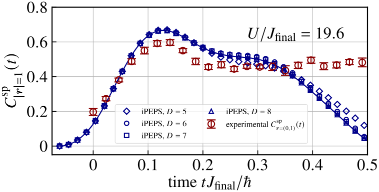
Simulating correlation-spreading dynamics in two-dimensional quantum many-body systems by the tensor-network method

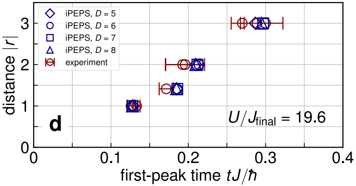
Ryui KANEKO

Dept. of Physics, Kindai Univ.

Collaborator: Ippei DANSHITA (Kindai Univ.)

R. Kaneko and I. Danshita, Commun. Phys. 5, 65 (2022)



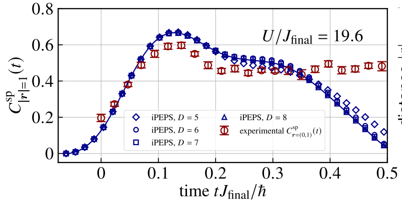


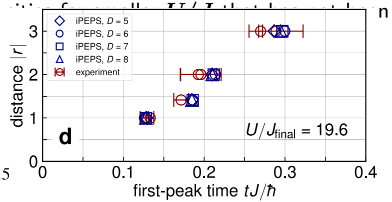
Outline

- Introduction
  - Quench dynamics by analog quantum simulation
  - Importance of comparison with numerical simulations
  - Numerical difficulty in simulating the dynamics of 2D quantum systems
- Bose-Hubbard model: quench from a Mott insulating state
  - Motivation
    - Lack of reliable 2D methods
    - How far one can go by tensor-network states in 2D?
  - Tensor-network method
    - Simple update, projected entangled pair states (PEPS)
  - Results
    - Good agreement with experimental results
    - Estimate group and phase velocities for smaller U/J that has not been investigated in the experiment
- Transverse-field Ising model: quench from a disordered state
  - Motivation
    - To what extent is PEPS useful?
  - Preliminary results

Outline

- Introduction
  - Quench dynamics by analog quantum simulation
  - Importance of comparison with numerical simulations
  - Numerical difficulty in simulating the dynamics of 2D quantum systems
- Bose-Hubbard model: quench from a Mott insulating state
  - Motivation
    - Lack of reliable 2D methods
    - How far one can go by tensor-network states in 2D?
  - Tensor-network method
    - Simple update, projected entangled pair states (PEPS)
  - Results
    - Good agreement with experimental results



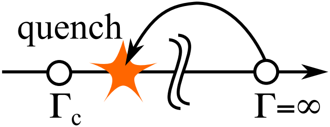


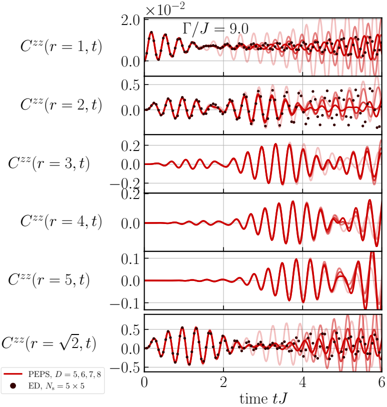
Outline

- Introduction
  - Quench dynamics by analog quantum simulation
  - Importance of comparison with numerical simulations
  - Numerical difficulty in simulating the dynamics of 2D quantum systems
- Bose-Hubbard model: quench from a Mott insulating state
  - Motivation
    - Lack of reliable 2D methods
    - How far one can go by tensor-network states in 2D?
  - Tensor-network method
    - Simple update, projected entangled pair states (PEPS)
  - Results
    - Good agreement with experimental results
    - Estimate group and phase velocities for smaller U/J that has not been investigated in the experiment
- Transverse-field Ising model: quench from a disordered state
  - Motivation
    - To what extent is PEPS useful?
  - Preliminary results

Outline

- Introduction
  - Quench dynamics by analog c
  - Importance of comparison wit
  - Numerical difficulty in simulat
- Bose-Hubbard model: quench frc
  - Motivation
    - Lack of reliable 2D metho
    - How far one can go by ter
  - Tensor-network method





- Transverse-field Ising model: quench from a disordered state
  - Motivation
    - To what extent is PEPS useful?
  - Preliminary results

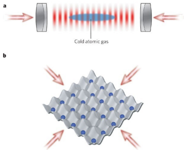
Introduction

Analog quantum simulators

Let the nature do the quantum simulations using highly controllable experimental devices

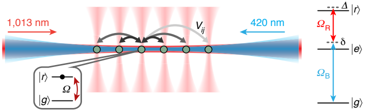
Ultracold atoms in optical lattices

[I.Bloch,Nature.453.1016('08); C.Gross,I.Bloch,Science.357.995('17); W.Hofstetter,T.Qin,J.Phys.B:At.Mol.Opt.Phys.51.082001('18)]



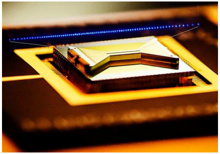
Rydberg atoms in optical tweezer arrays

[H.Bernien et al.,Nature.551.579('17); A.Keesling et al.,Nature.568.207('19)]



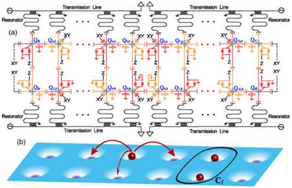
Trapped ion quantum computers

[R.Blatt,C.F.Roos,Nat.Phys.8.277('12); E.A.Martinez et al.,Nature.534.516('16); M.Gärtner et al.,Nat.Phys.13.781('17); `https://physicsworld.com/wp-content/uploads/2018/12/IonQ-chip.png`]



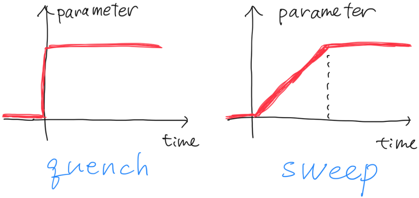
Superconducting quantum circuits

[R.Ma et al.,Nature.566.51('19); Y.Ye et al.,PRL.123.050502('19)]



What do we want to do using analog quantum simulators?

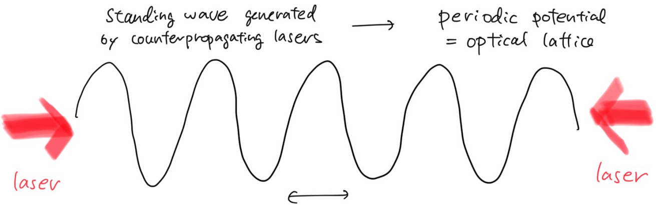
- Solve problems that are hard to tackle by classical computers
  - Prepare the Hamiltonian corresponding to the problem and obtain the equilibrium state (e.g. the ground state)
  - Simulate Schrödinger equation
    $\rightarrow$ Simulations of isolated quantum many-body systems have attracted much interest



∗ In experiments, quench is realized by very fast sweep

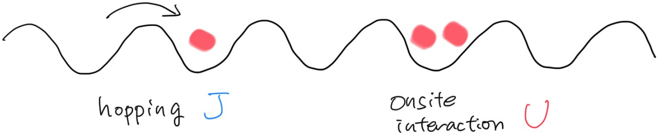
- In general, simulating time evolution requires all the information of eigenstates on classical computers
  $\rightarrow$ It is much harder than the ground-state calculation

In the case of ultracold atoms on optical lattices...



potential
$V(x) = V_0 \sin^2(kx)$
↑ intensity of laser

lattice spacing
$d = \frac{\pi}{k} \sim 500\text{nm}$ ($k = \frac{2\pi}{\lambda}$, λ: wave length)



Bose-Hubbard model : $\hat{H} = -J \sum_{\langle ij \rangle} \hat{a}_i^\dagger \hat{a}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1)$

In the case of ultracold atoms on optical lattices...

$$V(x) = V_0 \sin^2(kx)$$

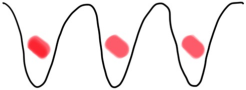
weaker V_0

U/J is small

⇓

superfluid

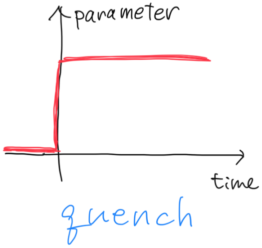
Stronger V_0



U/J is large

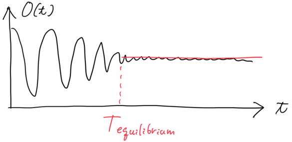
⇓

Mott insulator



What do we want to clarify by simulating time evolution?

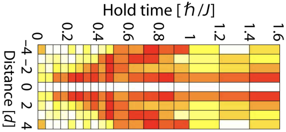
- How do isolated quantum many-body systems thermalize?



- What is the upper limit of the information propagation (= Lieb-Robinson bound)?

  cf. In relativistic system:
  Upper limit = speed of light

  Theoretical investigation is active recently
  cf. Light-cone-like behavior in Bose-Hubbard models
  [T.Kuwahara, K.Saito, PRL.127.070403('21)]



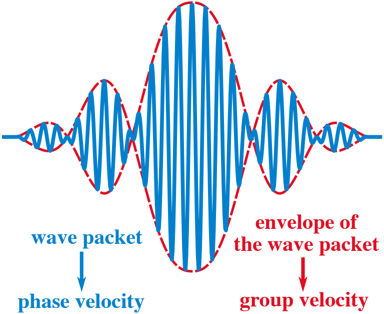
[Y.Takasu et al., sciadv.aba9255('20)]

Desirable to simulate the dynamics of correlation spreading
to answer these questions

→ Longer-time experimental and numerical simulations are important

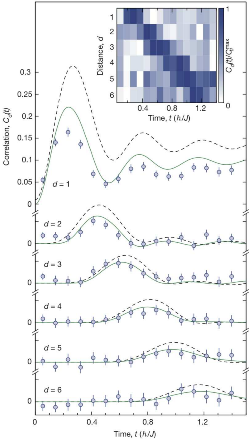
Propagation velocities can be obtained from equal-time correlations

- Two characteristic velocities
  - Phase velocity
  - Group velocity (≲ Lieb-Robinson bound)



- In 1D, tensor-network simulations with matrix product states (MPS) are popular

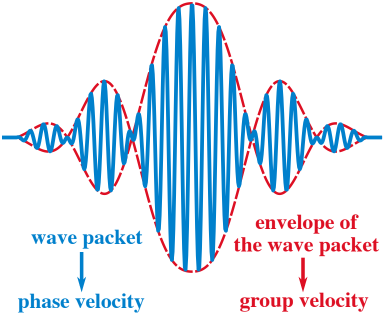
- e.g. 1D Bose-Hubbard simulator
  Correlations after a quench
  [M.Cheneau et al.,Nature.481.484('11)]



Comparisons between experimental and numerical simulations are desired

Propagation velocities can be obtained from equal-time correlations

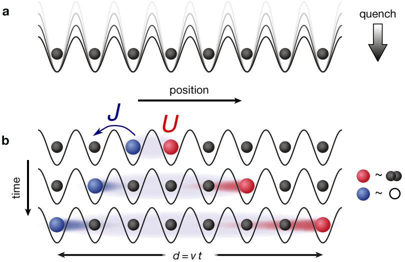
- Two characteristic velocities
  - Phase velocity
  - Group velocity ($\lesssim$ Lieb-Robinson bound)



- In 1D, tensor-network simulations with matrix product states (MPS) are popular

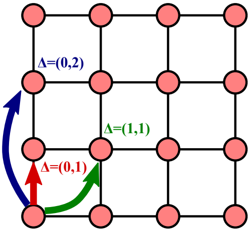
- e.g. 1D Bose-Hubbard simulator
  Correlations after a quench
  [M.Cheneau et al.,Nature.481.484('11)]

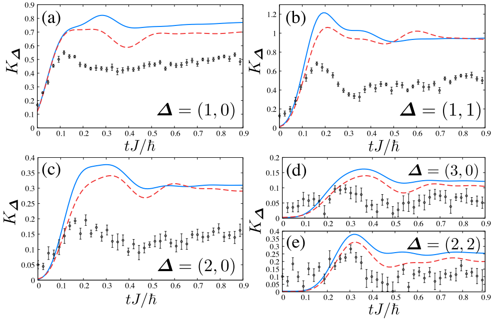
Quasiparticle picture



Dynamics of doublons and holons

Numerical simulations in 2D are extremely hard





[K.Nagao et al., PRR.3.043091('21)]

- e.g. Quench dynamics in the 2D Bose-Hubbard model
- Semiclassical approach (truncated Wigner approximation) is not powerful enough to reproduce the intensity of correlations
- Extend the 1D MPS wave functions to 2D
  Examine the accuracy of the 2D tensor-network method

Motivation

- Numerical simulations of time evolution on classical computers
- Crosscheck and predict experimental results
- Numerical simulations in 2D are extremely hard so far

- Focus on
  - 2D Bose-Hubbard model
  - 2D transverse-field Ising model

  to examine the accuracy of the 2D tensor-network method

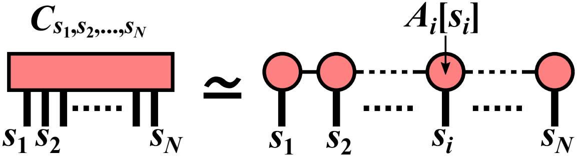
Tensor-network method

Tensor-network states: MPS and PEPS

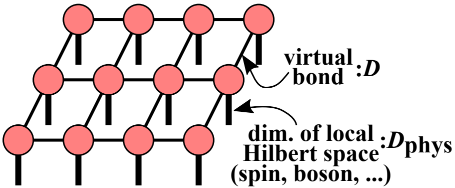
- Wave function for quantum spin systems:

$$|\psi\rangle = \sum_{\{s_i\}} C_{s_1,s_2,\ldots,s_N} |s_1, s_2, \ldots, s_N\rangle \qquad \#\text{elements} = O(e^N)$$

- In 1D: Matrix product state (MPS)



- In 2D: Projected entangled pair state (PEPS), tensor product state

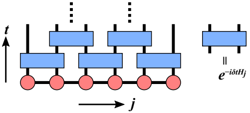


- $D_{\text{phys}} = 2S + 1$ for spin S (chosen to be sufficiently large for soft-core bosons)
- $D = 1$: direct product state
- $D \geq 2$: entangled state
- Wave functions are more accurate for larger D
- Translational invariant PEPS can treat infinite systems

[T.Nishino et al.,PTP.105.409('01); F.Verstraete, J.Cirac, arXiv:cond-mat/0407066]

Simulating real-time evolution by infinite PEPS

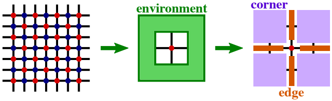
- Real-time evolution of infinite PEPS: $|\psi(t)\rangle = e^{-itH}|\psi(0)\rangle$



Time-evolving block decimation in 2D (= simple update) [comp. cost: $O(D^5)$]

[H.C.Jiang,Z.Y.Weng,T.Xiang('08); P.Corboz et al.('10)]

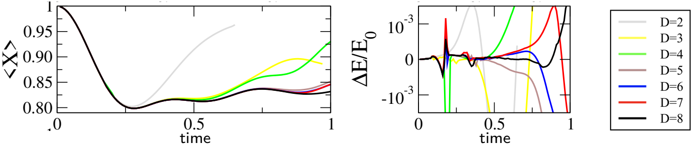
- Calculation of expectation values for infinite PEPS:



Corner transfer matrix renormalization group method [comp. cost $O(D^{10})$]

[R.J.Baxter('68); T.Nishino,K.Okunishi('96,'97); R.Orus,G.Vidal('09)]

- Previous studies on 2D quench dynamics:
  e.g. transverse-field Ising model (tr.-field: $h^x = \infty \to h^x_c$)
  Time $\lesssim \hbar/J$ accessible by increasing bond dimension D



[A.Kshetrimayum et al.,Nat.Commun.8.1291('17); P.Czarnik et al.,PRB.99.035115('19); C.Hubig,J.I.Cirac,SciPost.Phys.6,031('19)]

Quench dynamics in the Bose-Hubbard model

Motivation:

- Reproduce experimental results
- Examine the parameter region that has not been explored

Numerical setup: Wish to calculate $|\psi(t)\rangle = e^{-i\hat{H}t}|\psi_0\rangle$

- Square Bose-Hubbard model: $\hat{H} = \sum_{\langle ij \rangle} \hat{H}_{ij}$

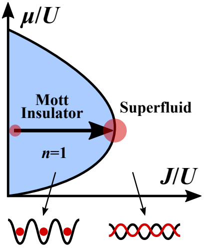
$$\hat{H}_{ij} = -J(\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i) + \frac{U}{2z}[\hat{n}_i(\hat{n}_i - 1) + \hat{n}_j(\hat{n}_j - 1)] - \frac{\mu}{z}(\hat{n}_i + \hat{n}_j) \ \ (z = 4)$$

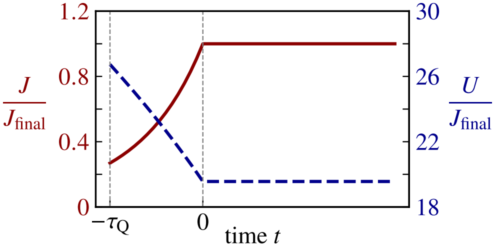
[V.Murg et al.,PRA('07); J.Jordan et al.,PRB('09); A.Kshetrimayum et al.,PRL('19); S.S.Jahromi and R.Orus,PRB('19); P.Schmoll et al.,PRL('20); W.-L.Tu et al.,JPCM('20); H.-K.Wu et al.,PRA('20); P.C.G.Vlaar and P.Corboz et al.,PRB('21)]

- Simple update by e.g. $e^{-idt\hat{H}/\hbar} \sim \prod_{\langle ij \rangle} e^{-idt\hat{H}_{ij}/\hbar}$

  (use second-order Suzuki-Trotter decomposition in practice)

- Very fast ($\tau_Q > 0$) and sudden ($\tau_Q = 0$) quenches from Mott insulator $\otimes_i |n_i = 1\rangle$
- Experimental setup: $U/J \sim 100 \to 19.6$ in $\tau_Q = 0.1$ms
  ($U/J = 19.6 > 16.74 = U_c/J$: Mott insulating region)



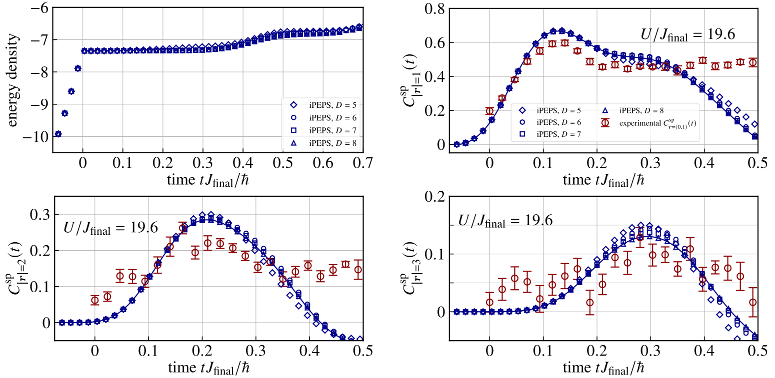


- Use tensor-network library TeNeS

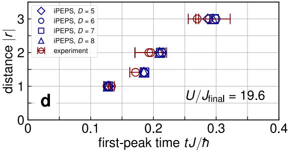
[Y.Motoyama et al., Comp.Phys.Commun.279.108437('22); `https://github.com/issp-center-dev/TeNeS`, `https://github.com/TsuyoshiOkubo/pTNS`]

Numerical results: Comparison with the experiment at $U/J = 19.6$

$$C_r^{\mathrm{sp}}(t) = \frac{1}{2N_s} \sum_{r_i - r_j = r} \langle \hat{a}_i^\dagger(t)\hat{a}_j(t) + \hat{a}_j^\dagger(t)\hat{a}_i(t)\rangle$$

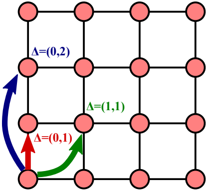


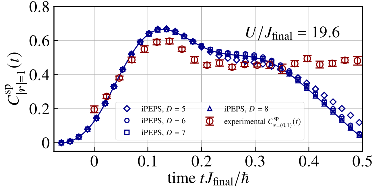
- Consider finite quench time as in the experiment
- Nearly conserved energy for $0 \leq tJ/\hbar \lesssim 0.4$
- Physical quantities are likely to be converged for this short time

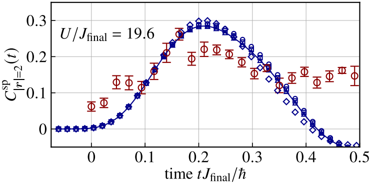


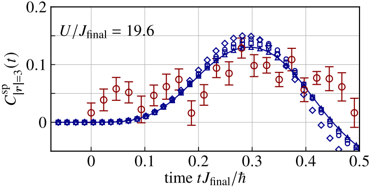
Numerical results: Comparison with the experiment at $U/J = 19.6$

$$C_r^{\mathrm{sp}}(t) = \frac{1}{2N_\mathrm{s}} \sum_{r_i - r_j = r} \langle \hat{a}_i^\dagger(t)\hat{a}_j(t) + \hat{a}_j^\dagger(t)\hat{a}_i(t)\rangle$$

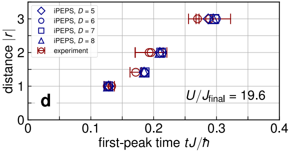




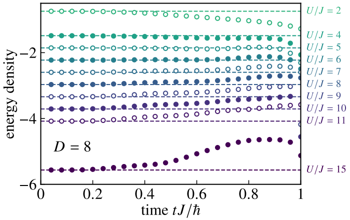


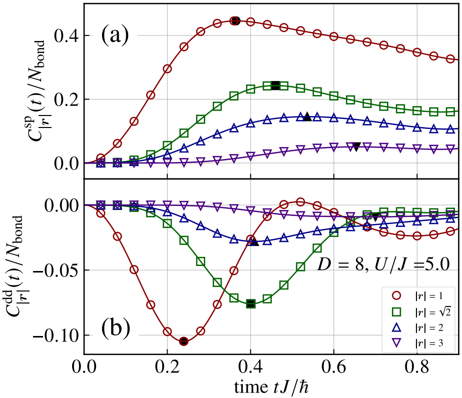


- Consider finite quench time as in the experiment
- Nearly conserved energy for $0 \leq tJ/\hbar \lesssim 0.4$
- Single-particle correlations agree very well
- How about other parameter regions?
- How does the propagation velocity behave?



Numerical results: Estimate propagation velocities from $\langle a_0^\dagger a_r \rangle$ and $\langle n_0 n_r \rangle$





Consider a sudden quench

Energy is conserved for longer time $tJ/\hbar \lesssim 0.9$ when $U/J \sim 5$

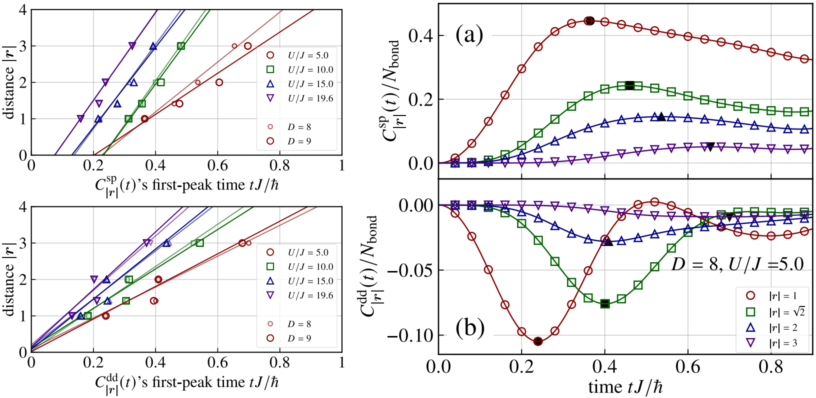
Can capture peaks up to $|r| \leq 3$

$$C_r^{\mathrm{sp}}(t) = \frac{1}{2N_{\mathrm{s}}} \sum_{r_i - r_j = r} \langle \hat{a}_i^\dagger(t)\hat{a}_j(t) + \hat{a}_j^\dagger(t)\hat{a}_i(t) \rangle$$

$$C_r^{\mathrm{dd}}(t) = \frac{1}{N_{\mathrm{s}}} \sum_{r_i - r_j = r} (\langle \hat{n}_i(t)\hat{n}_j(t) \rangle - 1)$$

- v_{phase}: captured by single-particle correlation $\langle a_0^\dagger a_r \rangle$
- v_{group}: captured by density-density correlation $\langle n_0 n_r \rangle$

Numerical results: Estimate propagation velocities from $\langle a_0^\dagger a_r \rangle$ and $\langle n_0 n_r \rangle$

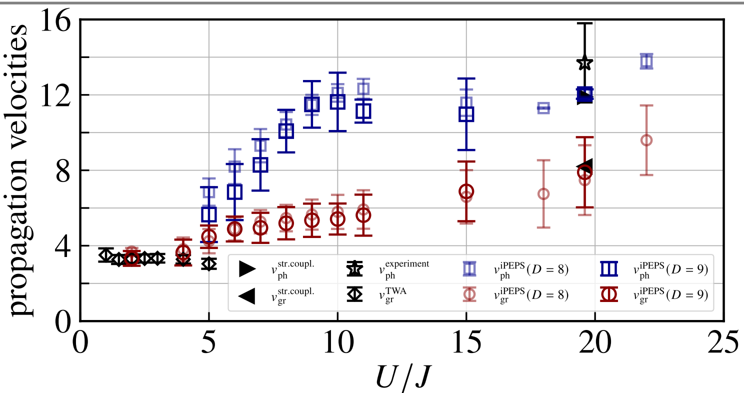


$$C_r^{\rm sp}(t) = \frac{1}{2N_{\rm s}} \sum_{r_i - r_j = r} \langle \hat{a}_i^\dagger(t)\hat{a}_j(t) + \hat{a}_j^\dagger(t)\hat{a}_i(t) \rangle$$

$$C_r^{\rm dd}(t) = \frac{1}{N_{\rm s}} \sum_{r_i - r_j = r} \left(\langle \hat{n}_i(t)\hat{n}_j(t) \rangle - 1 \right)$$

- $v_{\rm phase}$: captured by single-particle correlation $\langle a_0^\dagger a_r \rangle$
- $v_{\rm group}$: captured by density-density correlation $\langle n_0 n_r \rangle$

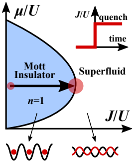
Numerical results: U dependence of velocity

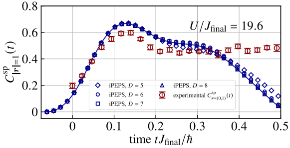


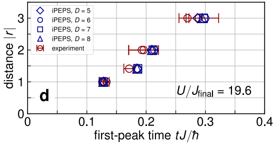
- For $U \lesssim zJ$ $(z = 4)$, single-particle picture (mean-field-like picture) holds
  $v_{\text{group}} \sim 4J/\hbar$ [K.Nagao et al.,PRA.99.023622('19)]
- For $U \gg J$, quasi-particle picture holds
  $v_{\text{group}} \sim 6J/\hbar \times [1 + \mathcal{O}(J^2/U^2)]$ [M.Cheneau et al.,Nature.481.484('11)]
- v_{group} estimated from $\langle n_0 n_r \rangle$ consistent with
  - single-particle group velocity deep in superfluid region
  - strong-coupling result near criticality
- v_{phase} and v_{group} gradually converge to the same value as U/J is decreased

Conclusions: Bose-Hubbard case

- Quench dynamics from Mott insulator in 2D Bose-Hubbard model
- Simulation by infinite PEPS using simple update
- Compare PEPS simulations with experiments
  $\rightarrow$ Good agreement for $tJ/\hbar \lesssim 0.4$ at $U/J = 19.6$



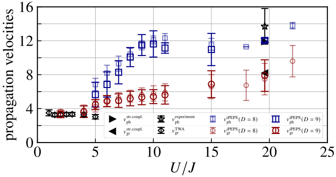




- Estimate velocity of correlation spreading for smaller U/J

$v_{\rm phase}$ and $v_{\rm group}$ gradually converge to the same value as U/J is decreased

Might be helpful for future experiments



R. Kaneko and I. Danshita, Commun. Phys. 5, 65 (2022)

Quench dynamics in the 2D transverse-field Ising model

Motivation:

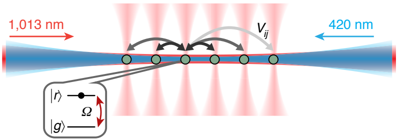
- How good is the 2D tensor-network method in this case?
- How does the group velocity for spin correlations look?
  (Compare with the recently updated Lieb-Robinson bound)

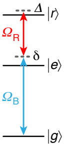
Analog quantum simulations of the quantum Ising model by Rydberg-atom arrays

[H.Bernien et al.,Nat.551.579('17); A.Keesling et al.,Nat.568.207('19); E.Guardado-Sanchez et al.,PRX.8.021069('18); V.Lienhard et al.,PRX.8.021070('18); D.Bluvstein et al.,Science.371.1355('21); P.Scholl et al.,Nat.595.233('21); S.Ebadi et al.,Nat.595.227('21); ...]

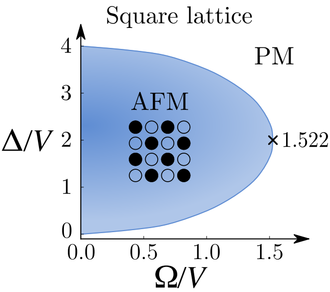
$$H = \Omega \sum_i S_i^x - \Delta \sum_i n_i + V \sum_{\langle ij \rangle} n_i n_j \quad \left(n_i = S_i^z + \frac{1}{2},\ D:\ \text{dim.} \right)$$

$$= \Omega \sum_i S_i^x - (\Delta - VD) \sum_i S_i^z + V \sum_{\langle ij \rangle} S_i^z S_j^z + \sum_i \left(\frac{VD}{4} - \frac{\Delta}{2} \right)$$





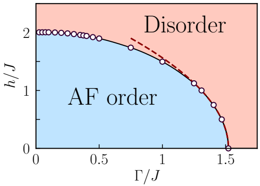
	Rydberg atoms	quantum Ising model
bases	$\lvert g\rangle$, $\lvert r\rangle$	$\lvert\downarrow\rangle$, $\lvert\uparrow\rangle$
Ω	Rabi frequency	transverse field
Δ	detuning	longitudinal field
V	van der Waals interaction	Ising spin interaction



Very recently, real-time dynamics for # qubits > 200

Numerical setup: 2D transverse-field Ising model

- Ground-state phase diagram [R.Kaneko et al.,JPSJ.90.073001('21)]

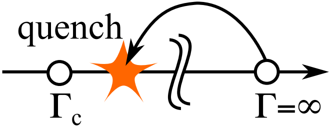


$$H = +J \sum_{\langle ij \rangle} S_i^z S_j^z - \Gamma \sum_i S_i^x - h \sum_i S_i^z$$

- For simplicity, focus on $h = 0$ case
  $\rightarrow$ Map to ferromagnetic model by appropriate unitary transformation

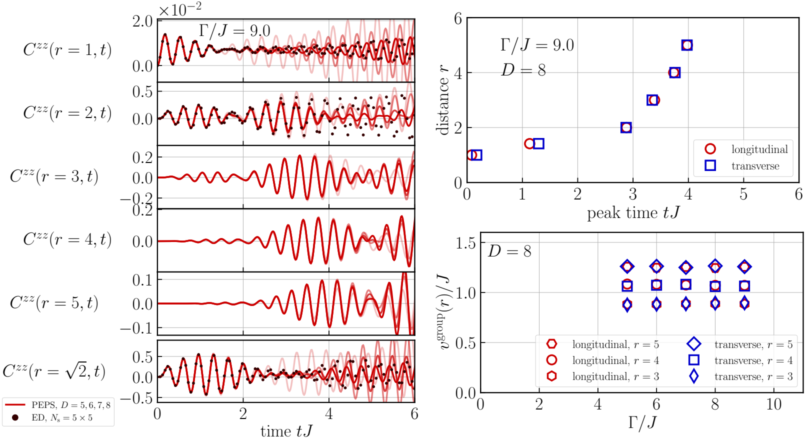
$$H = -J \sum_{\langle ij \rangle} S_i^z S_j^z - \Gamma \sum_i S_i^x$$

- Sudden quench from the $\Gamma = \infty$ ground state $|\rightarrow\rightarrow\cdots\rightarrow\rangle$



$$|\psi(t)\rangle = e^{-iHt/\hbar}|\rightarrow\rightarrow\cdots\rightarrow\rangle$$

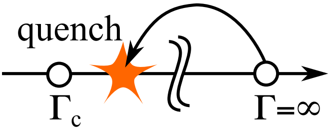
Numerical results: Extract group velocity from spin correlations

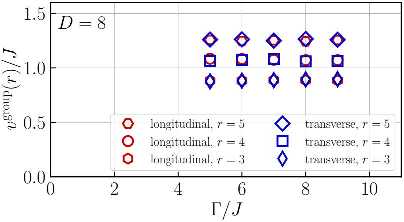


- Distances longer than exact diag are calculable
- Estimated group velocity for $\Gamma \gg J$: $v_{\text{spin}}/J = 1.07 \pm 0.20$
- Best Lieb-Robinson bound for any correlations in 2D TFIsing model for $\Gamma \gg J$: $v_{\text{LR}}/J = 7.55$ [Z.Wang, K.R.A.Hazzard, PRXQuantum.1.010303('20)]
- $v_{\text{spin}} \ll v_{\text{LR}}$
  $\rightarrow$ Our data is more meaningful when we need to compare the spin correlations

Conclusions: Ising case

- Quench dynamics from the disordered state in 2D transverse-field Ising model
- Simulation by infinite PEPS using simple update





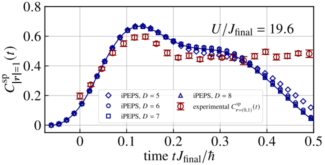
- Our estimate of the group velocity: $\boldsymbol{v_{\text{spin}}/J \sim 1}$
- This is much smaller than the current best Lieb-Robinson bound: $\boldsymbol{v_{\text{LR}}/J = 7.55}$
- Our group velocity and spin correlations are helpful for crosschecking experimental data

Conclusions

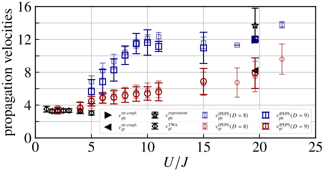
- Simulating the dynamics of 2D systems by the tensor-network method with iPEPS
- Focus on the quench in the 2D Bose-Hubbard and transverse-field Ising models

<u>Bose-Hubbard case</u>

- Good agreement with the experiment

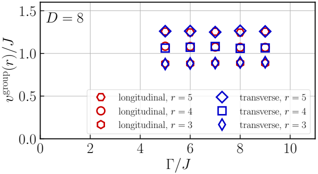


- Examine the parameter region that has not been explored



<u>Ising case</u>

- Group velocity satisfies the Lieb-Robinson bound (but the value is much smaller than the bound)



  - $v_{\mathbf{spin}} \ll v_{\mathbf{LR}}$ is intrinsic?
  - Recent $v_{\mathbf{LR}}$ is still loose?

- Provide numerical data that can be compared with future experiments