Emergent eigenstate solution to quantum dynamics far from equilibrium

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1. **Introduction**
   - An experiment with ultracold bosons in 1D lattices
     - Emergence of quasi-condensates at finite momentum

2. **Emergent eigenstate solution**
   - Noninteracting fermions and related models
   - Geometric quantum quench and emergent Hamiltonian

3. **Emergent Gibbs ensemble**
   - Effective cooling during the melting of a Mott insulator
   - Emergent Gibbs ensemble

4. **Fully interacting example**
   - Spinless fermions with nearest neighbor interactions (XXZ chain)

5. **Summary**
Experiments in the 1D regime

Effective one-dimensional $\delta$ potential
M. Olshanii, PRL 81, 938 (1998).

$$U_{1D}(x) = g_{1D} \delta(x)$$

where

$$g_{1D} = \frac{2\hbar a_s \omega_\perp}{1 - C a_s \sqrt{m \omega_\perp / 2\hbar}}$$

Lieb & Liniger ’63, Girardeau ’60 ($g_{1D} = \infty$)

$n(p)$: Momentum distribution
$n(x)$: Density distribution
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Lieb, Schulz, and Mattis ’61 ($U/J = \infty$)

B. Paredes et al.,

$n(p)$: Momentum distribution $\Leftrightarrow$

$n(x)$: Density distribution $\Leftrightarrow$
Emergence of quasi-condensates at finite momentum


Predicted theoretically in:
Emergence of quasi-condensates at finite momentum


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Introduction

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1. Spinless fermions with nearest neighbor interactions (XXZ chain)

Summary
Bose-Fermi mapping in a 1D lattice \((U \gg J)\)

Hard-core boson Hamiltonian in an external potential

\[
\hat{H} = -J \sum_i \left( \hat{b}_i^\dagger \hat{b}_{i+1} + \text{H.c.} \right) + \sum_i v_i \hat{n}_i
\]

Constraints on the bosonic operators

\[
\hat{b}_i^\dagger^2 = \hat{b}_i^2 = 0
\]
Bose-Fermi mapping in a 1D lattice \((U \gg J)\)

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\[\downarrow\]

Map to spins and then to fermions (Jordan-Wigner transformation)

\[
\hat{\sigma}_i^+ = \hat{f}_i^\dagger \prod_{\beta=1}^{i-1} e^{-i\pi \hat{f}_\beta^\dagger \hat{f}_\beta}, \quad \hat{\sigma}_i^- = \prod_{\beta=1}^{i-1} e^{i\pi \hat{f}_\beta^\dagger \hat{f}_\beta} \hat{f}_i
\]

\[\downarrow\]

Non-interacting fermion Hamiltonian

\[
\hat{H}_F = -J \sum_i \left( \hat{f}_i^\dagger \hat{f}_{i+1} + \text{H.c.} \right) + \sum_i v_i \hat{n}_i^f
\]
One-body density matrix

One-body Green’s function

\[ G_{ij} = \langle \Psi_{HCB} | \hat{\sigma}_i^- \hat{\sigma}_j^+ | \Psi_{HCB} \rangle = \langle \Psi_F | \prod_{\beta=1}^{i-1} e^{i\pi \hat{f}_\beta^\dagger \hat{f}_\beta} \hat{f}_i \hat{f}_j^\dagger \prod_{\gamma=1}^{j-1} e^{-i\pi \hat{f}_\gamma^\dagger \hat{f}_\gamma} | \Psi_F \rangle \]

Time evolution

\[ |\Psi_F(t)\rangle = e^{-i\hat{H}_F t} |\Psi_F^I\rangle = \prod_{\delta=1}^{N} \sum_{\sigma=1}^{L} P_{\sigma \delta}(t) \hat{f}_\sigma^\dagger |0\rangle \]

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Exact Green’s function

\[ G_{ij}(t) = \det \left[ (P^l(t))^\dagger P^r(t) \right] \]

Computation time \( \propto L^2 N^3 \rightarrow \text{study very large systems} \)

\[ \sim 10000 \text{ lattice sites,} \quad \sim 1000 \text{ particles} \]

1D lattice in equilibrium \((U \gg J)\)

Quasi-condensation in the presence of a trap

\[ n \]

\[ n_k \]

MR and A. Muramatsu, PRA 72, 013604 (2005).
1D lattice in equilibrium \((U \gg J)\)

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The Mott insulator in the presence of a trap

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Emergence of quasi-condensates at finite momentum

Density and momentum profiles during the expansion

Dynamics of the natural orbitals:
\[ \sum_j \langle \hat{b}^\dagger_i \hat{b}_j \rangle \phi_\eta(j) = \lambda_\eta \phi_\eta(i) \]

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Velocities of the quasi-condensate

\[ v_{NO} = \pm 2aJ = \frac{\partial \epsilon_k}{\partial k} \]

Dispersion in the lattice

\[ \epsilon_k = -2J \cos ka \implies k = \pm \pi/2a \]
Emergence of quasi-condensates at finite momentum

Quasi-condensate position

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Quasi-condensate occupation

\[ n_{k=\pm \pi/2}^{\text{max}} \sim \lambda_0^{\text{max}} \propto \sqrt{N} \]

One-body correlations

\[ |\rho_{ij}| \propto \frac{1}{\sqrt{|x_i - x_j|}} \implies \]

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Emergence of quasi-condensates (finite $U$)

Density and momentum profiles during the expansion ($U = 40J$)

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Quasi-condensate momenta

Gutzwiller mean-field theory for $U \gg J$ in 3D

Density profile

Momentum profile

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Spontaneous emergence of ground-state-like correlations
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Ground-state construction in inhomogeneous fields for correlations and entanglement entropy
Domain wall melting in 1D

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- **Ground-state construction in inhomogeneous fields for correlations and entanglement entropy**

- **Is the time-evolving state the ground state of a local Hamiltonian?**
  Free fermions (and related models) & spin-1/2 XXZ:
Domain wall melting in 1D

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- **Is the time-evolving state the ground state of a local Hamiltonian?**
  Free fermions (and related models) & spin-1/2 XXZ:

This is an example of a (geometric) quantum quench:

\[ |\psi_0\rangle \text{ is an eigenstate of some } \hat{H}_0(\text{local}), \text{ and } |\psi(t)\rangle = e^{-i\hat{H}t}|\psi_0\rangle \]
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Initial state:

\[(\hat{H}_0 - \lambda)|\psi_0\rangle = 0\]

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Time evolving state \(|\psi(t)\rangle = e^{-i\hat{H}t}|\psi_0\rangle\)

\[(e^{-i\hat{H}t}\hat{H}_0 e^{i\hat{H}t} - \lambda)|\psi(t)\rangle \equiv \hat{M}(t)|\psi(t)\rangle = 0\]

\(|\psi(t)\rangle\) is an eigenstate of \(\hat{M}(t)\).

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This is, in general, a useless observation as

\[\hat{M}(t) = \hat{H}_0 - \lambda - it[\hat{H}, \hat{H}_0] + \frac{(it)^2}{2!}[\hat{H}, [\hat{H}, \hat{H}_0]] + \ldots\]

is highly nonlocal. Note that \(\hat{M}_H(t) = \hat{H}_0 - \lambda\).

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Something remarkable occurs if

\[
[\hat{H}, \hat{H}_0] = ia_0\hat{Q} \quad \text{with} \quad [\hat{H}, \hat{Q}] = 0.
\]

We can define \(\hat{H}(t) \equiv \hat{H}_0 + a_0 t \hat{Q} - \lambda\), and \(|\psi(t)\rangle\) is an eigenstate of \(\hat{H}(t)\).

\(\hat{H}_H(t) = \hat{H}_0 - \lambda\), \(\hat{H}(t)\) is a local conserved quantity!

Noninteracting fermions (or models mappable to them)

The domain wall $|11\ldots1100\ldots00\rangle$ is the ground state of:

$$\hat{H}_0 = \sum_l l \hat{n}_l$$

The physical Hamiltonian is:

$$\hat{H} = -\sum_l (\hat{f}^\dagger_l \hat{f}_l + H.c.)$$

Which means that ($a_0 = -1$):

$$[\hat{H}, \hat{H}_0] = -i \hat{Q},$$

with

$$\hat{Q} = \sum_l (i \hat{f}^\dagger_l \hat{f}_l + H.c.)$$

$\hat{Q}$ is the charge current, which is “conserved” (up to boundary terms).

And the emergent Hamiltonian is

$$\hat{H}^E(t) = \sum_l l \hat{n}_l - t \hat{Q} - \lambda |\psi(t)\rangle$$

is the ground state of $\hat{H}^E(t)$ (up to corrections that vanish as $L \to \infty$).
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Boundary terms are responsible for the nonvanishing charge current

\[
[H, Q] = -2i(\hat{n}_1 - \hat{n}_L)
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This means that \( \langle \psi(t)|\hat{H}(t)|\psi(t)\rangle \neq 0 \).
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One can compute it! Writing \( \langle \psi_0|\hat{H}_H(t)|\psi_0\rangle \), one gets

\[
\sum_{n=1}^{\infty} \frac{(-n)i^n t^{n+1}}{(n + 1)!} \langle \psi_0|[\hat{H}, [\hat{H}, \ldots [\hat{H}, Q] \ldots]]|\psi_0\rangle.
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Quadratic term (\( n = 1 \)):

\[-(i/2)t^2 \langle \psi_0 | [\hat{H}, \hat{Q}] | \psi_0 \rangle = -t^2 \langle \psi_0 | (\hat{n}_1 - \hat{n}_L) | \psi_0 \rangle = -t^2 \]

Leads to a redefinition \( \lambda \rightarrow \lambda(t) = \lambda - t^2 \). Take particle number \( N = L/2 \).
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Leads to a redefinition \( \lambda \rightarrow \lambda(t) = \lambda - t^2 \). Take particle number \( N = L/2 \).

Higher orders vanish up to the term:

\[ \left((2N + 1)t^{2N+2} / (2N + 2)!\right) \times O(1), \]

The result is exponentially small for \( t \lesssim 2N/e \).
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Higher orders vanish up to the term:

\[ [(2N + 1)t^{2N+2}/(2N + 2)!] \times O(1), \]

The result is exponentially small for \( t \lesssim 2N/e \). Physically, for \( t \lesssim N/2 \) particles (holes) have not reached the edge of the lattice.
Noninteracting fermions (or models mappable to them)

Boundary terms are responsible for the nonvanishing charge current

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\sum_{n=1}^{\infty} \frac{(-n)\imath n t^{n+1}}{(n + 1)!} \langle \psi_0 | [\hat{H}, \hat{H}, \ldots [\hat{H}, \hat{Q}] \ldots] | \psi_0 \rangle.
\]

Numerical verification

\[ \hat{H} = -\sum_l (f_{l+1}^{\dagger} f_l + \text{H.c.}) \rightarrow |\psi(t)\rangle \]

\[ \hat{H}(t) = \sum_l l \hat{n}_l - t \hat{Q} - \lambda \rightarrow |\psi_t\rangle \]

Overlap

\[ |\langle \psi_t | \psi(t) \rangle| \quad \Rightarrow \quad \text{Overlap} \]

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### Summary
Dynamics of hard-core bosons at finite temperature

One-body density matrix (grand-canonical ensemble)

$$\rho_{ij}(t) = Z_0^{-1} \text{Tr} \left[ e^{i \hat{H} t} \hat{b}_i^\dagger \hat{b}_j e^{-i \hat{H} t} e^{-(\hat{H}_0 - \mu \hat{N})/T} \right] \quad \text{where} \quad Z_0 = \text{Tr}[e^{-(\hat{H}_0 - \mu \hat{N})/T}]$$

MR, PRA 72, 063607 (2005); W. Xu and MR, PRA 95, 033617 (2017).
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where \( Z_0 = \text{Tr}[e^{-(\hat{H}_0 - \mu \hat{N}) / T}] \)

Mapping to noninteracting fermions

\[ \rho_{ij}(t) = Z_0^{-1} \text{Tr} \left[ e^{i \hat{H} t} \left( \prod_{\alpha=1}^{i-1} e^{-i \pi \hat{f}_\alpha^\dagger \hat{f}_\alpha} \right) \hat{f}_i^\dagger \hat{f}_j \left( \prod_{\beta=1}^{j-1} e^{i \pi \hat{f}_\beta^\dagger \hat{f}_\beta} \right) e^{-i \hat{H} t} e^{-(\hat{H}_0 - \mu \hat{N}) / T} \right] \]

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Mapping to noninteracting fermions

\[ \rho_{ij}(t) = Z_0^{-1} \text{Tr} \left[ e^{i\hat{H}t} \left( \prod_{\alpha=1}^{i-1} e^{-i\pi \hat{f}_\alpha^\dagger \hat{f}_\alpha} \right) \hat{f}_i^\dagger \hat{f}_j \left( \prod_{\beta=1}^{j-1} e^{i\pi \hat{f}_\beta^\dagger \hat{f}_\beta} \right) e^{-i\hat{H}t} e^{-(\hat{H}_0 - \mu \hat{N})/T} \right] \]

Exact one-body density matrix

\[ \rho_{ij}(t) = \frac{(-1)^{i-j}}{Z} \left\{ \text{det} \left[ U_0^\dagger e^{i\hat{H}t} O_j (I - A) O_i e^{-i\hat{H}t} U_0 + e^{-(E_0 - \mu)/T} \right] \right\} \\
- \text{det} \left[ U_0^\dagger e^{i\hat{H}t} O_j O_i e^{-i\hat{H}t} U_0 + e^{-(E_0 - \mu)/T} \right] \}

Computation time \( \propto L^5 \): \( \sim 1000 \) sites

MR, PRA 72, 063607 (2005); W. Xu and MR, PRA 95, 033617 (2017).
Melting of a finite-temperature domain wall

Initial state is thermal equilibrium state of:

\[ \hat{H}_0 = - \sum_l (b_{l+1}^\dagger b_l + \text{H.c.}) + V_1 \sum_l l \hat{n}_l. \]

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\[ n(k) \text{ for: } (a) \ T = 0.1 \quad (b) \ T = 0.5 \quad (c) \ T = 1.0 \]

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Melting of a finite-temperature domain wall

Dynamics
- $T = 0$
- $T = 0.1$
- $T = 0.5$
- $T = 1.0$

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Melting of a finite-temperature domain wall

![Graph showing the dynamics and equilibrium of $[n_k]^m_{\text{max}}$ as a function of $N$ for different temperatures $T$. The graph illustrates the emergence of eigenstate solutions at $T = 0$.]

Dynamics Equilibrium

- $T = 0$
- $T = 0.1$
- $T = 0.5$
- $T = 1.0$

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Emergent Gibbs ensemble

Initial state:

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If \( \hat{\mathcal{M}}'(t) \) is a local operator, \( \hat{\mathcal{M}}'(t) \equiv \hat{\mathcal{H}}'(t) \):

\[ \hat{\Sigma}(t) = Z_0^{-1} e^{-\beta \hat{\mathcal{H}}'(t)}. \]

Then the time-evolving state is a thermal state of an emergent Hamiltonian. \textbf{Note that the temperature “remains” the same as in the initial state.}

Initial state with a finite hopping amplitude

Initial state is a stationary state of:

\[ \hat{H}_0 = -\sum_l (\hat{b}_{l+1}^\dagger \hat{b}_l + \text{H.c.}) + V_1 \sum_l l \hat{n}_l. \]

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\hat{\mathcal{H}}(t) = - \sum_l (\hat{f}_{l+1} \hat{f}_l + \text{H.c.}) - \lambda
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+ V_1 \left[ \sum_l l \hat{n}_l - t \sum_l (i \hat{f}_{l+1} \hat{f}_l + \text{H.c.}) + t^2 (\hat{n}_1 - \hat{n}_L) \right].
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\( \hat{H}(t) \) can be rewritten as (replacing \( \hat{n}_1 \rightarrow 1 \) and \( \hat{n}_L \rightarrow 0 \))

\[ \hat{H}(t) = - A(t) \sum_l (e^{-i \varphi(t)} \hat{f}_{l+1} \hat{f}_l + \text{H.c.}) + V_1 \sum_l l \hat{n}_l - (\lambda - V_1 t^2), \]

where \( A(t) = \sqrt{1 + (V_1 t)^2} \) and \( \varphi(t) = \arctan (V_1 t) \).

Effective Hamiltonian:

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\hat{H}_{\text{eff}}(t) = -\sum_{l} (e^{-i\varphi(t)} \hat{f}_{l+1}^{\dagger} \hat{f}_{l} + \text{H.c.}) + \frac{V_{1}}{\sqrt{1 + (V_{1}t)^{2}}} \sum_{l} l \hat{n}_{l},
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W. Xu and MR, PRA 95, 033617 (2017).
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Outline

1. Introduction
   - An experiment with ultracold bosons in 1D lattices
   - Emergence of quasi-condensates at finite momentum

2. Emergent eigenstate solution
   - Noninteracting fermions and related models
   - Geometric quantum quench and emergent Hamiltonian

3. Emergent Gibbs ensemble
   - Effective cooling during the melting of a Mott insulator
   - Emergent Gibbs ensemble

4. Fully interacting example
   - Spinless fermions with nearest neighbor interactions (XXZ chain)

5. Summary
Spinless fermions with nearest neighbor interactions

Physical Hamiltonian:

\[ \hat{H}(V) = \sum_{l=-N+1}^{N-1} \hat{h}_l(V), \text{ with } \hat{h}_l(V) = -(\hat{f}_{l+1}^\dagger \hat{f}_l + \text{H.c.}) + V(\hat{n}_l - 1/2)(\hat{n}_{l+1} - 1/2) \]
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\hat{Q}(V) = \sum_{l=-N+1}^{N-2} \left\{ (i\hat{f}_{l+2}^{\dagger} \hat{f}_l + \text{H.c.}) - V (i\hat{f}_{l+1}^{\dagger} \hat{f}_l + \text{H.c.})(\hat{n}_{l+2} - 1/2) - V (i\hat{f}_{l+2}^{\dagger} \hat{f}_{l+1} + \text{H.c.})(\hat{n}_l - 1/2) \right\}
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And the emergent Hamiltonian is:

\[ \hat{H}_V(t) = \hat{H}_0(V) + t \hat{Q}(V) \]
Spinless fermions with nearest neighbor interactions

Numerical verification

\[ \hat{H}(V) \rightarrow |\psi(t)\rangle \]

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Overlap

\[ |\langle \psi_t | \psi(t) \rangle| \]
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Site and momentum occupations

\[ \hat{n}_l = \hat{f}_l^\dagger \hat{f}_l \]
\[ n(q) = \frac{1}{2N + 1} \sum_{j,l} e^{iq(j-l)} \langle \hat{f}_j^\dagger \hat{f}_l \rangle \]
The emergent eigenstate solution explains why ground-state-like power-law correlations emerge during the meting of domain walls.
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The emergent Gibbs ensemble can be used to describe the dynamics of finite-temperature initial states.
Collaborators

- Deepak Iyer (Penn State → Bucknell)
- Ranjan Modak (Penn State → ICTP, Trieste)
- Lev Vidmar (Penn State → Jožef Stefan Institute)
- Wei Xu (Penn State → PayPal)

Collaborators in the Bose-Hubbard and Fermi-Hubbard projects

- Alejandro Muramatsu (Buenos Aires 1951- Stuttgart 2015)

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