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Geometry of quantum observables and thermodynamics of small systems

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We show that for classical and quantum observables, the integrability-to-ergodicity transition leaves constant the sum of (a) the ensemble variance of the temporal average and (b) the ensemble average of temporal variance. The induced Frobenius (Hilbert-Schmidt) geometry of quantum observables encodes how eigenstate thermalization appears, the inverse participation ratio decreases, and the integrals of motion disappear during the transition. We use it to optimize the set of conserved quantities entering the Generalized Gibbs Ensemble for integrable, near-integrable, or mesoscopic systems.

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Nonequilibrium dynamics of isolated quantum systems has received much attention [1–5] following the landmark experiment [6]. Much studied is the integrability-to-chaos transition (ICT) [2, 7, 8], linked to the Fock-space diffusion and localization in disordered interacting systems [2, 7, 8] and, in quantum field theory, to the confinement of topological excitations [7, 9] and the decay of higher-mass excitations [7, 10]. On the classical side, all began with the Fermi-Pasta-Ulam problem [11, 12], its legacy including solitons, dynamical chaos, and the Kolmogorov-Arnold-Moser (KAM) theorem. For quantum dynamics, we now know that chaos and thermalization happen within individual eigenstates (the eigenstate thermalization hypothesis (ETH) [2, 5, 13–15]). Much impetus came [15] from studying relaxation in integrable systems [2, 5, 16].

We will study the ICT in the following setting: let \hat{H}_0 be an integrable Hamiltonian, and \hat{V} a perturbation such that the full Hamiltonian $\hat{H} = \hat{H}_0 + g\hat{V}$ ($g \geq 0$) is non-integrable if $g > 0$. g varies from zero to large enough to just begin to fully ergodize the system, without changing the energetics. (Ergodicity normally emerges for interaction strengths still too weak to alter the thermal expectations of observables: e.g., the van der Waals interactions between the air molecules cause thermalization but do not modify the Maxwell distribution.) Let A be an observable, and \hat{A} the corresponding operator.

Below, we will: 1. show that the ICT obeys a “circle law”: the sum of certain two types of fluctuations is independent of g ; 2. motivated by this, introduce a geometry in the space of observables, based on the Hilbert-Schmidt inner product; 3. as an application of this new formalism for describing the ICT, show how to optimally choose the operators to be included into the Generalized Gibbs Ensemble (GGE) [16].

The “circle law” relates two fluctuation measures of A :

$$\text{Var}_{\text{MC}}[E_t[A]] \Big|_{\text{QM}} + E_{\text{MC}}[\text{Var}_t[A]] \Big|_{\text{QM}} = \text{const. independent of } g. \quad (1)$$

The text from here to the paragraph containing Eq. (2) is dedicated to explaining this statement.

Start classically: imagine a ball in a rectangular billiards with periodic boundary conditions and either with or without a localized obstacle. With no obstacle, the system is integrable; with the obstacle present, let the system be ergodized but with unchanged energetics (see above). Consider $A = v_x$ of the ball. Given an initial velocity \vec{v}_0 , compute the infinite-time

mean of A over a trajectory, $E_t[A]$, and the infinite-time average of the temporal fluctuations around this mean, $\text{Var}_t[A]$. Do this for all \vec{v}_0 ’s from a microcanonical (MC) hypersurface of a certain energy; compute the MC variance of $E_t[A]$ and the MC mean of $\text{Var}_t[A]$. Now: if the obstacle is absent, then $v_x = v_{x,0}$ for all t ; thus $E_t[A] = v_{x,0}$, while $\text{Var}_t[A] = 0$. So $\text{Var}_{\text{MC}}[E_t[A]]$ = the variance of A in the MC distribution, while $E_{\text{MC}}[\text{Var}_t[A]] = 0$. The obstacle reverses this [17]: no matter what \vec{v}_0 is, the infinite time average of v_x is zero, so $\text{Var}_{\text{MC}}[E_t[A]] = 0$; meanwhile, the temporal fluctuations in v_x are finite, so $E_{\text{MC}}[\text{Var}_t[A]]$ is finite, and in fact it *also* turns out to be equal to the variance of A in the MC distribution, consistent with Eq. (1). Figure 1a shows on an example that this law also holds for intermediate strengths of the obstacle.

Next we translate the classical quantities to quantum ones. Let $\hat{H}|\alpha_g\rangle = E_\alpha^g|\alpha_g\rangle$. The *MC window* [MC], which will be short for ‘maximal allowed MC window,’ is a certain heuristically determined energy interval centered on the mean energy of the system: plot $\langle\alpha_g|\hat{A}|\alpha_g\rangle$ versus E_α^g . Start zooming in to the part of the plot at the mean energy; once the plot starts to have no structure across the MC window (it should ‘look the same’ if it is flipped left-to-right), further decreases in window size would not decrease the MC variance. We make sure this window size works for both $g = 0$ and the maximal g of interest; the horizontal extent $[E_{\min}, E_{\max}]$ is then our [MC]. In our numerics below, the MC window is a fraction of the full width of the energy spectrum. ‘ $|\alpha_g\rangle, \alpha_g \in [\text{MC}]$ ’ mean that $E_\alpha^g \in [\text{MC}]$. The MC means and variances are the usual ones, over all $|\alpha_g\rangle \in [\text{MC}]$.

For us, the quantum analog of an ensemble of classical initial conditions is the ensemble of randomly chosen energy eigenstates [18]. So $\text{Var}_{\text{MC}}[E_t[A]] \Big|_{\text{QM}} = \text{Var}_{\text{MC}}[\langle\alpha|\hat{A}|\alpha\rangle]$:

$$\text{Var}_{\text{MC}}[E_t[A]] \Big|_{\text{QM}} \equiv \frac{1}{N_{\text{MC}}} \sum_{\alpha \in [\text{MC}]} (\langle\alpha|\hat{A}|\alpha\rangle - \langle A \rangle)^2,$$

where $\langle A \rangle = E_{\text{MC}}[A] \equiv (N_{\text{MC}})^{-1} \sum_{\alpha \in \text{MC}} \langle\alpha|\hat{A}|\alpha\rangle$, and N_{MC} the number of eigenstates in [MC]. For brevity, $|\alpha\rangle = |\alpha_g\rangle$. A sufficient condition for the emergence of ergodicity [13–15] is that $\text{Var}_{\text{MC}}[\langle\alpha|\hat{A}|\alpha\rangle] \rightarrow 0$ in the thermodynamic limit: this is ETH [19]. Below, in Eq. (3), we give a scale for this variance, determining to what extent A is thermalizable.

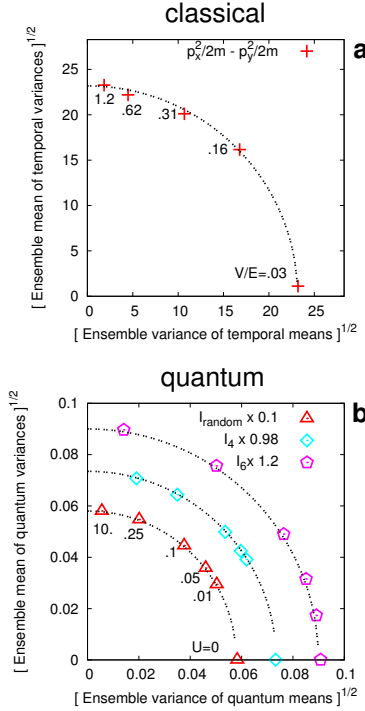


FIG. 1. The ‘circle law.’ **a**, A classical rectangular billiards perturbed by a soft-core barrier, with periodic boundary conditions (see Sec. SD6 of [22]). For all barrier heights \lesssim the kinetic energy, Eq. (1) holds, where $A = \frac{1}{2m}p_x^2 - \frac{1}{2m}p_y^2$. With no barrier, the ensemble mean energy is $E_0 = 33.7$. V is the barrier height and E is the mean energy of the ensemble (including the barrier energy). (V/E) point-to- (V/E) point, the phase-space volume of the MC ensemble ($W = 1184.3$), and that of the phase-space points with energies below the MC window ($W_b = 7895.7$), do not change. Such a set of ensembles is the closest classical analogue of a quantum set using the same window of quantum state *indices* for all perturbation strengths. **b**, A quantum example: three integrals of motion of a system of hard-core bosons. The integrability is gradually broken by a soft-core two-body repulsive potential, whose height is U at distances \leq four sites, and zero otherwise (see Sec. SD7 of [22]). There are $N = 4$ particles and $L = 16$ lattice sites, and open boundary conditions. The integrals of motion \hat{I}_4 and \hat{I}_6 are explained in the text. The ‘artificial’ integral of motion \hat{I}_{random} is, in the basis of the unperturbed eigenstates, a diagonal matrix whose entries are randomly and uniformly distributed between -1 and $+1$. For \hat{I}_{random} , the cosine-squared of the polar angle of a plotted point equals the inverse participation ratio η (up to corrections of $\mathcal{O}(N_{\text{MC}}^{-1})$; see Eq. (4)). \hat{I}_4 and \hat{I}_6 behave similarly.

To quantify $E_{\text{MC}}[\text{Var}_t[A]]|_{\text{QM}}$: for every t of interest, we repeatedly time-evolve the system from the same initial state until performing the measurement at t ; at the end we compute the variance. Reference [20] argued that in the ergodic case, these are in fact the *thermal* fluctuations [21]. Thus

$$E_{\text{MC}}[\text{Var}_t[A]]|_{\text{QM}} \equiv \frac{1}{N_{\text{MC}}} \sum_{\alpha \in [\text{MC}]} \left(\langle \alpha | \hat{A}^2 | \alpha \rangle - \langle \alpha | \hat{A} | \alpha \rangle^2 \right).$$

In Fig. 1b we test Eq. (1) on the 1D gas of lattice hard-core bosons perturbed by a two-body soft-core repulsive interaction (see Sec. SD7 of [22]). In 1D, both continuous-space and

lattice hard-core bosons are integrable: Girardeau’s map [23] and the Jordan-Wigner transformation, respectively, map the system eigenstates to those of a free Fermi gas, so that occupation numbers of the eigenstates of the one-body Hamiltonian for the underlying free fermions are integrals of motion. The integrals of motion we consider are \hat{I}_4 and \hat{I}_6 , which are easiest to understand using the \hat{a}_j s and \hat{a}_j^\dagger s of the underlying lattice free fermions (see also Sec. SD8 of [22]): note that the energy is the normalized sum over lattice sites j of $\hat{a}_j^\dagger \hat{a}_{j+1}$ (plus h.c.); then \hat{I}_{2k} is the normalized sum (modulo h.c. and boundary terms to accommodate the open boundary conditions) over j of $\hat{a}_j^\dagger \hat{a}_{j+k}$. Equivalently, up to boundary terms, $\hat{I}_{2k} \sim \cos k\hat{p}$, where \hat{p} is the momentum of the underlying fermions. As we ramp up the perturbation, \hat{I}_4 and \hat{I}_6 are gradually destroyed: while the quantum (=thermal [20]) fluctuations increase, the deviations from ergodicity decrease. However, the sum of the two variances remains constant. The square of the radius of the circles corresponds to the ensemble variance of the observable, over a series of *single* measurements, on a randomly chosen eigenstate.

To finally prove (1), we rearrange the terms in the definitions of $\text{Var}_{\text{MC}}[E_t[A]]|_{\text{QM}}$ and $E_{\text{MC}}[\text{Var}_t[A]]|_{\text{QM}}$ and write the left-hand-side (LHS) of (1) as the *ensemble variance* of \hat{A} :

$$\text{Var}_{\text{MC}}[E_t[A]]|_{\text{QM}} + E_{\text{MC}}[\text{Var}_t[A]]|_{\text{QM}} = \text{Var}_{\text{MC}}[A], \quad (2)$$

where $\text{Var}_{\text{MC}}[A] = E_{\text{MC}}[A^2] - E_{\text{MC}}[A]^2$, and so is a function of two ensemble means. Let us prove that as g is increased from zero up to a value where the system first becomes ergodic, the ensemble means remain constant. The integrability-breaking perturbation $g\hat{V}$ will need to satisfy two conditions: let $\delta E^0(g)$ be the typical shift in eigenenergies due to $g\hat{V}$; and let ΔE_V^0 be the characteristic energy interval such that \hat{V} appreciably couples only those eigenstates of \hat{H}_0 whose energy difference is less than ΔE_V^0 . We require that both $\delta E^0(g)$ and ΔE_V^0 be much smaller than the width of the MC window used to define the ensemble means. Now consider the eigenstates of the unperturbed system; the perturbation results in their mutual coupling, and some shifting of the eigenenergies. Because $\delta E^0(g)$ is small, as g is increased, almost all eigenenergies remain in the original MC window; and because ΔE_V^0 is small, we may neglect the coupling of states within the window to states outside the window. But then we may as well truncate our Hilbert space to just the states inside the window (obtaining a ‘truncated Hamiltonian’). Let us first truncate, and then turn on g . The eigenstates of the perturbed and unperturbed truncated Hamiltonians, being bases of the truncated space, are related by a unitary transformation. But the two ensemble means are traces, and thus do not change under unitary transformation of the basis; thus they do not depend on g , proving Eq. (1).

The system in Fig. 1b does satisfy the two requirements. We have $[\text{MC}] = [-2, 2]$; for the values of g used, when one plots the eigenenergies with $g = 0$ and $g \neq 0$, the energy shifts are not noticeable on the scale of this MC window. As

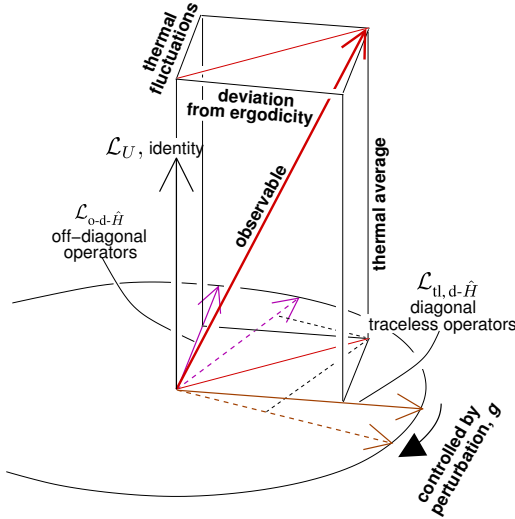


FIG. 2. The Hilbert-Schmidt geometry and quantum integrability-ergodicity transition. The N^2 -dimensional space of operators on an N -dimensional space is divided onto the sum of three subspaces \mathcal{L}_U , $\mathcal{L}_{tl, d, \hat{H}}$, and $\mathcal{L}_{o-d, \hat{H}}$ (see text). Varying the coupling constant g of the Hamiltonian $\hat{H} = \hat{H}_0 + g\hat{V}$ rotates the spaces $\mathcal{L}_{tl, d, \hat{H}}$ and $\mathcal{L}_{o-d, \hat{H}}$ but not the identity axis (the projection to which is proportional to the microcanonical (MC) average). An observable's HS vector also remains fixed (thus, so does the MC average). Observables with a large projection onto $\mathcal{L}_{tl, d, \hat{H}}$ are quasi-conserved (non-ergodic); those with a large projection onto $\mathcal{L}_{o-d, \hat{H}}$ are thermalizable (infinite time average equals the MC average). We have ergodicity when $\mathcal{L}_{o-d, \hat{H}}$ aligns with the traceless versions of all the observables of interest, e.g. with all few-body observables in a many-body system.

for the second requirement, let $\hat{H}_0|\alpha_0\rangle = E_{\alpha_0}^0|\alpha_0\rangle$; the rms energy distance between the $|\alpha_0\rangle$'s coupled by \hat{V} is ($V_{\alpha_0, \alpha'_0} = \langle\alpha_0|\hat{V}|\alpha'_0\rangle$):

$$\Delta E_V^0 \equiv \sqrt{\frac{\sum_{\alpha_0 \in [\text{MC}]} \sum_{\alpha'_0} |V_{\alpha_0, \alpha'_0}|^2 (E_{\alpha'_0}^0 - E_{\alpha_0}^0)^2}{\sum_{\alpha_0 \in [\text{MC}]} \sum_{\alpha'_0} |V_{\alpha_0, \alpha'_0}|^2}} = 0.3.$$

Equation (2) has a geometric interpretation: after we move $E_{\text{MC}}[A]^2$ to the LHS, the RHS becomes the norm-squared of a vector, and the new LHS is its decomposition over certain complementary subspaces that change with g . The relevant inner product is the Frobenius, or Hilbert-Schmidt (HS), product of matrices: $(\hat{A}|\hat{B}) \equiv \text{Tr}[\hat{A}^\dagger \hat{B}]$. Quantum observables (Hermitian matrices) form a linear space over the reals; the HS product is a real-valued inner product on this space. The unitary transformations $\hat{A} \mapsto \hat{U} \hat{A} \hat{U}^{-1}$ are a subgroup of the group of linear transformations preserving the product. Consider the MC window of eigenstates (a space of size N_{MC}), and the N_{MC}^2 -dimensional space (over the reals) of all Hermitian operators acting within the window. The HS product is an inner product on the latter space, which we decompose into the direct sum of three pairwise orthogonal subspaces: 1. the 1D space \mathcal{L}_U spanned by the identity operator \hat{I}_d ; the projection of \hat{A} onto this space is $\hat{P}_{\mathcal{L}_U} \hat{A} = (\text{Tr} \hat{A} / N_{\text{MC}}^2) \hat{I}_d$; 2. the $(N_{\text{MC}} - 1)$ -dimensional space $\mathcal{L}_{tl, d, \hat{H}}$ of all traceless *integrals of motion*, i.e. of traceless operators purely

diagonal in the basis of the eigenstates $|\alpha_g\rangle$: $\hat{P}_{\mathcal{L}_{tl, d, \hat{H}}} \hat{A} = \sum_{\alpha_g} |\alpha_g\rangle \langle \alpha_g| (\hat{A} - \hat{P}_{\mathcal{L}_U} \hat{A}) |\alpha_g\rangle \langle \alpha_g|$; 3. the $N_{\text{MC}}(N_{\text{MC}} - 1)$ -dimensional space $\mathcal{L}_{o-d, \hat{H}}$ of all purely off-diagonal operators in the same basis: $\hat{P}_{\mathcal{L}_{o-d, \hat{H}}} \hat{A} = \hat{I}_d - \hat{P}_{\mathcal{L}_U} - \hat{P}_{\mathcal{L}_{tl, d, \hat{H}}}$ (see Fig. 2).

The HS angle $\theta_{\mathcal{L}_{tl, d, \hat{H}}, \hat{A}_{tl}}$ between the traceless version of an observable ($\hat{A}_{tl} \equiv \hat{A} - \text{Tr}[\hat{A}] / N_{\text{MC}}$) and the space $\mathcal{L}_{tl, d, \hat{H}}$ quantifies the extent to which A is thermalizable:

$$\tan^2[\theta_{\mathcal{L}_{tl, d, \hat{H}}, \hat{A}_{tl}}] = E_{\text{MC}}[\text{Var}_t[A]] \Big|_{\text{QM}} / \text{Var}_{\text{MC}}[E_t[A]] \Big|_{\text{QM}} \quad (3)$$

(see Fig. 2). The HS angle between a vector \hat{B} and a hyperplane \mathcal{L} is given through $\cos^2(\theta_{\hat{B}, \mathcal{L}}) = \sum_i \cos^2(\theta_{\hat{B}, \hat{e}_i})$ $0 \leq \theta_{\hat{B}, \mathcal{L}} \leq \pi/2$, where $\{\hat{e}_i\}$ is any orthonormalized basis set in \mathcal{L} ; $\cos(\theta_{\hat{B}, \hat{e}_i}) = (\hat{B}|\hat{e}_i) / (\hat{B}|\hat{B})^{1/2}$. If eigenstate thermalization [13–15] holds, $\theta_{\mathcal{L}_{tl, d, \hat{H}}, \hat{A}_{tl}}$ approaches 90° .

The inverse participation ratio η , which governs the transition to thermalizability [8, 24, 25], defines the average angle between the projector to an eigenstate of \hat{H}_0 and the space of the integrals of motion of \hat{H} :

$$\eta \equiv N_{\text{MC}}^{-1} \sum_{\alpha_g, \alpha_0 \in [\text{MC}]} |\langle \alpha_0 | \alpha_g \rangle|^4 = \overline{\cos^2[\theta_{\mathcal{L}_{d, \hat{H}}, (|\alpha_0\rangle \langle \alpha_0|)}]}^{\alpha_0}, \quad (4)$$

where the space of diagonal operators $\mathcal{L}_{d, \hat{H}} = \mathcal{L}_{tl, d, \hat{H}} \oplus \mathcal{L}_U$ (compare with the discussion of \hat{I}_{random} in Fig. 1).

As an application, we now show how to optimize the set of conserved quantities to be used in a *predictively enhanced thermodynamics*, i.e. the GGE, valid for systems anywhere on the ICT continuum. In all examples studied so far [16, 26] there is a straightforward map between the integrable system and an underlying system of free particles, and so it is the occupation numbers of the one-body eigenstates of the latter that are included in the Gibbs exponent of the GGE [16, 27–30]. However: (a) it seems that for a disorder-induced *localization*, these occupation numbers do *not* improve the thermodynamic predictions [30]; (b) not every integrable system can be mapped to free particles; and (c) for systems in the middle of an ICT, the failure of the ETH is for all practical purposes, indistinct from that due to actual integrals of motion.

Recall that the MC ensemble prediction for the infinite time average of A , $E_{\text{MC}}[A]$, has the mean square error (MSE) $\text{Var}_{\text{MC}}[A_{\alpha, \alpha}]$ ($A_{\alpha, \alpha} = \langle \alpha | \hat{A} | \alpha \rangle$). Similarly, the MSE of the MC version of the GGE (where not only the energy, but additional quantities, normally integrals of motion, are constrained to lie in narrow windows; see Secs. SD3 of [22]) is $\text{Var}_{\text{GGE}}[A_{\alpha, \alpha}]$. Our procedure, which does not assume that there are any special conserved quantities, is based on the following exact result, where the HS structure naturally emerges:

$$\text{Var}_{\text{GGE}}[A_{\alpha, \alpha}] / \text{Var}_{\text{MC}}[A_{\alpha, \alpha}] \leq \sin^2 \Theta + |\cos \Theta| \mathcal{O}(\epsilon), \quad (5)$$

where $\Theta = \theta_{\hat{I}_{tl}, \hat{P}_{\hat{H}} \hat{A}_{tl}}$; $\epsilon = \Delta I / \sqrt{\text{Var}_{\text{MC}}[\langle \alpha | \hat{I} | \alpha \rangle]} \ll 1$; $\hat{P}_{\hat{H}}$ is the “super-operator” that removes the off-diagonal (with respect to the eigenbasis of \hat{H}) matrix elements; $\Delta I \equiv \max_j (I_{j+1} - I_j)$ is the maximal width of the MC window

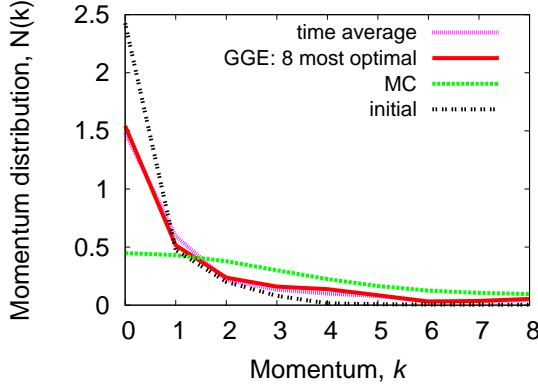


FIG. 3. Momentum distribution after a quench. The initial state is the ground state of a hard-core boson Hamiltonian for $N = 4$ atoms on $L = 16$ sites, with periodic boundary conditions. At $t = 0+$, a soft-core repulsion is turned on. The microcanonical (MC) ensemble contains $N_{MC} = 300$ lowest eigenstates. The GGE ensemble uses 8 most optimal integrals of motion, each of which was fixed to a window around its initial state value (except the first, which was strongly correlated with the energy). The half-width of each window was 10% of the corresponding MC standard deviation.

for the additional integral of motion; and $\{[I_{j+1} - I_j]\}$ is the set of intervals tiling the axis of the integral of motion I (see Secs. SD2-SD5 of [22]).

The procedure is: let $\mathcal{L}_{o.i.}$ be the linear space of the observables whose relaxations we wish to describe. Let $(\hat{I}_1)_{dl}$ be the diagonal traceless observable that minimizes the HS angle between itself and $\mathcal{L}_{o.i.}$; let $(\hat{I}_2)_{dl}$ be defined similarly, except that is restricted to lie in the space orthogonal to $(\hat{I}_1)_{dl}$; we keep doing this, always searching in the space orthogonal to all the integrals of motion previously chosen, till we reach the desired predictive power.

In Fig. 3 we study a system of 1D hard-core bosons, with and without an integrability-breaking perturbation by soft-core interactions (described in Sec. SD7 of [22]), undergoing a quench from the ground state in the integrable regime to a strongly perturbed regime ($\eta = .023$). The observable of interest is $N(k)$, the infinite time average of the momentum distribution of the bosons $\hat{N}(k) = \frac{1}{L} \sum_{j=1}^L \sum_{j'=1}^L e^{2\pi i k(j-j')/L} \hat{b}_j^\dagger \hat{b}_{j'}$, $k = 1, \dots, L/2$. The Figure shows that the optimal GGE is indeed superior to the MC ensemble. Section SD9 of [22] gives a detailed study of the bound (5) for this system.

Non-thermal behavior has been held to come from either (a) nontrivial symmetries or the Bethe ansatz [31, 32]; or (b) deviations from the ETH [15] due to small system size. In small systems the two are practically indistinct; there are no obvious candidates for the relevant conserved quantities. Our theory offers a unified approach, based on a “blind” optimization of the GGE. Our next application will be to study how fluctuations and imperfect thermalization impact the sensitivity and signal-to-noise ratio in matter-wave transistors [33, 34].

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