1. Original formulation of DMRG

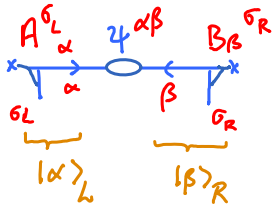
[White1992], [White1993], [Schollwöck2011, Sec 2.2]

Goal: finding ground state of infinite chain

Infinite-size DMRG (iDMRG)

Diagonalize small system (e.g. 2 sites), write ground state in the form

$$|\psi\rangle = \sum_{\alpha\beta} |\alpha\rangle_L |\beta\rangle_R \, \psi^{\alpha\beta} \qquad (1)$$

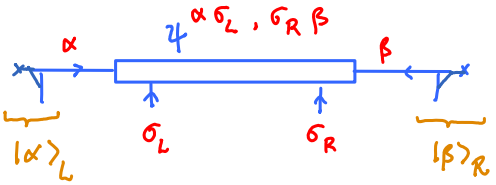


'Block L' describes left part of system, with basis $\{|\alpha\rangle_L\}$

'Block R' describes right part of system, with basis $\{|\beta\rangle_R\}$

Now add two sites between blocks L and R, and seek new ground state of $H_{L\bullet\bullet R}$ of the form

$$|\psi\rangle = |\alpha\rangle_L |\sigma_L\rangle |\sigma_R\rangle |\beta\rangle_R \; \psi^{\alpha\sigma_L,\sigma_R\beta} \qquad (2)$$

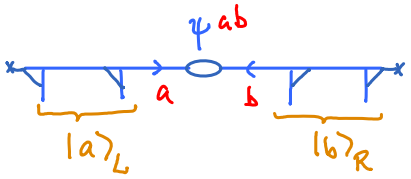


by minimizing (Lanzcos) $\dfrac{\langle\psi|\hat{H}_{L\bullet\bullet R}|\psi\rangle}{\langle\psi|\psi\rangle}$

Bond dimension has grown from $D\times D$ for $\psi^{\alpha\beta}$ to $Dd\times Dd$ for $\psi^{\alpha\sigma_L,\sigma_R\beta}$, so truncation is needed.
Split enlarged system in the middle, and call left side (new) block L, right side (new) block R.

Write ground state in the form

$$|\psi\rangle = |a\rangle_L |b\rangle_R \, \psi^{a,b} \qquad (3)$$



with composite indices $a = (\alpha, \sigma_L), b = (\beta, \sigma_R)$

of dimension $D_a = D_\alpha d$. White's truncation prescription: compute reduced DM of $L\bullet$,

$$\rho_{L\bullet} = \mathrm{Tr}_{\bullet R} |\psi\rangle\langle\psi| = |a'\rangle_L \underbrace{\psi^{a'b'} \overline{\psi}_{b'a}}_{(\rho_{L\bullet})^{a'}{}_{a}} {}_L\langle a| = \sum_c |\tilde{c}\rangle_L \rho_c {}_L\langle\tilde{c}| \qquad (4)$$

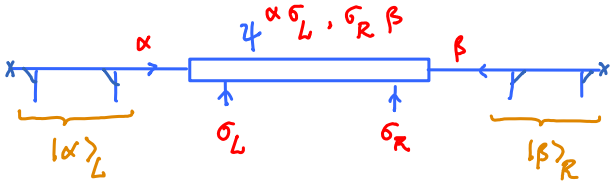
diagonalize

Construct truncated basis for block L , using the D eigenvectors $|\tilde{c}\rangle_L$ with the largest eigenvalues ρ_c . Rename: $|\alpha\rangle_L^{new} := |\tilde{c}\rangle_L$.

here truncation happens

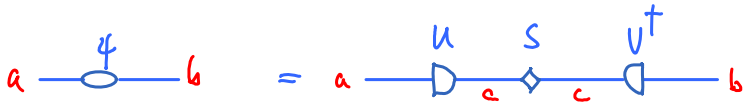
Ditto for block $\bullet$R.

Then iterate,: add two more sites,
seek ground state of larger system using
using similar Ansatz for wavefunction, etc.



(5)

Remark: we established early on (see TNB.6) that the eigenvalues ρ_c of reduced density matrix of L are obtained by SVD of ψ^{ab}

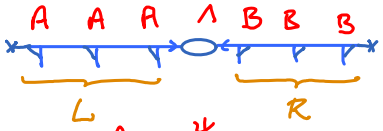


$$\Rightarrow \quad \rho_c = (S^c{}_c)^2 \qquad (6)$$

So retaining the ρ_L-eigenstates with largest ρ_c is equivalent to just doing SVD-truncation on ψ^{ab}.

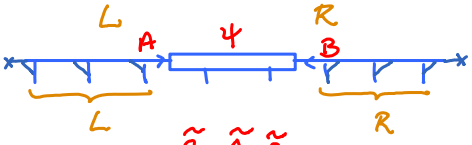
Modern formulation

Start with MPS in bond-canonical form:



(7)

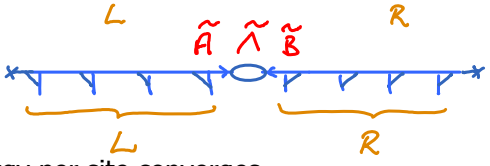
Add two central sites and find ground state (Lanczos):



(8)

Do SVD to split chain into two larger blocks, and truncate:

$\psi = USV^\dagger = \tilde{A}\,\tilde{\Lambda}\,\tilde{B}$

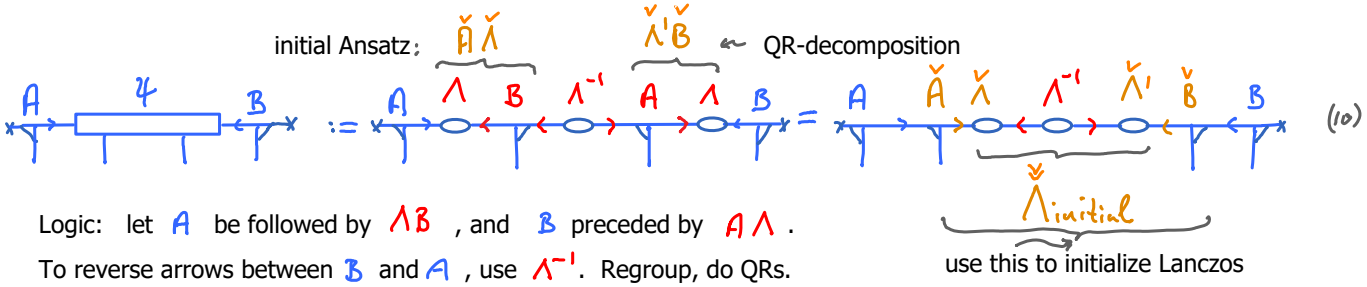


(9)

Iterate: make chain longer and longer, until ground state energy per site converges.

'iDMRG state prediction' [McCulloch2008], [Schollwöck2011, Sec. 10.1]

To speed up Lanczos search for ground state, construct initial guess for ψ from previous data:



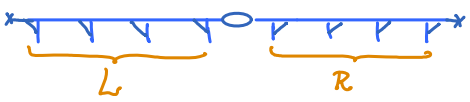
(10)

Logic: let A be followed by ΛB, and B preceded by $A\Lambda$.
To reverse arrows between B and A, use Λ^{-1}. Regroup, do QRs.

This leads to 'dramatic speedup' of iDMRG.

Finite-size DMRG

Grow chain to some length $\mathcal{L}$ using infinite-size DMRG algorithm.

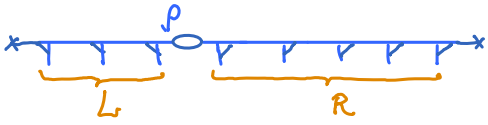


(11)

Then reduce L, enlarge R, optimize ψ:

(12)

Diagonalize ρ_L, truncate.



(13)

Iterate: sweep back and forth until convergence.

This is conceptually identical to variational optimization with two-site update.

Single-site DMRG is also possible ⟷ variational single-site update.

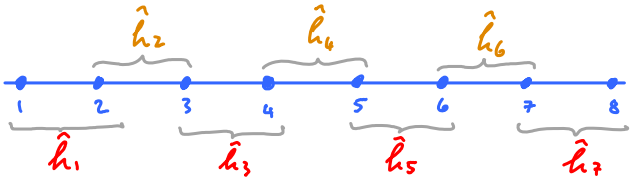
2. Time-dependent DMRG (tDMRG) [Daley2004], [White2004]

Invented 2004 by Daley, Kollath, Schollwöck, Vidal, and independently by White, Feiguin.

Goal: to compute $|\psi(t)\rangle = e^{-i\hat{H}t}|\psi\rangle$ (1)

Time-evolution operator for nearest-neighbor interactions (cf. iTEBD.1)

Even-odd decomposition of Hamiltonian:



$$\hat{H} = \sum_\ell \hat{h}_\ell = \hat{H}_o + \hat{H}_e \quad (2)$$

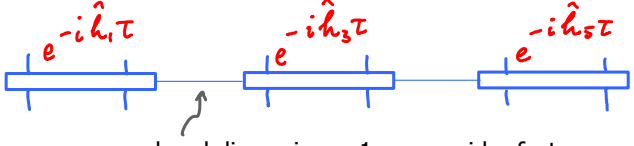
Trotterize: $t = \tau N_t$

$$\hat{U}(t) = e^{-i\hat{H}t} = (e^{-i\tau(\hat{H}_e + \hat{H}_o)})^{N_t} \simeq (\underbrace{e^{-i\tau\hat{H}_e}}_{\hat{U}_e}\ \underbrace{e^{-i\tau\hat{H}_o}}_{\hat{U}_o} + \mathcal{O}(\tau^2))^{N_t} \quad (3)$$

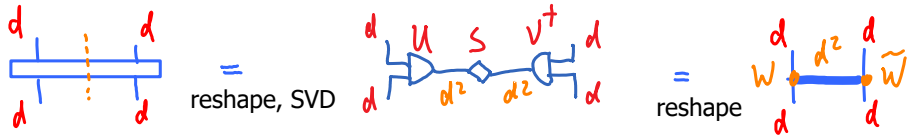
Time-evolution protocol [Schollwöck2011, Sec. 7.1-7.3]

Construct MPO representations for $\hat{U}_o$ and $\hat{U}_e$, compute $|\psi(t+\tau)\rangle = \hat{U}_o \cdot \hat{U}_e |\psi(t)\rangle$ (4)

(i) MPO $\hat{U}_o =$ (5)



bond dimension = 1, so consider factors separately



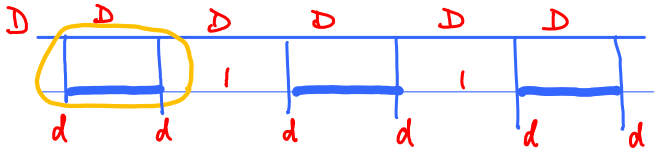
(6)

$$O^{\sigma_1'\sigma_2'}{}_{\sigma_1\sigma_2} = W^{\sigma_1'}{}_{\sigma_1\mu}\,\tilde{W}^{\mu\sigma_2'}{}_{\sigma_2}, \quad \mu = 1,\dots,d^2 \quad (7)$$

can be constructed explicitly — then SVD to yield

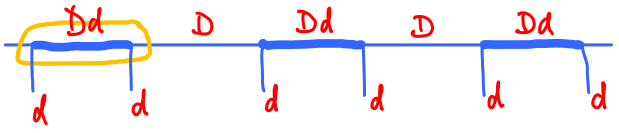
(ii) Evolve

$|\psi(t+\tau)\rangle = \hat{U}_o|\psi(t)\rangle =$



(8)

reshape, SVD =



(9)

(iii) Compress: either 'variationally' (global) or 'bond by bond' (local)

Variational compression: First apply full MPO for $\hat{U}_o$ to entire chain. Then variationally minimize

Variational compression: First apply full MPO for $\hat{U}_0$ to entire chain. Then variationally minimize

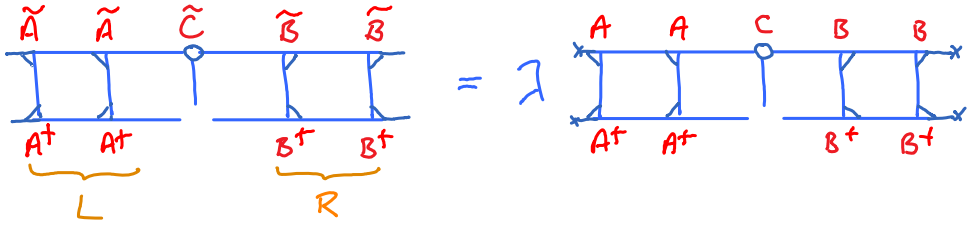
$$\| |\psi(t+\tau)\rangle - |\psi_{compressed}\rangle \|^2 \qquad (10)$$

target; bond dimension $D \cdot d$; D

. This yields optimal (in variational sense) way to compress $|\psi_{target}\rangle$ to $|\psi_{compressed}\rangle$ with given resources.

Explicitly:

$$\frac{\partial}{\partial A_\ell^\dagger}\left[\langle \psi_{compressed} | \psi_{target} \rangle - \lambda \langle \psi_{compressed} | \psi_{compressed} \rangle \right] = 0 \qquad (11)$$



(12)

$$L\,\tilde{C}\,R = \lambda C \qquad (13)$$

[λ is fixed by normalization condition: $\tilde{C}^\dagger \tilde{C} = 1$]

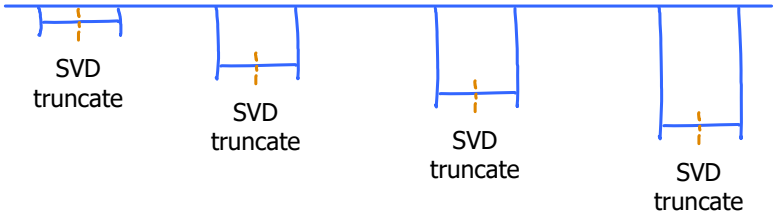
Sweep back and forth, until overlap $\langle \psi_{compressed} | \psi_{target} \rangle$ no longer changes. Then apply $\hat{U}_e$.

Bond by bond compression

Apply $\hat{U}_0$ to bond 1-2,

then reshape, SVD, truncate;

repeat for bond 3-4, then 5-6, etc.



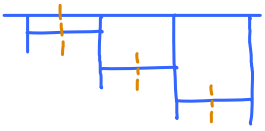
This protocal keeps bond dimensions low throughout, hence is cheaper. However, some interdependence of successive truncations may creep in, hence variational compression is, strictly speaking, cleaner.

The difference between variational and bond-by-bond compression strategies becomes negligible for sufficiently small τ, because then the state does not change much during a time step anyway, so truncations are benign.

With bond-to-bond compression, there is no need to split $\hat{H} = \hat{H}_0 + \hat{H}_e$, $\hat{U} = \hat{U}_e \cdot \hat{U}_0$ (14)

Instead, Trotterize as follows:

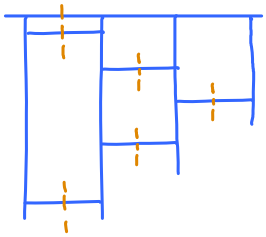
$$e^{-i\hat{H}\tau} = e^{-i\hat{h}_{\ell-1}\tau} \cdots e^{-i\hat{h}_2\tau} e^{-i\hat{h}_1\tau} + O(\tau^2) \qquad (15)$$



1st order Trotter

or

$$e^{-i\hat{H}\tau} = \left(e^{-i\hat{h}_1\tau/2} e^{-i\hat{h}_2\tau/2} \cdots e^{-i\hat{h}_{\ell-2}\tau/2}\right) e^{-i\hat{h}_{\ell-1}\tau} \left(e^{-i\hat{h}_{\ell-2}\tau/2} \cdots e^{-i\hat{h}_2\tau/2} e^{-i\hat{h}_1\tau/2}\right) + O(\tau^3) \qquad (16)$$



2nd order Trotter

Error analysis

$\varepsilon_{Trotter}$ = (error per step) (# of steps) $= \tau^{n+1} \frac{t}{\tau} = \tau^n t$ (17)

(for nth order Trotter scheme)

linear in time; controllable by reducing τ

Truncation error due to truncation of bond dimensions:

$\varepsilon_{trunc} \sim e^{\# t}$, grows exponentially! (until you 'hit the wall')

Reason: under time evolution, state becomes increasingly more entangled; on a bond 

entanglement entropy is

$$S_E = -\sum_\alpha (S^\alpha{}_\alpha)^2 \ln (S^\alpha{}_\alpha)^2 \quad (18)$$

This is maximal if all singular values on bond are equal, $(S^\alpha{}_\alpha)^2 = \frac{1}{D}$, $\Rightarrow S_E \leq \ln_2 D$ (19)

If Hamiltonian $H(t)$ is changed abruptly (quench) such that global energy changes extensively, then

$$S(t) \leq S(0) + ct \quad (20)$$

[For less dramatic changes (e.g. local perturbation), entanglement growth is slower; but still significant.]

Bond dimension needed to encode entanglement entropy S_E is given by $D(t) \gtrsim 2^{S(t)}$ (21)

If, however, bond dimension D is held fixed during time evolution, errors will grow exponentially.

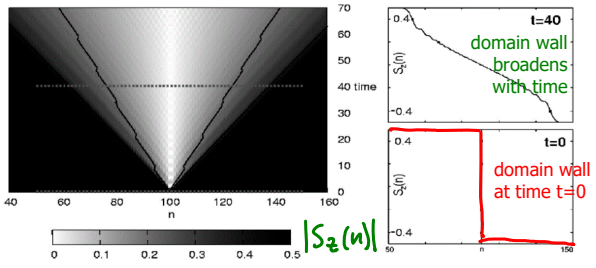
A quantitative error analysis has been performed by [Gobert2005] on the exactly solvable XX model:

$$H_{XX} = J \sum_l S^x_l S^x_{l+1} + S^y_l S^y_{l+1} \quad (22)$$

They performed quench, with initial state

$|\psi\rangle_{J=0} = \uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\downarrow$

For $t>0$: $J \neq 0$, domain wall widens...



[Gobert2005]

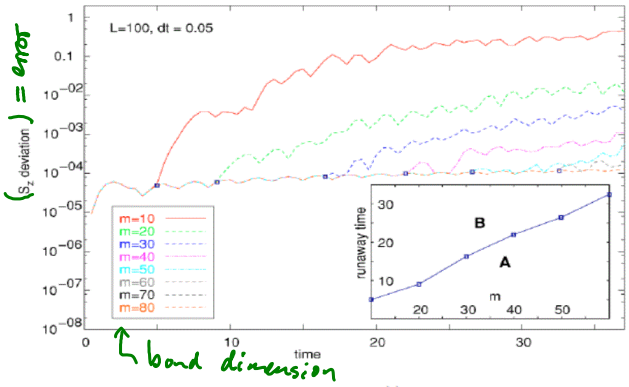


FIG. 6. Magnetization deviation $\Delta M(t)$ as a function of time for different numbers m of DMRG states. The Trotter time interval is fixed at dt=0.05. Again, two regimes can be distinguished: For early times, for which the Trotter error dominates, the error is slowly growing (essentially linearly) and independent of m (regime A); for later times, the error is entirely given by the truncation error, which is m-dependent and growing fast (almost exponential up to some saturation; regime B). The transition between the two regimes occurs at a well-defined "runaway time" t_R (small squares). The inset shows a monotonic, roughly linear dependence of t_R on m.

3. Exponential thermal renormalization group (XTRG)

[Chen2018a]

Goal: computation of the thermal density matrix, $\hat{\rho}(\beta) = e^{-\beta \hat{H}}$, $\beta = 1/T$ (1)

for arbitrary temperature T, in particular large to intermediate T, (i.e. small to intermediate β)

Once $\hat{\rho}$ is known, thermal expectation values follow from $\langle \hat{O} \rangle_\beta = Tr[\hat{\rho}(\beta)\hat{O}]$ (2)

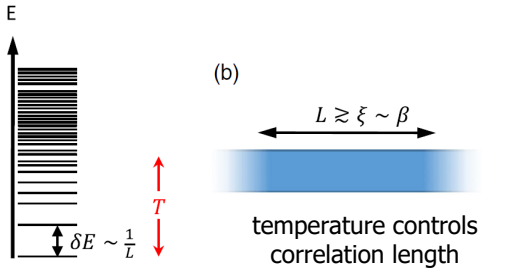
Further application: to obtain ground state projector, take $\beta \to \infty$.

One option: imaginary time evolution with Trotter decomposition, $\hat{\rho}(\beta) = [e^{-\tau \hat{H}}]^N$, $\tau = \beta/N$

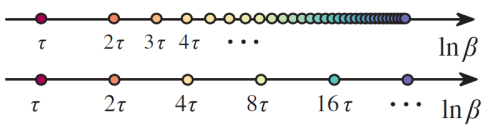
However, then number of time steps increases linearly with β, so reaching low T is numerically costly.

Key observation 1: If $\hat{\rho}(\beta)$ is represented as an MPO, the MPO entanglement entropy grows only logarithmically with decreasing temperature: [Barthel2017], [Dubail2017]

$S_E(\beta) \sim \ln(\beta)$ (for 1D systems) (4)



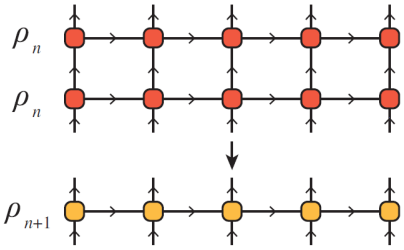
Thus, seek algorithm which lowers temperature in exponential steps!



Key observation 2: multiplying the density matrix by itself lowers the temperature by a factor of 2 :

$$e^{-2\beta\hat{H}} = e^{-\beta\hat{H}} \cdot e^{-\beta\hat{H}} \quad (3)$$

$$\Rightarrow \quad \boxed{\hat{\rho}(2\beta) = \hat{\rho}(\beta)\hat{\rho}(\beta)} \quad (4)$$

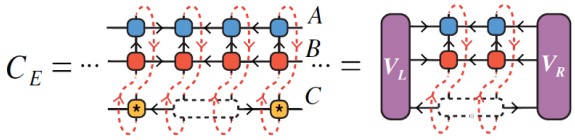


XTRG algorithm exploits this:

(i) Initialize density matrix at very high temperature, as an MPO (with small bond dimension):

$$\hat{\rho}(\beta_0) \simeq 1 - \beta_0 \hat{H}, \quad \beta_0 \simeq 10^{-6} \quad (5)$$

(ii) Compute $\hat{\rho}^\dagger(\beta)\hat{\rho}(\beta)$ via MPO multiplication.



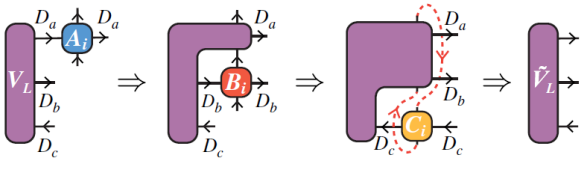
(iii) Reduce bond dimension by global variational optimization:

$$\frac{\partial}{\partial C^\dagger_{[s_i]}} \frac{\partial}{\partial C^\dagger_{[s_i]}} \| A \cdot B - C \|_F^2 = 0 \quad (7)$$

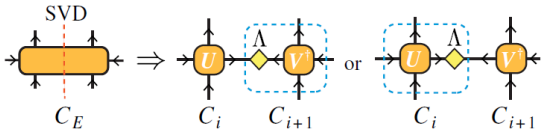
$\rho^\dagger(\beta)$ $\rho(\beta)$ $\rho(2\beta)$ Frobenius norm

(fat) input MPO, large bond dim

compressed MPO, smaller bond dim.



Compute environment of bond to be updated iteratively, use SVD to bring updated MPO bond into canonical form.



Iterate (ii,iii) until desired temperature is reached.

Application: XTRG for 2D Hubbard model at finite-temperature [Chen2020]

2D Hubbard model:

$$H = -t \sum_{\langle i,j\rangle,\sigma} (\hat{c}^{\dagger}_{i,\sigma}\hat{c}_{j,\sigma} + \text{H.c.}) + U \sum_{i} \hat{n}_{i\uparrow}\hat{n}_{i\downarrow} - \mu \sum_{i,\sigma} \hat{n}_{i,\sigma},$$

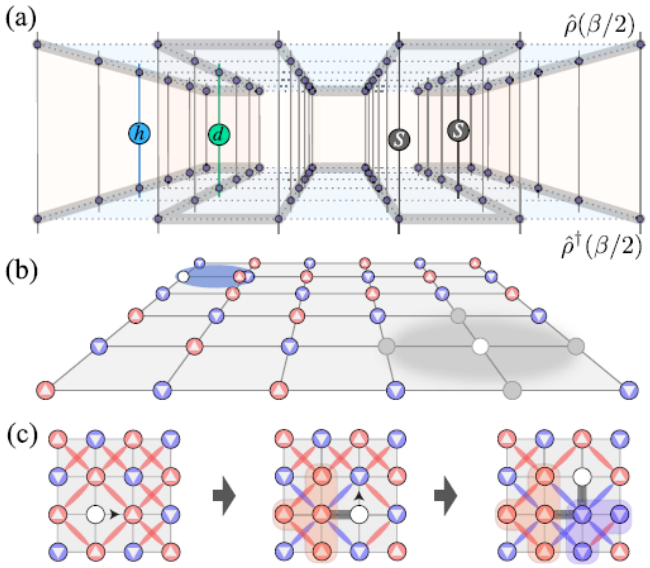


FIG. 1. (a) Bilayer calculation of the spin-spin $\langle \hat{S}_i \cdot \hat{S}_j \rangle$ and hole-doublon $\langle \hat{h}_i \cdot \hat{d}_j \rangle$ correlators by sandwiching corresponding operators in between $\hat{\rho}(\beta/2)$ and $\hat{\rho}^{\dagger}(\beta/2)$, where the snakelike ordering of sites for the XTRG is indicated by thick gray lines. (b) In the low-temperature AF background (blue down and red up spins), a magnetic polaron (gray shaded region) emerges around a moving hole, where the spins around the hole can be in a superposition of spin-up and -down states. The blue ellipse represents a hole-doublon pair showing a strong bunching effect. (c) A hole moves in the system along the path indicated by the gray string, leading to a sign reversal of the diagonal spin correlation. The red and blue shaded regions illustrate the deformed magnetic background due to the interplay between the hole and spins. Diagonal correlations are indicated red (aligned) or blue (antialigned).

$$C_S(d) \equiv \frac{1}{N_d} \sum_{|i-j|=d} \frac{\langle \hat{S}_i \cdot \hat{S}_j \rangle}{S(S+1)}$$

number of pairs of spins at distance

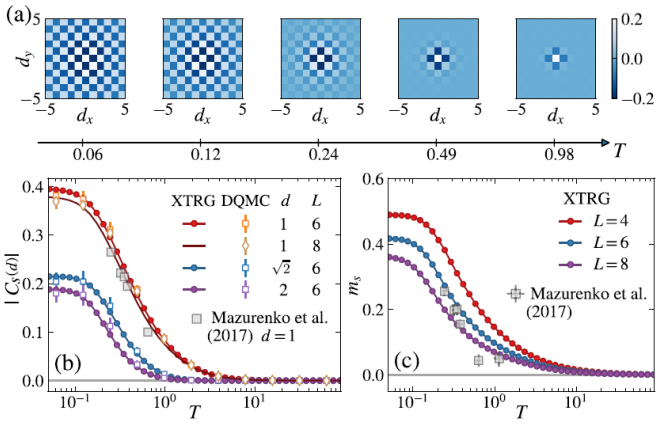


FIG. 2. Half-filled FHM with $U = 7.2$ and $L = 4, 6, 8$. (a) The finite-size AF order pattern is determined from the spin correlation $C_S(d)$ versus (d_x, d_y), which melts gradually as T increases. We show in (b) the spin correlation function $|C_S(d)|$ of various $d = 1, \sqrt{2}, 2$ and in (c) the finite-size spontaneous magnetization m_s. Excellent agreement between the calculated ($L = 8$) data and the experimental data [17] can be observed.

Inspiration for such computations comes from cold-atom experiments seeking to simulate the behavior in cuprates using a quantum gas microscope: [Koepsell2021a]

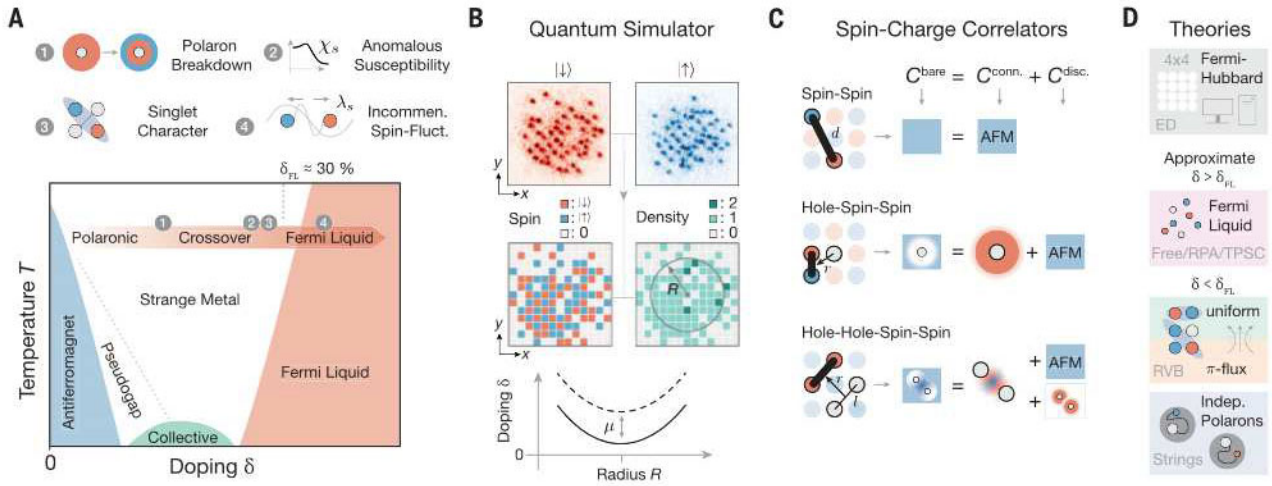


Fig. 1. Probing doped Mott insulators with spin-charge correlators. (**A**) Conjectured phase diagram of the 2D Fermi-Hubbard model upon hole doping δ and temperature *T*. Boundaries indicate crossovers between different regimes. Insets summarize our main experimental results. Incommen., incommensurate. (**B**) We independently image the two spin components of each Fermi-Hubbard realization with our quantum gas microscope. This enables reconstruction of the full spin and density (charge) information. The doping varies spatially in our harmonic trap and can be tuned by the total particle number to study the doping dependence of correlations. (**C**) Spin-spin, hole-spin-spin, and hole-hole-spin-spin correlators are analyzed in this work. As illustrated, bare multipoint correlations contain lower-order contributions and a connected part. For instance, in the magnetic polaron regime, a hole alters the antiferromagnetic environment in its vicinity. Therefore, bare hole-spin-spin correlations are reduced (white) close to the hole compared with the strong antiferromagnetic correlation at large distance (blue). The bare correlation (C^{bare}) can be decomposed into the genuine effect of the hole, that is, the connected part ($C^{conn.}$, red), and the antiferromagnetic (AFM) background value, that is, the disconnected part ($C^{disc.}$, blue). The sum of both parts corresponds to the bare correlation. Similarly, the genuine effect of a pair of holes on spin correlations (i.e., beyond single-hole effects) is quantified by the connected part of hole-hole-spin-spin correlations. This work focuses on connected correlations. (**D**) We compare experimental findings to exact diagonalization of 4×4 Fermi-Hubbard systems (top), mean-field–inspired approaches or free fermions approximating Fermi liquids at high doping (second from top), as well as three approaches (uniform-RVB, π-flux, and string), which are designed to capture the low-doping regime (bottom two panels). Indep., independent.

4. Finite temperature: purification [Verstraete2004b], [Schollwöck2011, Sec. 7.2.1] DMRG-II.3

General quantum-mechanical density matrix for a mixed state, $\hat{\rho} = \sum_{\mu\nu} |\mu\rangle_p \rho^{\mu}{}_{\nu} {}_p\langle\nu|$ (1)

'p' denotes 'physical'

has three defining properties:

(i) Hermiticity: $\hat{\rho}^\dagger = \hat{\rho}$ (2)

(ii) Positivity: Eigenvalues are non-negative: $\hat{\rho}_{\text{diagonalized}} = \sum_\alpha |\alpha\rangle_p \rho_\alpha {}_p\langle\alpha|$ (3), $\rho_\alpha \geq 0$

(iii) Normalized: $\mathrm{Tr}\,\hat{\rho} = 1 \Rightarrow \sum_\alpha \rho_\alpha = 1$ (4)

Expectation values: $\langle\hat{O}\rangle = \mathrm{Tr}(\hat{\rho}\hat{O})$ (5)

[or $\frac{\mathrm{Tr}(\hat{\rho}\hat{O})}{\mathrm{Tr}(\hat{\rho})}$ if one works with non-normalized $\hat{\rho}$]

'Purification'

Can we represent $\hat{\rho}$ in terms of a pure state?
Yes: double Hilbert space by introducing an 'auxiliary' state for each physical state, and define

'purified state': $|\Psi\rangle = \sum_\alpha |\alpha\rangle_a |\alpha\rangle_p \sqrt{\rho_\alpha} \in \mathcal{H}_a \otimes \mathcal{H}_p$ (6)

auxiliary, physical

This can be viewed as Schmidt decomposition of a pure state in doubled Hilbert space.

Norm yields trace: $\langle\Psi|\Psi\rangle = \sum_{\alpha'\alpha} \sqrt{\rho_{\alpha'}} {}_p\langle\alpha'| {}_a\langle\alpha'|\alpha\rangle_a |\alpha\rangle_p \sqrt{\rho_\alpha} = \sum_\alpha \rho_\alpha = \mathrm{Tr}\,\hat{\rho}_p$ (7), $\langle\alpha'|\alpha\rangle_a = \mathbb{1}^{\alpha'}{}_{\alpha}$

Tracing out auxiliary state space from $|\Psi\rangle\langle\Psi|$ (a pure DM in doubled Hilbert space) (7)
yields physical density matrix $\hat{\rho}_p$ (a mixed DM in physical Hilbert space):

$$\mathrm{Tr}_a |\Psi\rangle\langle\Psi| = \sum_\beta \sum_{\alpha'\alpha} {}_a\langle\beta|\alpha'\rangle_a |\alpha'\rangle_p \sqrt{\rho_{\alpha'}} \sqrt{\rho_\alpha} {}_p\langle\alpha| {}_a\langle\alpha|\beta\rangle_a \quad (8)$$

$\langle\beta|\alpha'\rangle_a = \mathbb{1}^{\beta}{}_{\alpha'}$, $\langle\alpha|\beta\rangle_a = \mathbb{1}^{\alpha}{}_{\beta}$

$$= \sum_\alpha |\alpha\rangle_p \rho_\alpha {}_p\langle\alpha| = \hat{\rho}_p \quad (9)$$

Purified-state expectation values in doubled Hilbert space yield thermal averages in physical space:

$$\langle\Psi| \mathbb{1}_a \otimes \hat{O}_p |\Psi\rangle = \sum_{\alpha'\alpha} \sqrt{\rho_{\alpha'}} {}_p\langle\alpha'| {}_a\langle\alpha'| \mathbb{1}_a \otimes \hat{O}_p |\alpha\rangle_a |\alpha\rangle_p \sqrt{\rho_\alpha} \quad (10)$$

$\mathbb{1}^{\alpha'}{}_{\alpha}$

$$= \sum_\alpha {}_p\langle\alpha|\hat{O}|\alpha\rangle_p \rho_\alpha = \mathrm{Tr}_p\, \hat{\rho}_p \hat{O}_p = \langle\hat{O}_p\rangle \quad (11)$$

If $\hat{\rho}$ is not normalized, use $\frac{\langle\Psi| \mathbb{1}_a \otimes \hat{O}_p |\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\mathrm{Tr}\,\hat{\rho}_p \hat{O}_p}{\mathrm{Tr}\,\hat{\rho}_p} = \langle\hat{O}_p\rangle$ (12)

Thermal density matrix

Thermal equilibrium is described by $\hat{\rho}_\beta = e^{-\beta \hat{H}_p} = \sum_\alpha |\alpha\rangle_p e^{-\beta E_\alpha} {}_p\langle\alpha|$ (13)

Not normalized: $\mathrm{Tr}_p \hat{\rho}_\beta = \sum_\alpha e^{-\beta E_\alpha} = Z(\beta) =$ partition function $\neq 1$ (14)

Purified version: $|\Psi_\beta\rangle = \sum_\alpha |\alpha\rangle_a |\alpha\rangle_p e^{-\beta E_\alpha/2} = e^{-\beta \hat{H}_p/2} \underbrace{\sum_\alpha |\alpha\rangle_a |\alpha\rangle_p}_{\equiv |\Psi_0\rangle}$ (15)

acts only on physical space!

$$|\Psi_0\rangle = \sum_{\vec{\sigma}} |\vec{\sigma}\rangle_a |\vec{\sigma}\rangle_p = \sum_{\vec{\sigma}} |\sigma_1\rangle_a |\sigma_1\rangle_p \ldots |\sigma_\ell\rangle_a |\sigma_\ell\rangle_p = \prod_{\ell=1}^{\mathcal{L}} \underbrace{\left(\sum_{\sigma_\ell} |\sigma_\ell\rangle_a |\sigma_\ell\rangle_p\right)}_{\text{maximal aux-phys entanglement}} \quad (16)$$

= product state, with each factor describing maximal aux-phys entanglement at site ℓ

Note: at $T = \infty$, i.e. $\beta = 0$, we have $|\Psi\rangle = |\Psi_0\rangle$ (all states $|\vec{\sigma}\rangle$ are equally likely).

Check:

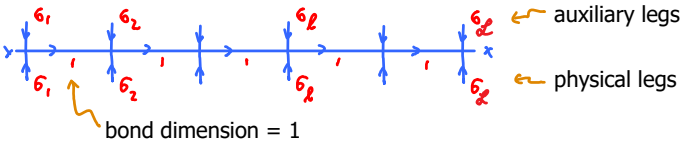
$$\langle \Psi_\beta | \hat{O}_p | \Psi_\beta \rangle = \sum_{\vec{\sigma}\vec{\sigma}'} {}_p\langle\vec{\sigma}| \underbrace{{}_a\langle\vec{\sigma}| e^{-\beta \hat{H}_p/2} \hat{O}_p e^{-\beta \hat{H}_p/2} |\vec{\sigma}'\rangle_a}_{\delta_{\vec{\sigma}\vec{\sigma}'}} |\vec{\sigma}'\rangle_p$$

$$= \sum_{\vec{\sigma}} {}_p\langle\vec{\sigma}| e^{-\beta \hat{H}_p/2} \hat{O}_p e^{-\beta \hat{H}_p/2} |\vec{\sigma}\rangle_p$$

$$= \mathrm{Tr}\left[e^{-\beta \hat{H}_p/2} \hat{O}_p e^{-\beta \hat{H}_p/2}\right] = \mathrm{Tr}\left[\hat{\rho}_p \hat{O}_p\right] \quad \checkmark$$

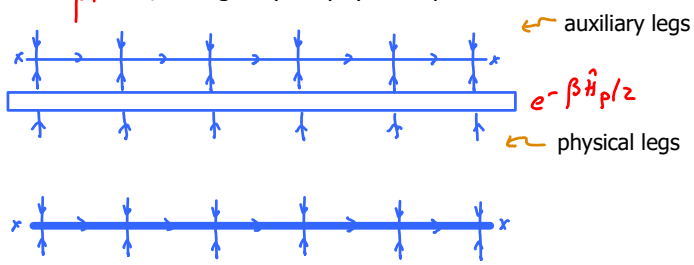
Protocol for finite-T DMRG calculations

Start from pure product state in doubled Hilbert space: $|\Psi_0\rangle =$ (17)



Perform imaginary-time evolution over a 'time' $\beta/2$, acting only on physical space:

$|\Psi_\beta\rangle = e^{-\beta \hat{H}_p/2} |\Psi_0\rangle =$ (Trotterize…)



compress $\simeq$

For thermal averages, trace out auxiliary space:

$$\langle \hat{O}_{[e]p} \rangle = \frac{\langle \Psi_\beta | \mathbb{1}_a \otimes \hat{O}_p | \Psi_\beta \rangle}{\langle \Psi_\beta | \Psi_\beta \rangle} =$$