Emergent eigenstate solution to quantum dynamics far from equilibrium

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Quantum Information and Thermodynamics

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Outline

1. Introduction
   - Experiments with ultracold gases in 1D
   - Emergence of quasi-condensates at finite momentum
2. Emergent eigenstate solution
   - Noninteracting fermions and related models
   - Spinless fermions with nearest neighbor interactions (XXZ chain)
3. Emergent Gibbs ensemble
   - Effective cooling during the melting of a Mott insulator
   - Emergent Gibbs ensemble
4. Maximal work from a "quantum battery"
   - Speed up (quasi-)adiabatic transformations
   - "Quantum battery"
5. Summary

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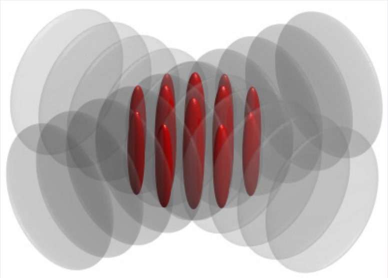
Experiments with ultracold gases in 1D



Effective one-dimensional δ potential

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

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

where

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

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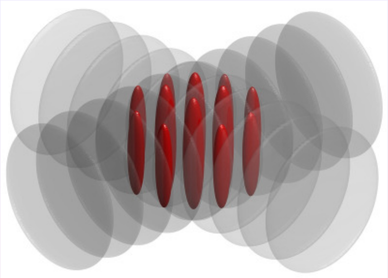

Girardeau '60, Lieb and Liniger '63

T. Kinoshita, T. Wenger, and D. S. Weiss, Science **305**, 1125 (2004).

T. Kinoshita, T. Wenger, and D. S. Weiss, Phys. Rev. Lett. **95**, 190406 (2005).

$\gamma_{\text{eff}} = \frac{m g_{1D}}{\hbar^2 \rho}$

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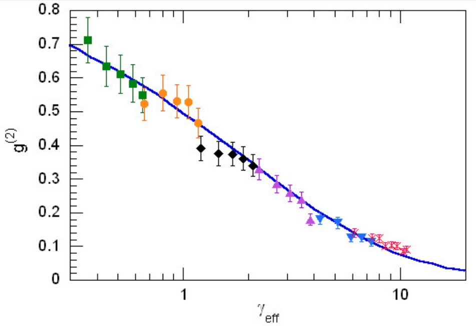

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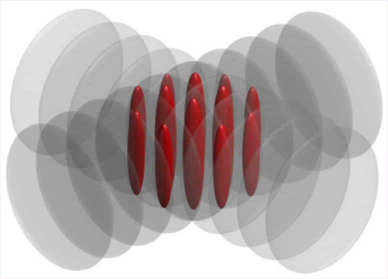

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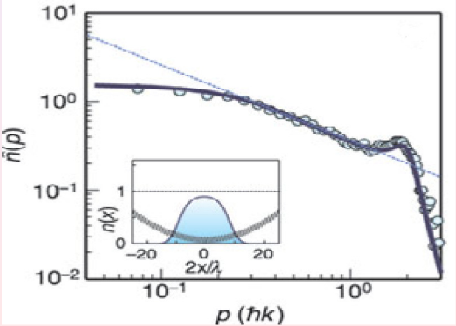
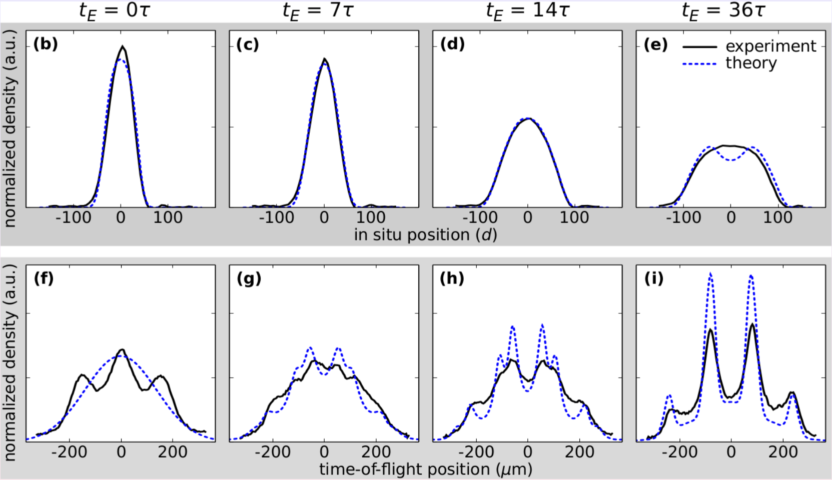
Lieb, Schulz, and Mattis '61

B. Paredes *et al.*,
Nature (London) **429**, 277 (2004).

$n(x)$: Density distribution
$n(p)$: Momentum distribution



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).

Theoretically predicted in:
MR and A. Muramatsu, PRL **93**, 230404 (2004).

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

Hard-core boson Hamiltonian in an external potential

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

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

$$\hat{H}_F = -J \sum_i \left(\hat{f}_i^\dagger \hat{f}_{i+1} + \text{H.c.} \right) + \sum_i \mu_i \, \hat{n}_i^f$$

One-particle density matrix

One-particle 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

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

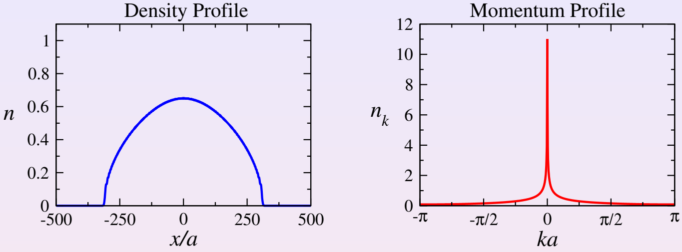
Computation time $\propto L^2 N^3 \to$ study very large systems

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

MR and A. Muramatsu, Mod. Phys. Lett. B **19**, 861 (2005).

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

Quasi-condensation in the presence of a trap



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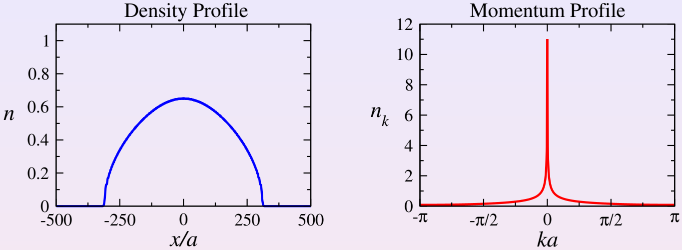
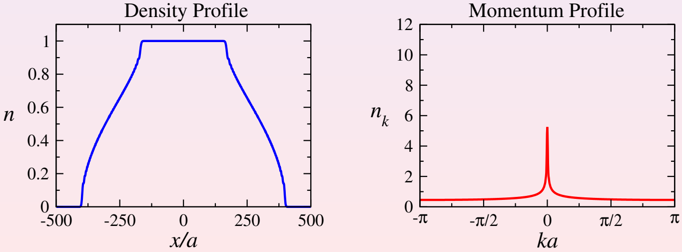


The Mott insulator in the presence of a trap



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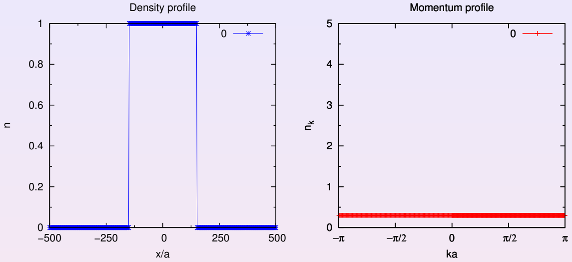
Emergence of quasi-condensates at finite momentum

Density and momentum profiles during the expansion



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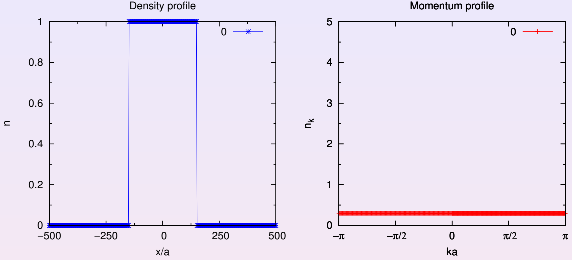
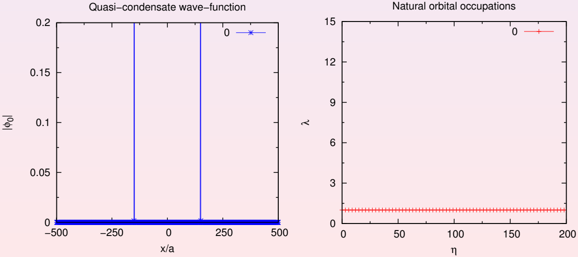


Dynamics of the natural orbitals: $\sum_j \langle \hat{b}_i^\dagger \hat{b}_j \rangle \phi_\eta(j) = \lambda_\eta \phi_\eta(i)$



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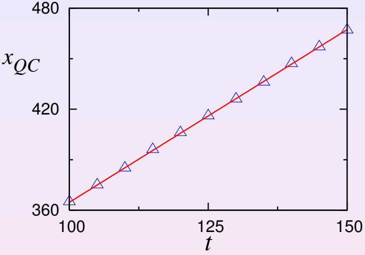
Emergence of quasi-condensates at finite momentum

Quasi-condensate position



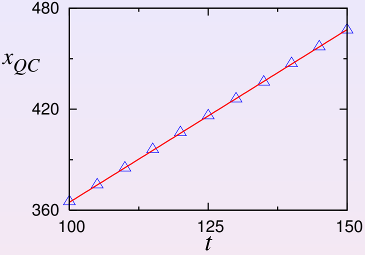
Velocity of the quasi-condensate

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

Dispersion in the lattice

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

Quasi-condensate position



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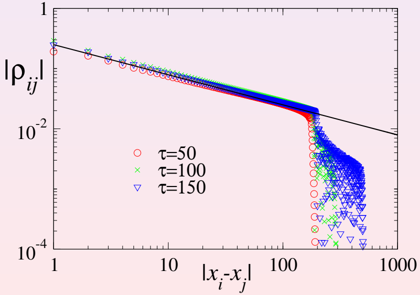
Quasi-condensate occupation

$$\lambda_0^{\text{max}} \propto \sqrt{N}$$

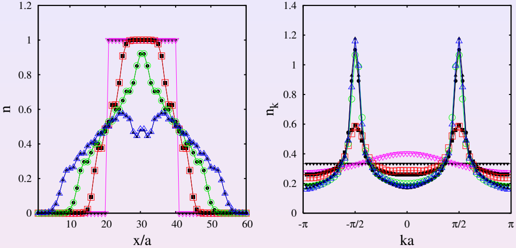
Spatial coherence

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



Emergence of quasi-condensates (finite U)

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



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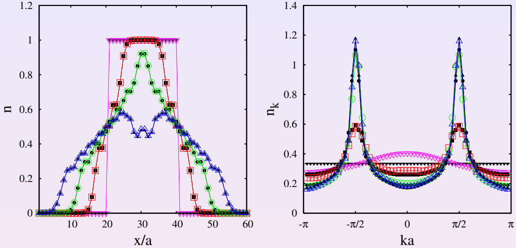
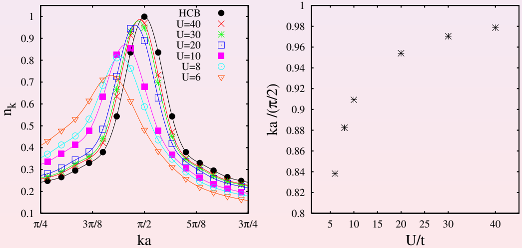


Quasi-condensate momenta



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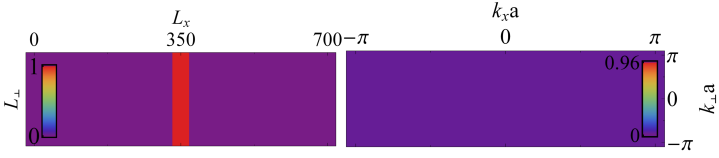
Gutzwiller mean-field theory for $U \gg J$ in 3D

Density profile | Momentum profile



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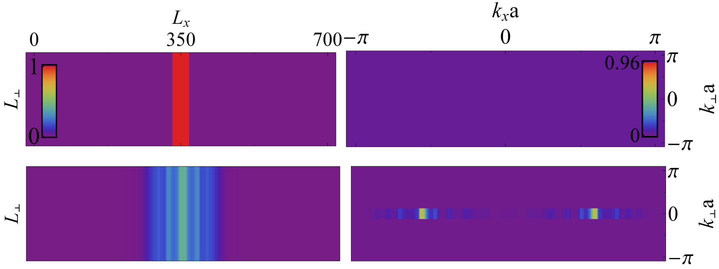

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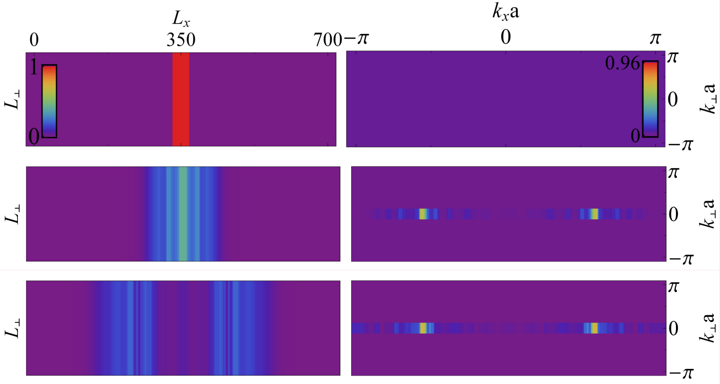

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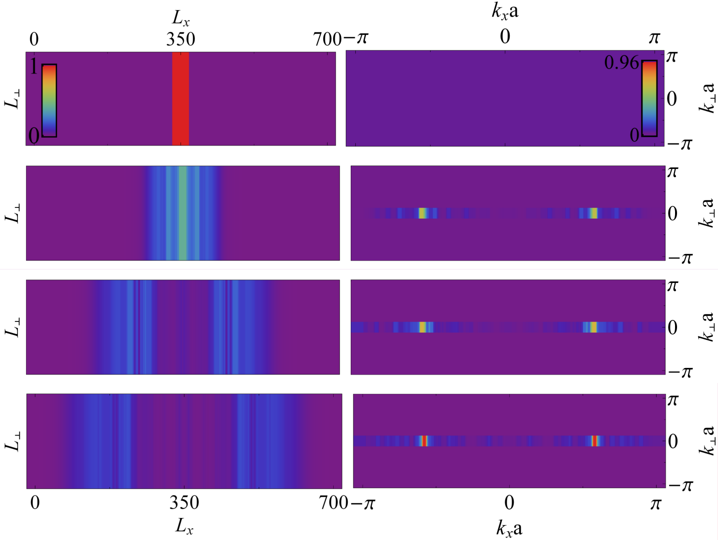

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Outline

Domain wall melting in 1D

- Spontaneous emergence of ground-state-like correlations
  Free fermions: Antal, Rácz, Rákos, and Schütz, PRE **59**, 4912 (1999).
  Hard-core bosons: MR and A. Muramatsu, PRL **93**, 230404 (2004).

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This problem is a classic example of a (geometric) quantum quench:

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

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 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 $\hat{M}_{\mathrm{H}}(t) = \hat{H}_0 - \lambda$.

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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!

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

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 ($a_0 = -1$):

$$[\hat{H}, \hat{H}_0] = -i\hat{Q}, \qquad \text{with} \qquad \hat{Q} = \sum_l (i\hat{f}^\dagger_{l+1}\hat{f}_l + \text{H.c.}).$$

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

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And

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

$|\psi(t)\rangle$ 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

$$[\hat{H}, \hat{Q}] = -2i(\hat{n}_1 - \hat{n}_L)$$

This means that $\langle\psi(t)|\hat{\mathcal{H}}(t)|\psi(t)\rangle \neq 0$.

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One can compute it! Writing $\langle\psi_0|\hat{\mathcal{H}}_{\mathsf{H}}(t)|\psi_0\rangle$, one gets

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

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

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

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

Higher orders vanish up to the term:

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

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

Noninteracting fermions (or models mappable to them)

Boundary terms are responsible for the nonvanishing charge current

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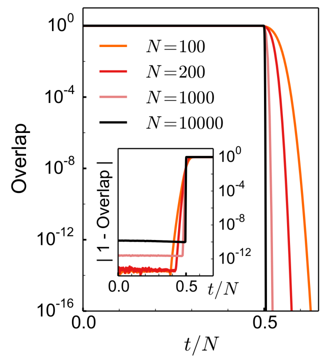
Numerical verification

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

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

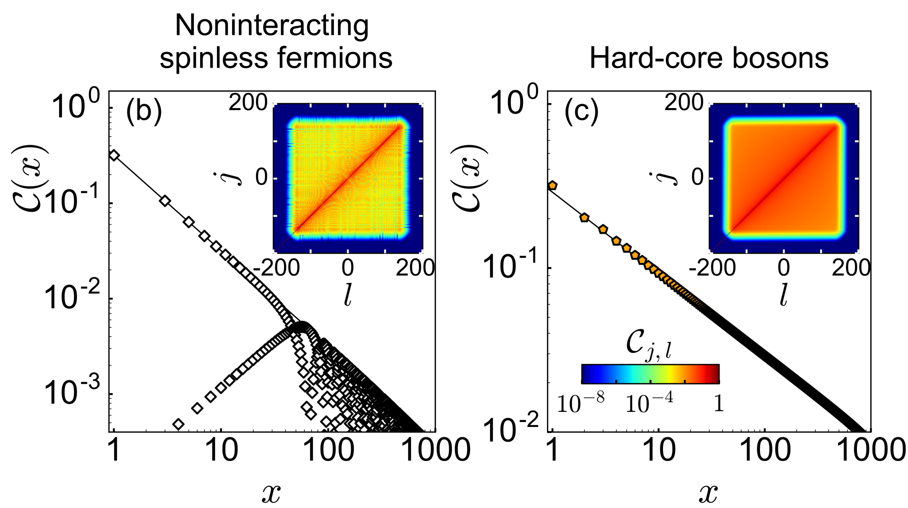
Overlap

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



Noninteracting fermions and hard-core bosons

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



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

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

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

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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

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

$$\hat{H}_V(t) \quad \rightarrow \quad |\psi_t\rangle$$

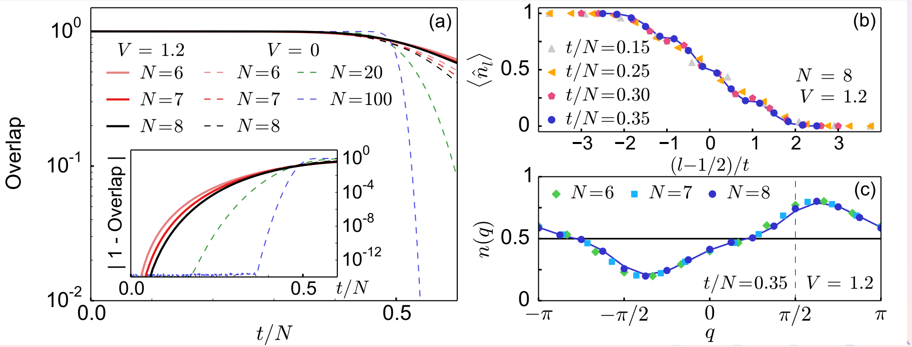
Overlap

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

Site and momentum occupations

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

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



Outline

Hard-core bosons at finite temperature

One-particle density matrix (grand-canonical ensemble)

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

MR, PRA **72**, 063607 (2005); W. Xu and MR, PRA **95**, 033617 (2017).

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Mapping to noninteracting fermions

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

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Exact one-particle density matrix

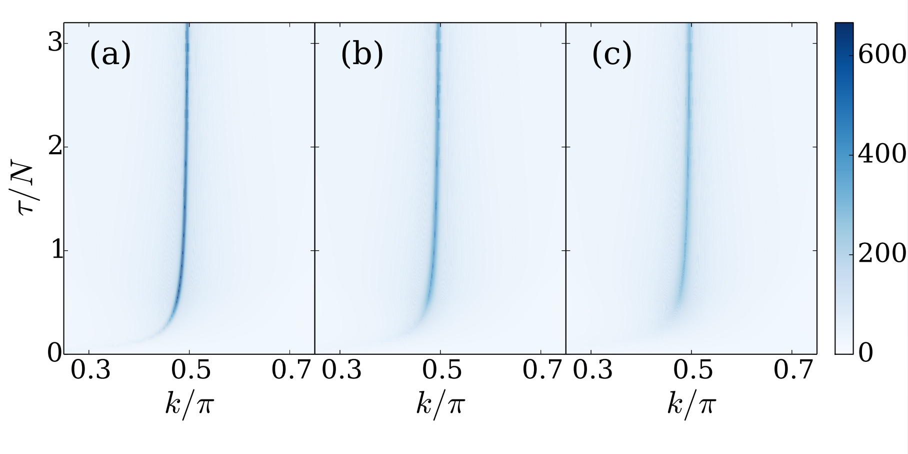
$$\begin{aligned}\rho_{ij}(t) \quad = \quad & \frac{(-1)^{i-j}}{Z}\left\{\det\left[U_0^\dagger e^{iHt} O_j (I+A) O_i e^{-iHt} U_0 + e^{-(E_0-\mu)/T}\right]\right. \\ & \left. -\det\left[U_0^\dagger e^{iHt} O_j O_i e^{-iHt} U_0 + e^{-(E_0-\mu)/T}\right]\right\}\end{aligned}$$

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 Mott insulator

(a) $T = 0.1$ (b) $T = 0.5$ (c) $T = 1.0$



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

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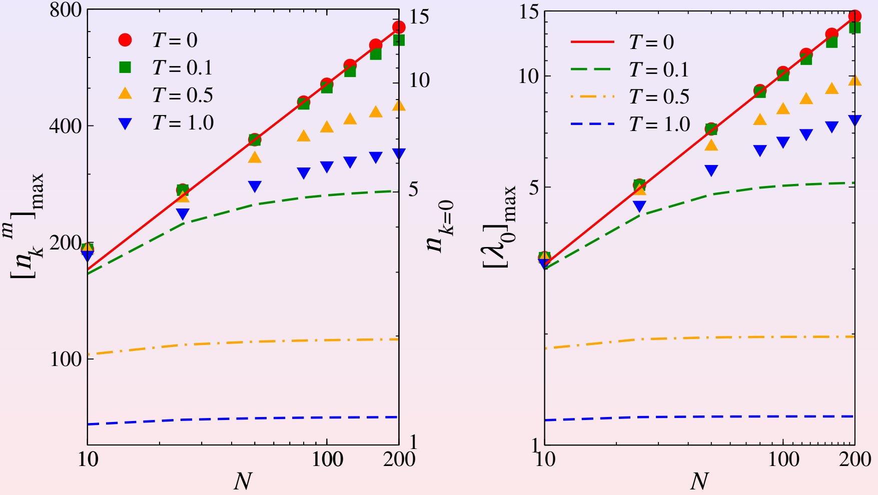

Outline

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).

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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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:

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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 remains the same as in the initial state.*

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

Effective temperature

Effective Hamiltonian:

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

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

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

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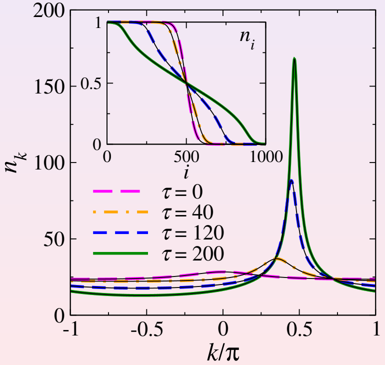

W. Xu and MR, PRA **95**, 033617 (2017).

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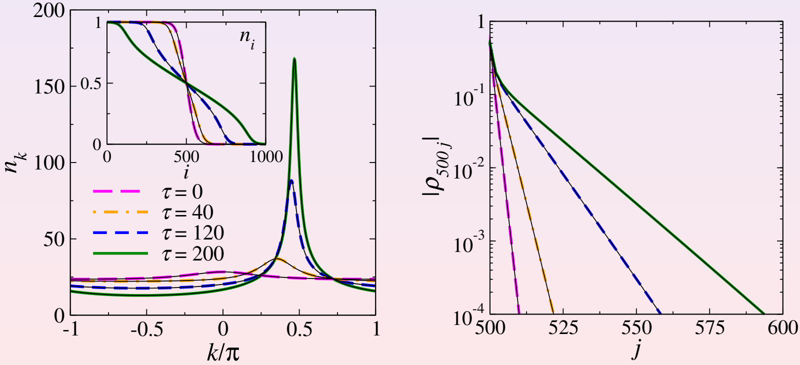
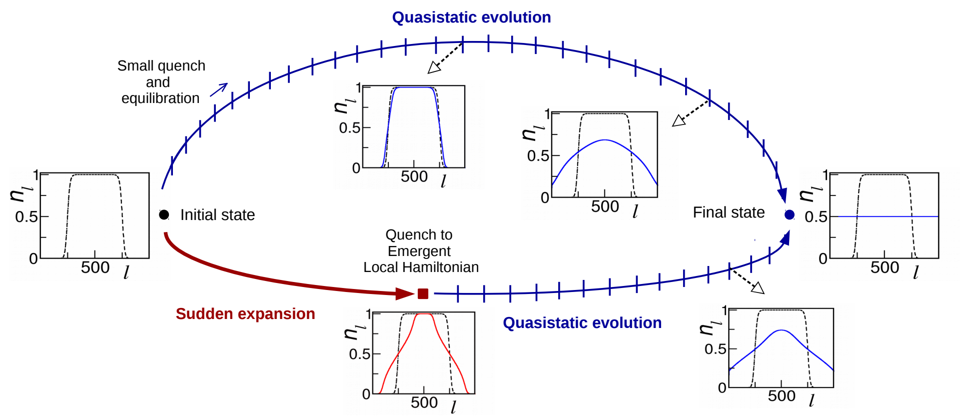


W. Xu and MR, PRA **95**, 033617 (2017).

Outline

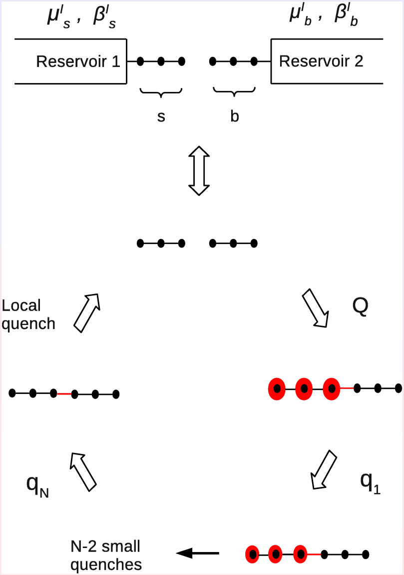
Transfer from power-law to box traps



R. Modak, L. Vidmar, and MR, arXiv:1608.08453.

Outline

“Quantum battery”



R. Modak and MR, PRE **95**, 062145 (2017)

“Quantum battery” made of band insulators

Initial state (two chains with $L/2$ sites)

$$|\psi_I\rangle = |\psi_I\rangle_1 \otimes |\psi_I\rangle_2, \text{ with } |\psi_I\rangle_1 = \prod_{l=1}^{L/2} \hat{c}_l^\dagger |\emptyset\rangle_1 \,, \text{ and } |\psi_I\rangle_2 = |\emptyset\rangle_2.$$

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Work extracted for $\hat{H}_\ell = -J\sum_{l=1}^{L/2-1}(\hat{c}_l^\dagger \hat{c}_{l+1} + \text{H.c.})$, $\ell = 1, 2$:

$$W = \text{Tr}\left[(\hat{\rho}^I - \hat{\rho}^F)\,(\hat{H}_1 + \hat{H}_2)\right].$$

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(i) Connect the chains. The time-evolving state is the ground state of

$$\hat{\mathcal{H}}(t) = -\sum_{l=1}^{L-1} (e^{i\pi/2} \hat{c}_l^\dagger \hat{c}_{l+1} + \text{H.c.}) + \frac{1}{t} \sum_{l=1}^{L} l\, \hat{n}_l\,,$$

so we quench to $\hat{\mathcal{H}}(t_Q)$ at time $t_Q < L/(2v_{\text{max}}) = L/4$.

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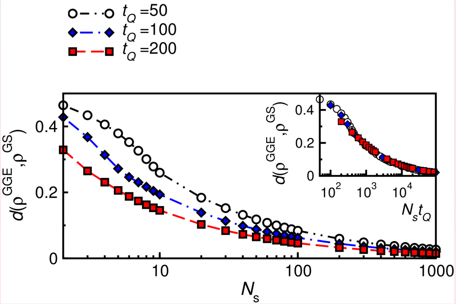
(ii) Transform $\hat{\mathcal{H}}(t_Q) \to \hat{H}_1 + \hat{H}_2$ quasi-statically:

We turn off the linear trap and the phase $\pi/2$ in N_s equal steps, then disconnect the chains. Assume relaxation to the GGE.

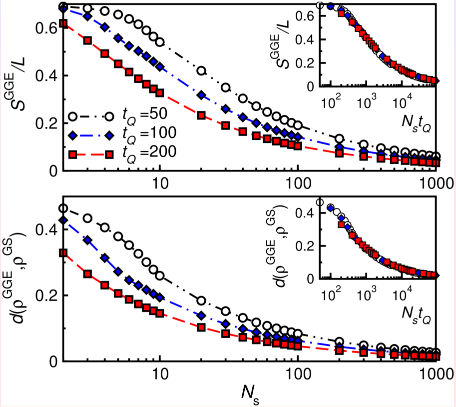
R. Modak, L. Vidmar, and MR, arXiv:1608.08453.

“Quantum battery” made of band insulators



$$d(\rho^{\mathsf{GGE}}, \rho^{\mathsf{GS}}) = \frac{1}{2N} \mathrm{Tr}\left[\sqrt{[\rho^{\mathsf{GGE}} - \rho^{\mathsf{GS}}]^2}\right].$$

"Quantum battery" made of band insulators



$$S = -\sum_{\alpha=1}^{L}[I_\alpha \ln I_\alpha + (1-I_\alpha)\ln(1-I_\alpha)] .$$

$$d(\rho^{\text{GGE}}, \rho^{\text{GS}}) = \frac{1}{2N}\text{Tr}\left[\sqrt{[\rho^{\text{GGE}} - \rho^{\text{GS}}]^2}\right] .$$

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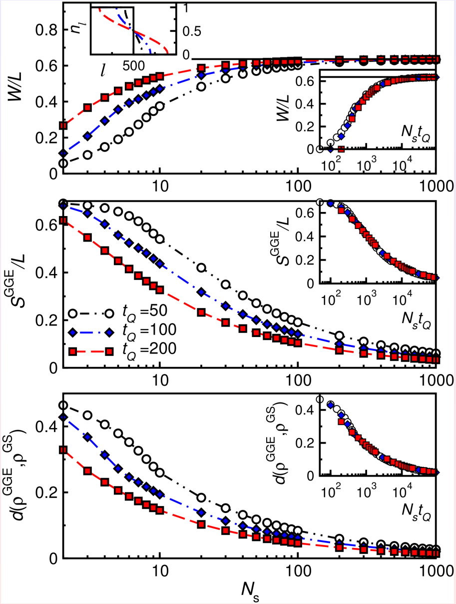

$$W = \mathrm{Tr}\left[(\hat{\rho}^I - \hat{\rho}^F)(\hat{H}_1 + \hat{H}_2) \right].$$

$$S = -\sum_{\alpha=1}^{L} [I_\alpha \ln I_\alpha + (1 - I_\alpha)\ln(1 - I_\alpha)].$$

$$d(\rho^{\mathrm{GGE}}, \rho^{\mathrm{GS}}) = \frac{1}{2N} \mathrm{Tr}\left[\sqrt{[\rho^{\mathrm{GGE}} - \rho^{\mathrm{GS}}]^2}\right].$$

Summary

- The emergent eigenstate solution explains why ground-state-like power-law correlations emerge during the meting of domain walls
- Only one conserved (or quasi-conserved) quantity is needed for the emergent Hamiltonian construction to work
  - Nonintegrable systems close to integrability?
  - More general nonintegrable systems?
- An effective cooling takes place during the melting of finite-T Mott insulators (internal energy is converted into center of mass energy).
- The emergent Gibbs ensemble can be used to describe the dynamics of finite-temperature initial states.
- Emergent Hamiltonians can be used to speed up adiabatic processes, and to speed up maximal work extraction.

Collaborators

- Deepak Iyer (Penn State $\longrightarrow$ Bucknell)
- Ranjan Modak (Penn State)
- Lev Vidmar (Penn State $\longrightarrow$ Jožef Stefan Institute)
- Wei Xu (Penn State)
- Collaborators in the Bose-Hubbard and Fermi-Hubbard projects
- Alejandro Muramatsu (Buenos Aires 1951- Stuttgart 2015)

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