2PI strong coupling approach to out of equilibrium dynamics of the clean and disordered Bose Hubbard model

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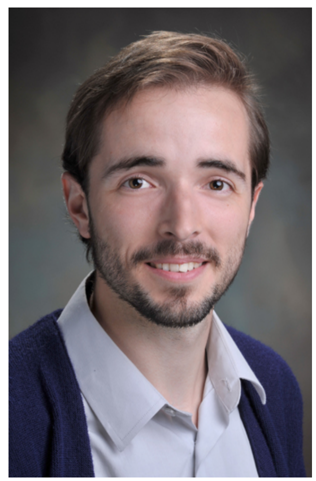


A. Mokhtari-Jazi and M. K., Phys. Rev. A 111, 043313 (2025).
A. Mokhtari-Jazi, M. Fitzpatrick and M. K., Nucl. Phys. B 997, 116386 (2023).
A. Mokhtari-Jazi, M. Fitzpatrick and M. K., Phys. Rev. A 103, 023334 (2021).
M. Fitzpatrick and M. K., Phys. Rev. A 98, 053618 (2018).
M. Fitzpatrick and M. K., Nucl. Phys. B 930, 1 (2018).

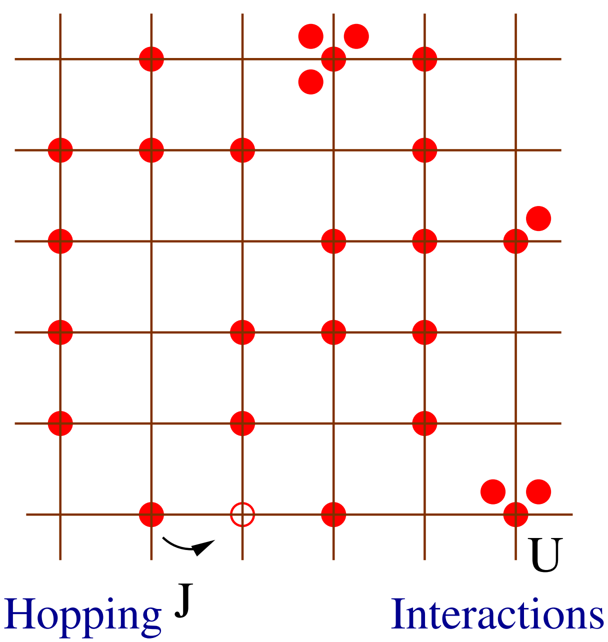
Motivation

- Experimental observations of out of equilibrium dynamics in the Bose Hubbard model (BHM)
  - Correlation spreading in 1D and 2D
  - Slow dynamics (Many Body Localization?) in disordered BHM in 2D
- Exact analytical and numerical methods give a good account of correlations in 1D
  - In higher dimensions, other methods are required

Bose Hubbard model

$$\hat{H}_{\mathrm{BHM}} = -J \sum_{<ij>} \left(\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i \right) - \mu \sum_j \hat{n}_j + \frac{U}{2} \sum_j \hat{n}_j (\hat{n}_j - 1),$$

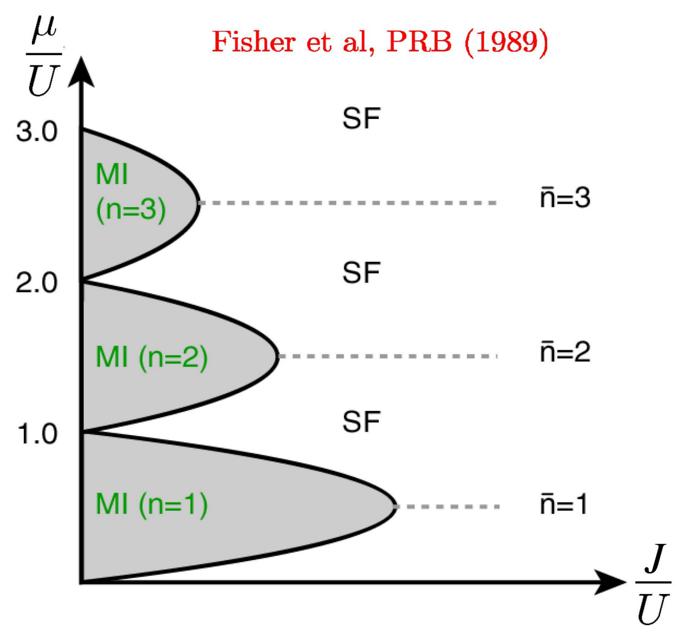
Hopping J, Chemical potential μ, Interaction strength U



- Cold atoms: can tune lattice depth V to vary J/U

Phase Diagram

- $U \ll J$: Superfluid
- $J = 0$: Mott insulator
- Finite J/U: Mott insulator to Superfluid transition

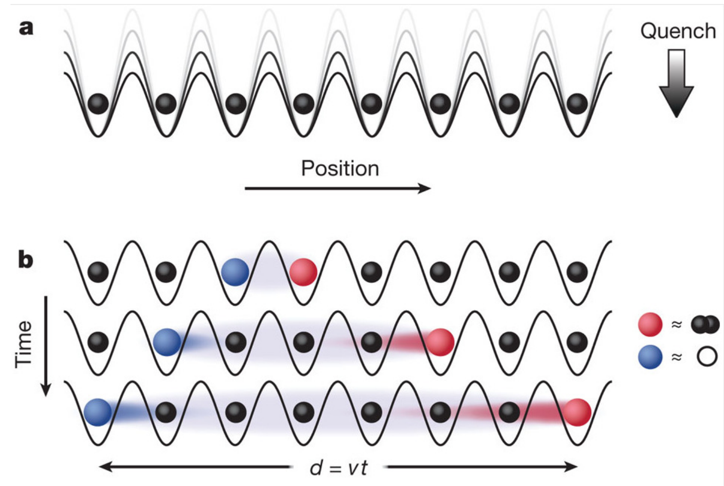


Correlation spreading after a quench

- **Single-site imaging of cold atoms allows imaging of correlations**

Lieb-Robinson bound:
Maximum speed for information spreading in a non-relativistic quantum system
[Lieb and Robinson, Commun. Math. Phys. (1972)]

Bose-Hubbard model:
Rigorous bounds for special initial states but not in general



[Cheneau *et al.*, Nature (2012)]

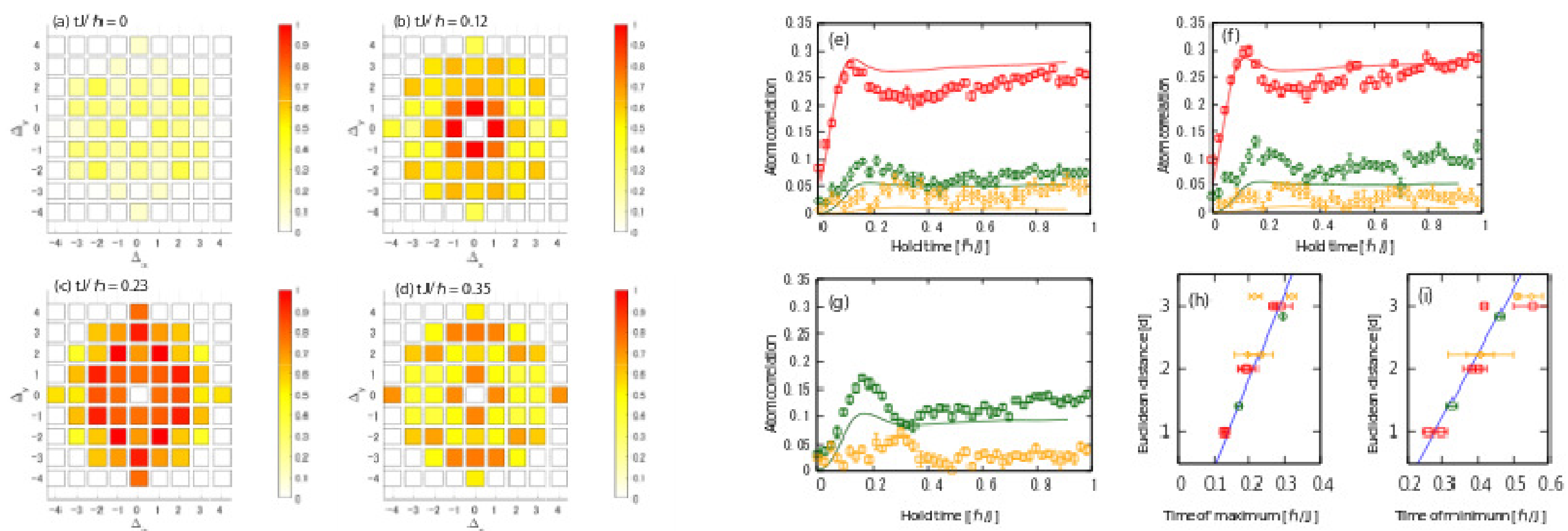
MI to MI quenches:

- Light-cone-like spreading of correlations in 1D systems
  Barmettler *et al.*, PRA 85, 053625 (2012); Cheneau *et al.* Nature 481, 484 (2012)

$$v_{\max}^{D=1} \simeq \frac{6Jd}{\hbar}\left[1 - \frac{16J^2}{U^2}\right]$$

Spreading of single particle correlations in $D = 2$

- Experiments on correlation spreading in $D = 2$: [Takasu *et al.*, Sci. Adv. **6**, eaba9255 (2020)]



- Propagation velocities extracted from first peak and trough:

$$v^{\rm peak} = 13.7(2.1)Jd/\hbar, \qquad v^{\rm trough} = 10.2(1.4)Jd/\hbar$$

- Estimates for $D = 2$:

$$v \simeq \frac{6Jd\sqrt{D}}{\hbar} \simeq 8.4Jd/\hbar$$

[Krutitsky *et al.*, Eur. Phys. J. Quant. Tech. **1**, 12 (2014)]

$$v = 8.1Jd/\hbar$$

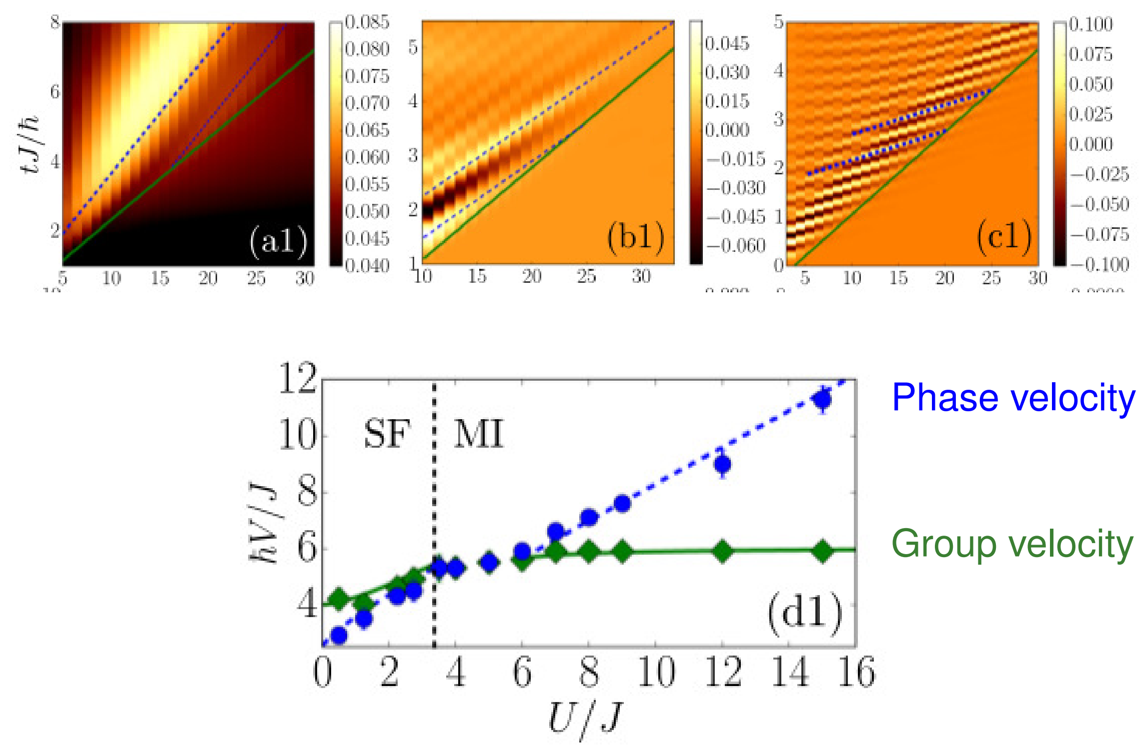
[Fitzpatrick and Kennett, PRA **98**, 053618 (2018)]

How do we reconcile this discrepancy?

Phase and group velocity in the BHM

- Takasu *et al.* suggested that the explanation is that there are two velocities, phase and group velocity and they observe the phase velocity

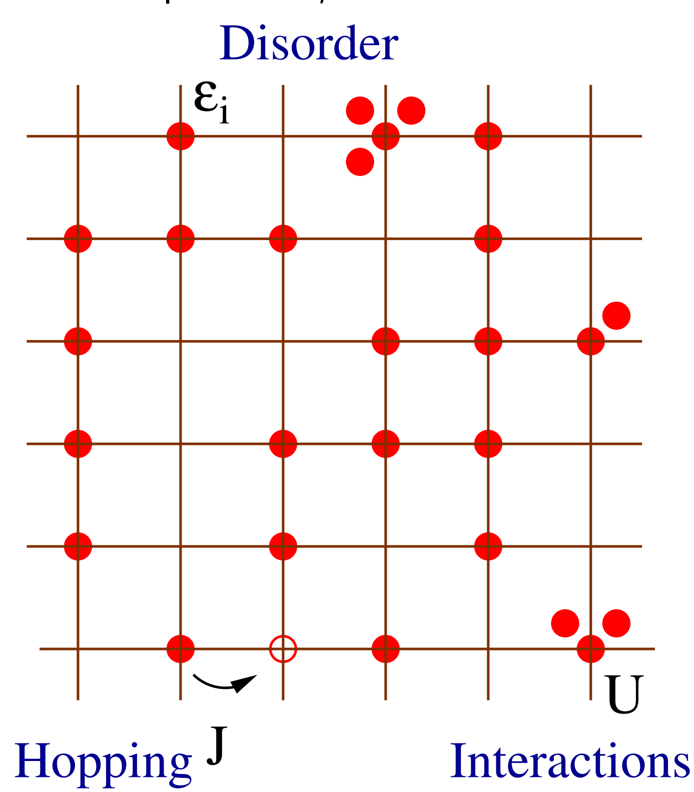
Spreading of single particle correlations in $D = 1$ calculated with MPS
[Despres *et al.*, Sci. Rep. 9, 4135 (2019)]



Disordered Bose Hubbard model

$$\hat{H}_{\mathrm{BHM}} = -J \sum_{<ij>} \left(\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i \right) + \sum_i \varepsilon_i \hat{n}_i + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i,$$

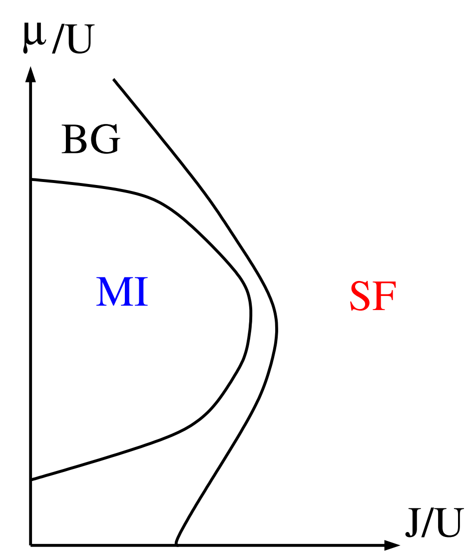
Hopping J, On-site disorder ε_i,
Interaction strength U,
Chemical potential μ



Phase Diagram

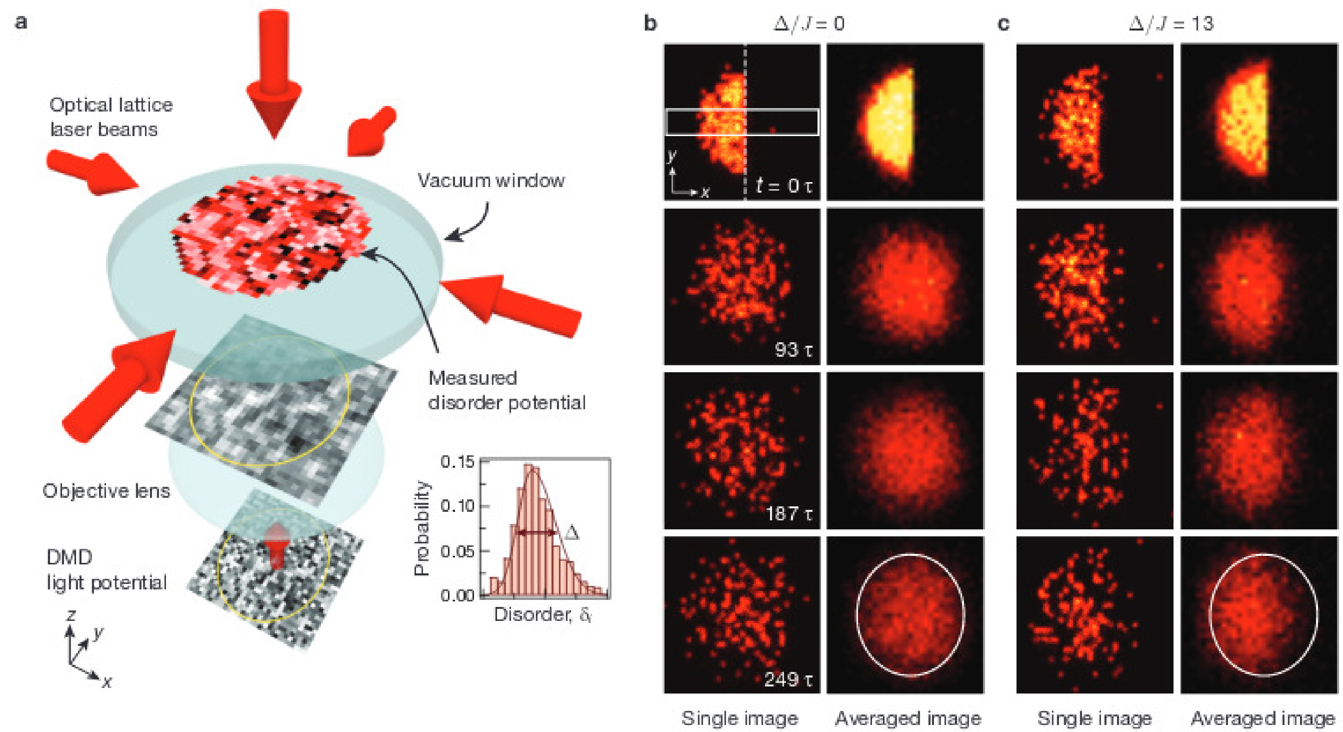
- $U \ll J$: Superfluid
- $J = 0$: Mott insulator
- Finite J/U: Mott insulator to Superfluid transition

Bose Glass?



Disordered BHM in two dimensions

- Disordered Bose Hubbard model in a 2 dimensional optical lattice:
  Choi *et al.*, Science **352**, 1547 (2016)



Started from an imbalanced initial condition, studied persistence of imbalance as a function of disorder strength (Δ/J)

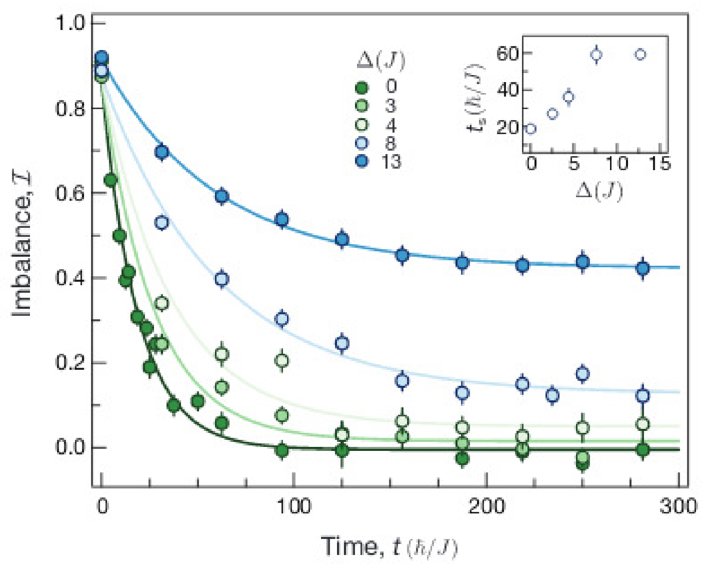
Evidence of a lack of thermalization? Many body localization (MBL)?

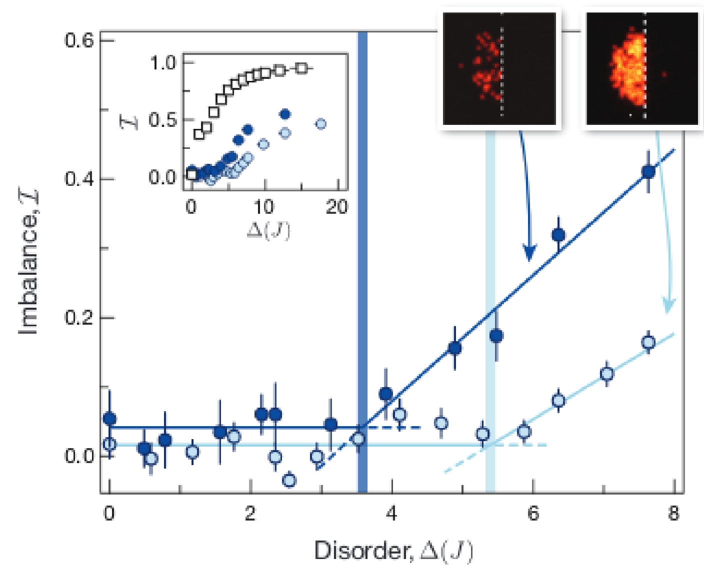
Does MBL exist in dimensions > 1? Experiment

- Imbalance

$$\mathcal{I} = \frac{N_L - N_R}{N_L + N_R}$$

as a function of time and disorder strength





- Potential MBL transition as a function of Δ/J

2PI Strong Coupling (2PISC) Formalism

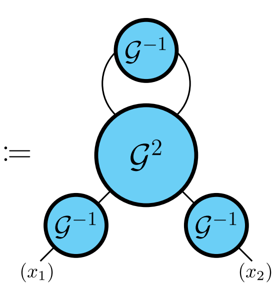
- Want to calculate equations of motion for:
  - Superfluid order parameter $\phi_i^a(t) = \langle \hat{a}_i^a(t) \rangle$
  - Two point Green's function $G_{ij}(t_1, t_2) = -i \left\langle \hat{a}_i(t_1)\hat{a}_j^\dagger(t_2) \right\rangle$

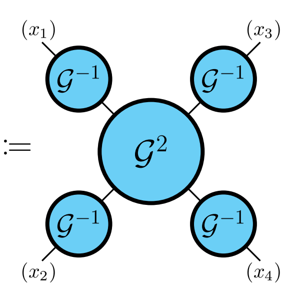
- Interacting out of equilibrium quantum problem: convenient to use closed time path techniques in conjunction with 2PI approach
  - Allows for zero temperature and finite temperature in the same formalism, also disorder averaging

- Generalize strong-coupling approach using two Hubbard-Stratonovich transformations $\Longrightarrow$ allows description of both SF and MI phases

- Action truncated to quartic order (z and a fields have same correlations)

$$S_{\mathrm{BHM}}[a] = \frac{1}{2!}\left(2J_{x_1x_2} + \left[\mathcal{G}^{-1}\right]_{x_1x_2} + \tilde{u}_{x_1x_2}\right) z_{x_1}z_{x_2} + \frac{1}{4!}u_{x_1\ldots x_4}z_{x_1}z_{x_2}z_{x_3}z_{x_4}$$

$\tilde{u}_{x_1x_2} :=$ 

$u_{x_1x_2x_3x_4} :=$ 

$\mathcal{G}$, $\mathcal{G}^{2c}$: atomic ($J = 0$) limit connected 1 and 2 particle Green's functions

- u-vertex generates "physical" and "anomalous" diagrams (those with internal lines of $\mathcal{G}^{-1}$) with anomalous terms cancelled by $\tilde{u}$ vertex

2PI Equations of Motion

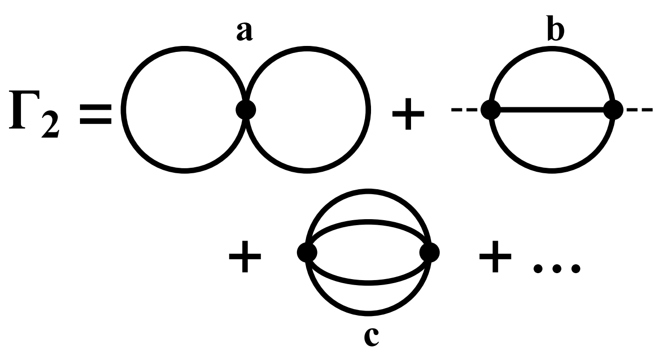
- Define mean field $\mathcal{V}^{\chi_1} = \langle \Phi^{\chi_1} \rangle$ and full propagator $i\mathcal{V}^{\chi_1\chi_2,c} = \langle \Phi^{\chi_1}\Phi^{\chi_2} \rangle$
- Equations of motion [Cornwall *et al.*, PRD **10**, 2428 (1974)]

$$0 = \frac{\delta S}{\delta \mathcal{V}^{\chi_1}} + \frac{i}{2}\left[\frac{\delta [D^{-1}]^{\chi_1\chi_2}}{\delta \mathcal{V}^{\chi_1}} \mathcal{V}^{\chi_1\chi_2,c}\right]$$

$$\left[\mathcal{V}^{-1}\right]^{\chi_1\chi_2,c} = \left[D^{-1}\right]^{\chi_1\chi_2} - \left[\Sigma^{(2PI)}\right]^{\chi_1\chi_2} \qquad \text{(Dyson's Equation)}$$

Action $S[\mathcal{V}^{\chi}]$; Inverse "bare" propagator $i\left[D^{-1}\right]^{\chi_1\chi_2} \equiv \frac{\delta^2 S[\mathcal{V}^{\chi}]}{\delta \mathcal{V}^{\chi_1}\delta \mathcal{V}^{\chi_2}}$

2PI Self energy: $\left[\Sigma^{(2PI)}\right]^{\chi_1\chi_2} = 2i\frac{\delta \Gamma_2\left[\mathcal{V}^{\chi}, \mathcal{V}^{\chi\chi',c}\right]}{\delta \mathcal{V}^{\chi_1\chi_2,c}}$



- : Interaction vertex

— : Propagator G

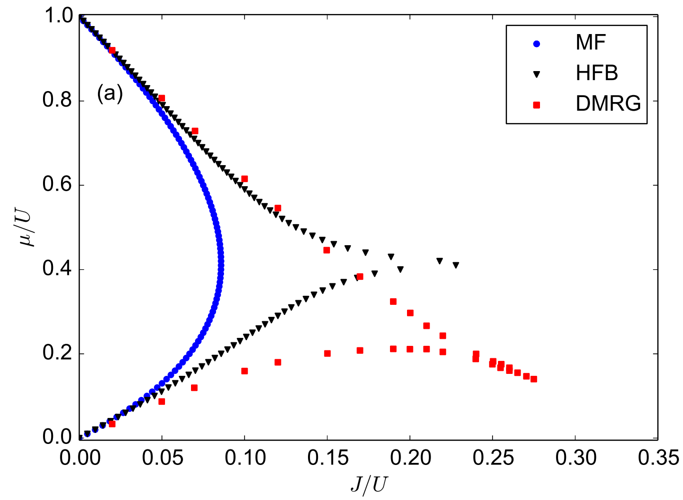
--: Mean field ϕ

Hartree-Fock Bogoliubov (HFB) approximation: only keep diagram "a"

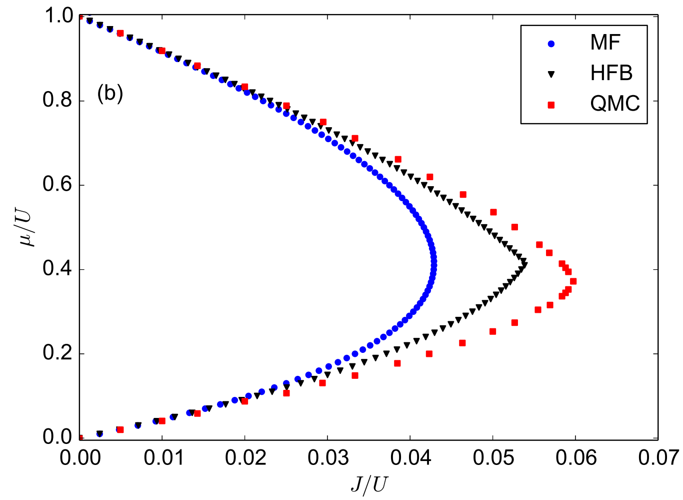
Equilibrium Results: no disorder

M. Fitzpatrick and M. K., Nucl. Phys. B 930, 1 (2018)

$d = 1$



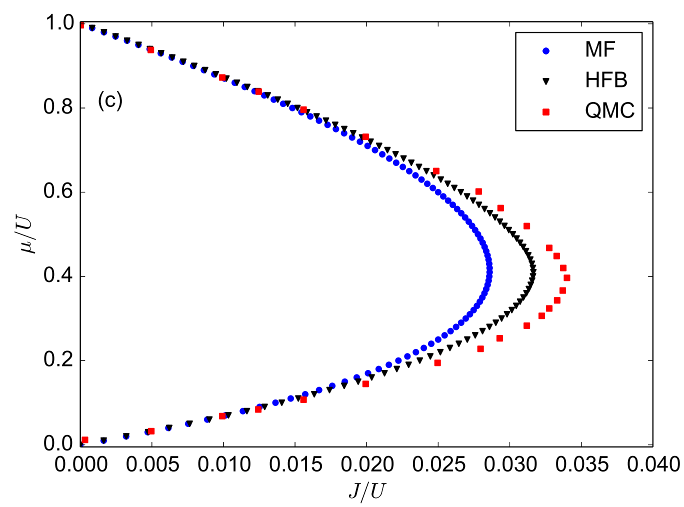
$d = 2$



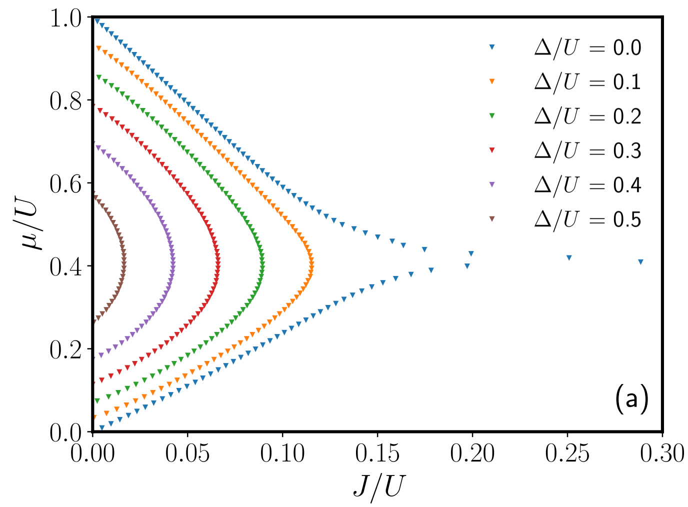
- $T = 0$ phase boundary
  HFB vs MF and exact results

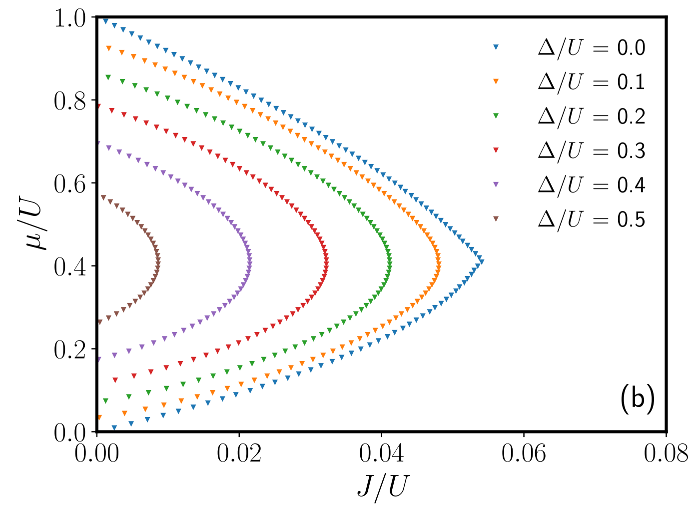
$d = 1$ DMRG:
PRB 58, 14741(R) (1998)
$d = 2$ QMC:
PRA 77, 015602 (2008)
$d = 3$ QMC:
PRA 75, 134302 (2008)

$d = 3$



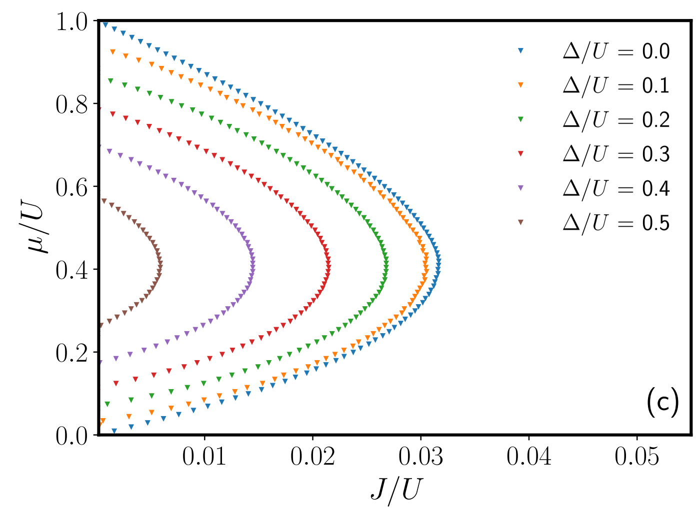
Effect of disorder on Mott insulator phase boundary





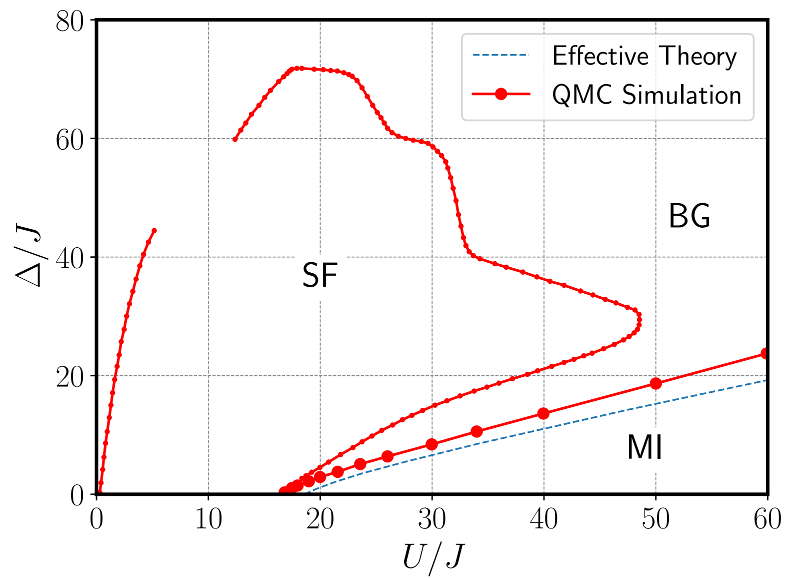
- $T = 0$ Mott insulator phase boundary

a) $d = 1$
b) $d = 2$
c) $d = 3$



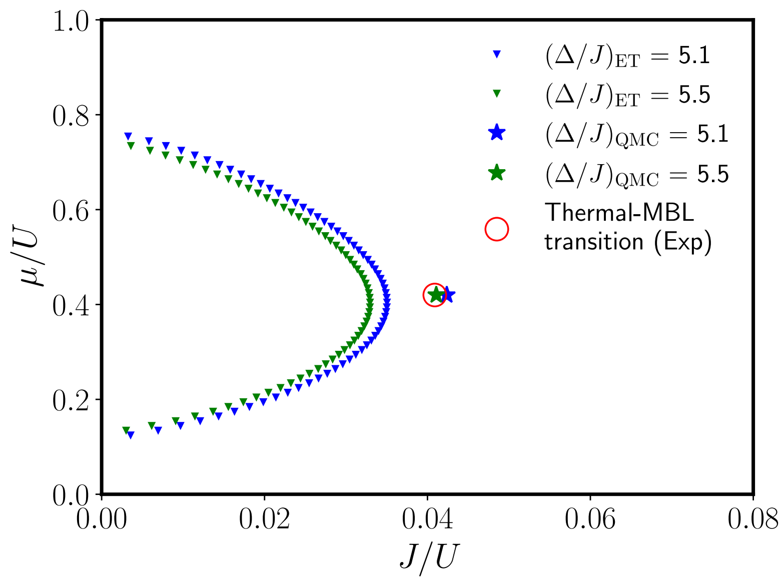
Comparison to Quantum Monte Carlo

$D = 2$



S. G. Söyler *et al.*, PRL **107**, 185301 (2011)

MBL in $D = 2$?



Putative MBL transition found by Choi *et al.*

appears to match MI-BG transition

Out of Equilibrium Results

- Focus on special case of quenches within MI regime

$$\Longrightarrow \langle \Phi^{(\dagger)}_{r_1,\alpha_1}(t_1)\rangle = \langle \Phi_{r_1,\alpha_1}(t_1)\Phi_{r_2,\alpha_2}(t_2)\rangle = \langle \Phi^{\dagger}_{r_1,\alpha_1}(t_1)\Phi^{\dagger}_{r_2,\alpha_2}(t_2)\rangle = 0$$

- Calculate single particle density matrix

$$\rho_1\left(\Delta\mathbf{r} = \mathbf{r}_i - \mathbf{r}_j, t\right) = \left\langle \hat{a}^{\dagger}_{\mathbf{r}_i}(t)\hat{a}_{\mathbf{r}_j}(t)\right\rangle,$$

- On a lattice can be written as

$$\rho_1\left(\Delta\vec{r}, t\right) \; = \tfrac{1}{2N_s}\sum_{\vec{k}} \cos\left(\vec{k}\cdot\Delta\vec{r}\right)\left\{iG^{(K)}_{\vec{k}}\left(t,t\right) - 1\right\},$$

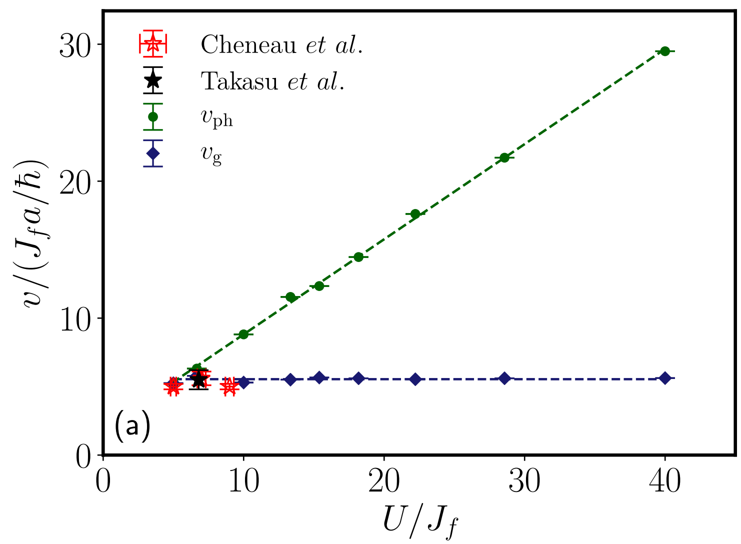
N_s: number of sites, $G^{(K)}_{\vec{k}}\left(t,t\right)$ is the equal time kinetic Green's function

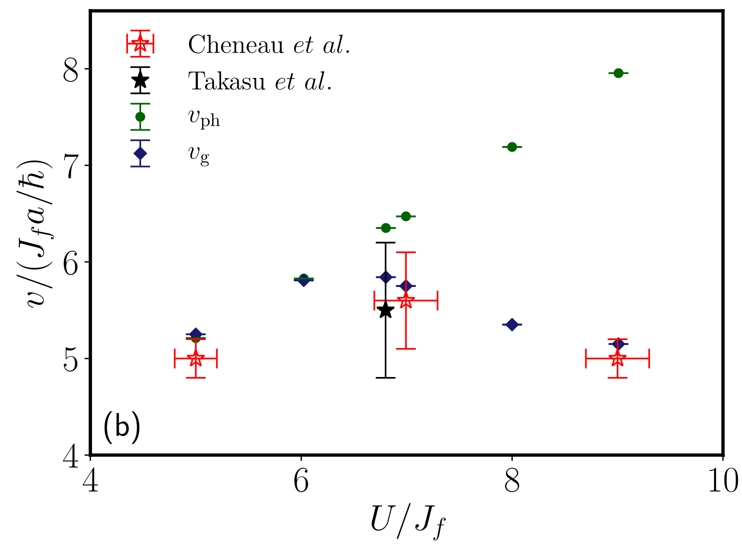
- Benchmarking:
  Agreement with exact results in 1 dimension
  [M. Fitzpatrick and M. K., Phys. Rev. A 98, 053618 (2018)]

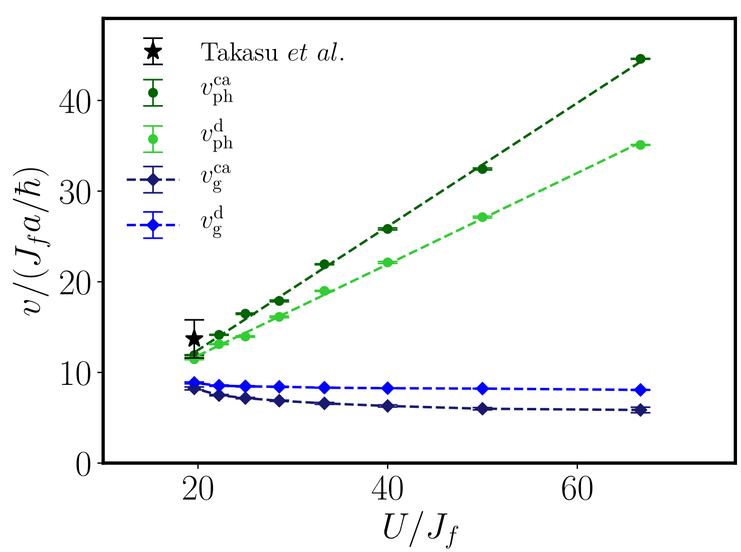
- Determine spreading of correlations after a quench: hopping $J_i \to J_f$

Phase and Group velocity in 1 and 2 D

Excellent agreement with experiments in 1d



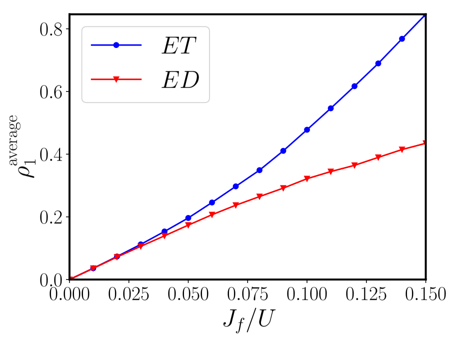


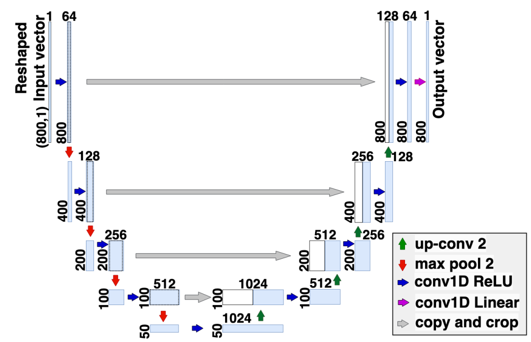


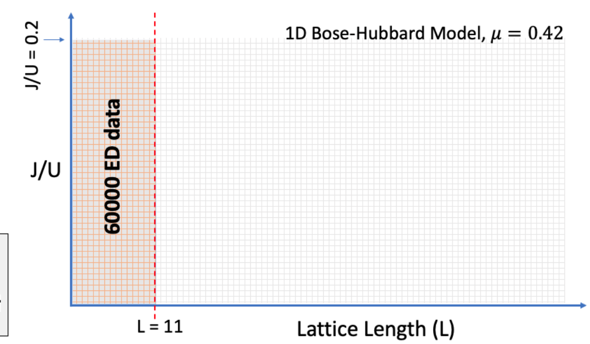
- Clear agreement between phase velocity and experiments in 2d
- Anisotropy in both phase (ph) and group (g) velocities between diagonal (d) and crystal axes (ca)

Machine learning out of equilibrium dynamics

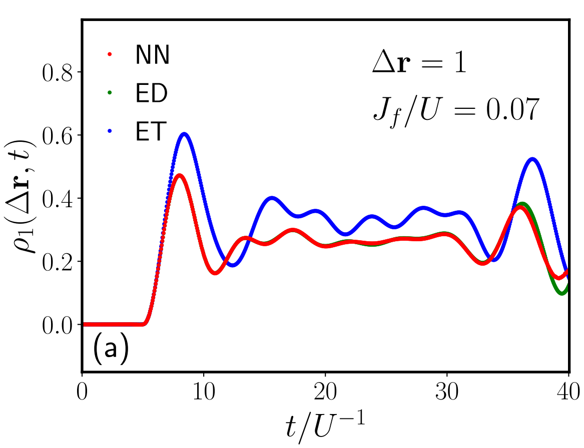
- Effective theory (ET) calculates phase accurately, less so for amplitude of single particle density matrix close to MI-SF transition
- Trained U-net neural network to take effective theory input to exact diagonalization output

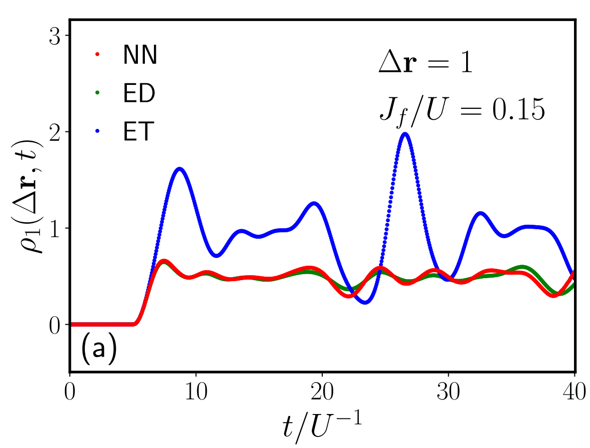






$D = 1$, $L = 14$, $J_f = 0.07$ and $L = 13$, $J_f = 0.15$ (outside training region)
– Large improvement over ET up to at least twice largest training size





Summary and Future Work

- Developed 2PI approach to study out of equilibrium correlations in the Bose Hubbard model

- Can be generalized to include disorder – equilibrium results match well with exact results

- Good agreement with speed with which correlations spread experimentally in 1 and 2 dimensions

- Out of equilibrium dynamics from effective theory can be improved with machine learning

- Future directions: multi-component BHM, extended BHM

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