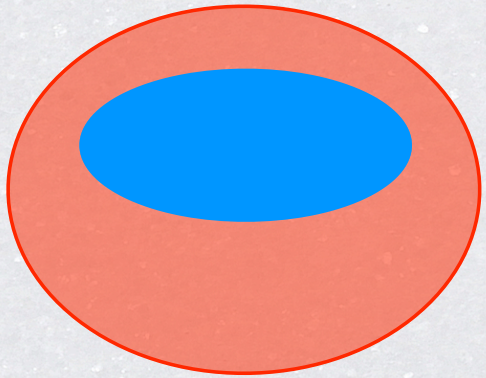
quantum dynamics of mixed states:
finite temperature

finite-temperature dynamics

- purification

  density matrix of physical system:
  pure state of physical system plus auxiliary system

$$\hat{\rho}_{phys} = \mathrm{Tr}_{aux} |\psi\rangle\langle\psi|$$



- finite-temperature dynamics

  evolution of pure state in enlarged state space

Verstraete, Garcia-Ripoll, Cirac, PRL ‘04

thermal density matrix

- auxiliary system: copy of physical system
  simulate ladders instead of chains
- purification of a completely mixed state (infinite temperature)

$$\hat{\rho}_0 = (1/2)[|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow|] \longleftarrow |\psi_0\rangle = (1/\sqrt{2})[|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle]$$

- thermal density matrix by imaginary-time evolution of pure state

$$\hat{\rho}_\beta = e^{-\beta H/2} \cdot 1 \cdot e^{-\beta H/2} = e^{-\beta H/2}\mathrm{Tr}_{\mathrm{aux}}|\psi_0\rangle\langle\psi_0|e^{-\beta H/2} = \mathrm{Tr}_{\mathrm{aux}}|\psi_\beta\rangle\langle\psi_\beta|$$

purification of $\hat{\rho}_\beta$ $\quad$ $\boxed{|\psi_\beta\rangle = e^{-\beta H/2}|\psi_0\rangle}$

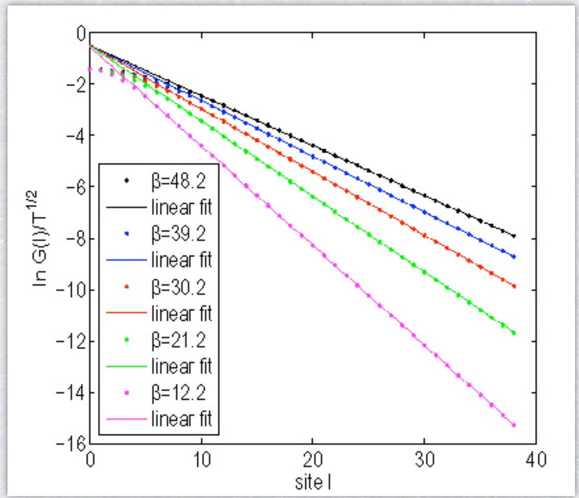
- real-time evolution of density matrix via pure state

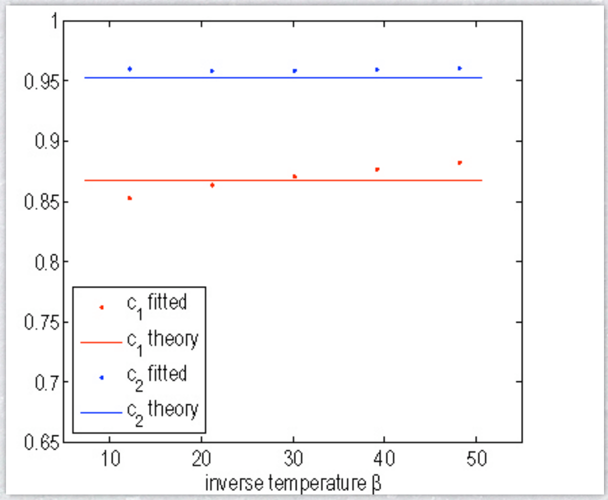
hardcore bosons at finite T

Barthel, McCulloch, US

- hardcore bosons, grandcanonical: $H = -\sum (b_i^\dagger b_{i+1} + b_{i+1}^\dagger b_i) - \mu \sum n_i$
- $\mu = -2$: quantum phase transition at T=0
- local and static quantities (thermodynamics): quasiexact
- nonlocal and static quantities (correlators):

$$\langle b_n^\dagger b_0 \rangle_\beta = c_1 \sqrt{T/2} \exp(-c_2 \sqrt{2T} n) \qquad c_1 = 0.8676\ldots \quad c_2 = 0.9528\ldots$$

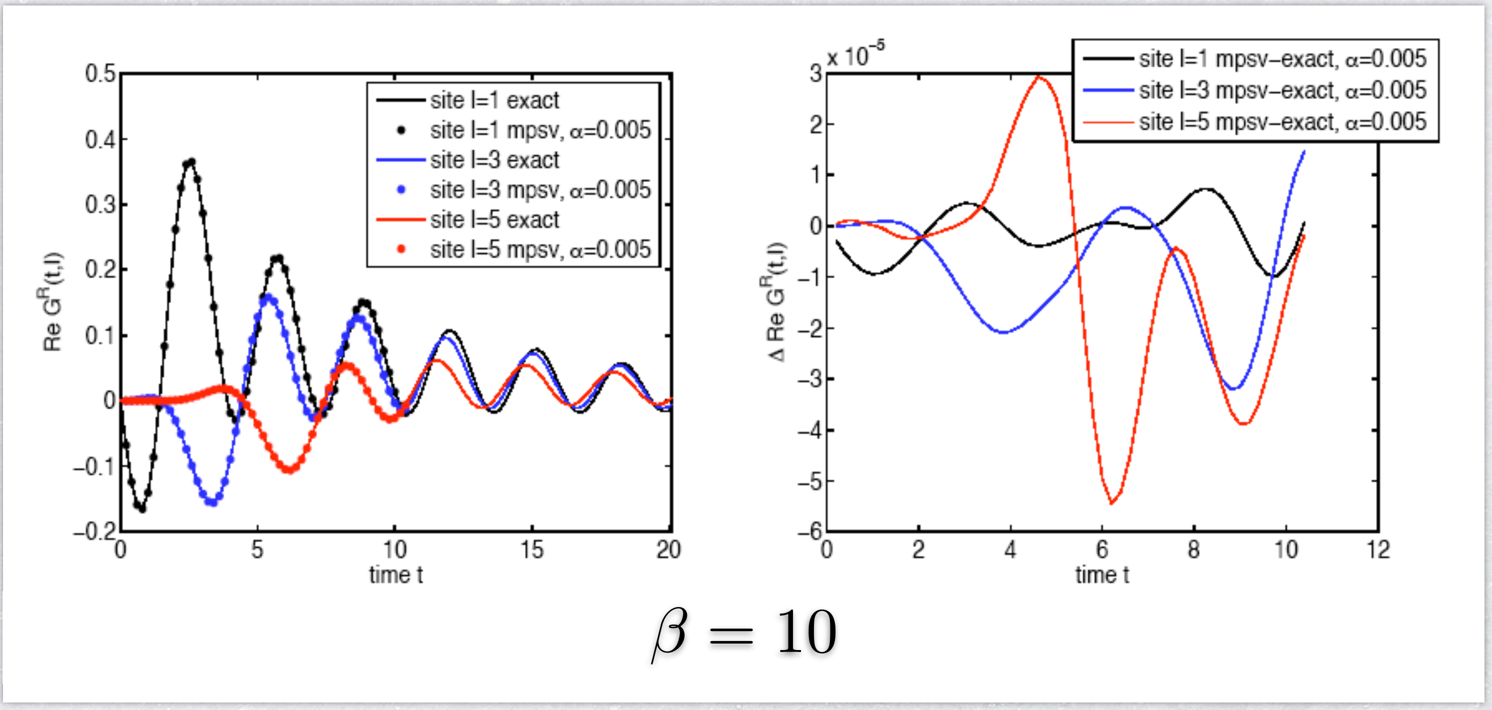




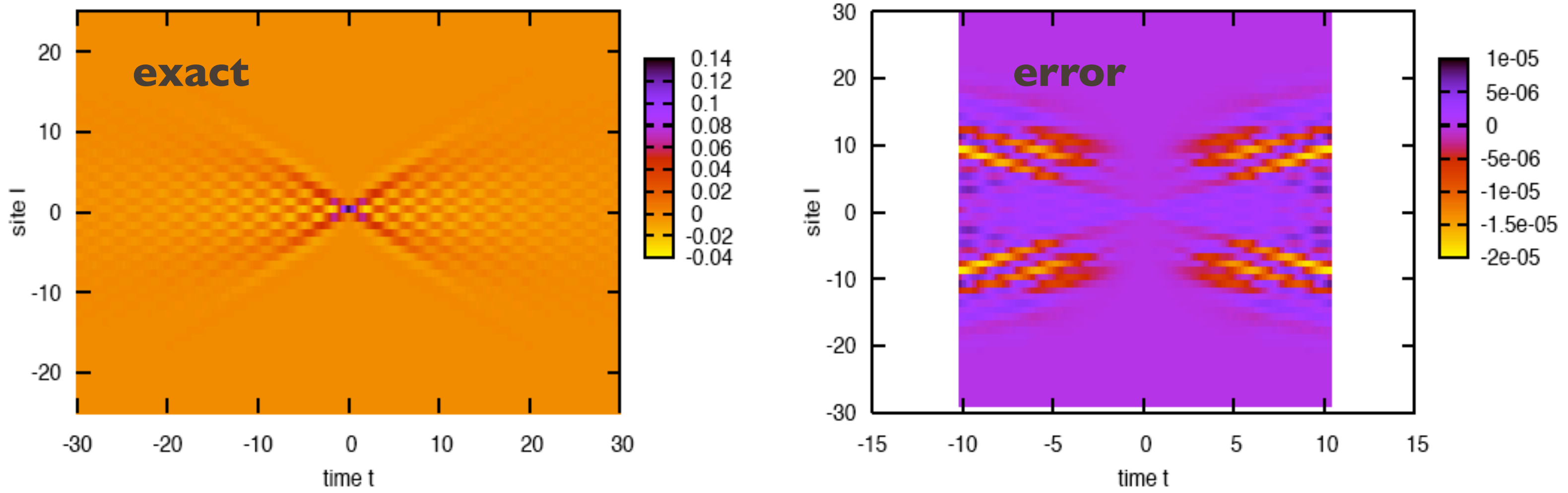
truncation:0.0001

retarded Green's function at finite T

$$\langle\psi|b_i^\dagger(t)b_j(0)|\psi\rangle = \langle\psi|e^{+\mathrm{i}Ht}b_i^\dagger e^{-\mathrm{i}Ht}b_j|\psi\rangle = \langle\psi(t)|b_i^\dagger|\phi(t)\rangle \quad |\phi\rangle = b_j|\psi\rangle$$



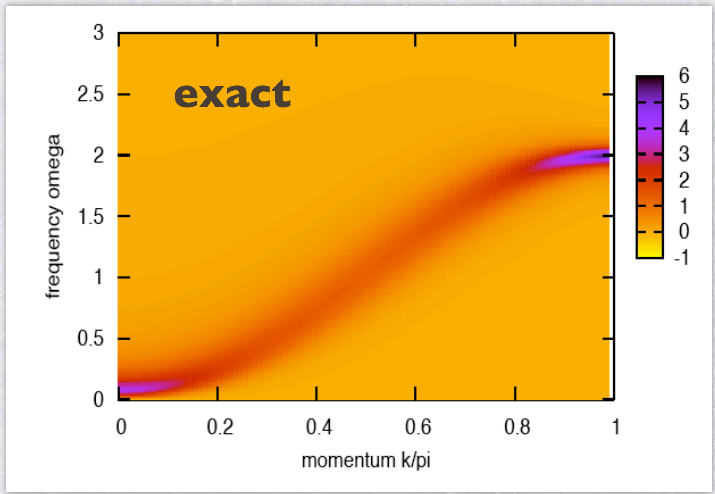
structure function: space-time

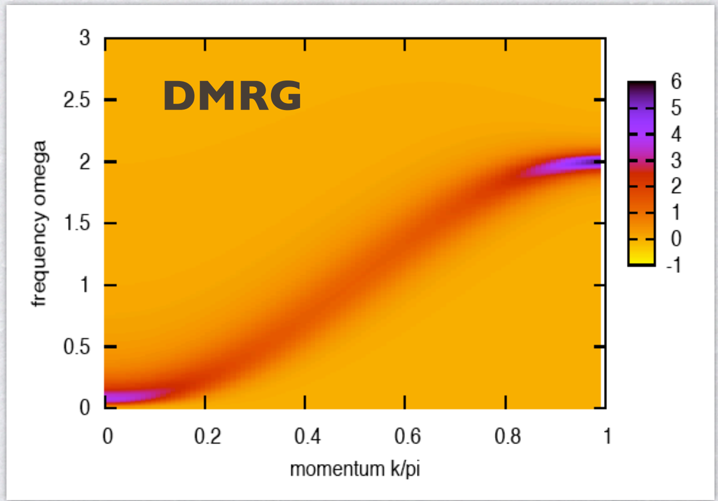


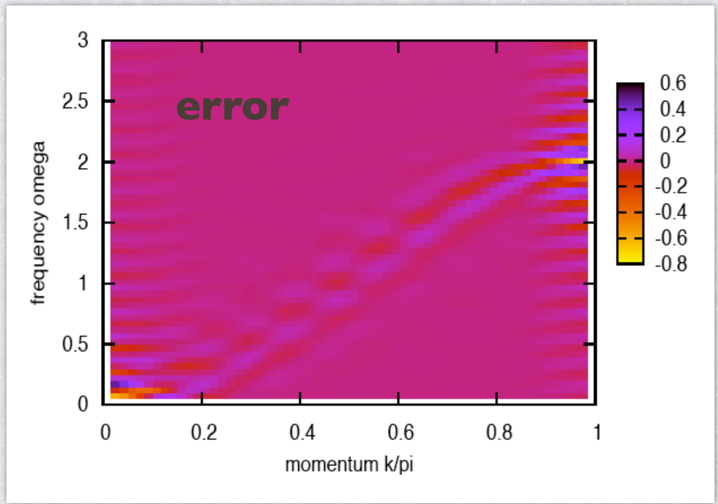
$$\beta = 10$$

- structure function at finite T in real space and time

structure function: momentum-frequency







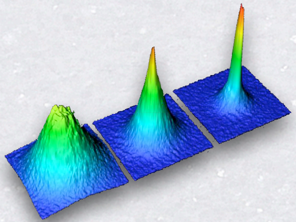
$\beta = 10 \qquad t_{max} = 35$

relative error < 0.01

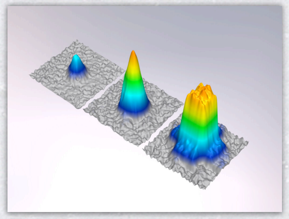
reachable time scales
with inverse temperature:
low T easier

conclusion

- cold atom toolbox: control and tunability in time

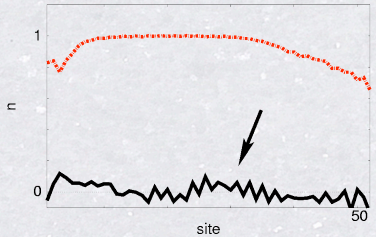


bosons

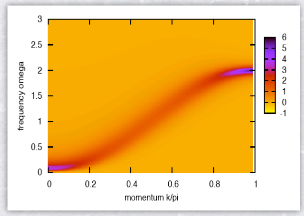


fermions

- new methods in quantum simulation



time evolution



finite temperature

- the best is yet to be!