Generalized thermalization in integrable lattice systems

Marcos Rigol

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Fifth Mandelstam Theoretical Physics School and Workshop Pilanesberg Game Reserve, South Africa

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L. Vidmar and MR, *Generalized Gibbs ensemble in integrable lattice models*, J. Stat. Mech. 064007 (2016).

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Video to be posted in the conference website!



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Outline



Introduction

- Experiments with ultracold gases in one dimension
- Classical and quantum integrability
- Hard-core bosons in one-dimensional lattices
- 2 Generalized Gibbs Ensemble (GGE)
 - Maximal entropy and the GGE
- 3 Generalized Thermalization
 - GGE vs quantum mechanics
 - Generalized eigenstate thermalization

Summary

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- Classical and quantum integrability
- Hard-core bosons in one-dimensional lattices
- Generalized Gibbs Ensemble (GGE
 Maximal entropy and the GGE
- 3 Generalized Thermalization
 - GGE vs quantum mechanics
 - Generalized eigenstate thermalization

Summary



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



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).

$$\eta^{(2)}(x) = rac{\langle \hat{\Psi}^{\dagger 2}(x) \Psi^2(x)
angle}{n_{1D}^2(x)}$$
 and $\gamma_{\mathsf{eff}} = rac{mg_{1D}}{\hbar^2 n_{1D}}$

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101 100 (d) 10-1 0 -20 0 20 2x/2 10-4 100 $D(\hbar k)$ 5/33 January 13, 2023

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

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

> n(p): Momentum distribution \Leftrightarrow n(x): Density distribution \Leftrightarrow

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T. Kinoshita, T. Wenger, and D. S. Weiss, Nature 440, 900 (2006).

MR, A. Muramatsu, and M. Olshanii, Phys. Rev. A 74, 053616 (2006).

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T. Kinoshita, T. Wenger, and D. S. Weiss, Nature **440**, 900 (2006).

 $\gamma = \frac{mg_{1D}}{\hbar^2 n_{1D}}$

 g_{1D} : Contact interaction strength n_{1D} : One-dimensional density

If $\gamma \gg 1$ the system is in the strongly correlated Tonks-Girardeau regime

If $\gamma \ll 1$ the system is in the weakly interacting regime

Review of related work in atom chips: T. Langen, T. Gasenzer, and J. Schmiedmayer, J. Stat. Mech. 064009 (2016).

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Outline



Classical chaos and integrability

Particle trajectories in a circular cavity and a Bunimovich stadium (scholarpedia)



- Integrability: A system is said to be integrable if it has as many constants of motion as degrees of freedom
- Chaos: exponential sensitivity of the trajectories to perturbations

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Liouville's integrability theorem (Classical)

Hamiltonian

$$H(p,q),$$
 coordinates $q = (q_1, \cdots, q_N)$
momenta $p = (p_1, \cdots, p_N)$

N independent constants of the motion, $I = (I_1, \cdots, I_N)$, in involution

$$\{I_{\alpha}, H\} = 0, \quad \{I_{\alpha}, I_{\beta}\} = 0, \qquad \{f, g\} = \sum_{i=1,N} \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i}$$

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There is a canonical transformation $(p,q) \rightarrow (\Theta, I)$ (action-angle variables)

$$H(p,q) = H'(I)$$

Equations of motion

$$\frac{dI_{\alpha}}{dt} = -\frac{\partial H'}{\partial \Theta_{\alpha}} = 0 \Rightarrow I_{\alpha} = \text{constant}$$
$$\frac{d\Theta_{\alpha}}{dt} = \frac{\partial H'}{\partial I_{\alpha}} = \Omega_{\alpha}(I) \Rightarrow \Theta_{\alpha} = \Omega_{\alpha}(I)t + \Theta_{\alpha}^{0}$$

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Impenetrable particles, interaction potential decays sufficiently fast, $x_1 \ll x_2 \ll x_3 \ll \ldots$, and $k_1 > k_2 > k_3 > \ldots$

B. Sutherland, Beautiful Models (World Scientific, Singapore, 2004).

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Two particles: $K = k_1 + k_2$, $E = \varepsilon(k_1) + \varepsilon(k_2)$, $\Psi(x_1, x_2) \rightarrow \psi(x_1, x_2)$ $\sum_{P} A(P) e^{i(k_{P1}x_1 + k_{P2}x_2)} = A(12) e^{i(k_1x_1 + k_2x_2)} + A(21) e^{i(k_2x_1 + k_1x_2)}$

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 $\begin{array}{ll} \text{Three particles:} & K = k_1 + k_2 + k_3, & E = \varepsilon(k_1) + \varepsilon(k_2) + \varepsilon(k_3) \\ \Psi(x_1, x_2, x_3) \rightarrow \sum_P A(P) \; e^{i(k_{P1}x_1 + k_{P2}x_2 + k_{P3}x_3)} + \; \text{diffractive scattering} \end{array}$

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B. Sutherland, Beautiful Models (World Scientific, Singapore, 2004).

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Outline



Introduction

Summary

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Bose-Fermi mapping in a 1D lattice

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

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

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

Non-interacting fermion Hamiltonian

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

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Bose-Fermi mapping in a 1D lattice

Hard-core boson Hamiltonian in an external potential

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Constraints on the bosonic operators

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

Set of conserved quantitites

(Occupations of the single-particle energy eigenstates of the noninteracting fermions)

$$\hat{H}_F \hat{\gamma}_m^{f\dagger} |0\rangle = E_m \hat{\gamma}_m^{f\dagger} |0\rangle$$
$$\left\{ \hat{I}_m^f \right\} = \left\{ \hat{\gamma}_m^{f\dagger} \hat{\gamma}_m^f \right\}$$

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

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

MR and A. Muramatsu, PRL 93, 230404 (2004).

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

 \sim 10000 lattice sites, $~~\sim$ 1000 particles

MR and A. Muramatsu, PRL 93, 230404 (2004).

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Dynamical fermionization during expansion in 1D

Dynamics after turning off the confining potential

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MR and A. Muramatsu, Phys. Rev. Lett. 94, 240403 (2005).

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J. M. Wilson, N. Malvania, Y. Le, Y. Zhang, MR, and D. S. Weiss, Science 367, 1461 (2020).



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Finite temperature

One-particle density matrix (grand-canonical ensemble)

$$\rho_{ij} \equiv \frac{1}{Z} \operatorname{Tr} \left\{ \hat{b}_i^{\dagger} \hat{b}_j e^{-\frac{\hat{H}_{HCB} - \mu \sum_m \hat{b}_m^{\dagger} \hat{b}_m}{k_B T}} \right\}, \quad Z = \operatorname{Tr} \left\{ e^{-\frac{\hat{H}_{HCB} - \mu \sum_m \hat{b}_m^{\dagger} \hat{b}_m}{k_B T}} \right\}$$

MR, PRA 72, 063607 (2005)

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Mapping to noninteracting fermions

$$\rho_{ij} = \frac{1}{Z} \operatorname{Tr} \left\{ \hat{f}_i^{\dagger} \hat{f}_j \prod_{k=1}^{j-1} e^{i\pi \hat{f}_k^{\dagger} \hat{f}_k} e^{-\frac{\hat{H}_F - \mu \sum_m \hat{f}_m^{\dagger} \hat{f}_m}{k_B T}} \prod_{l=1}^{i-1} e^{-i\pi \hat{f}_l^{\dagger} \hat{f}_l} \right\}$$

Exact one-particle density matrix

$$\rho_{ij} = \frac{1}{Z} \left\{ \det \left[\mathbf{I} + (\mathbf{I} + \mathbf{A}) \mathbf{O}_1 \mathbf{U} e^{-(\mathbf{E} - \mu \mathbf{I})/k_B T} \mathbf{U}^{\dagger} \mathbf{O}_2 \right] - \det \left[\mathbf{I} + \mathbf{O}_1 \mathbf{U} e^{-(\mathbf{E} - \mu \mathbf{I})/k_B T} \mathbf{U}^{\dagger} \mathbf{O}_2 \right] \right\}$$

Computation time $\sim L^5$: 1000 sites MR, PRA **72**, 063607 (2005)

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Outline



Summary

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Relaxation dynamics in an integrable system



MR, V. Dunjko, V. Yurovsky, and M. Olshanii, PRL 98, 050405 (2007).

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Relaxation dynamics in an integrable system



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Thermal equilibrium

$$\hat{\rho} = Z^{-1} \exp\left[-\left(\hat{H} - \mu\hat{N}\right)/k_BT\right]$$
$$Z = \operatorname{Tr}\left\{\exp\left[-\left(\hat{H} - \mu\hat{N}\right)/k_BT\right]\right\}$$
$$E = \operatorname{Tr}\left\{\hat{H}\hat{\rho}\right\}, \quad N = \operatorname{Tr}\left\{\hat{N}\hat{\rho}\right\}$$

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MR, FRA 12, 003007 (2003)

Conserved quantities

(underlying noninteracting fermions)

$$\hat{H}_F \hat{\gamma}_m^{f\dagger} |0\rangle = E_m \hat{\gamma}_m^{f\dagger} |0\rangle$$

$$\left\{ \hat{I}_m \right\} = \left\{ \hat{\gamma}_m^{f\dagger} \hat{\gamma}_m^f \right\}$$



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Generalized Gibbs ensemble

$$\hat{\rho}_{\text{GGE}} = Z_c^{-1} \exp\left[-\sum_m \lambda_m \hat{I}_m\right]$$
$$Z_c = \text{Tr}\left\{\exp\left[-\sum_m \lambda_m \hat{I}_m\right]\right\}$$
$$\text{Tr}\left\{\hat{I}_m \hat{\rho}_{\text{GGE}}\right\} = \langle \hat{I}_m \rangle_{\tau=0}$$





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Outline



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Exact results from quantum mechanics

If the initial state is not an eigenstate of \widehat{H}

 $|\psi_{\rm ini}\rangle \neq |\alpha\rangle \quad {\rm where} \quad \widehat{H}|\alpha\rangle = E_\alpha |\alpha\rangle \quad {\rm and} \quad E = \langle \psi_{\rm ini}|\widehat{H}|\psi_{\rm ini}\rangle,$

then observables \hat{O} evolve in time:

$$O(\tau) \equiv \langle \psi(\tau) | \hat{O} | \psi(\tau) \rangle \quad \text{where} \quad |\psi(\tau)\rangle = e^{-i\hat{H}\tau} |\psi_{\text{ini}}\rangle.$$

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What is it that we call generalized thermalization?

$$O(\tau > \tau^*) \simeq O(I_1, \ldots, I_L).$$

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One can rewrite

$$O(\tau) = \sum_{\alpha,\beta} C^{\star}_{\alpha} C_{\beta} e^{i(E_{\alpha} - E_{\beta})\tau} O_{\alpha\beta} \quad \text{using} \quad |\psi_{\mathrm{ini}}\rangle = \sum_{\alpha} C_{\alpha} |\alpha\rangle.$$

Taking the infinite time average (diagonal ensemble $\hat{\rho}_{DE} \equiv \sum_{\alpha} |C_{\alpha}|^2 |\alpha\rangle \langle \alpha |$)

$$\overline{O(\tau)} = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau d\tau' \langle \Psi(\tau') | \hat{O} | \Psi(\tau') \rangle \stackrel{?}{=} \sum_{\alpha} |C_{\alpha}|^2 O_{\alpha \alpha} \equiv \langle \hat{O} \rangle_{\rm DE},$$

which depends on the initial conditions through $C_{\alpha} = \langle \alpha | \psi_{\text{ini}} \rangle$.

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Entropies after quenches in a superlattice potential



S_{DE} & S_{GGE} are extensive but different! Santos, Polkovnikov, and MR, Phys. Rev. Lett. **107**, 040601 (2011).

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"Thermalization" in Integrable Systems

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The transverse-field Ising model

$$\hat{H}_{\text{TFIM}} = -\sum_{j} \hat{S}_{j}^{x} \hat{S}_{j+1}^{x} - h \sum_{j} \hat{S}_{j}^{z}$$

Entropies after quenches in the translationally invariant case

$$S_{\text{GGE}} = 2S_{\text{DE}}$$

Gurarie, J. Stat. Mech. P02014 (2013); Kormos, Bucciantini & Calabrese, EPL 107, 40002 (2014).

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Generalized eigenstate thermalization:

A. C. Cassidy, C. W. Clark, and MR, PRL 106, 140405 (2011).

L. Vidmar and MR, J. Stat. Mech. 064007 (2016).

Behind generalized thermodynamic Bethe ansatz approaches: J.-S. Caux and F. H. L. Essler, PRL **110**, 257203 (2013). B Pozsgay, J. Stat. Mech. P09026 (2014).

Weight of eigenstate expectation values after equilibration



L. Vidmar and MR, J. Stat. Mech. 064007 (2016).

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Weight of eigenstate expectation values in the GGE



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Variance of observable $\hat{\mathcal{O}}$ after quenches $h_0 \to h$ (ENS = DE, GGE)

$$\Sigma_{\hat{\mathcal{O}},\mathsf{ENS}}^2 = \sum_n \rho_n^{\mathsf{ENS}} \langle n | \hat{\mathcal{O}} | n \rangle^2 - \left(\sum_n \rho_n^{\mathsf{ENS}} \langle n | \hat{\mathcal{O}} | n \rangle \right)^2$$

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For all local observables for which $\Sigma^2_{\hat{\mathcal{O}}, \mathrm{ENS}}$ was calculated analytically

$$\frac{\Sigma_{\hat{\mathcal{O}},\text{DE}}^2}{\Sigma_{\hat{\mathcal{O}},\text{GGE}}^2} = 2, \quad \text{and} \quad \Sigma_{\hat{\mathcal{O}},\text{ENS}} \sim \frac{1}{\sqrt{L}}$$

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For example, for quenches across the critical field:

$$\Sigma_{\hat{S}_{j}^{x}\hat{S}_{j+1}^{x},\text{DE}}^{2} = \begin{cases} \frac{1}{64L} \left[1 + h_{0}^{2} - \frac{2h_{0}}{h} \right] & \text{if} \quad h > 1, \ h_{0} < 1 \\ \\ \frac{1}{64L} \left[4 - 3h^{2} - \left(\frac{h}{h_{0}}\right)(4 - 2h^{2}) + \left(\frac{h}{h_{0}}\right)^{2} \right] & \text{if} \quad h < 1, \ h_{0} > 1 \end{cases}$$

L. Vidmar and MR, J. Stat. Mech. 064007 (2016).

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 Few-body observables in integrable systems equilibrate
 ★Recurrences occur but most of the time observables are described by the diagonal ensemble

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 Recurrences occur but most of the time observables are described by the diagonal ensemble
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★ Microcanonical discussion: Cassidy, Clark & MR, PRL 106, 140405 (2011).

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The assumption of local equilibration to the GGE is a starting point for generalized hydrodynamics theories
 ★O. A. Castro-Alvaredo, B. Doyon, T. Yoshimura, PRX 6, 041065 (2016).
 ★B. Bertini, M. Collura, J. De Nardis, M. Fagotti, PRL 117, 207201 (2016).

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- David Weiss & group (Penn State)

Vladimir Yurovsky (Tel Aviv U)

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