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Constructing the generalized Gibbs ensemble after a quantum quench

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Using a numerical renormalization group based on exploiting an underlying exactly solvable nonrelativistic theory, we study the out-of-equilibrium dynamics of a 1D Bose gas (as described by the Lieb-Liniger model) released from a parabolic trap. Our method allows us to track the post-quench dynamics of the gas all the way to infinite time. We also exhibit a general construction, applicable to all integrable models, of the thermodynamic ensemble that has been suggested to govern this dynamics, the generalized Gibbs ensemble. We compare the predictions of equilibration from this ensemble against the long time dynamics observed using our method.

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Understanding non-equilibrium quantum quench behavior in low-dimensional systems is a difficult theoretical challenge. Because one is initializing the system in a state that is not an eigenstate, this behavior is determined not merely by the system's ground state (or a small number of excited states), but rather by some coherent sum of a large number of eigenstates. If one wants to explore the emergence of a resulting steady state, the time evolution of this coherent sum must then be tracked over long periods of time. This problem confronts theorists who wish to understand dynamics in perturbed quantum gases [1, 2], ultrafast phenomena in superconductors [3], and questions of thermalization in integrable systems [4].

This last set of questions arise because of the surprising experimental finding that a perturbed one-dimensional Bose gas retains memory of its initial non-equilibrium state over long periods of time [1] and does not appear to relax to a state of thermodynamic equilibrium. To understand this, it was proposed [4] that equilibriation does occur but not as described by a grand canonical ensemble (GCE). Instead the ensemble describing equilibriation needs to take into account the additional, non-trivial conserved quantities that, at least according to the theoretical minimal model of the gas (the Lieb-Liniger (LL) model [5]), are present in the system. This new ensemble has been dubbed the generalized Gibbs ensemble (GGE). The GGE takes as the density matrix

$$\hat{\rho}_{GGE} = Z^{-1}\exp(-\sum_i \beta_i Q_i) \tag{1}$$

where the Q_i form an independent, complete sequence of conserved quantities in the system and β_i correspond to a set of generalized (inverse) temperatures. Computation of this density matrix is non-trivial and has only been successfully accomplished in certain special limits. Most of these limits are in models where interactions (though not necessarily correlation functions) correspond to a free model (the hard core limit of the interacting Bose gas [4], quadratic Hamiltonians [6], Luttinger liquids [7], the sine-Gordon model at the free-fermion point and in the semi-classical limit [8], and the quantum Ising model in the absence of a longitudinal field [9, 10]). A notable exception was the study of Fioretto and Mussardo [11] where it was possible to study quenches in general interacting integrable models but with the restriction to a very special set of quench protocols.

It is against this backdrop that we present a general methodology able to study non-equilibrium behavior and quench dynamics of low-dimensional interacting models, both integrable and non-integrable. This method is predicated on a numerical renormalization group (NRG) able to study models which can be represented as perturbed integrable and conformal field theories (CFT) [12]:

$$H = H_{Integrable/CFT} + V_{perturbation}. \tag{2}$$

The LL model in a trapping potential takes this form. We believe that this methodology is a valuable addition to other general methodologies used to study dynamics in low-dimensional systems such as the time-dependent density matrix renormalization group [13–17]. At least for a subset of quenches, where we quench into an integrable system (say by turning off the trapping potential in a LL system), we can track the dynamics for all times.

Concomitant with the introduction of this tool to study quench dynamics, we present a general methodology to compute the density matrix of the GGE using information arising from the application of the NRG. We show how one can write down a simple set of equations governing the GGE and how the entire infinite set of generalized temperatures, $\{\beta_i\}_{i=1}^{\infty}$ can be readily determined.

The specific example we consider is the LL model perturbed by a one-body parabolic trap $V(x) = m\omega^2 x^2/2$,

$$H = -\frac{\hbar^2}{2m}\sum_{j=1}^{N}\frac{\partial^2}{\partial x_j^2} + 2c\sum_{\langle i,j\rangle}\delta(x_i - x_j) + \sum_i V(x_i), \tag{3}$$

(we will work in units where $2m = \hbar = 1$). In running the NRG, we use the basis of eigenstates of the LL model and their matrix elements with respect to the trapping potential. Both the description of the states and the computation of matrix elements in the LL model are much more complicated than the examples of relativistic field theories where the NRG has been applied previously. The states in the LL model consist of N strongly interacting particles and not few-particle excitations above the true vacuum state, while the matrix elements do not see a chiral factorization as in a relativistic gapless theory but are N-dimensional determinants [18]. To tackle this, we took recourse to a highly optimized set of routines known as ABACUS [19] which solves and evaluates all equations needed to characterize both the necessary eigenstates and their matrix elements. This package has been shown to be able to successfully compute dynamical response functions for the LL model [19].

We first use the NRG to extract the ground state of the LL model in a trap [20]. The NRG produces the ground state of the gas, $|\psi\rangle_{GS}$, as a linear combination of exact eigenstates, $|s\rangle$, of the LL model: $|\psi\rangle_{GS} = \sum_s c_s|s\rangle$. In order to accurately describe the ground state in the NRG procedure we typically consider on the order of $10^4 - 10^5$ states. We then consider a sudden release of the trap, that is we will study the gas where we quench into an integrable model. For these types of quenches our methodology gives us the ability to study the evolution of the gas for arbitrary times. Each state, $|s\rangle$, appearing in the ground state is characterized by a set of N (one for each particle) rapidities (quasi-momenta) $\{\lambda_n\}_{n=1}^N$. These rapidities are solutions to the Bethe equations,

$$e^{i\lambda_n L} = \prod_{m\neq n} \frac{\lambda_n - \lambda_m + ic}{\lambda_n - \lambda_m - ic}, \qquad (4)$$

and can be readily obtained to arbitrary accuracy. With the NRG we can compute the coefficients c_s with reasonably high accuracy [20]. Time evolution under the post-quench Hamiltonian (the unperturbed LL model) is extremely simple. If E_s is the energy of state $|s\rangle$, the time evolution is described by $|\psi(t)\rangle_{GS} = \sum_s c_s e^{-iE_s t}|s\rangle$. Because each state's energy, E_s, is given in terms of the λ_n's as $\sum_n \lambda_n^2$, we can compute the phases appearing in the above sum to arbitrary accuracy for arbitrary time.

To characterize the evolution of the gas in the long time limit we compute the momentum distribution function (MDF) $n_k = \langle\psi_k^\dagger\psi_k\rangle$ in the diagonal ensemble (DE). An observable $\mathcal{O}^\dagger\mathcal{O}$ in this ensemble is simply given by

$$\langle\mathcal{O}^\dagger\mathcal{O}\rangle_{DE} \equiv \sum_s |c_s|^2\langle s|\mathcal{O}^\dagger\mathcal{O}|s\rangle. \qquad (5)$$

To compute this correlation function we insert a resolution of the identity between $\mathcal{O}^\dagger$ and $\mathcal{O}$ and use a specially-designed version of ABACUS for excited states to compute all of the necessary matrix elements [20].

In Fig. 1 we plot the MDF in the DE of the gas post-release for two values of c ($c = 10$ and $c = 7200$) and for a variety of system sizes, with ωL fixed and keeping

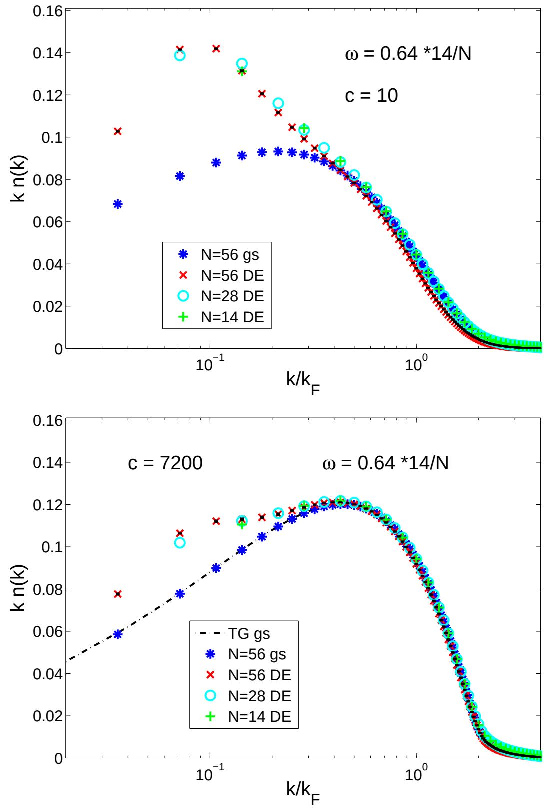


FIG. 1: The MDF in the DE of the gas after release from a trap for $c = 10$ (top) and $c = 7200$ (bottom). Shown are the gases at $(N = L = 14, \omega = 0.64)$, $(N = L = 28, \omega = 0.32)$, and $(N = L = 56, \omega = 0.16)$. Error bars are given for the $N = L = 56$ data alone and are estimated from the speed of convergence of the NRG (see [20]) – we believe the $N = L = 14, 28$ data is completely converged. The MDF of the untrapped gas $(N = L = 56)$ is shown for comparison as is the analytic expression available for the Tonks-Girardeau gas $c = \infty$ from Ref. [21].

$N = L$. For comparison we also plot the MDF of the gas in its ground state.

We see, as expected, that the MDF of the gas is perturbed from that of the ground state at low momenta but remains unchanged from the ground state MDF at higher momenta. The relative insensitivity to different values of $N = L, \omega$ is consistent with a perturbative (in ω) computation of the MDF in the DE at $c = \infty$ which shows $n(k)_{DE} = n(k)_{GS} + (\frac{\omega L}{2\pi})^4(\frac{N}{L})^{1/2}\frac{m^2\sqrt{2\pi}B_0}{8v_F^2 k^{5/2}} + \mathcal{O}(\omega^8)$. Here $n(k)_{GS}$ is the MDF of the ground state, the constant $B_0 \approx 0.5124$ [22], and v_F is the velocity of the gas. The scaling with N, L, and ω indicated by this expression implies that variations in $n(k)_{DE}$ between different system sizes in Fig. 1 are due to finite size corrections which are small (on the order of the symbol size). As an important check of our results, the high momenta tails of the MDF's at $c = 7200$ behave as the predicted k^{-4} [21, 23, 24].

While the diagonal ensemble tells us what the final steady state of the gas is after its release, a question of primary interest is whether the steady state can be associated with some ensemble. It has been postulated [4] that for a quench into an integrable system the correct ensemble to use is the GGE ensemble in Eqn. 1. The Q_i's are here non-trivial polynomials in the field operators (and their derivatives) [25]. The action of the Q_i's on the states, $|s\rangle$, is straightforward. With each state, $|s\rangle$, characterized by a set of N rapidities, λ_i, the action of the Q_i upon $|s\rangle$ is $Q_i|s;\lambda_1,\cdots,\lambda_N\rangle = \sum_j \lambda_j^i|s;\lambda_1,\cdots,\lambda_N\rangle$, that is to say, Q_i acts on the state like an i-th power sum. This shows that the Q_i's are both a complete and independent set of charges inasmuch as the polynomials form a complete and independent basis in the space of single variable functions.

To compute $\hat{\rho}_{GGE}$ the most straightforward path is to compute $\langle Q_i\rangle$ at $t = 0$ and insist that the set of β_i's is such that $\mathrm{Tr}(\hat{\rho}_{GGE}Q_i)$ gives the same answer. In the case of the hard core limit this is readily doable as the Q_i's can be written in terms of a more amenable basis, the momentum occupation numbers: $Q_i = \sum_\lambda \lambda^i n_\lambda$, where n_λ tells you whether there is a particle with rapidity of the form $\lambda = 2\pi m/L$ for $m \in \mathbb{Z}$. In this basis of charges, $\langle n_\lambda\rangle_{GGE}$ simplifies to $\mathrm{Tr}(\exp(-\beta_\lambda n_\lambda)n_\lambda)/\mathrm{Tr}\exp(-\beta_\lambda n_\lambda)$, i.e. for such expectation values the ensemble factorizes, and β_λ is readily computed. This simplification, however, does not exist away from the hard core limit and we are instead left with a complicated non-linear minimization problem which on the face of it does not obviously have a solution. We now show that it does and that the β_i's can be computed readily. We do so through a (generalized) thermodynamic Bethe ansatz [26].

Because the action of the charges Q_i on the states, $|s\rangle$, are given simply in terms of the rapidities, λ_i, identifying the state, to ask that $\langle Q_i\rangle_{t=0} = \langle Q_i\rangle_{GGE}$ amounts to asking whether there is a set of λ's, $\{\tilde{\lambda}_j\}_{j=1}^N$, such that

$$\langle Q_i\rangle_{t=0} = \sum_j \tilde{\lambda}_j^i, \quad i = 1, 2, \cdots .$$

There is in fact such a set. We can moreover determine its rapidity distribution, which we will call $\rho_{GGE}(\lambda)$, directly from $|\psi\rangle_{GS}$. To each state, $|s;\lambda_{s1},\cdots,\lambda_{sN}\rangle$, we associate a distribution, $\rho_s(\lambda)$, governing the λ's of that particular state: $\rho_s(\lambda) = \frac{1}{L}\sum_i \delta(\lambda-\lambda_{si})$. Then $\rho_{GGE}(\lambda)$ is the weighted sum of the $\rho_s(\lambda)$'s:

$$\rho_{GGE}(\lambda) = \sum_s |c_s|^2\rho_s(\lambda).$$

In particular $\int d\lambda \rho_{GGE}(\lambda)\lambda^i = L\langle Q_i\rangle_{t=0}$.

ρ_{GGE} contains, implicitly, all the information to characterize the action of $\hat{\rho}_{GGE}$ on a eigenstate of the LL model [26]. A distribution of λ's must be consistent with

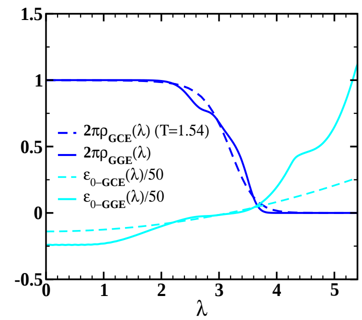


FIG. 2: $\varepsilon_0(\lambda)$ and $\rho(\lambda)$ for both the GGE and GCE ensembles for a gas with $N = L = 56$, $c = 7200$, and a prequench trap strength, $\omega = 0.256$. For the GCE ensemble the effective temperature is $T = 1.54$. The quantities plotted are symmetric about $\lambda = 0$.

the Bethe equations (Eqn. 4). In the continuum limit, these equations can be rewritten as [5, 27]

$$\rho_{GGE}(\lambda) + \rho^h_{GGE}(\lambda) = \frac{1}{2\pi} + \int \frac{d\lambda'}{2\pi}K(\lambda-\lambda')\rho_{GGE}(\lambda), \tag{6}$$

where $\rho^h_{GGE}(\lambda)$ is the density of holes in the λ-distribution and $K(\lambda) = 2c/(c^2+\lambda^2)$. Now the GGE is derived by the same principles as the grand canonical ensemble: namely entropy is maximized subject to the constraints of fixed conserved charges (energy for the grand canonical ensemble, all the charges, Q_i, for the GGE). Thus associated with GGE is a generalized free energy $F_{GGE} = \int d\lambda \rho_{GGE}(\lambda)\varepsilon_{0-GGE}(\lambda) - S$, where $\varepsilon_{0-GGE}(\lambda) \equiv \sum_i \beta_i\lambda^i$ is a generalized energy. It corresponds to the action of $\hat{\rho}_{GGE}$ on a state $|s;\lambda_1,\cdots,\lambda_N\rangle$:

$$\hat{\rho}_{GGE}|s;\lambda_1,\cdots,\lambda_N\rangle = \frac{e^{-\sum_i\varepsilon_{0-GGE}(\lambda_i)}}{Z}|s;\lambda_1,\cdots,\lambda_N\rangle. \tag{7}$$

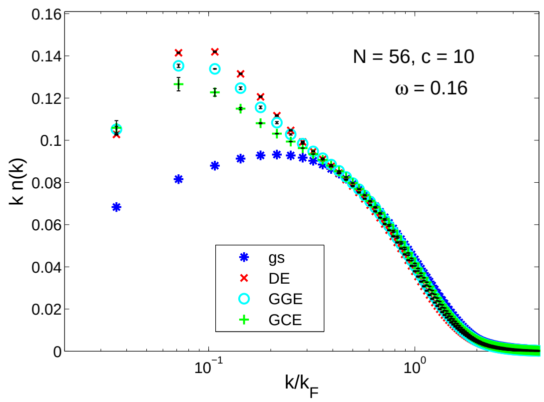
In particular knowing ε_{0-GGE} then allows us to compute general expectation values in the GGE. While ε_{0-GGE} differs from its form in the grand canonical ensemble, S is the standard entropy [27] of a system with a given distribution of particles, ρ_{GGE}, and holes, ρ^h_{GGE}:

$$S = \int d\lambda\Big[(\rho_{GGE}+\rho^h_{GGE})\log(\rho_{GGE}+\rho^h_{GGE}) - \rho_{GGE}\log\rho_{GGE} - \rho^h_{GGE}\log\rho^h_{GGE}\Big]. \tag{8}$$

We now show that we can express ε_{0-GGE} in terms of ρ_{GGE} that we derived from $|\psi\rangle_{GS}$.

If we minimize the generalized free energy we arrive at a constraint between the particle and hole distributions and ε_{0-GGE}:

$$\varepsilon(\lambda) = \varepsilon_{0-GGE}(\lambda) - \int \frac{d\lambda'}{2\pi}K(\lambda-\lambda')\log(1+e^{-\varepsilon(\lambda)}), \tag{9}$$



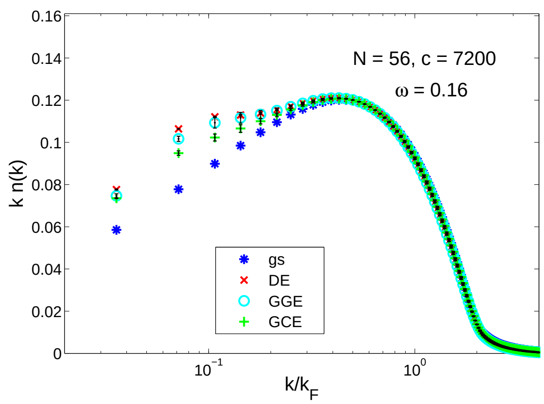


FIG. 3: The MDF (for $N = L = 56$) in the GCE and GGE for the gas after release from a trap of strength $\omega = 0.16$ for $c = 10$ (top) and $c = 7200$ (bottom). We again show the MDF of the untrapped gas for comparison (blue stars).

where $\varepsilon = \log(\rho^h_{GGE}/\rho_{GGE})$. Thus to determine ε_{0-GGE} we take our knowledge of $\rho_{GGE}(\lambda)$ obtained from $|\psi\rangle_{GS}$, use Eqn. (6) to determine ρ^h_{GGE} which then gives us $\varepsilon(\lambda)$. From Eqn. (9), we then can fix ε_{0-GGE}.

Following this procedure we plot in Fig. 2 ρ_{GGE} and ε_{0-GGE} for the gas in the hard core limit. For comparison we plot what these quantities would be if instead of a generalized Gibbs ensemble, the thermodynamics was governed by the grand canonical ensemble. (In this case we use the standard thermodynamic Bethe ansatz equations [27] to determine what ρ_{GCE} and $\varepsilon_{0-GCE} = \beta(\lambda^2 - \mu)$ need to be, i.e. what the effective temperature needs to be, if they are to reproduce the correct density and average energy of the system ${}_{GS}\langle\psi|H|\psi\rangle_{GS}$.) We see that both ρ_{GGE} and ε_{0-GGE} have considerably more structure than that of their grand canonical counterparts.

We now use this ability to compute $\varepsilon_{0-GGE}(\lambda)$, to compute various expectation values of observables in the GGE. In Fig. 3 we plot the MDF as computed in the DE and in both the GGE and GCE. The error estimate is computed similarly as in Fig. 1 (see [20] for details). For the data at hand, we see that for low momenta the two ensemble averages, GGE and GCE, disagree with the DE. However the GGE provides a considerably better match to the DE than does the ordinary thermal ensemble GCE. From the finite size comparison (see Fig. 3 of [20]), it can be argued (although not conclusively) that at small but finite k, this difference will vanish with increasing system size.

The disagreement between ensembles in the data is not entirely surprising. The logic of the GGE is such that it is expected to describe correlations that are local in space (and that involve a distance scale significantly smaller than the system size). We thus do not expect the correlations at $k \sim 1/L$ to be particularly well described by the GGE. However there is the possibility that the differences between ensembles will remain at finite $k > 1/L$ even in the infinite volume limit. In recent work [28] the entropy associated with the DE was shown to be considerably smaller than that of the GGE implying that the DE is more tightly constrained than the GGE, i.e. the GGE seems to be missing correlations. It would be interesting to understand if this missing entropy is solely associated with non-local correlations.

In conclusion, we have demonstrated how an NRG based on exploiting the integrability of the LL model can be used to study the time-dependent evolution after a quantum quench where a 1D gas is released from a parabolic trap. We have also demonstrated how to use the information arising from the NRG to construct the corresponding GGE which has been suggested as a possibility for governing the post-quench dynamics. While we have focused on the LL model, this methodology is applicable to any non-relativistic integrable theory of which the Heisenberg and XXZ spin chains are two prominent examples.

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