Breakdown of the generalized Gibbs ensemble for current–generating quenches

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We establish a relation between two hallmarks of integrable systems: the relaxation towards the generalized Gibbs ensemble (GGE) and the dissipationless charge transport. We show that the former one is possible only if the so called Mazur bound on the charge stiffness is saturated by local conserved quantities. As an example we show how a non–GGE steady state with a current can be generated in the one-dimensional model of interacting spinless fermions with a flux quench. Moreover an extended GGE involving the quasi-local conserved quantities can be formulated for this case.

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Recent advances in experiments on ultracold atoms together with new computational techniques have significantly broadened our understanding of relaxation processes in closed many-body quantum systems. It is commonly accepted that in generic macroscopic systems the long–time averages of local observables coincide with the results for the statistical Gibbs ensemble [1–4] and are uniquely determined by few parameters related to conserved quantities, in particular the system’s energy and particle number. Due to the presence of macroscopic number of conserved quantities such a simple scenario is not applicable to integrable systems [5–7]. However, there is a large and still growing evidence that relaxation in the latter systems is consistent with the generalized Gibbs ensemble (GGE) [8–12], where the density matrix is determined not only by the Hamiltonian $H$ and particle number $N$ but also by other local conserved quantities $Q_i$, i.e., $\rho_{GGE} \sim \exp[-\beta (H - \mu N) - \sum_i \lambda_i Q_i]$.

In this Letter we focus on the relaxation dynamics of one of the most studied integrable models: the model of interacting spinless fermions, being equivalent to the anisotropic Heisenberg ($XXZ$) model for which the set of $Q_i$ has been established [13–14]. We show that $\rho_{GGE}$ as generated only by local integrals of motion $Q_i$ doesn’t exhaust all generic stationary states in the metallic (easy plane) regime. Instead, there are cases for which one should lift the requirement of locality of the conserved quantities and allow also for quasi–local integrals of motion [15–16]. In this Letter we call them non–GGE states, however we stress that these states can be viewed also as “extended GGE”, where the extension concerns the locality of operators. Such operators have the parity opposite to local ones $Q_i$. We identify one of such quasi–local quantities as the time–averaged particle current operator and we construct as well as verify it explicitly.

It has been well recognized that integrable systems in spite of interaction reveal anomalous transport properties at finite inverse temperatures $\beta = 1/T$, e.g. the dissipationless particle current. This property is manifested by a nonvanishing charge stiffness $D(\beta < \infty) [17–19]$, which in turn is bounded from below by the local conservation laws via the Mazur bound [18–20]. The dissipationless transport and the relaxation towards GGE are probably the most prominent hallmarks of integrability, still they have been studied independently of each other so far. While it has been clear that in certain regimes the standard Mazur bound with only local $Q_i$ does not exhaust the phenomenon of dissipationless transport and $D(\beta < \infty) > 0$ [15] we show in this Letter that GGE should be extended by taking into account quasi–local conserved quantities of different parity, in particular the time averaged current, which saturate $D(\beta \rightarrow \infty)$ within the Mazur bound.

We study a prototype one-dimensional (1D) model of interacting particles, the tight-binding model of spinless fermions on $L$ sites at half filling (with $N = L/2$ particles) and with periodic boundary conditions [21–24].

$$H(t) = -t_h \sum_{j=1}^{L} (e^{i\phi(t)} c_{j+1}^\dagger c_j + \text{h.c.}) + V \sum_{j=1}^{L} \tilde{n}_j \tilde{n}_{j+1}, \quad (1)$$

where $n_j = c_{j}^\dagger c_j$, $\tilde{n}_j = n_j - 1/2$, $t_h$ is the hopping integral and $V$ is the repulsive interaction on nearest neighbors. The model [1] is equivalent to the anisotropic Heisenberg ($XXZ$) model with the exchange interaction $J = 2t_h$ and the anisotropy parameter $\Delta = V/2t_h$. However, we stay within the fermionic representation, where the phase $\phi(t)$ has a clear physical meaning: it represents the time-dependent magnetic flux which induces the electric field $F(t) = -\partial_t \phi(t)$. Further on we use $h = k_B = 1$ and units in which $t_h = 1$. We consider here the metallic (easy–plane) regime $V < 2 (\Delta < 1)$ where the system exhibits a ballistic particle (spin) transport at $T > 0$ [17–19,25–32].

The charge stiffness $D(T) > 0$ has been introduced via the $T > 0$ generalization of the Kohn’s [33] argument of the level curvatures $\epsilon_n(\phi) [17–34]$. It is still a challenging problem since it cannot be derived from local conservation laws [18–35]. To explore this relation we study in the following the standard particle current $J = \sum_j (ie^{i\phi(t)} c_{j+1}^\dagger c_j + \text{h.c.})$ as well as a less common cur-
from the initial value \( \phi \) evolution shown in Fig. 1 has been obtained by the Lanczos method [18]. Such a quench is equivalent to a pulse of the electric field \( F = \phi_0/(2\pi) \) and the regular (dissipative) part of conductivity becomes irrelevant in the long-time regime. Then we get within the LR, i.e., for \( \phi_0 \ll 1 \),

\[
\lim_{t \to \infty} \langle J(t) \rangle = 2LD\phi_0.
\]

An important message following from LR, Eq. (5), is that the non–GGE component of the density matrix has to contain contributions which are linear in \( \phi_0 \) and, therefore, can be singled out already within the first-order perturbation expansion in \( \phi_0 \). The unperturbed Hamiltonian \( H_0 = H(t < 0) \) is given by Eq. (1) with \( \phi(t) \) replaced by \( \phi_0 \), while the perturbation reads \( H'(t) = H(t) - H_0 = (\phi(t) - \phi_0)J_0 \), where \( J_0 = J(t < 0) \), so that \( H'(t > 0) = \phi_0J_0 \). For the sake of clarity all quantities obtained with the flux \( \phi_0 \) will be marked with a label "0", in particular the eigenvalues \( E_{m0} \) and the eigenvectors \( |m0\rangle \) of \( H_0 \). The degeneracy of energy levels plays an important role and should not be neglected. Hence, we diagonalize the current operator in each subspace spanned by degenerate eigenstates and take the eigenvectors of \( J \) as the basis vectors of this subspace, i.e., \( \langle m|J|n\rangle \propto \delta_{mn} \) if \( E_m = E_n \) (within a subspace only).

We assume that the system is initially in a thermal state, i.e., \( \rho_0 = \sum_m p_{m0}|m0\rangle\langle m0| \) with \( p_{m0} = \exp(-\beta E_{m0})/Z_0 \). Then, in the Schrödinger picture one obtains

\[
\rho(t > 0) = \sum_m p_{m0}e^{-iH_0t}U(t)|m0\rangle\langle m0|U^\dagger(t)e^{iH_0t},
\]

\[
U(t > 0) = T_i \exp\left(-i\int_0^t dt'H_i^\dagger(t')\right),
\]

where \( H_i^\dagger(t') \) is the perturbation in the interaction picture. Our aim is to explicitly express \( \bar{\rho} \) within the LR to the quench \( \phi_0 \). A straightforward calculation of Eqs. (3), (6) to first order in \( \phi_0 \) yields

\[
\bar{\rho} \simeq \rho_0 + \phi_0 \sum_{E_{m0} \neq E_{n0}} \frac{p_{m0} - p_{m0}}{E_{m0} - E_{n0}} \langle m0|J_0|n0\rangle|m0\rangle\langle n0|.
\]

We should also take into account the change of current operator due to flux, hence

\[
J = J(t > 0) = J_0 - \phi_0H_0^{k},
\]
where $H^k_0$ is the kinetic part of $H_0$, Eq. (1). Using Eqs. (7), (8), (5) one then restores the LR result for the equilibrium charge stiffness [17, 34]

$$D = \frac{1}{2L} \left[ -\langle H^k_0 \rangle + \sum_{E_m \neq E_n} \frac{p_m - p_n}{E_m - E_n} \langle m|J_0|n \rangle \rangle^2 \right].$$

Eq. (7) does not yet accomplish our aim of decomposing $\bar{\rho}$ into odd and even parts with respect to $\phi$ after the quench, i.e. at $\beta \to 0$. We achieve this by using again the first–order perturbation theory for $H_0 = H - \phi_0 J$ and $J_0 = J + \phi_0 H^k$, where now $H, H^k$ and $J$ are the operators after the quench, i.e. at $\phi = 0$. Substituting

$$E_{n0} = E_n - \phi_0 \langle n|J|n \rangle, \quad |n\rangle = |n\rangle - \phi_0 \sum_{m, E_m \neq E_n} \frac{\langle m|J|n \rangle}{E_n - E_m} |m\rangle,$$

into Eq. (7), and assuming that there is no particle current in the initial thermal state, we finally obtain

$$\bar{\rho} = \sum_n p_n |n\rangle \langle n| \left( 1 + \beta \phi_0 \bar{J} \right),$$

where $\bar{J}$ is the time-averaged steady–current operator

$$\bar{J} = \lim_{\tau \to \infty} \frac{1}{\tau} \int_0^\tau dt e^{iHt} J e^{-iHt} = \sum_n \langle n|J|n\rangle \langle n|n\rangle.$$

The LR results [Eq. (3)] is immediately restored, however this time with the alternative form of the charge stiffness but equivalent for $\beta < \infty$ and in the thermodynamic limit [15]

$$D = \frac{\beta}{2L} \sum_n p_n \langle n|J|n\rangle^2.$$

By definition $\bar{J}$ is an integral of motion $[H, \bar{J}] = 0$. It is important to note that $\text{Tr} J^2 / N \propto L$ where $N = \text{Tr} 1$ is the dimension of the Hilbert space, already implies that $\bar{J}$ is a quasi–local quantity. Since at $\beta \to 0$,

$$\frac{1}{N} \text{Tr} J^2 = 2LD, \quad \text{where} \quad D = \lim_{\beta \to 0} D(\beta)/\beta,$$

the quasi-local character of $\bar{J}$ is consistent with the well established fact that the charge stiffness is an intensive quantity.

We now turn to the question of whether $\bar{\rho}$ is compatible with $\rho_{\text{GGE}}$ and the answer is clearly negative. A necessary and a sufficient condition for such compatibility, to leading order in the quench $\phi_0$, would be a decomposition in terms of local conserved $Q_i$,

$$\bar{J} = \sum_i \alpha_i Q_i,$$

holding for some set of $\alpha_i$. Assuming that $\text{Tr} \{Q_i Q_j\} \propto \delta_{ij}$ we can employ the inequality

$$\text{Tr} \{(\bar{J} - \sum i a_i Q_i)^2\} \geq 0,$$

which holds for any $a_i$ and becomes an equality only for the GGE state with $a_i = \alpha_i$. Now we can follow original steps by Mazur [20]. We minimize the lhs of Eq. (16) with respect to $a_i$,

$$a_i = \frac{\text{Tr} \{J_i Q_i \}}{\text{Tr} \{Q_i^2 \}} = \frac{\text{Tr} \{J_i Q_i \}}{\text{Tr} \{Q_i^2 \}},$$

and substitute this result in (16) to obtain the Mazur inequality for $\beta \to 0$

$$\text{Tr} \{J^2\} \geq \sum_i \text{Tr} \{J_i Q_i^2 \} / \text{Tr} \{Q_i^2 \},$$

which is the Mazur bound on charge stiffness at $T \to \infty$ [see Eq. (14)]. Since this inequality turns into equality for GGE states, so should the Mazur bound. In other words relaxation towards GGE is possible provided the Mazur bound saturates the charge stiffness. This relation holds for an arbitrary filling $N/L$. In particular for $N/L = 1/2$ one finds $\text{Tr} \{Q_i J\} = 0$ due to the symmetry (2), hence the rhs of (18) vanishes, and our quenched dynamics does not relax to GGE.

As has been shown in Refs. [15, 16], another set of non-local, but quasi-local conserved Hermitian operators $\{Q(\varphi)\}$ exists for a dense set commensurate interactions $\Delta = \cos(\pi l/m)$, with $l, m$ integers, densely covering the range $|V| < 2$. They are all odd under (2), $Q(\varphi) \to -Q(\varphi)$. Quasi-locality implies linear extensivity $\text{Tr} \{Q(\varphi)^2\} / N \propto L$, similarly as for the local conserved operators $Q_i$, while $\text{Tr} \{Q(\varphi)/\langle L N \rangle = \text{const}, making them suitable for implementing the Mazur bound. For $\Delta = \cos(\pi l/m)$ for which $T \to \infty$ limit of the Bethe ansatz result [25] is available it has been shown [16] to agree precisely with the Mazur bound, so one may conjecture that the latter is now indeed saturated. Hence our argument [15, 18] can be used to argue that the complete time-averaged current can be expressed in terms of an integral

$$\bar{J} = \int_{D_m} d^2 \varphi f(\varphi) Q(\varphi)$$

where $f(\varphi) = c_m / |\sin \varphi|^4$ for a suitable constant $c_m$ (see [19]) and $D_m$ is a vertical strip in the complex plane with $|Re \varphi - \pi/2| < \pi/(2m)$. After straightforward calculation, again using the notation and machinery of [16], one arrives at the explicit matrix-product expression for $\bar{J} = i(J_+ - J_-^\dagger)$ in terms of local operators

$$J_+ = \sum_j \sum_{r \geq 2} J_+^{(r)}$$
with
\[ J_1^{(r)} = \sum_{s_2, \ldots, s_{r-1}} g_{s_2, \ldots, s_{r-1}} (B^{s_2} \ldots B^{s_{r-1}})_{11} \sigma^+_{s_1} \sigma^{-s_2} \ldots \sigma^{-s_{r-1}} \sigma^+_r, \]
\[ g_{s_2, \ldots, s_{r-1}} := \sum_{j \in s} \left( \#_{+} \{ s_i \} \right) I_j + \frac{1}{2} \#_{+} \{ s_i \} \]
where \#_{+} \{ s_i \} denotes the number of indices of the set \{ s_i \} having a value \( s \). Here \( I_k := \int \frac{d^2 \varphi}{\pi} (\varphi) (\cot \varphi)^2 \) are elementary integrals which can be evaluated as
\[ I_k = -\frac{2\pi}{m(2k+1)} \frac{2\pi}{m} \sum_{j=0}^{2k+1} \binom{2k+1}{j} (-1)^j \times \]
\[ \left( \cos \frac{\pi}{m} \right)^{2k+1-j} \left( \sin(\pi(j+1)/m) - \sin(\pi(j-1)/m) \right), \]
and \( I_{k+1/2} = 0 \) for \( k \) integer. The coefficient of Eq. \((21)\) \((B^{s_2} \ldots B^{s_{r-1}})_{11}\) is the \((1,1)\)-component of a product of \((m-1) \times (m-1)\) matrices \( B^s \), related to modified Lax operator \( \tilde{B} \),
\[ B^0_{jk} = \cos(\pi j/m) \delta_{j,k}, \quad B^1_{jk} = -\sin(\pi j/m) \delta_{j,k}, \]
\[ B^2_{jk} = \sin(\pi j/m) \delta_{j+1,k}, \quad B^3_{jk} = -\sin(\pi j/m) \delta_{j,k+1}. \]
Pauli matrices \( \sigma^j \) are related to fermion operators via Jordan-Wigner transformation \( c_j = (\prod_{i=1}^{j-1} \sigma_i^-) \sigma_j^+ \). The result \((21)\) is derived in the limit \( L \to \infty \) and is valid up to corrections of order \( O(1/L) \) for a finite periodic ring. Explicitly, \( \tilde{J} \) to all terms up to order four \( (r \leq 4) \) reads
\[ \tilde{J} = \tilde{D} (8J + 2VJ') + \sum_j \left( i\kappa c_{j+3}^j c_j + i\kappa' c_{j+3}^j + 2c_{j+2} c_{j+1} c_j + i c_j \right) + \ldots \] (23)
For example, for \( V = 1 \), \( (\Delta = \cos \frac{\pi}{2}) \), one has explicitly
\[ \tilde{D} = \frac{1}{8} - \frac{3\sqrt{3}}{32\pi}, \quad \kappa = \frac{1}{4} - \frac{9\sqrt{3}}{16\pi}, \quad \kappa' = \frac{9\sqrt{3}}{8\pi} - 1, \]
while \( \kappa'' = \tilde{D} V^2 / 2 \) in general.

Above analytical results are nicely corroborated by exact numerical simulations in finite systems shown in Fig. 2. From Eq. \((23)\) one finds that the ratio of two currents should be given as \( \text{Tr} \{ \tilde{p} J' \} / \text{Tr} \{ \tilde{p} J \} = V/4 \) as confirmed in Fig. 2a. Furthermore, one can define the stiffness with respect to current \( J' \) as \( \tilde{D}' = \langle \beta J'^2 \rangle / (2L) \). Formula \((23)\) immediately implies that \( \tilde{T} = (V/4) \tilde{J} \), and so the two stiffnesses should have a simple ratio \( \tilde{D}' / \tilde{D} = V / 4 \) (see Fig. 2a).

In conclusion, we have proposed a class of global quantum quench dynamics of integrable spin chains for which the state at asymptotic times does not relax to GGE. We argue that, at least for weak quenches where linear response theory is applicable, the validity of GGE ensemble is in one-to-one correspondence with the saturation of the Mazur bound expressed in terms of strictly local conserved operators. However, if one extends the GGE ensemble by including the quasi-local conserved operators from the opposite parity sector – having linearly extensive Hilbert-Schmidt norm – then the latter can be used to describe exactly the steady state density operator after the quench. Our theory has been demonstrated in the 1D model of interacting spinless fermions (XXZ spin model) within the metallic regime.

It should be noted that our results are expected to have further implications on other relevant quantities of integrable systems besides the charge stiffness. The flux–quench induced steady current \( \langle \tilde{J} \rangle = 2 \sum_k \sin(k) \langle \bar{n}_k \rangle \neq 0 \) is reflected into the fermion momentum–distribution function \( \langle \bar{n}_k \rangle \) which also does not comply to the standard GGE. The latter quantity is the one typically measured in cold–atom experiments \([10, 11]\) as well most frequently studied in connection with the GGE concept \([3, 8, 10]\). The inclusion of the quasi–local conserved quantity \( J \) fully fixes the steady state \( \langle \bar{n}_k \rangle \) within our quench protocol via extended GGE form Eq. \((11)\). It is still tempting to construct and consider further (presumably conserved) quantities from the same polarity sector which would fix this and related quantities for an arbitrary quench.

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