

# テンソルネットワークによる 量子系の実時間シミュレーション

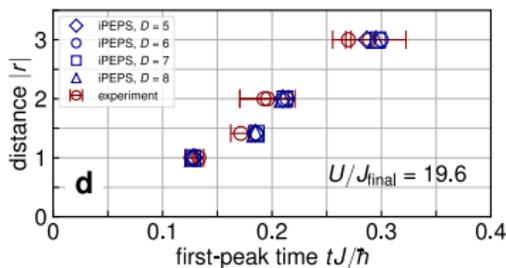
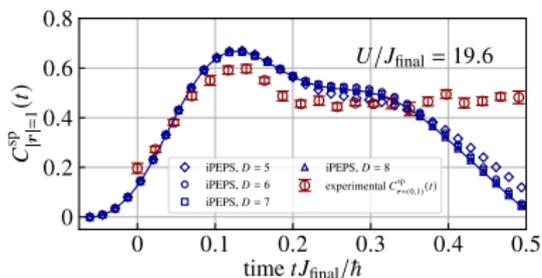
## Simulating the real-time evolution of quantum systems by tensor networks

Ryui KANEKO (金子 隆威)

Dept. of Physics, Sophia Univ. (上智大学)

Collaborator: Ippei DANSHITA (Kindai Univ.)

R. Kaneko and I. Danshita, *Commun. Phys.* **5**, 65 (2022)  
R. Kaneko and I. Danshita, *Phys. Rev. A* **108**, 023301 (2023)



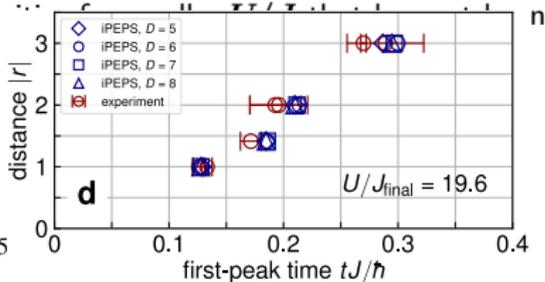
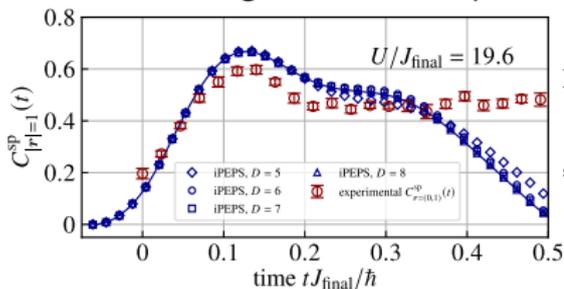
# Outline

---

- 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



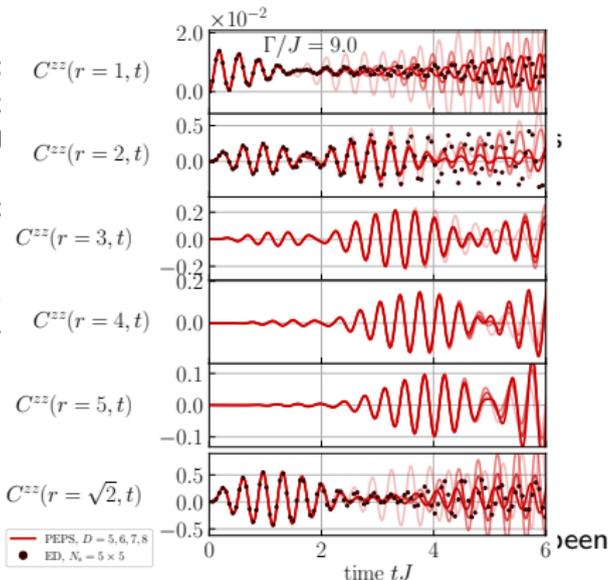
# Outline

---

- 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?
  - Estimate group velocity and compare it with the current best estimate

# 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?
  - Estimate group velocity and compare it with the current best estimate

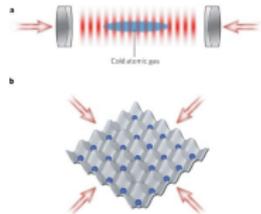
# Introduction

# Analog quantum simulators

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

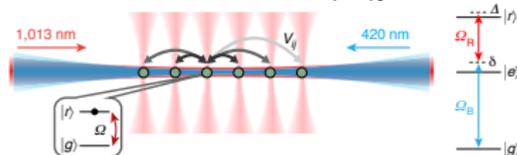
## Ultracold atoms in optical lattices

[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

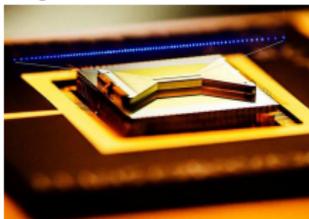
[H. Bernien et al., Nature.551.579('17); A. Keesling et al., Nature.568.207('19)]



## Trapped ion quantum computers

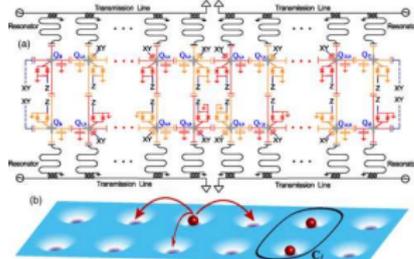
[R. Blatt, C. F. Roos, Nat. Phys. 8.277('12); E. A. Martinez et al., Nature.534.516('16); M. Gärtner et al., Nat. Phys. 13.781('17);

<https://physicsworld.com/wp-content/uploads/2018/12/IonQ-chip.png>



## Superconducting quantum circuits

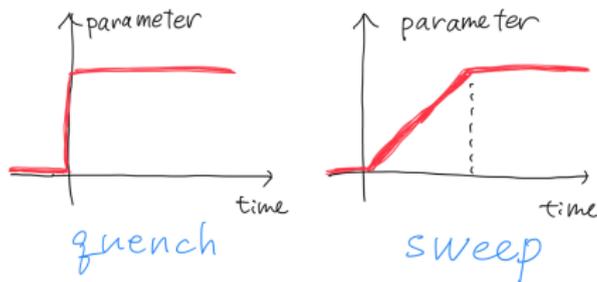
[R. Ma et al., Nature.566.51('19); Y. Ye et al., PRL.123.050502('19)]



## What do we want to do using analog quantum simulators?

---

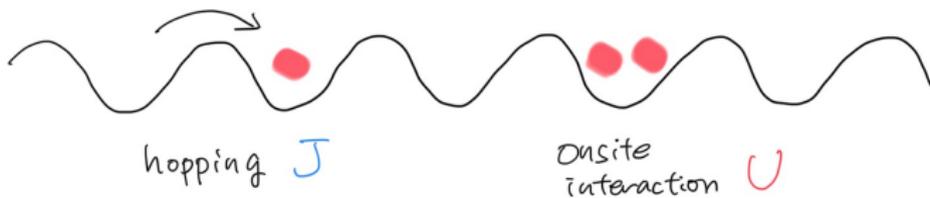
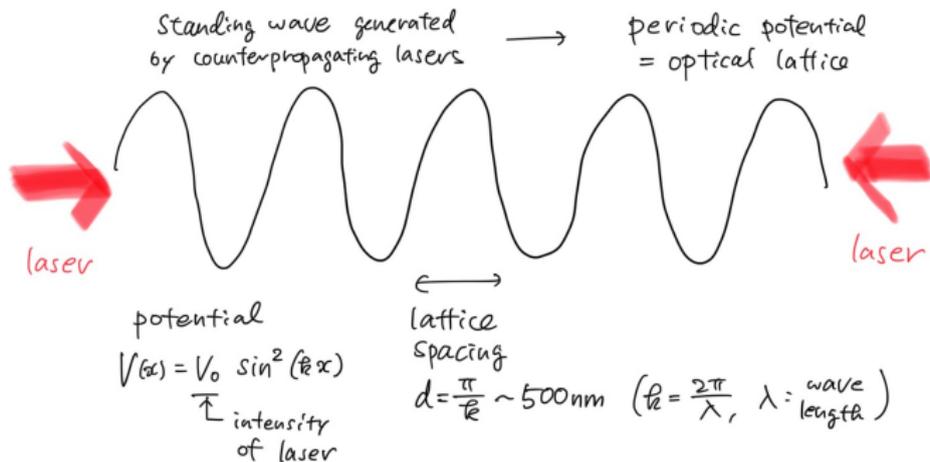
- Solve problems that are hard to tackle by classical computers
  - Prepare the Hamiltonian corresponding to the problem and obtain the **equilibrium state** (e.g. the ground state)
  - Simulate **Schrödinger equation**
    - Simulations of isolated quantum many-body systems have attracted much interest



\* In experiments, quench is realized by very fast sweep

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

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



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

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

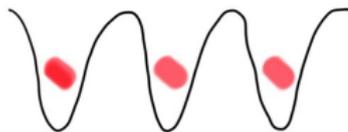
$$V(x) = V_0 \sin^2(kx)$$

weaker  $V_0$

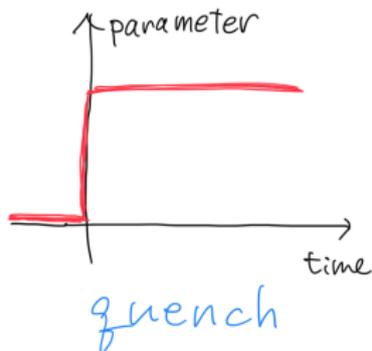


$U/J$  is small  
 $\Downarrow$   
superfluid

Stronger  $V_0$



$U/J$  is large  
 $\Downarrow$   
Mott insulator

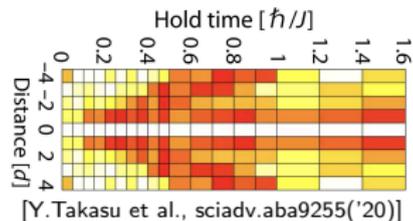
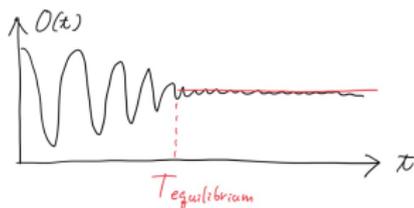


## What do we want to clarify by simulating time evolution?

- 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)]



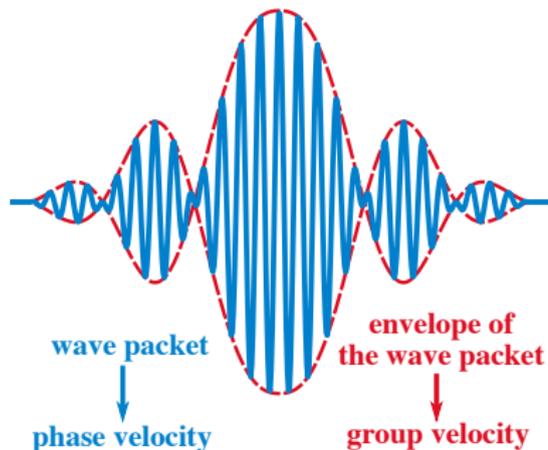
Desirable to simulate the dynamics of correlation spreading  
to answer these questions

→ Longer-time experimental and numerical simulations are important

## Comparisons between experimental and numerical simulations are desired

Propagation velocities can be obtained from equal-time correlations

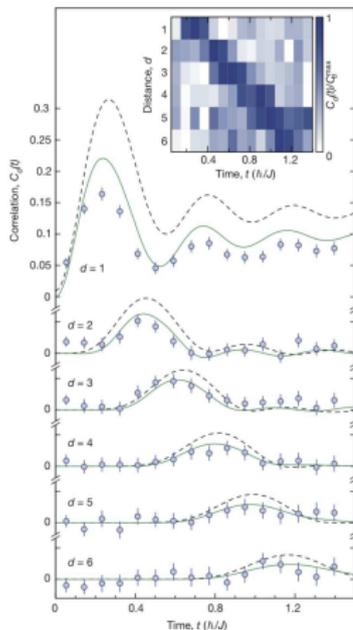
- Two characteristic velocities
  - Phase velocity
  - Group velocity ( $\leq$  Lieb-Robinson bound)



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

- e.g. 1D Bose-Hubbard simulator
- Correlations after a quench

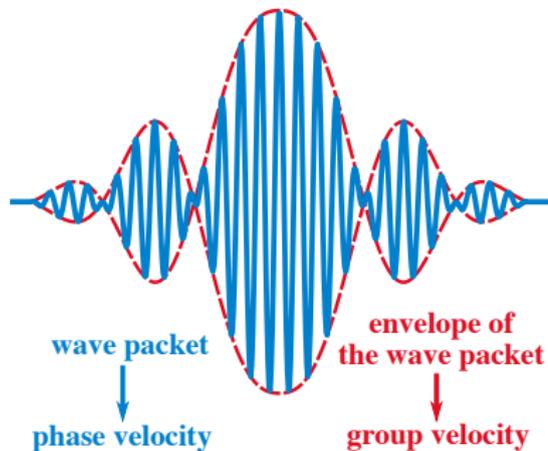
[M.Cheneau et al., Nature.481.484('11)]



## Comparisons between experimental and numerical simulations are desired

Propagation velocities can be obtained from equal-time correlations

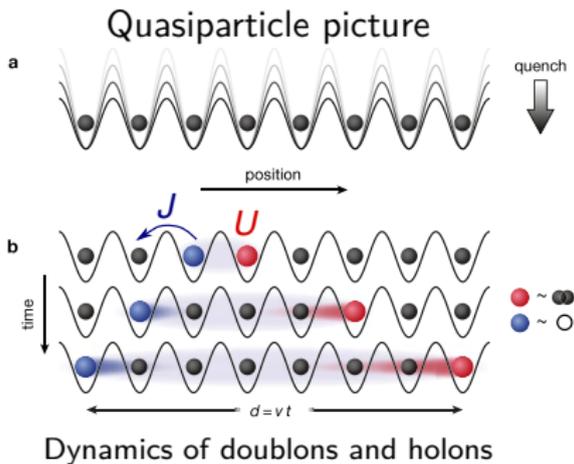
- Two characteristic velocities
  - Phase velocity
  - Group velocity ( $\leq$  Lieb-Robinson bound)



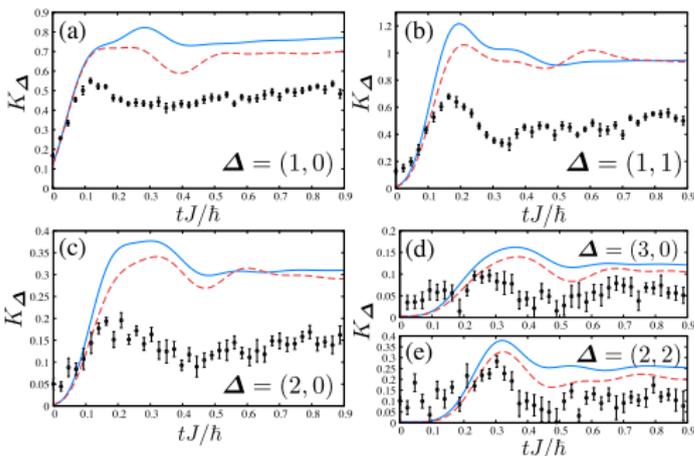
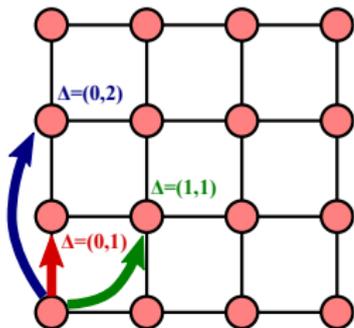
- In 1D, tensor-network simulations with matrix product states (MPS) are popular

- e.g. 1D Bose-Hubbard simulator  
Correlations after a quench

[M.Cheneau et al., Nature.481.484('11)]



## 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

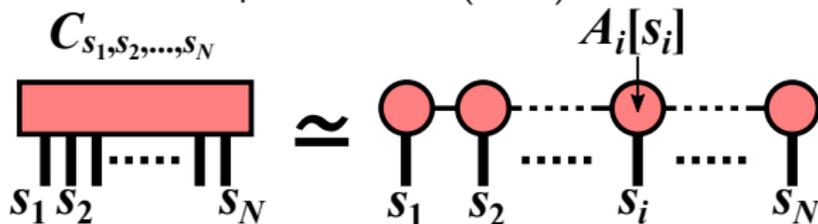
Tensor-network method

## Tensor-network states: MPS and PEPS

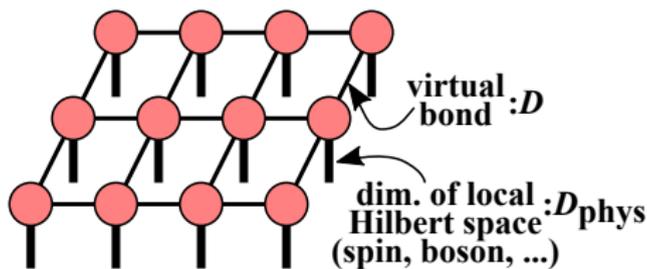
- Wave function for quantum spin systems:

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

- In 1D: Matrix product state (MPS)



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

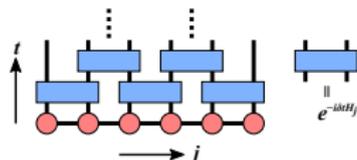


- $D_{\text{phys}} = 2S + 1$  for spin  $S$  (chosen to be sufficiently large for soft-core bosons)
- $D = 1$ : direct product state
- $D \geq 2$ : entangled state
- Wave functions are more accurate for larger  $D$
- Translational invariant PEPS can treat infinite systems

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

## Simulating real-time evolution by infinite PEPS

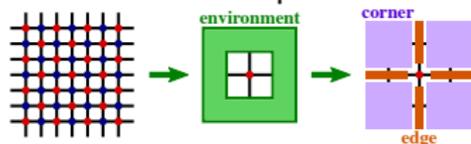
- Real-time evolution of infinite PEPS:  $|\psi(t)\rangle = e^{-itH}|\psi(0)\rangle$



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)]

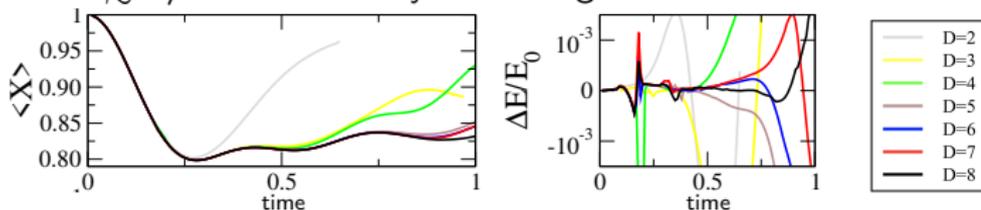
- Calculation of expectation values for infinite PEPS:



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 (full update):  
e.g. transverse-field Ising model (tr.-field:  $h^x = \infty \rightarrow h_c^x$ )  
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:  $\hat{H} = \sum_{\langle ij \rangle} \hat{H}_{ij}$

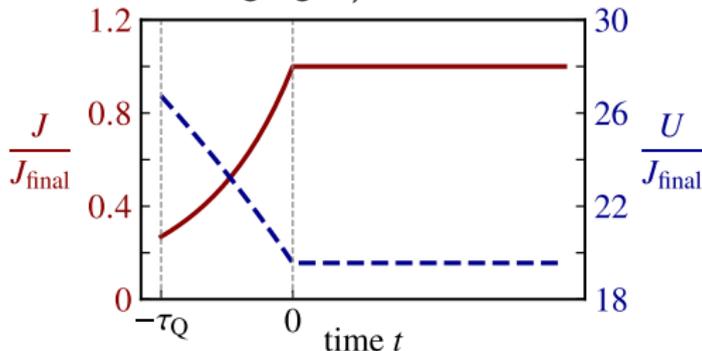
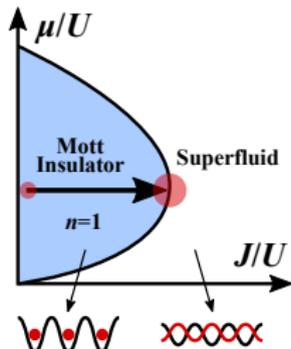
$$\hat{H}_{ij} = -J(\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i) + \frac{U}{2z} [\hat{n}_i(\hat{n}_i - 1) + \hat{n}_j(\hat{n}_j - 1)] - \frac{\mu}{z} (\hat{n}_i + \hat{n}_j) \quad (z = 4)$$

[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.Corbos 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:  $U/J \sim 100 \rightarrow 19.6$  in  $\tau_Q = 0.1\text{ms}$   
( $U/J = 19.6 > 16.74 = U_c/J$ : Mott insulating region)

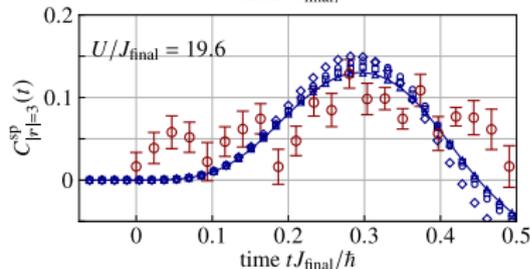
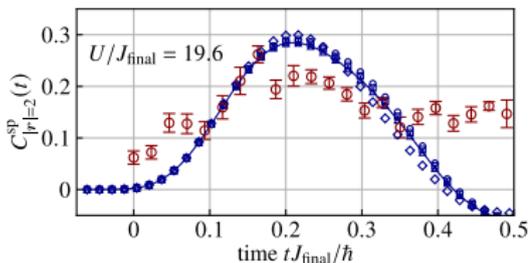
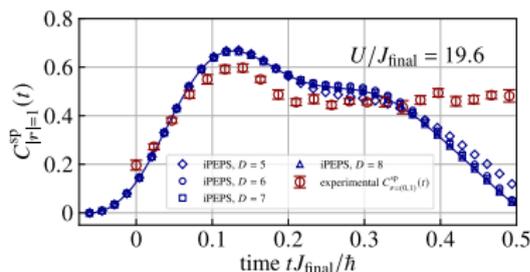
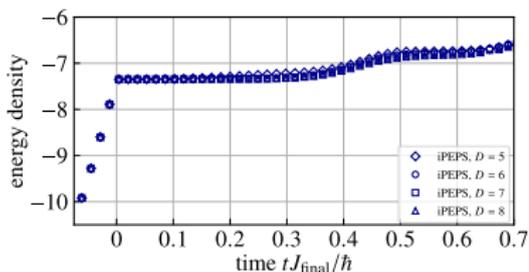


- Use tensor-network library TeNeS

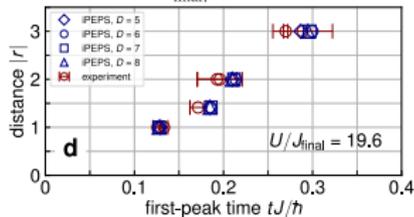
[Y.Motoyama et al., Comp.Phys.Commun.279.108437('22); <https://github.com/iissp-center-dev/TeNeS>, <https://github.com/TsuyoshiOkubo/pTNS>]

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

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

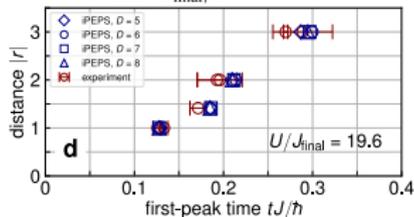
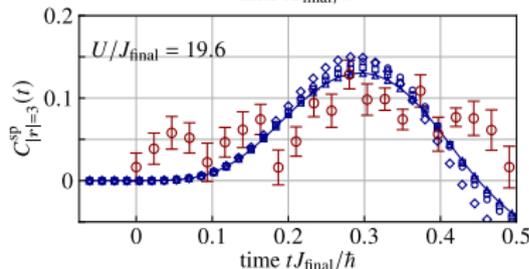
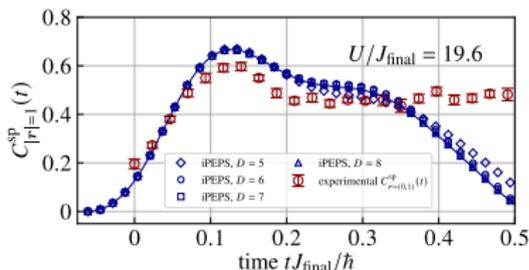
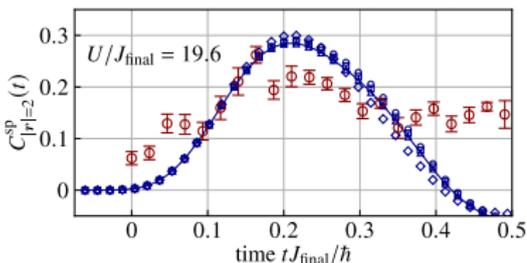
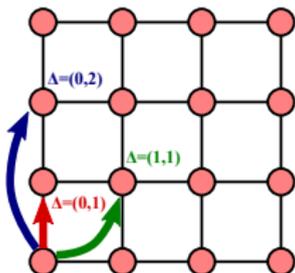


- Consider finite quench time as in the experiment
- Nearly conserved energy for  $0 \leq tJ/\hbar \lesssim 0.4$
- Physical quantities are likely to be converged for this short time



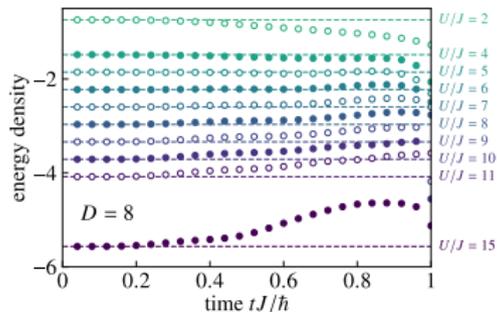
# Numerical results: Comparison with the experiment at $U/J = 19.6$

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



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

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



Consider a sudden quench

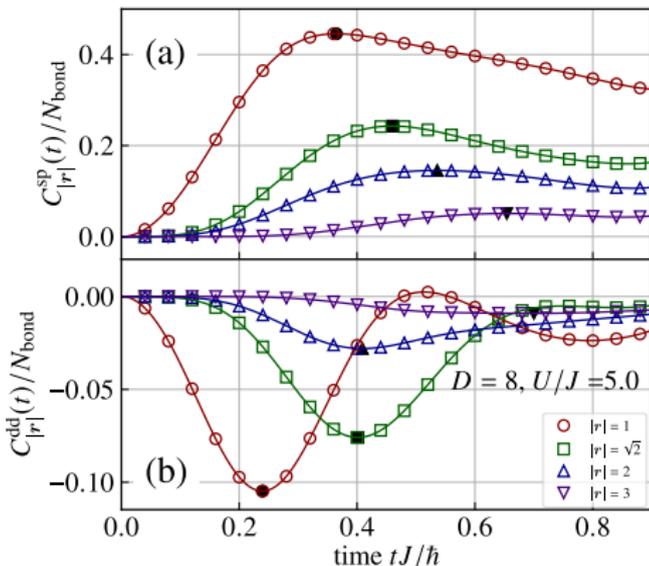
Energy is conserved for longer time  
 $tJ/\hbar \lesssim 0.9$  when  $U/J \sim 5$

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

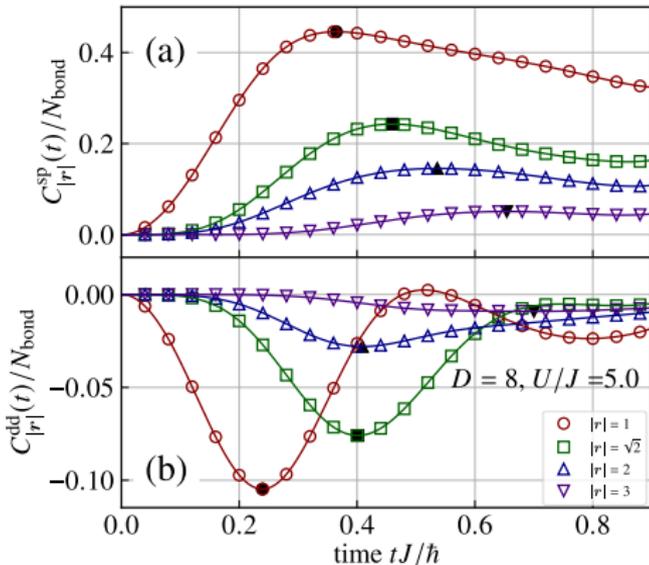
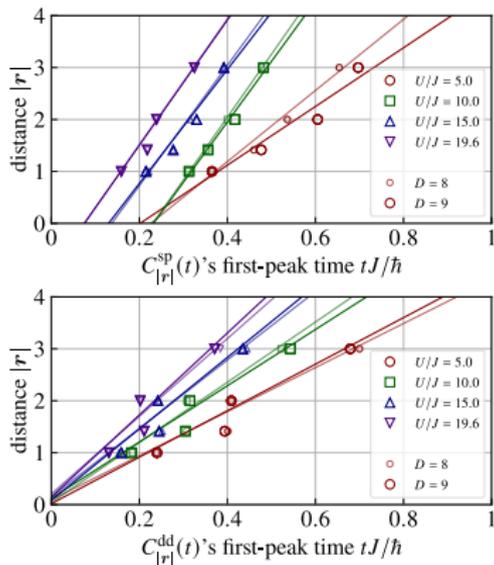
$$C_r^{\text{sp}}(t) = \frac{1}{2N_s} \sum_{r_i - r_j = r} \langle \hat{a}_i^\dagger(t) \hat{a}_j(t) + \hat{a}_j^\dagger(t) \hat{a}_i(t) \rangle$$

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

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

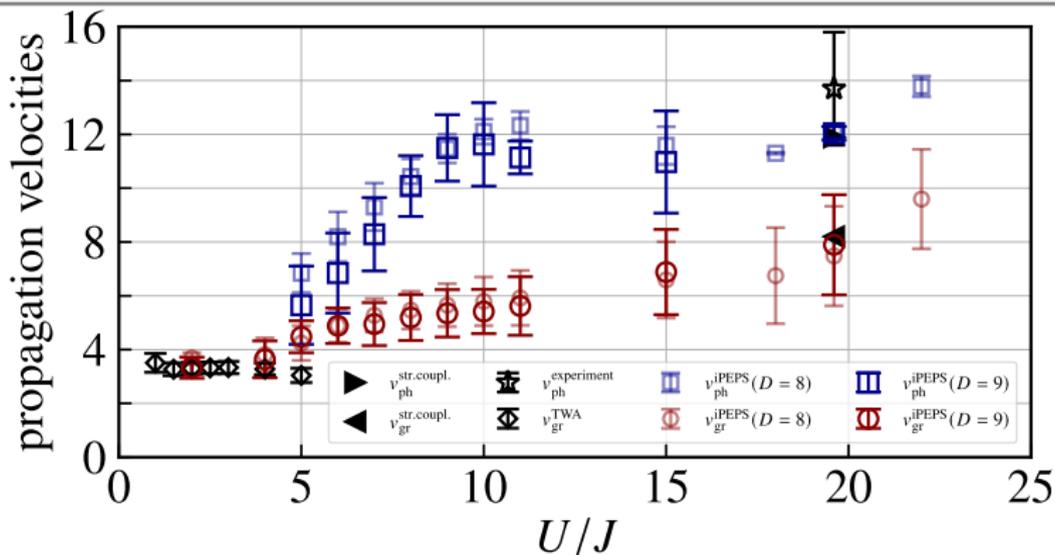


$$C_r^{\text{sp}}(t) = \frac{1}{2N_s} \sum_{r_i - r_j = r} \langle \hat{a}_i^\dagger(t) \hat{a}_j(t) + \hat{a}_j^\dagger(t) \hat{a}_i(t) \rangle$$

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

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

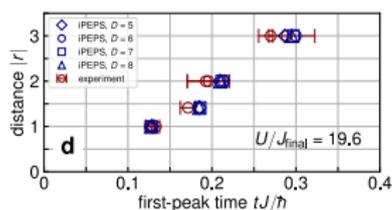
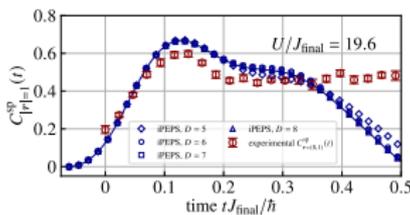
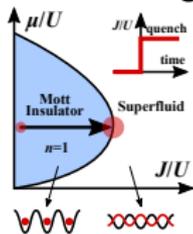
## Numerical results: $U$ dependence of velocity



- For  $U \lesssim zJ$  ( $z = 4$ ), single-particle picture (mean-field-like picture) holds  $v_{group} \sim 4J/\hbar$  [K.Nagao et al.,PRA.99.023622('19)]
- For  $U \gg J$ , quasi-particle picture holds  $v_{group} \sim 6J/\hbar \times [1 + \mathcal{O}(J^2/U^2)]$  [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

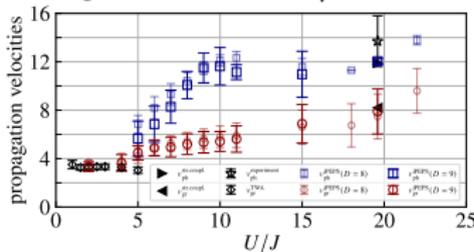
- Quench dynamics from Mott insulator in 2D Bose-Hubbard model
- Simulation by infinite PEPS using simple update
- Compare PEPS simulations with experiments  
 → Good agreement for  $tJ/\hbar \lesssim 0.4$  at  $U/J = 19.6$



- Estimate velocity of correlation spreading for smaller  $U/J$

$v_{\text{phase}}$  and  $v_{\text{group}}$  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:

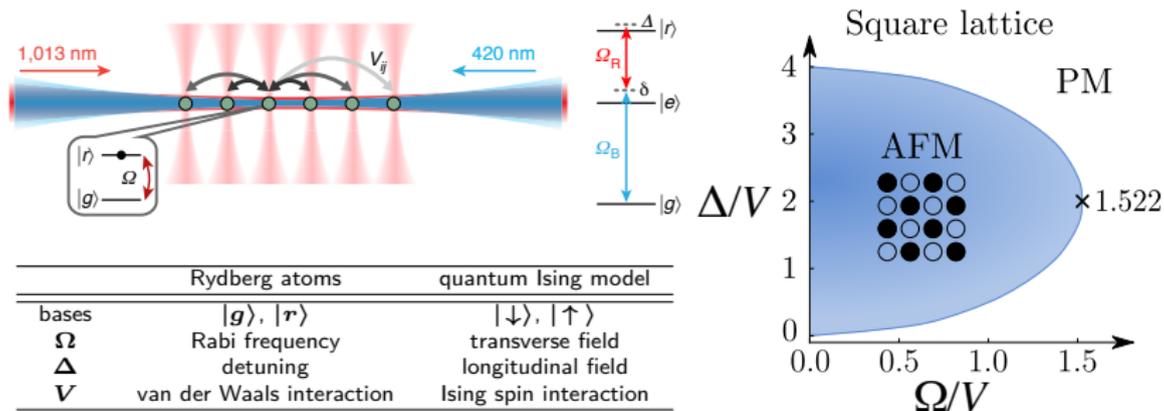
- How good is the 2D tensor-network method in this case?
- How does the group velocity for spin correlations look?  
(Compare with the recently updated Lieb-Robinson bound)

# 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); ...]

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

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

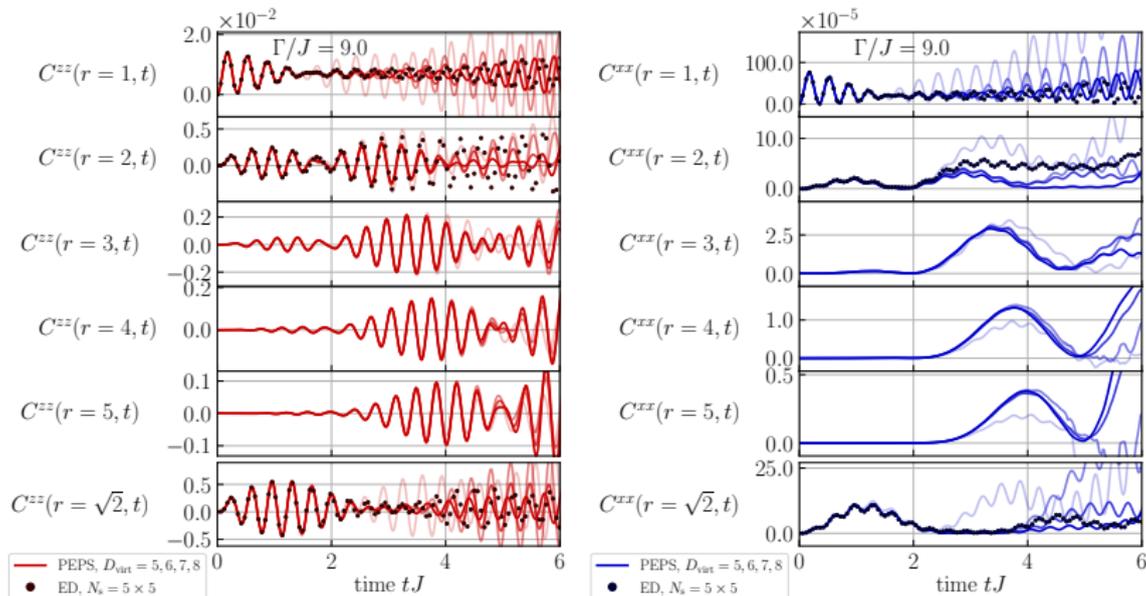


Very recently, real-time dynamics for # qubits > 200  
How does information propagate?

## Numerical results: 2D, iPEPS

$$C^{zz}(r, t) = \langle \psi(t) | \hat{S}_r^z \hat{S}_0^z | \psi(t) \rangle$$

$$C^{xx}(r, t) = \langle \psi(t) | \hat{S}_r^x \hat{S}_0^x | \psi(t) \rangle - \langle \psi(t) | \hat{S}_r^x | \psi(t) \rangle \langle \psi(t) | \hat{S}_0^x | \psi(t) \rangle$$

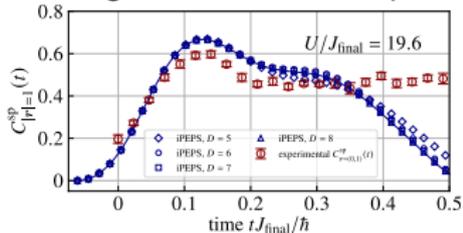


Distances longer than those by the exact diagonalization method are calculable

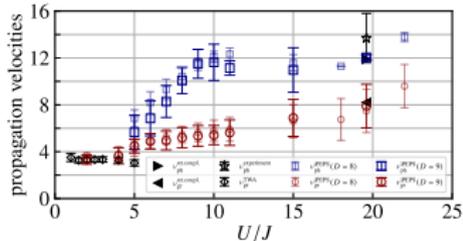
# Conclusions

- 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
  - Bose-Hubbard case
  - Ising case

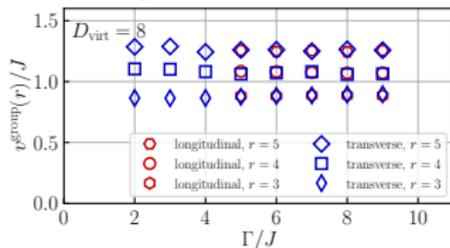
- Good agreement with the experiment



- Examine the parameter region that has not been explored



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



- $v_{\text{spin}}/J \approx 1$  both in 1D and 2D
- Recent estimate  $v_{\text{LR}}/J = 5.672$  is still loose?
- Provide numerical data that can be compared with future experiments

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

R. Kaneko and I. Danshita,  
Phys. Rev. A 108, 023301 (2023)



Backup slides

## Quench dynamics in the 2D transverse-field Ising model

### Motivation:

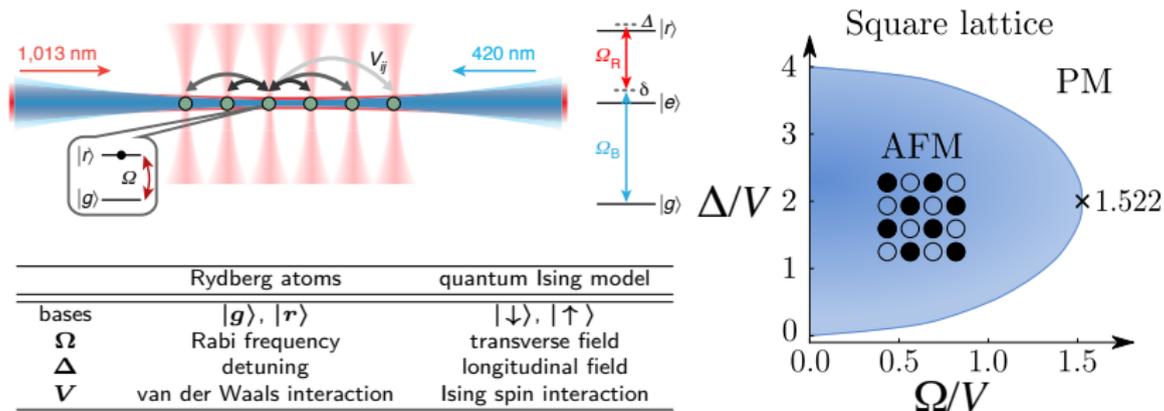
- How good is the 2D tensor-network method in this case?
- How does the group velocity for spin correlations look?  
(Compare with the recently updated Lieb-Robinson bound)

# 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); ...]

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

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



Very recently, real-time dynamics for # qubits > 200  
How does information propagate?

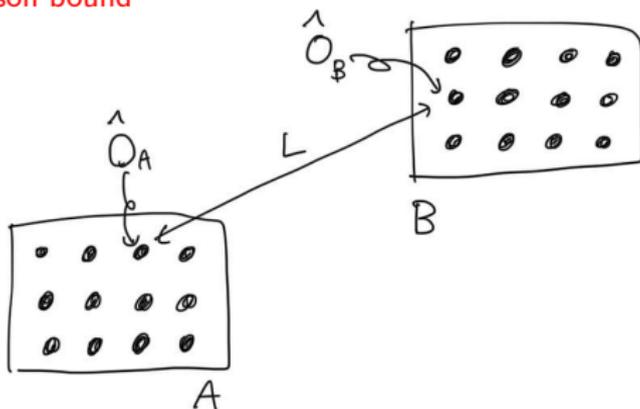
## Lieb-Robinson bound: Upper limit of group velocity for any correlations

---

- Consider regions  $A$  and  $B$  in a lattice system with short-range interaction
- Commutator of any operators  $O_A$  and  $O_B$  in regions  $A$  and  $B$  satisfies

$$||[O_A(t), O_B]|| \leq \text{const.} \times \exp\left(-\frac{L - vt}{\xi}\right)$$

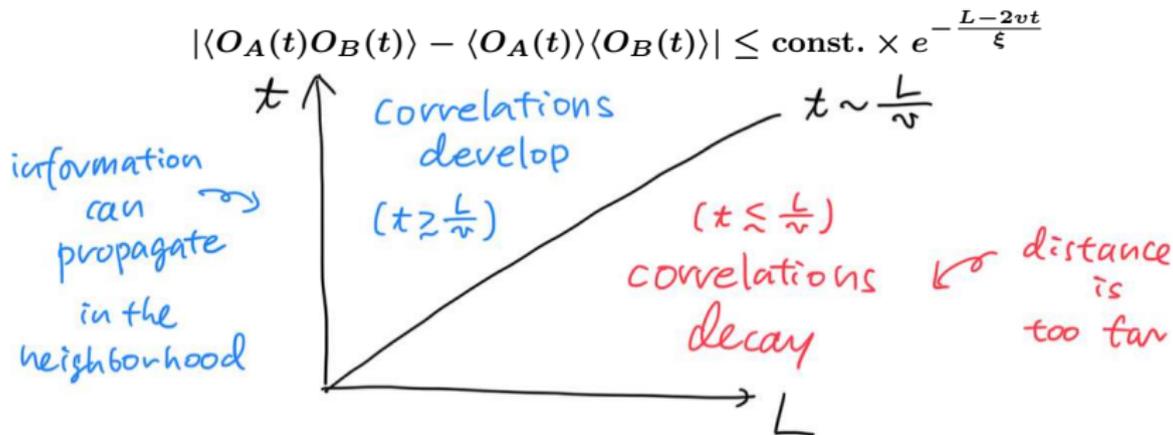
- $O_A(t) = e^{iHt}O_Ae^{-iHt}$ ,  $L$ : distance between  $A$  and  $B$ ,  $\xi$ : const.
- $v$ : Lieb-Robinson bound



- Information from  $A$  is transmitted to  $B$  up to  $t \sim L/v$
- It tells the **presence of bound**, but not the value itself

## Light-cone-like spreading of time-dependent correlations

- Corollary: For a state with finite correlation length  $\xi$ 
  - Bound for **any** equal-time correlations:  
[S.Bravyi et al., PRL.97.050401('06)]

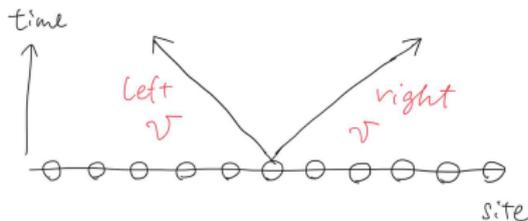


- Velocity  $v$ : Lieb-Robinson bound
- Exact Lieb-Robinson bound is known only for a few lattice models (e.g. 1D systems)
- Lieb-Robinson bound gets tighter very recently  
[Z.Wang, K.R.A.Hazzard, PRXQuant.1.010303('20)]

## How to get/estimate Lieb-Robinson velocity

- Bound for **any** equal-time correlations: [S.Bravyi et al., PRL.97.050401('06)]

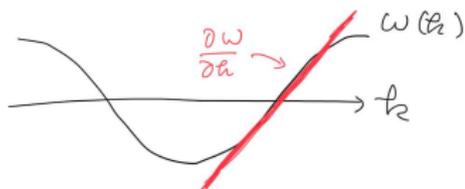
$$|\langle O_A(t)O_B(t) \rangle - \langle O_A(t) \rangle \langle O_B(t) \rangle| \leq \text{const.} \times e^{-\frac{L-2vt}{\xi}}$$



- Intuitively, prefactor **2** comes from left and right moving quasiparticles

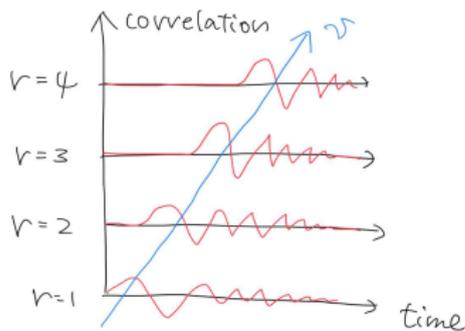
From dispersion

- $v = \max_k \frac{d\omega(k)}{dk}$
- In 1D TFIing,  $\omega(k)$  is exactly known and the exact  $v$  is obtained
- Precise shape of dispersion  $\omega(k)$  is not known in general



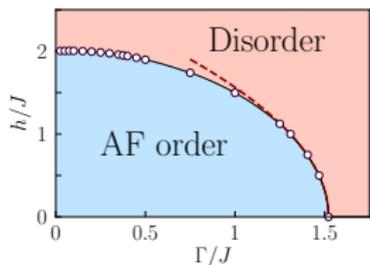
From peak localtions in correlations

- $v_{\text{experiment}} = 2v$
- Useful in experiments



## Numerical setup: Transverse-field Ising model

- Ground-state phase diagram in 2D [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  
 → 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  $|\rightarrow\rightarrow\cdots\rangle$



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

$$\begin{aligned} \Gamma_{c,1D}/J &= 0.5 \\ \Gamma_{c,2D}/J &\approx 1.522 \end{aligned}$$

- How does the group velocity for spin correlations look?

## Numerical setup: Considered dimensions and methods

---

Estimate  $v_{\text{experiment}} = 2v$  numerically from peak locations

For comparison, we also consider the 1D case

	exact	tensor network	spin wave approx.
1D	✓	✓(MPS*)	✓
2D	✗	✓(iPEPS)	✓

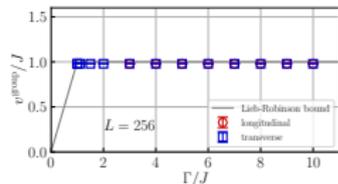
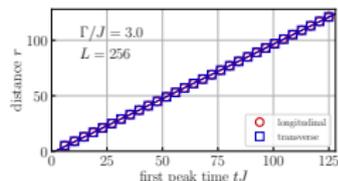
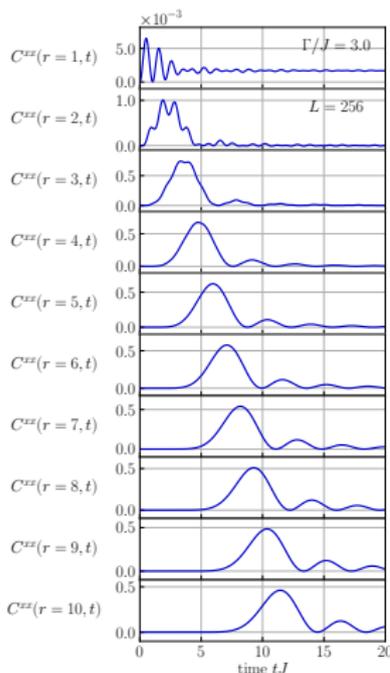
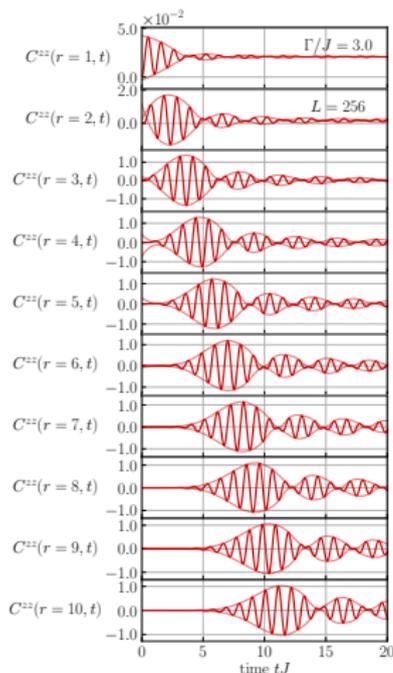
\* The data is not shown because it was consistent with the exact result

- 1D, exact
  - Jordan-Wigner transformation: Spin  $\rightarrow$  Fermion
  - Time-dependent correlations: Pfaffian ( $= \pm\sqrt{\text{determinant}}$ ) of the matrix containing two-body correlations of fermions
- 1D, 2D, spin wave approx.
  - Holstein-Primakoff transformation: Spin  $\rightarrow$  Boson (magnon)
  - Time-dependent correlations: Function of magnon dispersions

# Numerical results: 1D, exact

$$C^{zz}(r, t) = \langle \psi(t) | \hat{S}_r^z \hat{S}_0^z | \psi(t) \rangle$$

$$C^{xx}(r, t) = \langle \psi(t) | \hat{S}_r^x \hat{S}_0^x | \psi(t) \rangle - \langle \psi(t) | \hat{S}_r^z | \psi(t) \rangle \langle \psi(t) | \hat{S}_0^z | \psi(t) \rangle$$



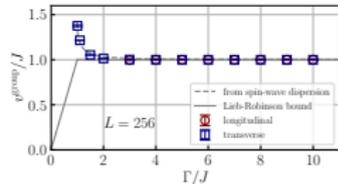
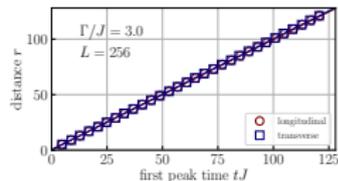
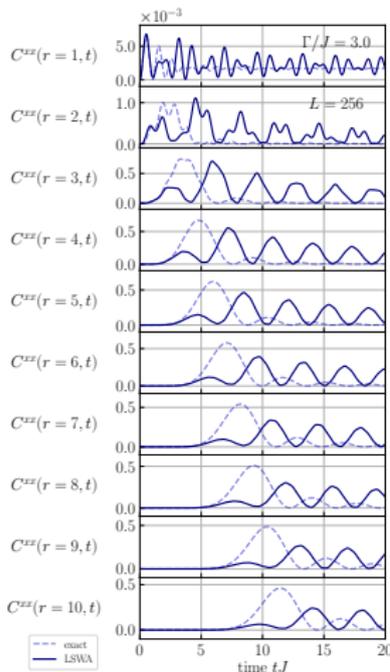
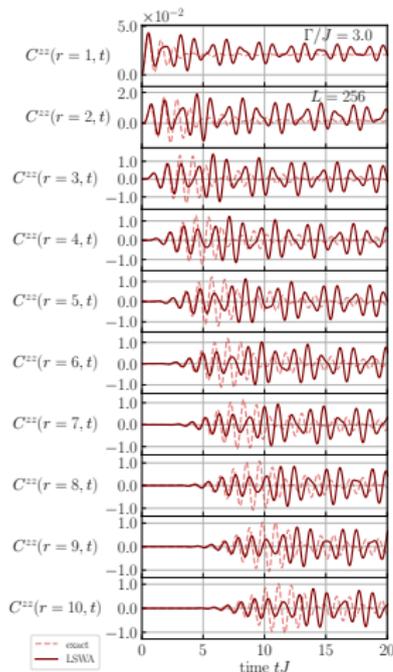
- Light-cone-like spreading of correlations
- Group velocity of spin-spin correlations = Lieb-Robinson velocity ( $v/J = 1$ )
- Quasiparticles with the fastest propagation velocity are responsible for the spreading of spin-spin correlations

# Numerical results: 1D, approximate method

## Focus on the spin wave approx.

$$C^{zz}(r, t) = \langle \psi(t) | \hat{S}_r^z \hat{S}_0^z | \psi(t) \rangle$$

$$C^{xx}(r, t) = \langle \psi(t) | \hat{S}_r^x \hat{S}_0^x | \psi(t) \rangle - \langle \psi(t) | \hat{S}_r^y | \psi(t) \rangle \langle \psi(t) | \hat{S}_0^y | \psi(t) \rangle$$

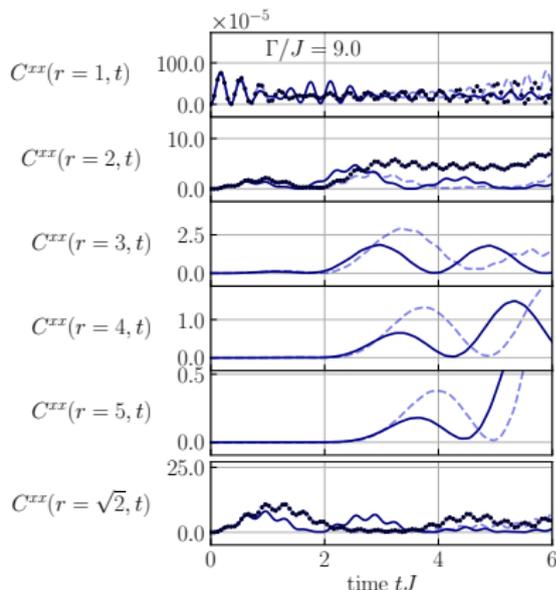
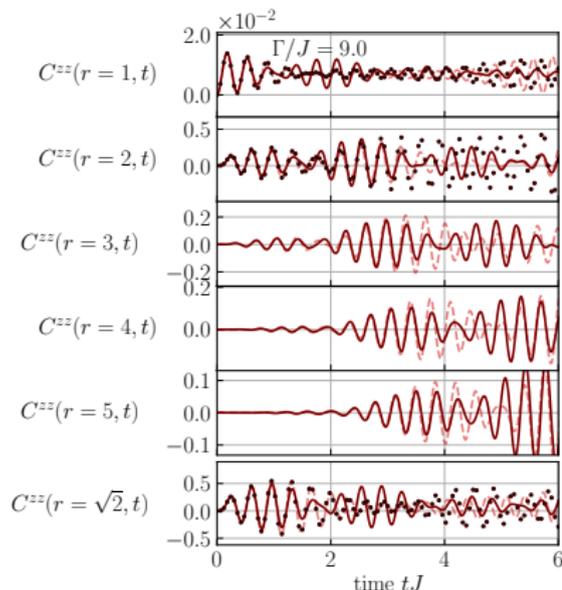


- Accurate up to the point where they begin to increase
- Group velocity of spin-spin correlations  $\rightarrow$  Lieb-Robinson velocity ( $v/J = 1$ ) when  $\Gamma \gg J$
- For a small quench ( $\Gamma = \infty$  to  $\Gamma \gg J$ ), few quasiparticles are involved, and SW approx. is good

# Numerical results: 2D, spin wave approx. (should be good for higher dimensions)

$$C^{zz}(r, t) = \langle \psi(t) | \hat{S}_r^z \hat{S}_0^z | \psi(t) \rangle$$

$$C^{xx}(r, t) = \langle \psi(t) | \hat{S}_r^x \hat{S}_0^x | \psi(t) \rangle - \langle \psi(t) | \hat{S}_r^y | \psi(t) \rangle \langle \psi(t) | \hat{S}_0^y | \psi(t) \rangle$$



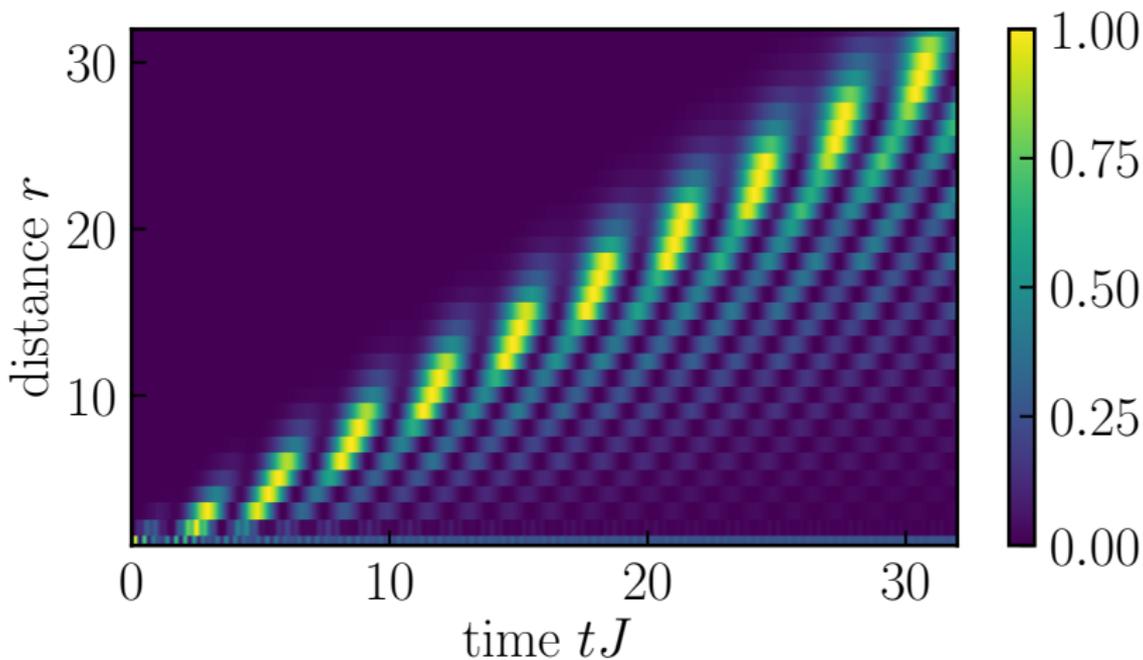
--- PEPS,  $D_{\text{virt}} = 8$     ● ED,  $N_s = 5 \times 5$     — LSWA,  $N_s = 128 \times 128$

--- PEPS,  $D_{\text{virt}} = 8$     ● ED,  $N_s = 5 \times 5$     — LSWA,  $N_s = 128 \times 128$

Agreement is slightly better than in 1D

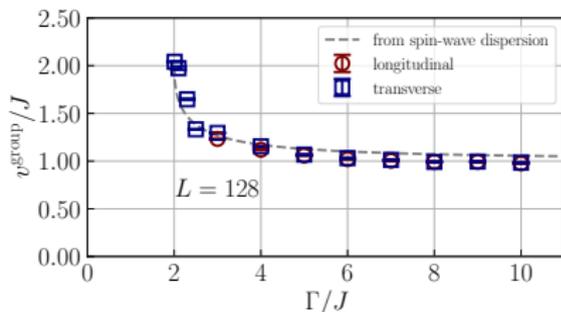
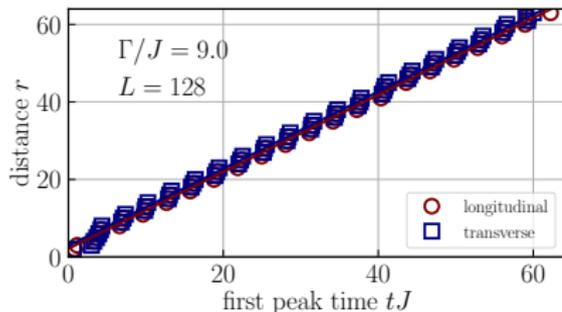
## Numerical results: 2D, spin wave approx.

normalized correlation function  
 $C^{xx}(r, t) / \max_{t \in [0, L/(2J)]} C^{xx}(r, t) \in [0, 1]$



Areas of high intensity are not continuously connected  
(Complex interference effects in 2D?)

## Numerical results: 2D spin wave approx.



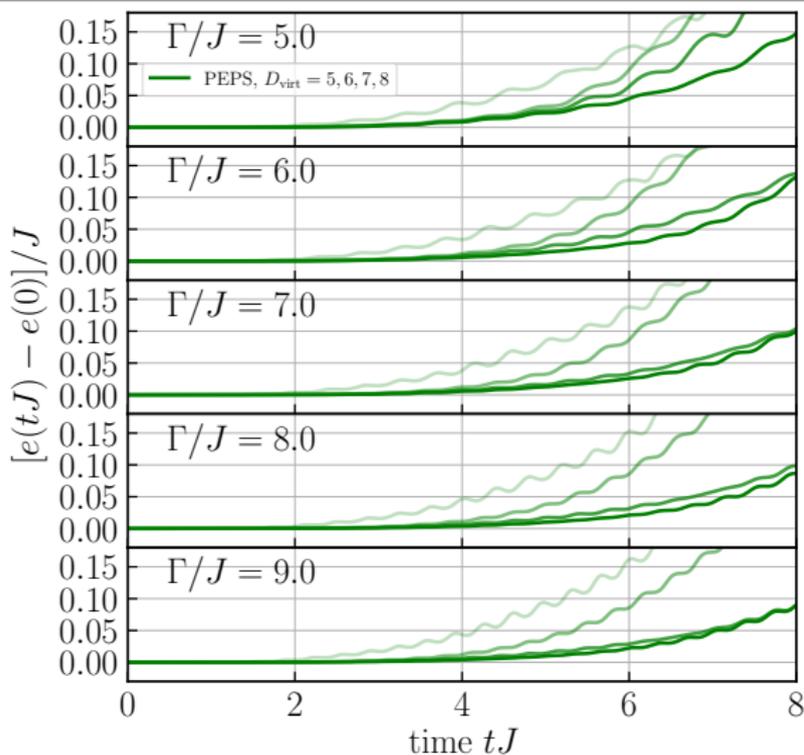
- Light-cone-like spreading of correlations in 2D as well
- For  $\Gamma/J \gg 1$ , the group velocity estimated from the peak location is  $v/J \approx 1$
- The group velocity estimated from the SW dispersion

$$\Omega_{\mathbf{k}} = \sqrt{\Gamma^2 - \frac{z}{2}\Gamma J \gamma_{\mathbf{k}}} \quad (\gamma_{\mathbf{k}} = \frac{1}{D} \sum_{\nu=1}^D \cos k_{\nu}, \quad z = 2D, \quad D: \text{dimension})$$

$$v^{\text{SW}}/J = (1 - J/\Gamma + \sqrt{1 - 2J/\Gamma})^{-1/2} / \sqrt{2},$$

which also approaches  $v/J \approx 1$  for  $\Gamma/J \gg 1$

## Numerical results: 2D, iPEPS

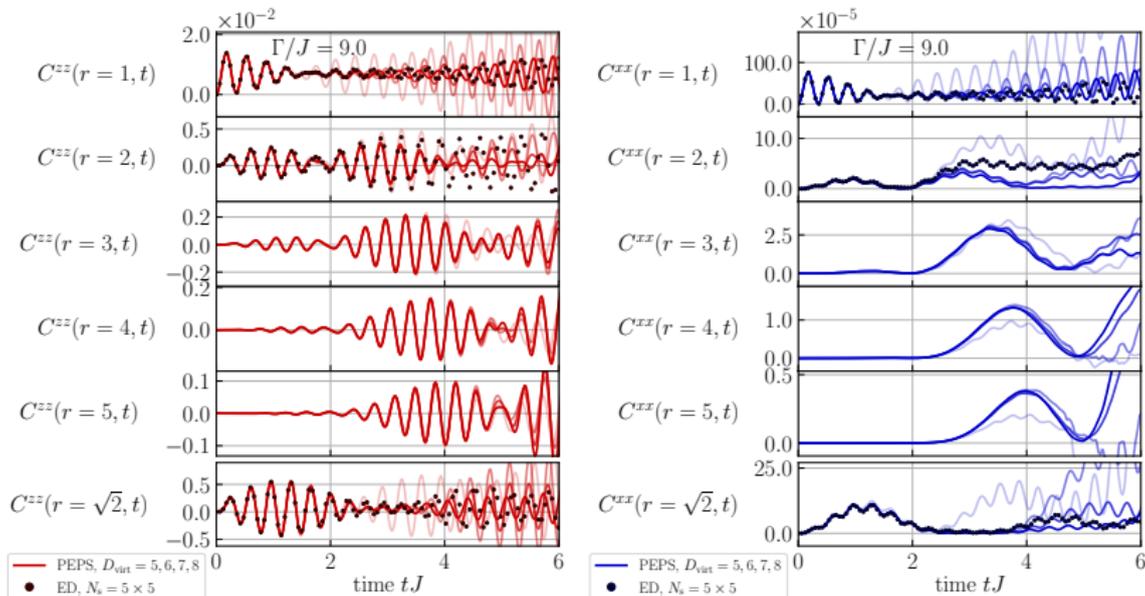


The energy is nearly conserved for  $D_{\text{virt}} \geq 6$   
in a time frame  $tJ \in [0, 4]$

## Numerical results: 2D, iPEPS

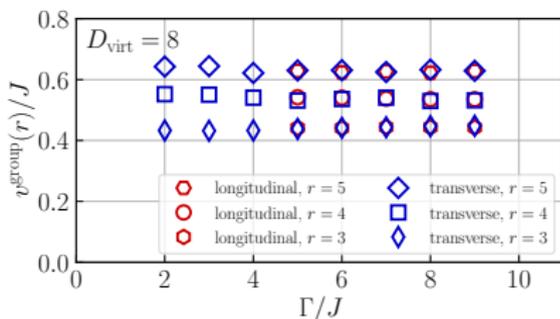
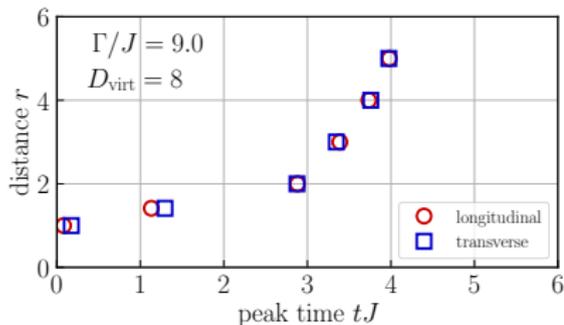
$$C^{zz}(r, t) = \langle \psi(t) | \hat{S}_r^z \hat{S}_0^z | \psi(t) \rangle$$

$$C^{xx}(r, t) = \langle \psi(t) | \hat{S}_r^x \hat{S}_0^x | \psi(t) \rangle - \langle \psi(t) | \hat{S}_r^x | \psi(t) \rangle \langle \psi(t) | \hat{S}_0^x | \psi(t) \rangle$$



Distances longer than those by the exact diagonalization method are calculable

## Numerical results: 2D, iPEPS



- Since the energy is conserved for a short time, accessible time is limited
- Not easy to estimate the group velocity from iPEPS data
- Assume light-cone-like spreading of correlations (as in SW approx.) exists and the peak location eventually grows linearly with the peak time
- Estimate  $v = r/t(r)$  for each distance  $r$ :  $v/J \in [0.86, 1.3]$

## Comparison of group velocities $v/J$ at $\Gamma/J \gg 1$

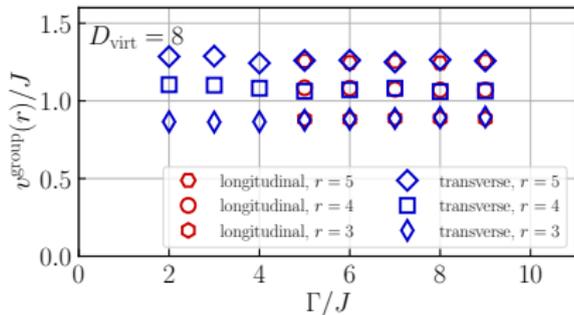
	from dispersion (fermion or magnon)	from peak location ( $C^{zz,xx}(\mathbf{r})$ )	from recent inequality* (any correlations)
1D, exact	<b>1 (exact)</b>	<b>1.0</b>	<b><math>\leq 3.02</math></b>
1D, SW	<b>1.0</b>	<b>1.0</b>	
2D, PEPS	N/A	$\in [0.86, 1.3]$	<b><math>\leq 5.672</math></b>
2D, SW	<b>1.0</b>	<b>1.0</b>	

\* [Z.Wang,K.R.A.Hazzard,PRXQuant.1.010303('20)]

- In 1D, the spin correlation provides the group velocity corresponding to the fastest quasiparticle (identical to exact Lieb-Robinson bound)
- If this is so in 2D as well, LR bound in 2D TFIsing would also be  $v/J = 1 \rightarrow$  **Room for improvement in LR bound?**

## 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:  $v_{\text{spin}}/J \sim 1$
- This is much smaller than the current best Lieb-Robinson bound:  $v_{\text{LR,horiz}}/J = 5.672$
- Our group velocity and spin correlations are helpful for crosschecking experimental data

R. Kaneko and I. Danshita, Phys. Rev. A 108, 023301 (2023)