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Time Evolution of Local Observables After Quenching to an Integrable Model

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We consider quantum quenches in integrable models. We argue that the behavior of local observables at late times after the quench is given by their expectation values with respect to a single representative Hamiltonian eigenstate. This can be viewed as a generalization of the eigenstate thermalization hypothesis to quantum integrable models. We present a method for constructing this representative state by means of a generalized thermodynamic Bethe ansatz (GTBA). Going further, we introduce a framework for calculating the time dependence of local observables as they evolve towards their stationary values. As an explicit example we consider quantum quenches in the transverse-field Ising chain and show that previously derived results are recovered efficiently within our framework.

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Introduction.—Recent years have witnessed dramatic progress in the study of isolated quantum systems out of equilibrium, in particular, in systems of optically trapped ultracold atomic gases. Key to these advances is the weak coupling to the environment, which allows the realization of essentially unitary time evolution on long time scales [1–6]. The experimental results have stimulated intense theoretical efforts aimed at answering fundamental questions such as: Do observables relax to time-independent values? What are the principles determining these values? How can one describe the relaxation towards stationary behavior?

There is compelling evidence that nonequilibrium time evolution is strongly affected by dimensionality and the presence of conservation laws. The experiments of [2] on trapped ⁸⁷Rb atoms established that three-dimensional condensates rapidly relax to a stationary state characterized by an effective temperature, whereas constraining the motion of atoms to one dimension greatly reduces the relaxation rate of the momentum distribution function. These results spurred a flurry of theoretical activity aimed at shedding light on the precise effects of integrability on the nonequilibrium dynamics of many-body quantum systems (see [7–38] and references therein).

So far two basic paradigms have emerged in translationally invariant models: at late times subsystems either thermalize, i.e., are characterized by a Gibbs distribution with an effective temperature, or they are described by a generalized Gibbs ensemble (GGE) [8]. When the time evolution occurs under the action of an integrable Hamiltonian, the GGE is applicable. Questions regarding the approach towards the steady state long after the quench remain difficult to tackle. Short and intermediate times can be efficiently studied by algorithms based on matrix-product states [5,13–15], while numerical methods based on integrability have allowed to access arbitrary times in finite systems [16–18]. The only cases which have been

largely understood are noninteracting theories such as the transverse field Ising chain (TFIC) [19–24].

It is our purpose here to develop an efficient framework for the description of the out-of-equilibrium dynamics of a system evolving under an integrable Hamiltonian $H(h)$, where h is a system parameter such as an interaction strength or a magnetic field. Our approach applies equally to quantum spin chains and to continuum theories like the Lieb-Liniger model. The situation we have in mind is that of a quantum quench: a given system is prepared in the ground state $|\Psi\rangle$ of the short-ranged Hamiltonian $H(h_0)$, which itself may not be integrable. At time $t = 0$ the system parameter is suddenly changed from h_0 to h , and the system evolves unitarily under $H(h)$ for all $t > 0$, i.e., $|\Psi(t)\rangle = e^{-iH(h)t}|\Psi\rangle$. Our main focus is the calculation of the expectation values of generic, local (in space) operators \mathcal{O}

$$\langle \mathcal{O}(t) \rangle = \frac{\langle \Psi(t) | \mathcal{O} | \Psi(t) \rangle}{\langle \Psi(t) | \Psi(t) \rangle}. \quad (1)$$

Examples of \mathcal{O} would be products of spin operators located in a finite segment of a spin chain, or density or field operators in quantum gases.

Our main result is to show that in the thermodynamic limit $L \rightarrow \infty$, at fixed particle density N/L and for local observables, the expectation value (1) can be expressed in a simple way in terms of projections onto a *single* judiciously chosen representative “saddle point” eigenstate $|\Phi_s\rangle$ of $H(h)$:

$$\lim_{N \rightarrow \infty} \langle \mathcal{O}(t) \rangle = \lim_{N \rightarrow \infty} \left[\frac{\langle \Psi | \mathcal{O}(t) | \Phi_s \rangle}{2 \langle \Psi | \Phi_s \rangle} + \Phi_s \leftrightarrow \Psi \right]. \quad (2)$$

In the stationary state, i.e., the limit $t \rightarrow \infty$, the averages of local observables are simply given by the expectation value in the eigenstate $|\Phi_s\rangle$

$$\lim_{t \rightarrow \infty} \lim_{N \rightarrow \infty} \langle \mathcal{O}(t) \rangle = \lim_{N \rightarrow \infty} \frac{\langle \Phi_s | \mathcal{O} | \Phi_s \rangle}{\langle \Phi_s | \Phi_s \rangle}. \quad (3)$$

We stress that no time averaging is involved in (3), which can be thought of as a generalization of the eigenstate thermalization hypothesis [39] (which states that single eigenstate expectation values can reproduce averages over a thermal ensemble) to local observables in integrable models, valid in the thermodynamic limit. A consequence of (3) is that the ensemble defined by the density matrix $\rho = |\Phi_s\rangle\langle\Phi_s|$ is locally indistinguishable from the GGE corresponding to the initial state $|\Psi\rangle$ (globally the two ensembles are different, see also [21]). Our description of the stationary state is closely related to the generalization of the eigenstate thermalization hypothesis proposed in [37], which is based on a generalized microcanonical ensemble, and to the single-state averages discussed in [34]. We emphasize that the description (3) of the steady state and the representation (2) for the time evolution offer a dramatic reduction in computational complexity as compared to earlier approaches.

GTBA approach to nonequilibrium evolution.—Let us consider a quantum integrable model with Hamiltonian H solvable by Bethe ansatz. Let $\{|\Phi\rangle\}$ be a complete set of eigenstates, i.e., $H|\Phi\rangle = \omega_\Phi|\Phi\rangle$. The time evolution of an arbitrary initial state $|\Psi\rangle$ is then given by

$$|\Psi(t)\rangle = \sum_{\Phi} e^{-\mathcal{E}_\Phi} e^{-i\omega_\Phi t} |\Phi\rangle, \quad (4)$$

where \mathcal{E}_Φ are constant, complex-valued overlaps

$$\mathcal{E}_\Phi \equiv -\ln\langle\Phi|\Psi\rangle. \quad (5)$$

Substituting (4) into the numerator of (1) gives a spectral representation of the form

$$\langle\Psi|\mathcal{O}(t)|\Psi\rangle = \sum_{\Phi, \Phi'} e^{-\mathcal{E}_\Phi^* - \mathcal{E}_{\Phi'}} e^{i(\omega_\Phi - \omega_{\Phi'})t} \langle\Phi|\mathcal{O}|\Phi'\rangle. \quad (6)$$

This double sum over a full Hilbert space basis is a serious bottleneck. To proceed further, we look to the thermodynamic limit. In the thermodynamic Bethe ansatz (TBA) approach to equilibrium thermodynamics [40] (see [41] for detailed expositions), a summation over states is recast as a functional integral over root densities ρ

$$|\Phi\rangle \rightarrow |\rho\rangle, \quad \sum_{\Phi} (\dots) \rightarrow \int \mathcal{D}[\rho] e^{S_\rho} (\dots). \quad (7)$$

Here, S_ρ is the entropy of all states characterized by a given root density and (\dots) represents quantities with well-defined thermodynamic limits. Using (7) once, we can formally recast (6) in the form

$$\int \mathcal{D}[\rho] e^{S_\rho} \sum_{\Phi} \left[e^{-\mathcal{E}_\Phi^* - \mathcal{E}_\rho} e^{i(\omega_\Phi - \omega_\rho)t} \frac{\langle\Phi|\mathcal{O}|\rho\rangle}{2} + \Phi \leftrightarrow \rho \right]. \quad (8)$$

The reason for using (7) only once is that we are interested in local operators \mathcal{O} . These have the property that $\langle\Phi|\mathcal{O}|\Phi'\rangle \neq 0$ only if both $|\Phi\rangle$ and $|\Phi'\rangle$ scale to the same distribution ρ up to microscopic differences [42]. In the thermodynamic limit the denominator in (1) becomes

$$\langle\Psi|\Psi\rangle = \int \mathcal{D}[\rho] e^{-2\text{Re}(\mathcal{E}_\rho) + S_\rho} \quad (9)$$

and can be evaluated by the method of steepest descent. The right-hand side of (9) can be viewed as the partition function of an integrable model with “generalized free energy”

$$\mathcal{F}_\rho \equiv 2\text{Re}(\mathcal{E}_\rho) - S_\rho. \quad (10)$$

Here, S_ρ is the usual Yang-Yang entropy of the integrable Hamiltonian $H(h)$. In the simplest scalar case, realized, e.g., in the Lieb-Liniger model, it takes the form $S_\rho = N \int d\lambda [(\rho + \rho^h) \ln(\rho + \rho^h) - \rho \ln \rho - \rho^h \ln \rho^h]$. The hole density ρ^h is related to the particle density ρ by the thermodynamic form of the Bethe equations

$$\rho(\lambda) + \rho^h(\lambda) = \frac{1}{2\pi} + \int d\lambda' K(\lambda - \lambda') \rho(\lambda'), \quad (11)$$

where $K(\lambda)$ is a known function for a given integrable model. The first term in (10) plays the role of an effective energy per temperature and hence acts as the “driving term” in a generalized thermodynamic Bethe ansatz (for details, see [18,43]). Since the effective overlaps (5) are strictly bounded from below, there exists a saddle point at ρ_s , i.e., $\delta\mathcal{F}_\rho/\delta\rho|_{\rho_s} = 0$ [44]. In the thermodynamic limit, fluctuations around the saddle point are negligible and thermodynamic averages can be calculated with respect to the energy eigenstate characterized by ρ_s . Given that the expectation values of all local integrals of motion in this state are by construction the same as those of the generalized Gibbs ensemble corresponding to $H(h)$ and $|\Psi(t=0)\rangle$, the saddle-point average of local observables precisely reproduces the GGE average in the sense of [21]. The functional integrals in (8) can be evaluated analogously: Given that $\langle\Phi|\mathcal{O}|\rho\rangle$ is nonzero only for states $\langle\Phi|$ such that $\omega_\Phi - \omega_\rho$ and $\mathcal{E}_\Phi^* + \mathcal{E}_\rho$ are intensive, the first term in (8) is dominated by the same saddle point ρ_s . The second term is treated analogously. Putting everything together we obtain the thermodynamic limit of (2). In practice we consider the theory in a large, finite volume L (at fixed density N/L) and a particular, representative eigenstate $|\Phi_s\rangle$ that reduces to $|\rho_s\rangle$ in the thermodynamic limit. The corresponding spectral representation is then

$$\langle\mathcal{O}(t)\rangle = \lim_{N \rightarrow \infty} \sum_{\Phi} \left[e^{\mathcal{E}_{\Phi_s}^* - \mathcal{E}_\Phi + i(\omega_\Phi - \omega_{\Phi_s})t} \frac{\langle\Phi|\mathcal{O}|\Phi_s\rangle}{2} + e^{\mathcal{E}_{\Phi_s} - \mathcal{E}_\Phi - i(\omega_\Phi - \omega_{\Phi_s})t} \frac{\langle\Phi_s|\mathcal{O}|\Phi\rangle}{2} \right]. \quad (12)$$

The gain in efficiency in (12) as compared to the “bare” spectral representation (6) is apparent: only a single sum remains, which, moreover, in practice needs to be carried out only over the subset of states with non-negligible matrix elements. As we did not have to assume t to be large we conjecture that (12) describes the time evolution of local observables in the thermodynamic limit, at arbitrary times after the quench. Importantly, in the limit $t \rightarrow \infty$ the integrals in the sum over Φ can be carried out by a stationary phase approximation. This shows that in the stationary state only the expectation value in $|\Phi_s\rangle$ survives in (12); i.e.,

$$\lim_{t \rightarrow \infty} \langle \mathcal{O}(t) \rangle = \lim_{N \rightarrow \infty} \frac{\langle \Phi_s | \mathcal{O} | \Phi_s \rangle}{\langle \Phi_s | \Phi_s \rangle}. \quad (13)$$

It is clear from our construction that the state $|\Phi_s\rangle$ is not unique. However, different choices give identical results for (12) and (13), in the thermodynamic limit.

The physical content of (12) is summarized as follows: in the thermodynamic limit, the relaxation of $\langle \mathcal{O}(t) \rangle$ towards its steady state is fully determined by quantum interference effects between eigenstates situated within a basin around the saddle point $|\rho_s\rangle$.

An explicit example: The transverse field Ising chain.—The Hamiltonian of the TFIC is given by

$$H(h) = -J \sum_{j=1}^L [\sigma_j^x \sigma_{j+1}^x + h \sigma_j^z], \quad (14)$$

where σ_j^α are Pauli matrices at site j of a one-dimensional chain and we consider $J, h > 0$. At zero temperature and in the thermodynamic limit, the TFIC exhibits ferromagnetic long-range order along the x direction for $h < 1$, while it is in a paramagnetic phase for $h > 1$ [45]. The two phases are separated by a quantum critical point in the Ising universality class. It is well known that $H(h)$ can be diagonalized by combined Jordan-Wigner and Bogoliubov transformations [45]

$$H(h) = \sum_p \varepsilon_h(p) \left(\alpha_p^\dagger \alpha_p - \frac{1}{2} \right), \quad (15)$$

where the single-particle energy is given by $\varepsilon_h(k) = 2J\sqrt{1+h^2-2h\cos k}$. Our quench protocol is as follows: we prepare the system in the ground state $|\Psi\rangle$ for an initial value h_0 of the transverse magnetic field. At time $t = 0$ we instantaneously change the field from h_0 to h . The state of the system at times $t > 0$ is obtained by evolving with respect to the new Hamiltonian $H(h)$,

$$|\Psi(t)\rangle = e^{-iH(h)t} |\Psi\rangle. \quad (16)$$

The reduced density matrix of a subsystem A at time t after the quench is given by $\rho_A(t) = \text{Tr}_{\bar{A}} \rho(t) = \text{Tr}_{\bar{A}} |\Psi(t)\rangle \langle \Psi(t)|$, in which \bar{A} is the complement of A . For quenches originating in the paramagnetic phase, i.e., $h_0 > 1$, the \mathbb{Z}_2

symmetry of rotations by π around the z axis remains unbroken and it is possible to express $\rho_A(t)$ in the form [46]

$$\rho_A(t) = \frac{1}{2^\ell} \sum_{\mu_l=0,1} \left\langle \prod_{l=1}^{2\ell} a_l^{\mu_l} \right\rangle \left(\prod_{l=1}^{2\ell} a_l^{\mu_l} \right)^\dagger \propto e^{a_l W_l a_m / 4}. \quad (17)$$

Here the expectation value is with respect to the state $|\Psi(t)\rangle$ and a_{2n} and a_{2n-1} are Majorana fermion operators fulfilling anticommutation relations $\{a_j, a_k\} = 2\delta_{j,k}$, which are related to the lattice spins by a Jordan-Wigner transformation

$$a_{2n-1} = \left[\prod_{m < n} \sigma_m^z \right] \sigma_n^x, \quad a_{2n} = \left[\prod_{m < n} \sigma_m^z \right] \sigma_n^y. \quad (18)$$

The matrix W is given by $\tanh(W/2) = \Gamma$ [47], where

$$\Gamma_{jk} = \text{Tr}[\rho(t) a_k a_j] - \delta_{j,k} = -\Gamma_{kj}. \quad (19)$$

In the thermodynamic limit, the correlation matrix is given by [22] $\Gamma_{2n-1, 2j-1} = \Gamma_{2j, 2n} = f_{j-n}$, $\Gamma_{2n-1, 2j} = g_{n-j}$ with

$$g_l = -i \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{-ikl} \frac{h - e^{ik}}{\sqrt{1+h^2-2h\cos k}} \times [\cos \Delta_k - i \sin \Delta_k \cos(2\varepsilon_h(k)t)], \quad (20)$$

$$f_l = \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{-ikl} \sin \Delta_k \sin(2\varepsilon_h(k)t),$$

where $\cos \Delta_k = 4J^2(1+hh_0 - (h+h_0)\cos k)/\varepsilon_h(k)\varepsilon_{h_0}(k)$. The reduced density matrix (17) is Gaussian, and hence multipoint correlation functions are obtained by Wick's theorem. Concomitantly all local correlation functions in the stationary state are fully specified by the two-point averages (19) and (20), in the limit $t \rightarrow \infty$. So far we have considered only the case $h_0 > 1$. For quenches originating in the ferromagnetic phase, i.e., $h_0 < 1$, the reduced density matrix $\rho_A(t)$ is not Gaussian [46]. However, as shown in [22], $\rho_A(\infty)$ is again given by the $t \rightarrow \infty$ limit of (17).

Stationary behavior.—We will now show how to recover these results in the GTBA framework. The simplest way to obtain the solution of the GTBA equations for the TFIC is to note that the mode occupation numbers constitute conserved quantities $[\alpha_k^\dagger \alpha_k, H(h)] = 0$. Hence, the root density in the stationary state is simply given by

$$\rho(k) = \frac{\langle \Psi | \alpha_k^\dagger \alpha_k | \Psi \rangle}{2\pi} = \frac{1 - \cos \Delta_k}{4\pi}, \quad (21)$$

and the particle density is $D = \int_{-\pi}^{\pi} dk \rho(k)$. The corresponding Hamiltonian eigenstate at density $D = 2N/L$ in a large, finite volume is then

$$|\Phi_s\rangle = \prod_{j=1}^N \alpha_{\kappa_j}^\dagger \alpha_{\kappa_j}^\dagger |0; h\rangle, \quad (22)$$

where $|0; h\rangle$ is the fermionic vacuum state and the momenta $\kappa_j > 0$ are distributed according to the density (21),

i.e., $\kappa_{j+1} = \kappa_j + 1/[L\rho(\kappa_j)]$. Changing the values of a finite number of κ_j leads to slightly different alternative representative states. Calculating the expectation values of local operators in these states gives rise to differences that disappear in the limit $N, L \rightarrow \infty$. The density matrix corresponding to the state (22) is $\rho_s = |\Phi_s\rangle\langle\Phi_s|$ and by virtue of the product form (22) it is Gaussian. This means that it can be represented in the form (17) and is completely determined by its correlation matrix (19). The only non-vanishing matrix elements are

$$(\Gamma_s)_{2l-1, 2l-2n} = -\frac{i}{L} \sum_k \frac{e^{-ink}(h - e^{ik})(1 - 2\delta_{k, \kappa_j})}{\sqrt{1 + h^2 - 2h \cos k}}. \quad (23)$$

Turning the sum over momenta into an integral by means of the Euler-Maclaurin sum formula, we find that $\Gamma_s = \Gamma(\infty)$ and hence $\lim_{t \rightarrow \infty} \rho_A(t) = \rho_{s,A}$. This proves that the GTBA formalism reproduces the correct stationary state for the reduced density matrix for any finite subsystem in the thermodynamic limit, and hence for all local correlation functions.

Relaxation behavior.—Our general formalism suggests that the time evolution of local (in space) operators is given by (2), where the state $|\Phi_s\rangle$ is defined in the previous paragraph. We now demonstrate the validity of (2) for any local operator \mathcal{O} in the case where the quench originates in the paramagnetic phase, such that the \mathbb{Z}_2 symmetry is unbroken. The proof is as follows: we start by defining two density matrices $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$ and $\rho_s(t) = |\Phi_s(t)\rangle\langle\Phi_s(t)|$. Crucially, both of these density matrices are Gaussian as a Wick's theorem holds for averages calculated with respect to both of them. The right-hand side of (2) can be written in the form

$$\left[\frac{\text{Tr}[\rho_s(t)\rho(t)\mathcal{O}]}{2\text{Tr}[\rho_s(t)\rho(t)]} + \rho \leftrightarrow \rho_s \right] \equiv \text{Tr}[\hat{\rho}(t)\mathcal{O}]. \quad (24)$$

Because each term in $\hat{\rho}$ is a product of two Gaussian density matrices, it is Gaussian itself, and hence fully characterized by its correlation matrix

$$\hat{\Gamma}_{jk} = \text{Tr}[\hat{\rho}(t)a_k a_j] - \delta_{j,k}. \quad (25)$$

The two-point functions in (25) are easily calculated, and as shown in the supplementary material we have $\lim_{N \rightarrow \infty} \hat{\Gamma}(t) = \Gamma(t)$. This proves that for any local observable \mathcal{O} (such as products of spin operators contained in a finite subsystem) in the thermodynamic limit $\lim_{N \rightarrow \infty} \text{Tr}[\hat{\rho}(t)\mathcal{O}] = \text{Tr}[\rho(t)\mathcal{O}]$, and establishes Eq. (2).

Our line of arguments breaks down for quenches originating in the ferromagnetic phase, because the density matrix $\rho(t)$ is no longer Gaussian [46]. In order to verify the validity of (2) in this case, we have analyzed the relaxation of the order parameter one-point function $\langle\Psi(t)|\sigma_\ell^x|\Psi(t)\rangle$ for quenches with $h_0, h < 1$ in the regime where the density of excitations of the postquench

Hamiltonian $H(h)$ in the initial state is small, i.e., $\langle\Psi|\alpha_k^\dagger\alpha_k|\Psi\rangle \ll 1$. The result for $Jt \gg 1$ in this case is [21]

$$\langle\Psi(t)|\sigma_\ell^x|\Psi(t)\rangle \approx (1 - h^2)^{1/8} \times \exp\left[-2t \int_0^\pi \frac{dk}{\pi} \varepsilon'_h(k) K^2(k)\right]. \quad (26)$$

This result is recovered from (2) in a very efficient way as follows. Taking into account boundary conditions in a large, finite volume, the appropriate form of (2) for the order parameter expectation value is

$$\langle\Psi(t)|\sigma_\ell^x|\Psi(t)\rangle = \text{Re}\left[\frac{\text{R}\langle\Psi(t)|\sigma_\ell^x|\Phi_s(t)\rangle_{\text{NS}}}{\text{NS}\langle\Psi|\Phi_s\rangle_{\text{NS}}}\right]. \quad (27)$$

Here R/NS correspond to periodic or antiperiodic boundary conditions on the fermions respectively, see, e.g., [21]. As shown in [21], the state $\text{R}\langle\Psi(t)|$ can be written as a linear superposition of energy eigenstates with n pairs of fermions $\text{R}\langle\Psi(t)| = \sum_{n=0}^{L/2} \text{R}\langle\Psi_n(t)|$. The late-time behavior of (27) is determined by states with N pairs, i.e., the term with $n = N$. Retaining only this contribution, and using the known form of matrix elements of the order parameter [48], one readily obtains [49] the result (26) by means of the techniques developed in [21].

Conclusions.—We have argued that averages of local operators in the steady state reached long after a quantum quench to an integrable model can be described as expectation values with respect to a single simultaneous eigenstate of all local conservation laws [Eqs. (3) and (13)]. This state can be constructed by means of a generalized thermodynamic Bethe ansatz. Going further, we have shown that the time evolution of local observables is governed by states in the vicinity of this saddle point through Eqs. (2) and (12). The spectral representation (12) allows us to identify the physical mechanism underlying the relaxation for a given observable at late times. Our approach paves the way for analyzing quantum quenches in interacting integrable models and applications to the Lieb-Liniger and the sine-Gordon model are in progress. Given the regularity assumptions in our GTBA analysis, an important question concerns the range of initial states that can be analyzed by our method. One requirement is that the probability distributions of all local conservation laws becomes very narrow as the thermodynamic limit is approached. An interesting application of our approach would be to quenches involving “integrable” disorder [50], where the GGE appears to no longer apply.

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