Failure of the local GGE for integrable models with bound states

Garry Goldstein and Natan Andrei

Department of Physics, Rutgers University and
Piscataway, New Jersey 08854

In this work we study the applicability of the local GGE to integrable one dimensional systems with bound states. We find that the GGE, when defined using only local conserved quantities, fails to describe the long time dynamics for most initial states including eigenstates. We present our calculations studying the attractive Lieb-Liniger gas and the XXZ magnet, though similar results may be obtained for other models.

I. INTRODUCTION

Recent years have witnessed spectacular advances in the theory of unitary nonequilibrium dynamics, particularly in systems of optically trapped atomic gases. Key to this advance is the extremely weak coupling to the environment which allows for essentially Hamiltonian dynamics. These experimental advances have spurred many theoretical questions: does a steady state emerge, how do local observables equilibrate, is there any principle which allows us to relate the steady state to the initial conditions?

One of the most surprising recent experimental [1], and theoretical [2] results is that there is a relation between the initial state and the long time steady state for integrable models. It was shown that after a quench integrable models retain memory of their initial state and do not appear to relax to thermodynamic equilibrium. This was ascribed to the fact that integrable models possess an infinite family of local conserved charges in involution, \{I_i\}, which include the Hamiltonian \(H\), typically identified with \(I_2\):

\[
[H, I_i] = [I_i, I_i^c] = 0, \quad H = I_2
\]  

(1)

These conserved quantities in turn imply that there is a complete system of eigenstates for the Hamiltonian which may be parametrized by sets of rapidities \(\{k\}\) and which simultaneously diagonalize all charges. To understand the equilibration of this system it was recently proposed that it is insufficient to consider only thermal ensembles but it is also necessary to include these nontrivial conserved quantities. It was proposed [3] that the system relaxes to a state given by the generalized Gibbs ensemble GGE with its density matrix being given by

\[
\rho_{\text{GGE}} = \frac{1}{Z} \exp \left( - \sum \alpha_i I_i \right)
\]

(2)

where the \(I_i\) are the local conserved quantities; the \(\alpha_i\) are the generalized inverse temperatures and \(Z\) is a normalization constant insuring \(\text{Tr}[\rho_{\text{GGE}}] = 1\). The \(\alpha_i\) are chosen in such a way as to insure that the conserved quantities \(I_i\) remain constant, namely, \(\langle I_i \rangle_{\text{final}} = \text{Tr} \langle \rho_{\text{GGE}} I_i \rangle = \langle I_i \rangle_{\text{initial}} = I_i^0\). Moreover it was proposed that expectation values of local operators and of correlation functions of an integrable model may be computed at long times by taking their expectation value with respect to the GGE density matrix, e.g. \(\langle \Theta (t \to \infty) \rangle = \text{Tr} [\rho_{\text{GGE}} \Theta]\). Recent numeric and theoretical works have, however, put this assumption into question [4].

Here we would like to show that the GGE hypothesis, based on local conserved quantities, fails in general for the class of integrable models possessing bound states, or string eigenstates. Bound states in integrable models are described, in the thermodynamic limit, by rapidities forming \(n\)-strings, [5]: 

\[
k_j^\alpha = k_0 + \mu (n-2j), \quad j = 0, 1, 2, \ldots, n\]

with \(n\) an arbitrary integer and \(\mu\) a coupling constant in the Hamiltonian. We will show that for such models the GGE hypothesis fails to reproduce the long time dynamics for most states and in particular for eigenstates of the Hamiltonian. We will focus in detail on the attractive Lieb-Liniger model, and repeat our arguments more briefly for the XXZ model. Our results are also applicable to other models with bound states.

The Lieb Liniger hamiltonian is given by:

\[
H_{\text{LL}} = \int_{-\infty}^{\infty} dx \left\{ \partial_x b^\dagger (x) \partial_x b (x) + c (b^\dagger (x) b (x))^2 \right\},
\]

(3)

Here \(b^\dagger (x)\) is the bosonic creation operator at the point \(x\) and \(c\) is the coupling constant. The eigenstates of the Hamiltonian are parametrized by rapidities \(\{|k\}\). In the basis of the Bethe rapidities, \(\{|k\}\), the local conserved quantities \(I_i\) are diagonalized and take the form, \(I_i |\{k\}\rangle = \sum k^i \{|k\}\rangle\). It was pointed out recently [6] that when not acting on eigenstates (or on a finite linear combination of them) the charges may generate divergences in the form of powers and derivatives of Dirac-deltas. Great care must then be taken to define their action. Here we assume an appropriate renormalization scheme has been implemented [7].

We consider the attractive Hamiltonian with the coupling constant taken to be negative \(c < 0\). In this case bound states are formed and the rapidities fall into \(n\)-string configurations \(k_j = k_0 + \frac{c}{2} (n-2j)\), with strings of arbitrary length length \(n = 1, 2, 3 \cdots\). The contribution an \(n\)-string centered at \(k_0\) to the conserved charge \(I_i\) is
given by:
\[ \varepsilon_i^n (k_0) = \sum_{j=0}^{n} \left( k_0 + \frac{i}{2} (n - 2j) \right)^i = \sum_{i=0}^{n} k_0^{i-1} \left( \frac{i}{2} \right)^i \sum_{j=1}^{n} (n - 2j)^i \]
(4)

We will show here explicitly for the Lieb-Liniger and the XXZ models (the proof can be extended to other models with bound states such as the Hubbard model or the Anderson model) that when the system is quenched from a non-equilibrium initial state \( \Phi_0 \) and allowed to evolve for a long time, the GGE hypothesis fails and for most initial states \( \Phi_0 \), including eigenstates, does not provide a correct description of the equilibrated system.

The rest of the paper is organized as follows. In Section II we present the outline of the proof of this result; in subsection IIIA we present some properties of the conserved quantities of the states used in Section II, in subsection IIIB we present some results concerning the GGE used in Section II, in Section III we briefly discuss the XXZ model and in Section IV we conclude.

II. OUTLINE OF PROOF

For the attractive Lieb-Liniger gas we may introduce densities of string excitations; for a given eigenstate \( \{ \{ k \} \} \) we denote by \( \rho_p^n (k) \) the Bethe density of \( n \)-strings, so that \( L_p^n (k) \) is the number of \( n \)-strings in the interval \([k, k + dk]\). Similarly \( \rho_h^n (k) \) denotes the \( n \)-strings hole density and \( \rho_t^n (k) = \rho_p^n (k) + \rho_h^n (k) \) the total \( n \)-string density. The Yang-Yang entropy associated with the densities \( \{ \rho_p^n (k), \rho_h^n (k) \} \), measures the number of states \( \{ \{ k \} \} \) consistent with the densities. It is given by:
\[ S (\{ \rho^n \}) = \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} dk \left( \rho_p^n (k) \ln \left( \frac{\rho_p^n (k)}{\rho_h^n (k)} \right) + \rho_h^n (k) \ln \left( \frac{\rho_h^n (k)}{\rho_t^n (k)} \right) \right) . \]
(5)

With this notation our proof of the failure of the GGE, based on local conserved quantities, will be based on two main results which we prove below: (1) For the attractive Lieb-Liniger model for a given set of conserved quantities \( I_i \), there is an infinite number of densities \( \{ \rho_p^n \} \) satisfying \( I_i \{ \rho_p^n \} = I_i \), (2) The GGE corresponds to a pure state whose Bethe densities \( \{ \rho^n \} \) maximizes the entropy \( S (\{ \rho^n \}) \) subject to the thermodynamic Bethe Ansatz equation and the constraints \( I_i \{ \rho_p^n \} = I_i \).

It follows then that while in the repulsive Lieb-Liniger model the quantities \( I_i \), fixed by the initial state, uniquely determine the Bethe density \( \rho_h \) such that \( I_i \{ \rho_h \} = I_i \), no such shortcut is available in the case of the attractive model. An infinite number of densities are required its description and the conditions \( I_i \{ \rho_p^n \} = I_i \) are insufficient to determine the densities and hence the GGE. The full time evolution is required. In more detail, point (1) indicates that there are many states with different particle densities \( \{ \rho_p^n \} \) that give the same GGE.

However states with different densities have different local correlations [9] so cannot correspond to the same density matrix. This is sufficient to show the failure of the GGE for most eigenstates, see Fig. 1. The point (2) identifies which eigenstates correspond to the GGE. For these eigenstates and these eigenstates only the GGE is a good description of the state.

If furthermore we assume the o-TBA hypothesis [10] then most states correspond to eigenstates and we get that the GGE fails for most states. We note that we do not need an o-TBA assumption to show that GGE based on local conserved quantities fails.

In Section II A we prove property (1) and in Section II B we prove property (2).

A. Properties of the states

We would like to show that for a given set of conserved quantities \( \{ I_i \} \) there is an infinite set of different densities \( \{ \rho_p^n \} \) that satisfy \( I_i \{ \rho_p^n \} = I_i \). In order to accomplish this we introduce the notation \( J_i^n = \int dk \rho_p^n (k) k^i \). These are the moments of the distributions \( \rho_p^n \). There is a one to one correspondence between a distribution and its moments. Then using Eq. (4) the equation \( I_i \{ \rho_p^n \} = I_i \) may be written as:
\[ \sum_{n=0}^{\infty} \sum_{l=0}^{i} J_i^n \left( \frac{ic}{2} \right)^i l \sum_{j=0}^{n} (n - 2j)^l = I_i^n . \]
(6)
We need to choose a change in the last moment to do this. Then in order for Eq. (6) to be satisfied all moments of the form $\rho^{n}$ are chosen such that this pure state satisfies $I_{i} (\{ \rho_{i} \}) = \sum_{l = 0}^{\infty} \sum_{m = 0}^{l} \text{dk} \rho_{i+l}(k) e_{i+l}(k) = I_{i}$. We note that $M_{l}$ is lower triangular with all the diagonal entries equal to $n + 1$ hence invertible. Since $J_{l}^{m-\alpha} = 0$ and is in the interior of the set of allowed moments and $\delta J_{l}^{m}$ is small we have the moments $J_{l}^{m-\alpha} + \delta J_{l}^{m}$ also correspond to a real density $\rho^{n}$. As such there is an infinite number of densities corresponding to each set of conserved moments.

### B. Properties of the GGE

We now show that the GGE density matrix corresponding to the moments $I_{l}^{n}$ corresponds to the pure state with the same moments that maximizes the entropy given in Eq. (5). To do so we use the result in [10] that the GGE, based on local conserved quantities, corresponds to a pure state that maximizes the functional $\Xi (\{ \rho_{i} \}) \equiv -\sum_{l = 0}^{\infty} \sum_{m = 0}^{\infty} \int \text{dk} \rho_{i+l}(k) e_{i+l}(k) + S (\rho^{n})$, subject to the constraint of the Thermodynamic Bethe Ansatz. The quantities $\alpha_{i}$ are chosen such that this pure state satisfies $I_{i} (\{ \rho_{i} \}) = \sum_{l = 0}^{\infty} \sum_{m = 0}^{\infty} \int \text{dk} \rho_{i+l}(k) e_{i+l}(k) = I_{i}$ so the maximization happens when this is satisfied. Within this subspace the functional $\Xi (\{ \rho^{n} \})$ simplifies to $\Xi (\{ \rho^{n} \}) = -\sum_{l = 0}^{\infty} \sum_{m = 0}^{\infty} \text{dk} \rho_{l+i}(k) e_{l+i}(k) + S (\{ \rho^{n} \})$. Therefore the GGE corresponds to the pure state that has the prescribed conserved quantities and maximizes the quantity $S (\{ \rho^{n} \})$ subject to the TBA and the constraint that $I_{i} (\{ \rho_{i} \}) = I_{i}$. Therefore for fixed conserved quantities the GGE corresponds to a single pure state and only reproduces the long time dynamics of that pure state.

### III. XXZ MODEL

We will briefly discuss how to extend our results to the XXZ model. The XXZ Hamiltonian is given by:

$$H_{\text{XXZ}} = -J \sum_{i = -\infty}^{\infty} \left[ \sigma_{i}^{x} \sigma_{i+1}^{x} + \sigma_{i}^{y} \sigma_{i+1}^{y} + \Delta (\sigma_{i}^{z} \sigma_{i+1}^{z} - 1) \right]$$

Here $\sigma_{i}^{x,y,z}$ is the Pauli matrix at the site $i$, we will focus on the case where $\Delta > 1$. This Hamiltonian is integrable and has an infinite number of conserved quantities $I_{i}$. The eigenstates may be parametrized by rapidities $\{ \{ \lambda \} \}$. The rapidities may be arranged into strings where each string is composed of the rapidities given by $\lambda_{j} = \lambda + \frac{\pi}{2} (n - 2 j)$ with $j = 0, 1, 2, \ldots, n$ and $\lambda \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ and $\Delta = \cosh \eta$. We would like to repeat our proof of the failure of the GGE for eigenstates for the case of the XXZ Hamiltonian. To do so we need to prove two statements akin to what was done in section [11]: (1) That for a given set of conserved quantities $I_{i}$ there is an infinite number of possible quasiparticle densities $\{ \rho^{n} \}$. (2) The GGE corresponds to a single choice of these densities $\rho^{n}$ which maximizes the entropy see Eq. (5). To prove (2) we note that according to the result in [10] that the GGE corresponds to a pure state that maximizes the functional $\tilde{\Xi} (\{ \rho^{n} \}) \equiv -\sum_{l = 0}^{\infty} \sum_{m = 0}^{\infty} \int \text{dk} \rho_{l+i}(k) e_{l+i}(k) + S (\rho^{n})$ subject to the constraint of the Thermodynamic Bethe Ansatz. Here $\tilde{E}_{l}^{n}$ is the value of the $i$th conserved quantities when acting on a string and $S (\rho^{n})$ is completely analogous to Eq. (5). We know that the quantities $\alpha_{i}$ are chosen such that this pure state satisfies $\tilde{I}_{i} (\{ \rho_{i} \}) \equiv \sum_{l = 0}^{\infty} \sum_{m = 0}^{\infty} \int \text{dk} \rho_{l+i}(k) e_{l+i}(k) = I_{i}$. Within this subspace the functional $\tilde{\Xi} (\{ \rho^{n} \})$ simplifies to $\tilde{\Xi} (\{ \rho^{n} \}) = -\sum_{l = 0}^{\infty} \sum_{m = 0}^{\infty} \text{dk} \rho_{l+i}(k) e_{l+i}(k)$. Therefore the GGE corresponds to the pure state that has the right conserved quantities and maximizes the quantity $S (\{ \rho^{n} \})$ subject to the TBA. To prove the observation (1) we note that the quantities $\tilde{E}_{l}^{n}$ have convergent power series in $\sin (2 \lambda)$ and $\cos (2 \lambda)$ and therefore may be expressed as a linear function in the quantities $\{ \sin (2 \lambda) \}$ and $\{ \cos (2 \lambda) \}$. This means that the quantities $\tilde{E}_{l}^{n}$ may be related to the Fourier coefficients of $\rho^{n}$. To reproduce values of the conserved quantities $I_{i}$ we obtain equations similar to Eq. (6) where the quantities $J_{l}^{m}$ are replaced by the Fourier coefficients $F_{l}^{n}$ of the quantities $\rho^{n}$. These equations are once again vastly underdetermined with infinitely more variables then constraints. As such, in a completely analogous way as before we obtain that there is infinite number of solutions to these equations and as a result the GGE fails for pure states for the XXZ Hamiltonian.

### IV. CONCLUSIONS

We have shown that for integrable models with bound states the GGE based on local conserved quantities does
not represent the long time dynamics of many states, in particular most eigenstates. This result is based on two observations we have proven: (1) for any set of conserved quantities $I_0^i$ there are many states $|\{k\}\rangle$ such that $I_i(|\{k\}\rangle) = I_0^i$, (2) The GGE corresponds to a specific state with fixed $I_0^i$. We have verified these statements explicitly for the case of the attractive Lieb-Liniger gas and the XXZ magnet though similar verifications may be done for other integrable models with bound states.

The question whether the local charges form a complete set is of great interest. For the repulsive case they appear to be complete, as the GGE with local charges represents the long time limit of the model. However the GGE with local charges fails to do so when the coupling constant changes sign. Would new non-local charges be required for the attractive Lieb-Liniger model? For the XXZ Heisenberg model such charges were recently proposed [11] to treat another aspect of completeness in the context of the Mazur inequality. Whether they also repair the GGE is an open question.

Acknowledgments: This research was supported by NSF grant DMR 1006684 and Rutgers CMT fellowship. We would like to thank M. Rigol and J.-S. Caux and Marton Kormos for useful discussions and comments.

Appendix: Regularization schemes

We would like to describe how to regularize the GGE for the attractive Lieb-Liniger model. Multiple regularizations are possible [6]. For example a regularization scheme for the GGE for the Lieb Liniger gas may be the following. Consider the conserved quantities:

$$\tilde{I}_i |\{k\}\rangle = \sum k^i \exp (-\lambda k^2) |\{k\}\rangle$$  \hspace{1cm} (8)

These are semi local in the sense that they have convergent powerseries with the expansion coefficients being the usual conserved quantities $I_i |\{k\}\rangle = \sum k^i |\{k\}\rangle$. Here $\lambda$ is a positive real number. We can define a GGE with these conserved quantities, that is we write $\rho_{GGE} = \frac{1}{Z} \exp (-\sum \alpha_i I_i)$ such that $tr \{\rho_{GGE} \tilde{I}_i\} = \tilde{I}_i (t=0)$. The $\tilde{I}_i$ have finite expectation values for any $\lambda$. Furthermore the matrix $\rho_{GGE}$ is independent of $\lambda$. Indeed for any $\lambda$ the $\tilde{I}_i$ are linear combinations of the $I_i$. Furthermore this linear transformation $\tilde{I}_i \rightarrow I_i$ is invertible (the matrix of the transformation is upper triangular with all ones on the diagonal). By composing the transformation $\tilde{I}^\lambda \rightarrow \tilde{I}^\nu$ is also invertible. Conservation of one set of charges for one $\lambda$ is completely equivalent to conservation of another set of charges for a different $\lambda$. With this regularization it is in principle possible to define the GGE for any state. Another regularization scheme is to average the local density for the conserved charges over a small interval, thereby obtaining a finite result, use these conserved quantities to calculate the GGE and then take the limit where the averaging goes to zero.

[1] T. Kinoshita, T. Wenger, and D. S. Weiss, Nature (London) 440, 900 (2006)
[2] Kai He and M. Rigol, Phys. Rev. A 87, 043615 (2013); G. Goldstein and N. Andrei, arXiv 1309.7029
[3] M. Rigol, V. Dunjko, V. Yurovsky and M. Olshanii, Phys. Rev. Lett. 98, 050405 (2007).
[4] B. Wouters, M. Brockmann, J. De Nardis, D. Fioretto, J.-S. Caux, arXiv:1405.0172, B. Pozsgay, M. Mestyán, M. A. Werner, M. Kormos, G. Zaránd, G. Takács arXiv:1405.2843
[5] M. Takahashi, Thermodynamics of one-dimensional solvable models, (Cambridge University Press, 1999).
[6] M. Kormos, A. Shashi, Y.-Z. Chou, J.-S. Caux, Adilet Imambekov Phys. Rev. B 88, 205131 (2013)
[7] See appendix
[8] V. E. Korepin, N. M. Bogoliubov and A. G. Izergin, Quantum inverse scattering and correlation functions, (Cambridge University Press, 1993).
[9] J. De Nardis, B. Wouters, M. Brockmann and J.-S. Caux, Phys. Rev. A 89, 033601 (2014).
[10] J. Mossel, J.-S. Caux, J. Phys. A: Math. Theor. 45, 255001, (2012).
[11] M. Mierzejewski, P. Prelovsek, and T. Prosen arXiv 1405.2557