Emergent eigenstate solution of quantum transport far from equilibrium

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Spin and Heat Transport in Quantum and Topological Materials

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In collaboration with:

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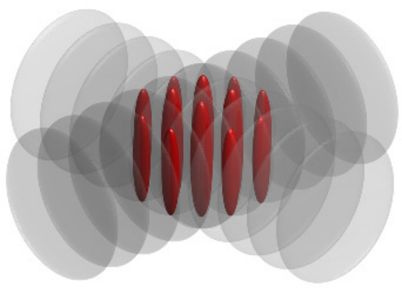
David Weiss, Wei Xu & Yicheng Zhang (Penn State)

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

Experiments in the 1D regime



Effective one-dimensional δ potential

M. Olshanii, PRL **81**, 938 (1998).

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

where

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

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

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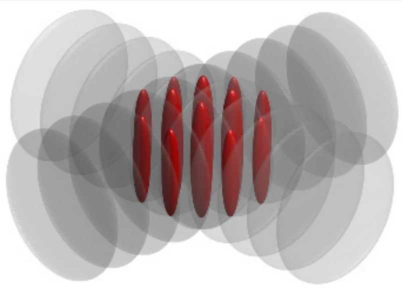

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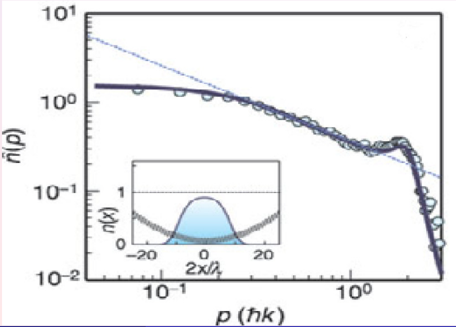
Lieb, Schulz, and Mattis '61 ($U/J \to \infty$)

B. Paredes *et al.*,

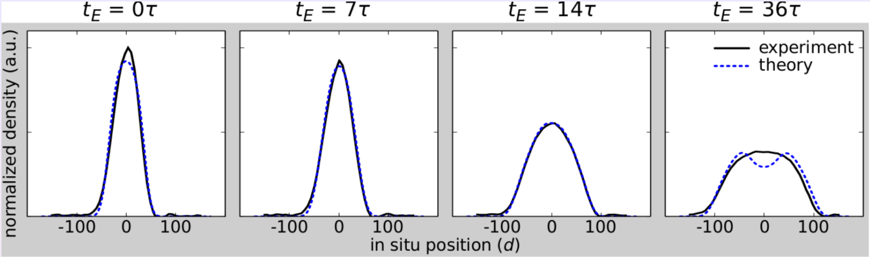
Nature (London) **429**, 277 (2004).

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

$n(x)$: Site occupations $\Leftrightarrow$



Emergence of quasi-condensates at finite momentum



L. Vidmar, J. P. Ronzheimer, M. Schreiber, S. Braun, S. S. Hodgman, S. Langer, F. Heidrich-Meisner, I. Bloch, U. Schneider, PRL **115**, 175301 (2015).

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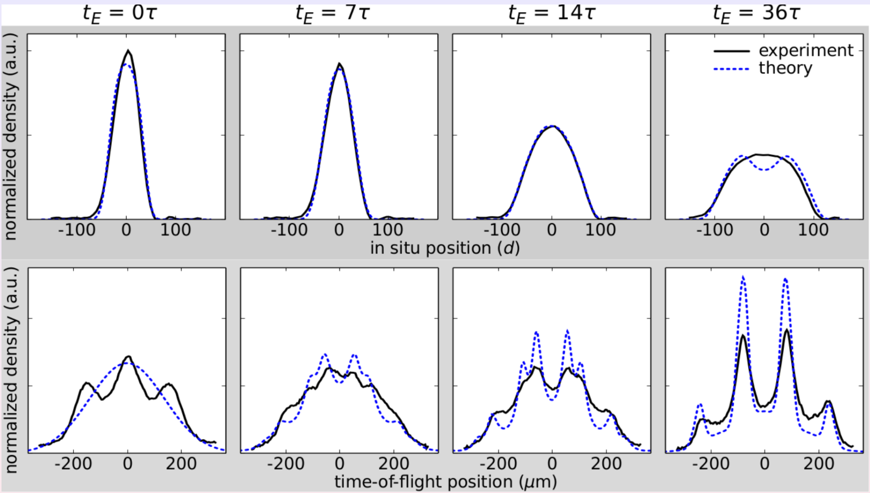

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Bose-Fermi mapping in a 1D lattice ($U \gg J$)

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

$$\hat{b}_i^{\dagger 2} = \hat{b}_i^2 = 0$$

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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

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

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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

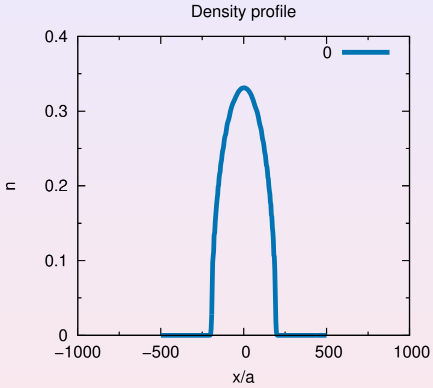
$$G_{ij}(t) = \det \left[\left(\mathbf{P}^i(t) \right)^\dagger \mathbf{P}^j(t) \right]$$

Computation time $\propto L^2 N^3 \rightarrow$ study very large systems

$$\sim 10000 \text{ lattice sites}, \qquad \sim 1000 \text{ particles}$$

MR and A. Muramatsu, PRA **70**, 031603(R) (2004); PRL **93**, 230404 (2004).

Dynamical fermionization



M. Rigol and A. Muramatsu, Phys. Rev. Lett. **94**, 240403 (2005).

“Problem” with TOF: B. Sutherland, Phys. Rev. Lett. **80**, 3678 (1998).

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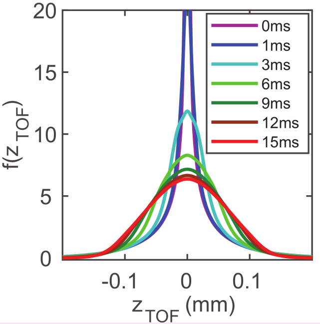

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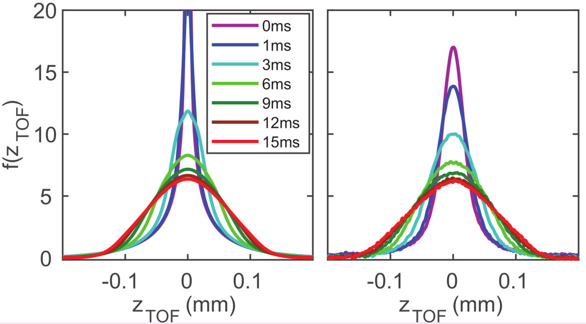

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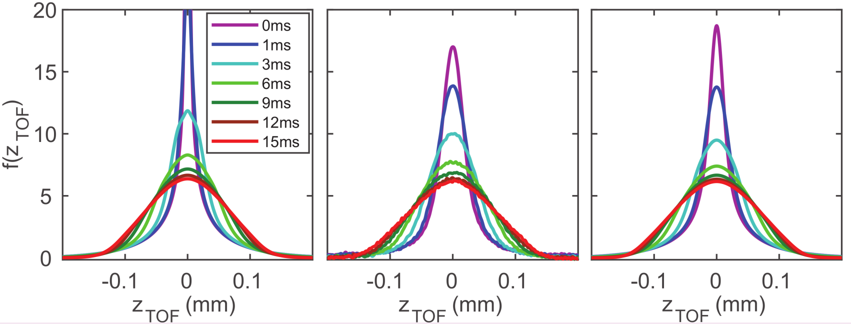

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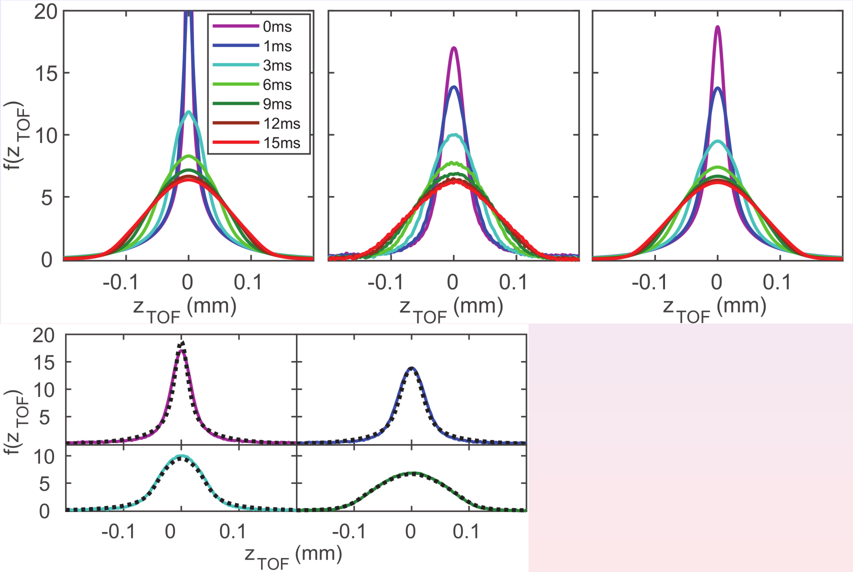

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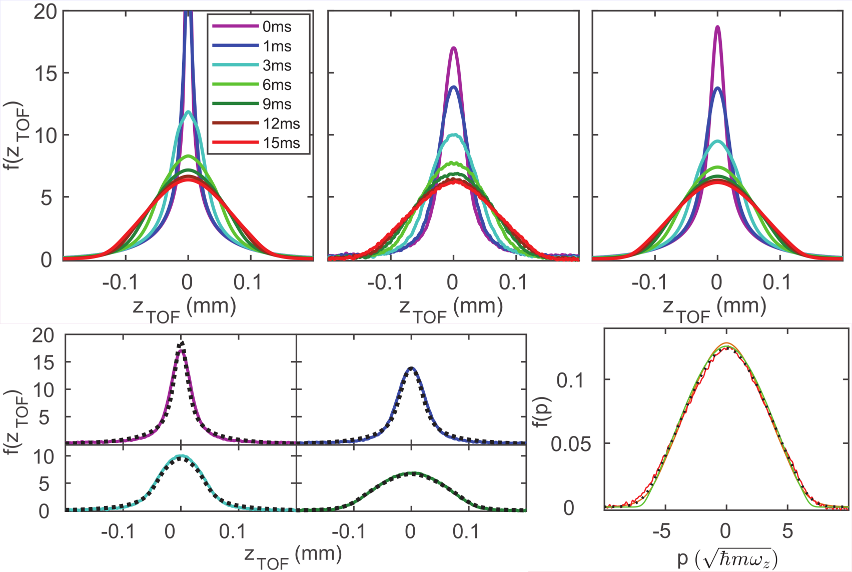

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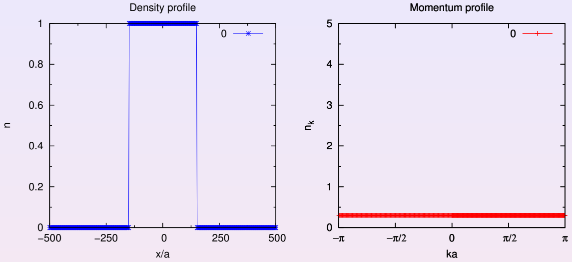
Emergence of quasi-condensates at finite momentum

Density and momentum profiles during the expansion



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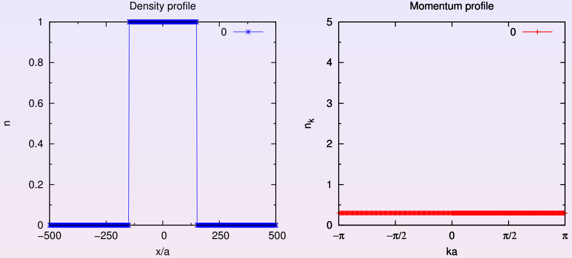
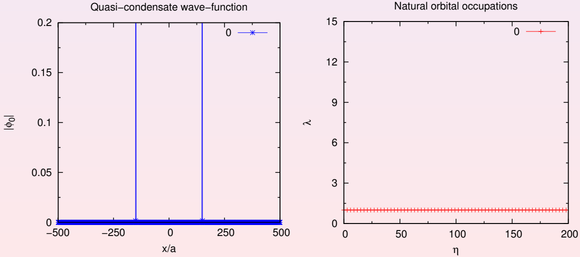


Dynamics of the natural orbitals: $\sum_j \langle \hat{b}_i^\dagger \hat{b}_j \rangle \phi_\eta(j) = \lambda_\eta \phi_\eta(i)$



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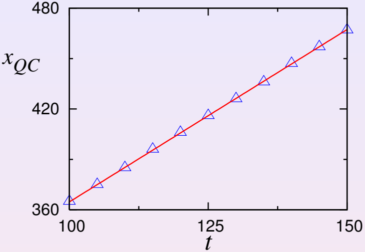
Quasi-condensate position



Velocity of the quasi-condensate

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

Dispersion in the lattice

$$\epsilon_k = -2J\cos ka \implies k = \pm\pi/2a$$

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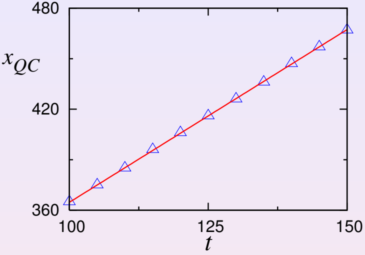

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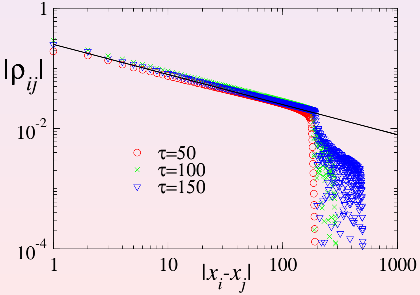
Quasi-condensate occupation

$$n^{\text{max}}_{k=\pm\pi/2} \sim \lambda^{\text{max}}_0 \propto \sqrt{N}$$

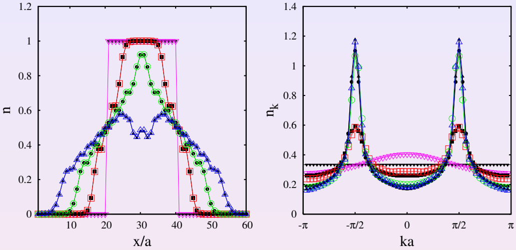
One-body correlations

$$|\rho_{ij}| \propto 1/\sqrt{|x_i - x_j|} \quad \Longrightarrow$$



Emergence of quasi-condensates (finite U/J)

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



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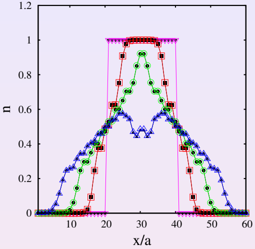
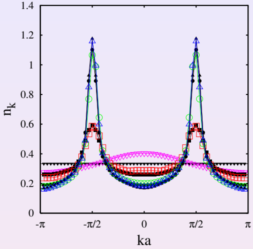
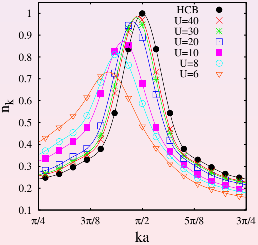
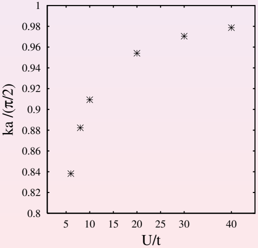




Quasi-condensate momenta





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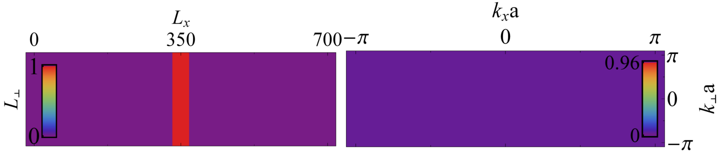
Gutzwiller mean-field theory for $U \gg J$ in 3D

Density profile   Momentum profile



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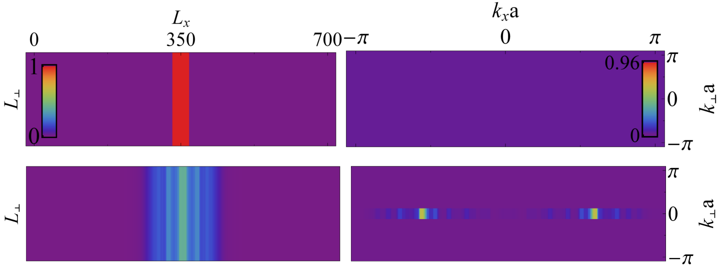

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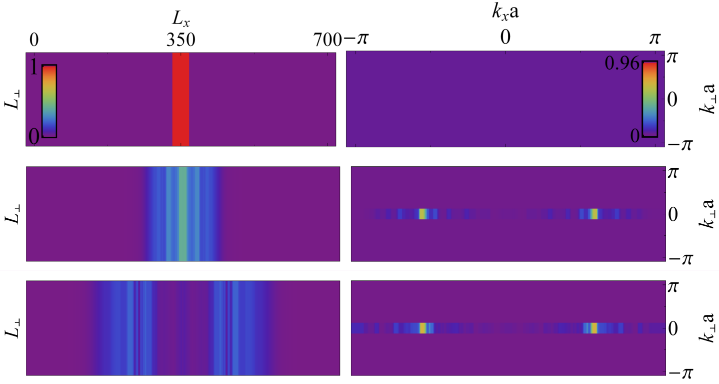

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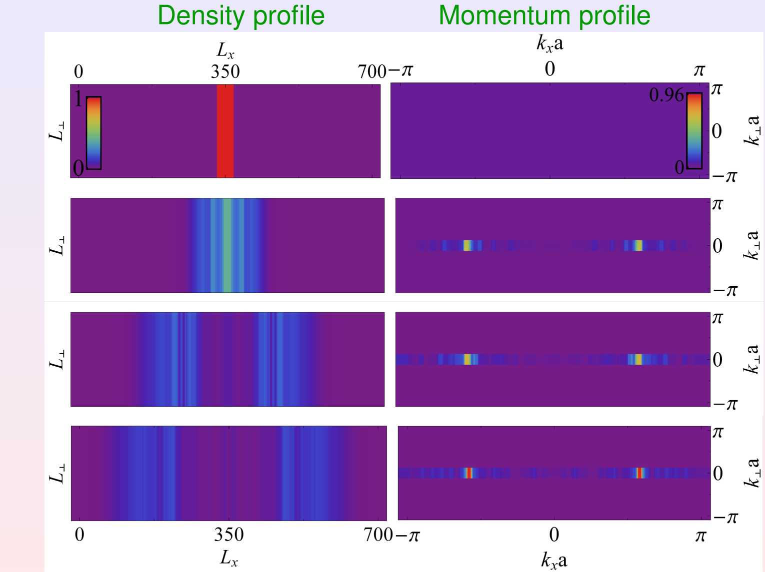

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Domain wall melting in 1D

- Spontaneous emergence of ground-state-like correlations
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This is an example of a (geometric) quantum quench:

$|\psi_0\rangle$ is an eigenstate of some $\hat{H}_0$(local), and $|\psi(t)\rangle = e^{-i\hat{H}t}|\psi_0\rangle$

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Emergent eigenstate solution

Initial state:

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

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

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

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This is, in general, a useless observation because

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

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

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Something remarkable occurs if

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

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

$\hat{\mathcal{H}}_{\mathsf{H}}(t) = \hat{H}_0 - \lambda$, $\hat{\mathcal{H}}(t)$ is a local conserved quantity!

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Noninteracting fermions (or models mappable to them)

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

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

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

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

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And the emergent Hamiltonian is

$$\hat{\mathcal{H}}(t) = \sum_l l\,\hat{n}_l - t\,\hat{Q} - \lambda$$

$|\psi(t)\rangle$ is the ground state of $\hat{\mathcal{H}}(t)$ (up to corrections that vanish as $L \to \infty$).

Noninteracting fermions (or models mappable to them)

Boundary terms are responsible for the nonvanishing charge current

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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 $\lambda \to \lambda(t) = \lambda - t^2$. Take particle number $N = L/2$.

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

The result is exponentially small for $t \lesssim 2N/e$.

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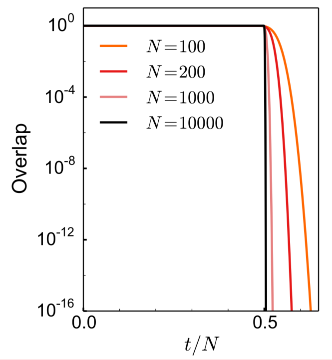
Numerical verification

$$\hat{H} = -\sum_l (\hat{f}^\dagger_{l+1} \hat{f}_l + \mathrm{H.c.}) \quad \rightarrow \quad |\psi(t)\rangle$$

$$\hat{\mathcal{H}}(t) = \sum_l l\, \hat{n}_l - t\, \hat{Q} - \lambda \quad \rightarrow \quad |\psi_t\rangle$$

Overlap

$$|\langle \psi_t|\psi(t)\rangle| \qquad \Longrightarrow$$



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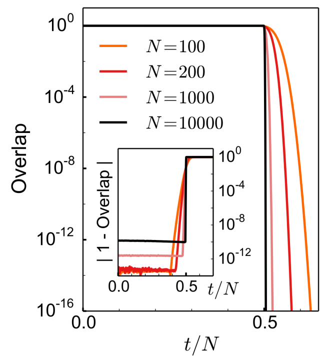
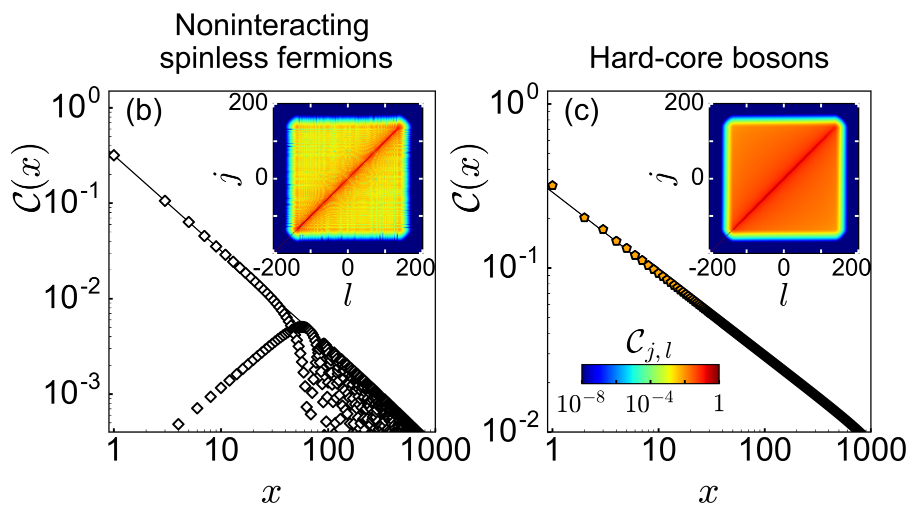


Noninteracting fermions and hard-core bosons

$$\mathcal{C}_{j,l} = |\langle \hat{f}_j^\dagger \hat{f}_l \rangle| \qquad \mathcal{C}_{j,l} = |\langle \hat{b}_j^\dagger \hat{b}_l \rangle|$$



Outline

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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Mapping to noninteracting fermions

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

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Exact one-body density matrix

$$\begin{aligned}\rho_{ij}(t) \quad = \quad \frac{(-1)^{i-j}}{Z}\Big\{&\det\left[U_0^\dagger e^{iHt}O_j(I-A)O_i e^{-iHt}U_0 + e^{-(E_0-\mu)/T}\right] \\ &-\det\left[U_0^\dagger e^{iHt}O_jO_i e^{-iHt}U_0 + e^{-(E_0-\mu)/T}\right]\Big\}\end{aligned}$$

Computation time $\propto L^5$: ~ 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:

$$\hat{H}_0 = -\sum_l (\hat{b}^\dagger_{l+1}\hat{b}_l + \text{H.c.}) + V_1 \sum_l l\,\hat{n}_l\,.$$

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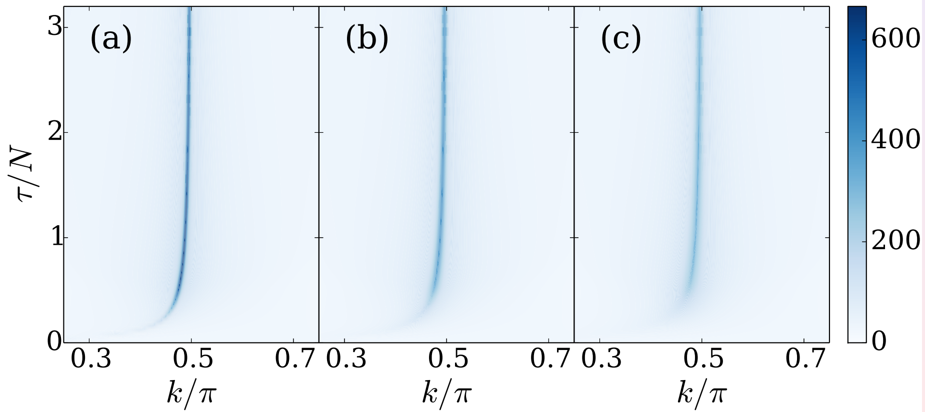
$n(k)$ for: (a) $T = 0.1$ (b) $T = 0.5$ (c) $T = 1.0$



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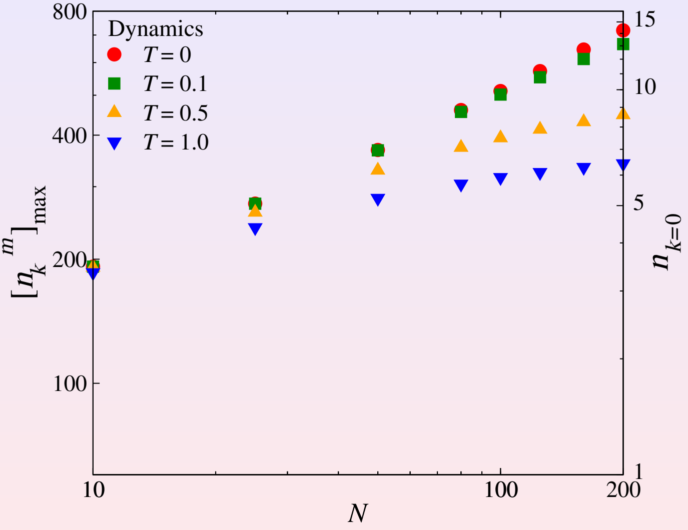

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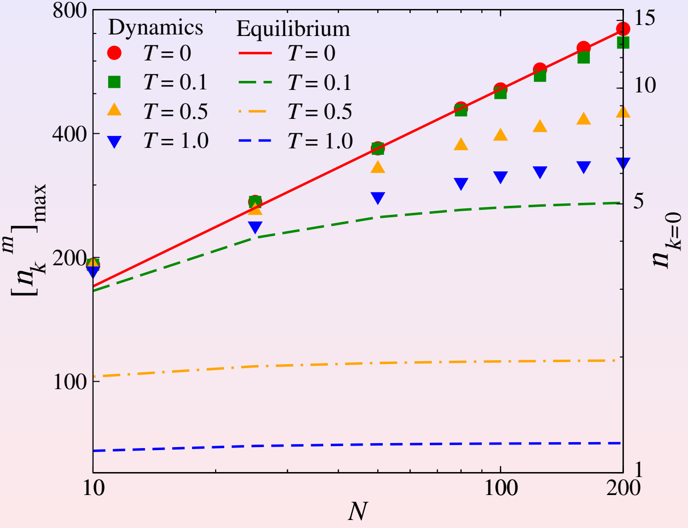

Outline

Emergent Gibbs ensemble

Initial state:

$$\hat{\rho}_0 = Z_0^{-1}\, e^{-\beta \hat{H}_0}, \quad \text{where} \quad Z_0 = \mathrm{Tr}[e^{-\beta \hat{H}_0}]$$

L. Vidmar, W. Xu, and MR, PRA **96**, 013608 (2017).

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$$\hat{\rho}(t) = Z_0^{-1} e^{-i\hat{H}t} e^{-\beta \hat{H}_0} e^{i\hat{H}t} = Z_0^{-1} \exp\left(-\beta\left[e^{-i\hat{H}t}\hat{H}_0 e^{i\hat{H}t}\right]\right).$$

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Again, one can introduce an operator $\hat{\mathcal{M}}'(t) \equiv e^{-i\hat{H}t} \hat{H}_0 e^{i\hat{H}t}$ so that:

$$\hat{\rho}(t) = Z_0^{-1} e^{-\beta \hat{\mathcal{M}}'(t)}.$$

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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.
Note that the temperature "is the same" as that in the initial state.

L. Vidmar, W. Xu, and MR, PRA **96**, 013608 (2017).

Initial state with a finite hopping amplitude

Initial state is a stationary state of:

$$\hat{H}_0 = -\sum_l (\hat{b}^\dagger_{l+1}\hat{b}_l + \text{H.c.}) + V_1 \sum_l l\,\hat{n}_l\,.$$

L. Vidmar, D. Iyer, and MR, PRX **7**, 021012 (2017).

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$$\begin{aligned}\hat{\mathcal{H}}(t) &= -\sum_l (\hat{f}^\dagger_{l+1}\hat{f}_l + \text{H.c.}) - \lambda \\ &\quad + V_1 \left[\sum_l l\,\hat{n}_l - t\sum_l (i\hat{f}^\dagger_{l+1}\hat{f}_l + \text{H.c.}) + t^2(\hat{n}_1 - \hat{n}_L)\right].\end{aligned}$$

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$\hat{\mathcal{H}}(t)$ can be rewritten as (replacing $\hat{n}_1 \to 1$ and $\hat{n}_L \to 0$)

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

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

L. Vidmar, D. Iyer, and MR, PRX **7**, 021012 (2017).

Effective temperature

Effective Hamiltonian:

$$\hat{\mathcal{H}}_{\text{eff}}(t) = -\sum_l (e^{-i\varphi(t)} \hat{f}^\dagger_{l+1} \hat{f}_l + \text{H.c.}) + \frac{V_1}{\sqrt{1+(V_1 t)^2}} \sum_l l\, \hat{n}_l,$$

and effective temperature $T_{\text{eff}}(t) = T/\sqrt{1+(V_1 t)^2}$.

W. Xu and MR, PRA **95**, 033617 (2017).

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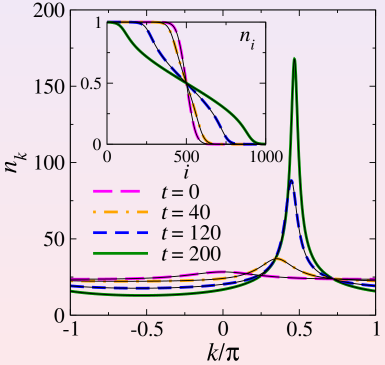

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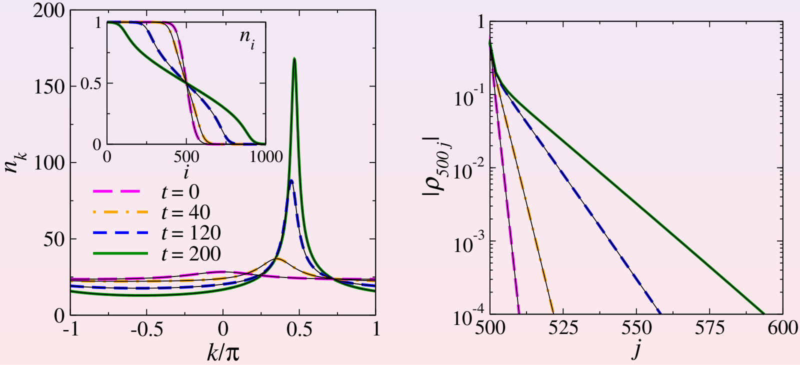

W. Xu and MR, PRA **95**, 033617 (2017).

Outline

Spinless fermions with nearest neighbor interactions

Physical Hamiltonian:

$$\hat{H}(V) = \sum_{l=-N+1}^{N-1} \hat{h}_l(V), \text{ with } \hat{h}_l(V) = -(\hat{f}^\dagger_{l+1}\hat{f}_l + \text{H.c.}) + V(\hat{n}_l - 1/2)(\hat{n}_{l+1} - 1/2)$$

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The domain wall is a highly excited eigenstate of the “boost” operator:

$$\hat{H}_0(V) = \sum_{l=-N+1}^{N-1} l\,\hat{h}_l(V)$$

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The commutator $[\hat{H}(V), \hat{H}_0(V)] = -i\hat{Q}(V)$ results in:

$$\begin{aligned}\hat{Q}(V) \quad = \quad & \sum_{l=-N+1}^{N-2} \Big\{ (i\hat{f}^\dagger_{l+2}\hat{f}_l + \text{H.c.}) - \\ & V(i\hat{f}^\dagger_{l+1}\hat{f}_l + \text{H.c.})(\hat{n}_{l+2} - 1/2) - V(i\hat{f}^\dagger_{l+2}\hat{f}_{l+1} + \text{H.c.})(\hat{n}_l - 1/2) \Big\}\end{aligned}$$

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And the emergent Hamiltonian is:

$$\hat{\mathcal{H}}_V(t) = \hat{H}_0(V) + t\,\hat{Q}(V)$$

Spinless fermions with nearest neighbor interactions

Numerical verification

$$\hat{H}(V) \quad \rightarrow \quad |\psi(t)\rangle$$

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Overlap

$$|\langle\psi_t|\psi(t)\rangle|$$

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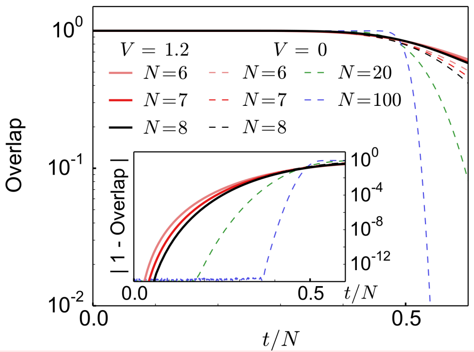

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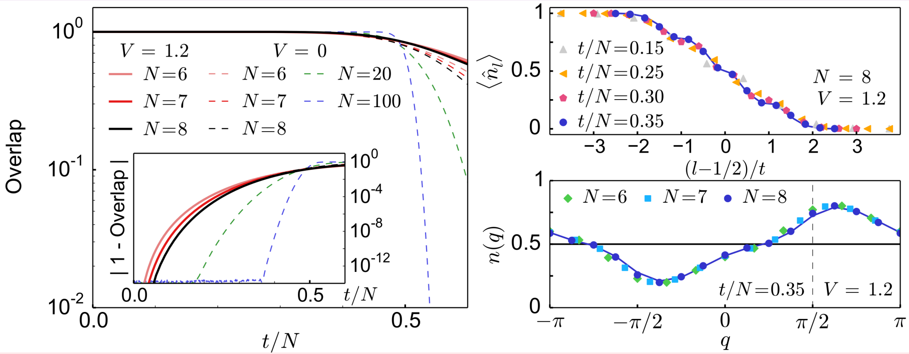
Site and momentum occupations

$$\hat{n}_l = \hat{f}_l^\dagger \hat{f}_l$$

$$n(q) = \frac{1}{2N+1}\sum_{j,l} e^{iq(j-l)}\langle \hat{f}_j^\dagger \hat{f}_l\rangle$$



Summary

- Geometric quenches (resulting in transport far from equilibrium) can produce states that are eigenstates of emergent local Hamiltonians

Publications exploring these ideas:

- L. Vidmar, D. Iyer, and MR. *Emergent Eigenstate Solution to Quantum Dynamics Far from Equilibrium*. Phys. Rev. X **7**, 021012 (2017).
- W. Xu and MR. *Expansion of one-dimensional lattice hard-core bosons at finite temperature*. Phys. Rev. A **95**, 033617 (2017).
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- R. Modak, L. Vidmar, and MR. *Quantum adiabatic protocols using emergent local Hamiltonians*. Phys. Rev. E **96**, 042155 (2017).
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Summary

- Geometric quenches (resulting in transport far from equilibrium) can produce states that are eigenstates of emergent local Hamiltonians
- For initial thermal states such quenches result in states that can be described by emergent Gibbs ensembles

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Summary

- Geometric quenches (resulting in transport far from equilibrium) can produce states that are eigenstates of emergent local Hamiltonians
- For initial thermal states such quenches result in states that can be described by emergent Gibbs ensembles
- Only one conserved (or quasi-conserved) quantity is needed for the emergent Hamiltonian construction to work
  - Nonintegrable systems?

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Collaborators

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- Ranjan Modak (Penn State $\longrightarrow$ ICTP, Trieste)
- *Lev Vidmar (Penn State $\longrightarrow$ Jožef Stefan Institute)*
- David Weiss & group (Penn State)
- *Wei Xu (Penn State $\longrightarrow$ PayPal)*
- *Yicheng Zhang (Penn State)*
- Alejandro Muramatsu (Buenos Aires 1951- Stuttgart 2015)

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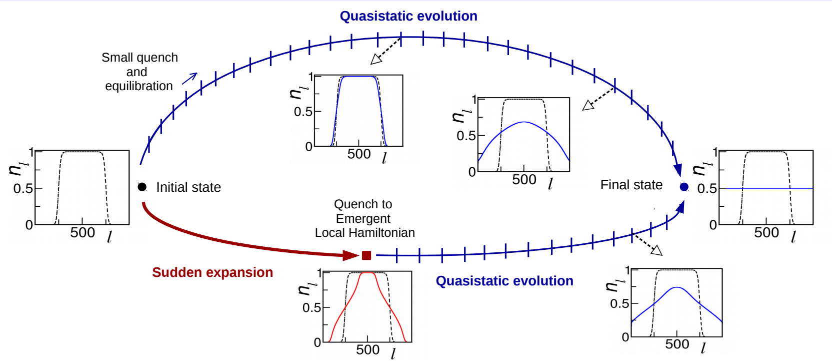
Quasi-adiabatic transfer from power-law to box traps



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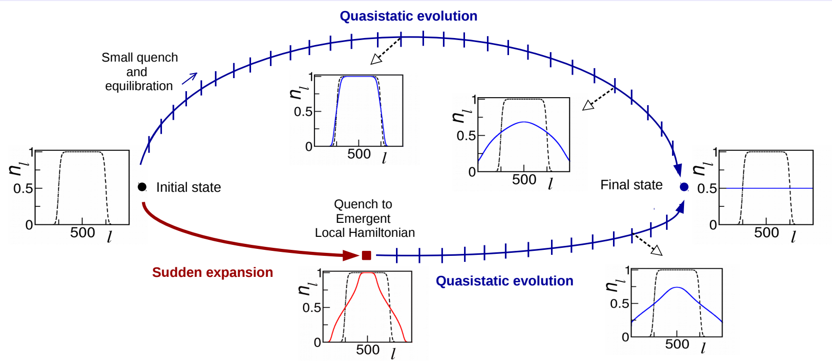

The emergent Hamiltonian for an initial harmonic trap takes the form:

$$\hat{\mathcal{H}}^{(2)}(t) = \frac{1}{R^2}\sum_{l=1}^{L}\tilde{l}^2\,\hat{n}_l - \left(\frac{t}{R}\right)^2 \sum_{l=1}^{L-2}(\hat{c}_l^\dagger\hat{c}_{l+2} + \text{H.c.}) - \sum_{l=1}^{L-1} A^{(2)}(t,l)(e^{i\phi^{(2)}(t,l)}\hat{c}_l^\dagger\hat{c}_{l+1} + \text{H.c.})$$

$$\tilde{l} = l - (L+1)/2, \;\; A^{(2)}(t,l) = \sqrt{1 + [(2t/R^2)(l+1/2)]^2}, \;\; \phi^{(2)}(t,l) = \arctan\left[2t(l+1/2)/R^2\right]$$

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