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Chapter 7

Generalized TBA for generalized Gibbs

In this chapter we discuss the generalized Gibbs ensemble in the thermodynamic limit. We show that a saddle-point approximation for the partition function is possible, therefore avoiding the computation of the Gibbs trace. Specializing to the Lieb-Liniger model, we generalize the well-known thermodynamic Bethe ansatz (TBA) for the generalized Gibbs ensemble. Writing down equations describing the saddle-point (pseudo-equilibrium) state of the infinite system, we prove the existence and uniqueness of solutions, provided simple requirements are met. As an example, we discuss interaction quenches in the Lieb-Liniger model. For concreteness, we illustrate the method using a worked-out example for a chain of coupled harmonic oscillators. This chapter is based on the results published in [55].

7.1 The Lieb-Liniger model in the thermodynamic limit

We start this chapter by reviewing how one can formulate the Bethe equation for the Lieb-Liniger model in the thermodynamic limit. While for a finite size system states could be labeled by a set of rapidities \( \{\lambda_j\} \) (or equivalently by a set of quantum numbers \( \{I_j\} \), in the thermodynamic limit it is more convenient to work with distributions that satisfy certain integral equations instead. We first recall the Bethe equations for the Lieb-Liniger model in case of finite size (2.29),

\[
\lambda_j = \frac{2\pi}{L} I_j - \frac{1}{L} \sum_{l=1}^{N} \phi(\lambda_j - \lambda_k). \tag{7.1}
\]

We can write this as an integral equation in terms of a function \( \lambda(x) \) such that \( \lambda(x = I_j/L) = \lambda_j \). In order to replace the sum in the equation above with an
7.1 The Lieb-Liniger model in the thermodynamic limit

integral we introduce the density function

$$\rho(x) = \frac{1}{L} \sum_{j=1}^{N} \delta(x - \frac{I_j}{L}),$$ (7.2)

so

$$\lambda(x) = 2\pi x - \int_{-\infty}^{\infty} \phi(\lambda(x) - \lambda(y)) dy.$$ (7.3)

Note that this equation also defines $\lambda(x)$ for $xL \notin \{I_j\}$, the so-called unoccupied quantum numbers. The quantum numbers $\{I\}$ take values on $\mathbb{Z}$ if $N$ is odd and on $\mathbb{Z} + 1/2$ for even $N$. Therefore, the unoccupied quantum numbers $\{\tilde{I}\}$ are defined as $\mathbb{Z}/\{I\}$ for odd $N$ and $(\mathbb{Z} + 1/2)/\{I\}$ for even $N$. We will introduce the terminology that an occupied quantum corresponds to a particle and an unoccupied one corresponds to a hole. The particle and hole densities are then defined as

$$\rho(x) = \frac{1}{L} \sum_{n \in \{I\}} \delta(x - n/L), \quad \rho_h(x) = \frac{1}{L} \sum_{n \in \{\tilde{I}\}} \delta(x - n/L).$$ (7.4)

Obviously, the density for all quantum numbers is simply $\rho_t(x) = \rho(x) + \rho_h(x)$. One can also write the corresponding densities as function of the the rapidity $\lambda$

$$\rho(\lambda) = \rho(x(\lambda)) \frac{dx(\lambda)}{dk}, \quad \rho_h(\lambda) = \rho_h(x(\lambda)) \frac{dx(\lambda)}{dk}, \quad \rho_t(x) = \frac{dx(\lambda)}{dk}.$$ (7.5)

Note that, in contrast with $\rho_t(x)$, $\rho_t(k)$ is a non-trivial function. We can write (7.3) as

$$\lambda = 2\pi x(\lambda) - \int_{-\infty}^{\infty} \phi(\lambda - \mu) \rho(\mu) d\mu.$$ (7.6)

We can write an equation without $x(\lambda)$ by differentiating with respect to $\lambda$

$$2\pi(\rho(\lambda) + \rho_h(\lambda)) = 1 + 2\pi \int_{-\infty}^{\infty} a_2(\lambda - \mu) \rho(\mu) d\mu.$$ (7.7)

Here, we have defined the kernel

$$a_2(\lambda) = \frac{1}{2\pi} \frac{d\phi(\lambda)}{d\lambda} = \frac{1}{\pi} \frac{c}{\lambda^2 + c^2}.$$ (7.8)

Using the standard convolution notation $f * g(\lambda) \equiv \int_{-\infty}^{\infty} d\lambda' f(\lambda - \lambda') g(\lambda')$, we can write the equation above as [56]

$$\rho(\lambda) + \rho_h(\lambda) = \frac{1}{2\pi} + a_2 * \rho(\lambda).$$ (7.9)

Since this equation involves the unknown functions $\rho(\lambda)$ and $\rho_h(\lambda)$, an additional functional equation is required to have a unique solution. A special case is the ground state which we will discuss below. More general states can be obtained using the generalized TBA equations which we will introduce in section 7.2.
The ground state

The ground state of the Lieb-Liniger model is a filled Fermi sea in terms of quantum numbers. In rapidity space this is equivalent to defining a Fermi momentum $\lambda_F$ and defining

$$\rho(\lambda) = \begin{cases} \rho_t(\lambda), & -\lambda_F \leq \lambda \leq \lambda_F, \\ 0, & \text{otherwise} \end{cases}$$

(7.10)

$$\rho_h(\lambda) = \begin{cases} \rho_t(\lambda), & |\lambda| > \lambda_F, \\ 0, & \text{otherwise}. \end{cases}$$

(7.11)

The equation (7.9) is now simply

$$\rho(\lambda) = \frac{1}{2\pi} + \int_{-\lambda_F}^{\lambda_F} a_{2}(\lambda - \mu)\rho(\mu)d\mu$$

(7.12)

which is known as the Lieb equation. One can solve this equation by numerical integration.

7.2 Generalized TBA for the Lieb-Liniger model

The effectiveness of the GGE for free models is that the partition functions factorize, which allows an efficient computation for the Lagrange multipliers $\beta_k$ and the computation of expectation values. In the fully interacting case, the implementation of the GGE is much more complicated, since now the partition function does not factorize. This has two important consequences. The first is that the Lagrange multipliers $\beta_k$ now depend on each other and have to be fixed simultaneously. The second problem is that now one has to take the trace in the partition function over all eigenstates that are assigned a significant weight. This would make the GGE completely useless, as it would be in the same order of computation complexity as constructing the diagonal ensemble explicitly. However, we know from ordinary statistical mechanics that in the thermodynamic limit saddle-point approximations can be used for the computation of local observables (for the Lieb-Liniger model see for instance [66, 65]). In this section we show that these results can be generalized to the GGE and obtain generalized TBA equations.

For concreteness, we will illustrate the ideas by considering the Lieb-Liniger model, for which the Hamiltonian is

$$H_0 = \int_0^L dx \left\{ \partial_x \Psi^\dagger(x) \partial_x \Psi(x) + c \Psi^\dagger(x) \Psi^\dagger(x) \Psi(x) \Psi(x) \right\}.$$  

(7.13)

We restrict ourselves to the case of positive coupling constant $c > 0$, in which energies per unit length remain finite in the thermodynamic limit.

The eigenvalues of $\hat{N}$, $\hat{P}$ and $\hat{H}_0$ on an eigenstate $|\{\lambda_j\}\rangle$ are respectively $Q_0 = N = \sum_j \lambda_j^0$, $Q_1 = \sum_j \lambda_j$ and $Q_2 = \sum_j \lambda_j^2$. The logic extends to all higher conserved charges $\hat{Q}_n$, whose eigenvalues are simply given by the power sum symmetric polynomials

$$\hat{Q}_n|\{\lambda\}\rangle = Q_n|\{\lambda\}\rangle, \quad Q_n \equiv \sum_j \lambda_j^n.$$  

(7.14)
The generalized Hamiltonian is therefore diagonalized according to
\[ H(\{\beta\},\{\lambda\}) = E(\{\beta\},\{\lambda\}), \quad E(\{\beta\},\{\lambda\}) = \sum_{n=0}^{\infty} \sum_{j=1}^{N} \beta_n \lambda^n_j = \sum_{j=1}^{N} \varepsilon_0(\lambda_j) \] (7.15)
in which we have defined the function
\[ \varepsilon_0(\lambda) \equiv \sum_{n=0}^{\infty} \beta_n \lambda^n \] (7.16)
by interpreting the coefficients \( \beta_n \) as those of its power series. For a given \( \rho(\lambda) \) one can then easily compute the expectation values of the conserved charges as [65]
\[ Q_n = L \int_{-\infty}^{\infty} d\lambda \lambda^n \rho(\lambda). \] (7.17)

Following the arguments given by Yang and Yang [66], we now consider a generalized partition function
\[ Z = \int \mathcal{D}[\rho] e^{-G[\rho,\rho_h[\rho]]} \] (7.18)
(note that we have explicitly written \( \rho_h \) as a functional of \( \rho \) by using the Bethe equations (7.9)) in which the measure is given by a generalized Gibbs ‘free energy’\(^1\) functional
\[ G[\rho,\rho_h] = \sum_{n=0}^{\infty} \beta_n Q_n - S[\rho,\rho_h] \] (7.19)
where the entropy is given to leading order in system size as [66, 173]
\[ S = L \int_{-\infty}^{\infty} d\lambda [(\rho + \rho_h) \ln(\rho + \rho_h) - \rho \ln \rho - \rho_h \ln \rho_h]. \] (7.20)

As Yang and Yang themselves point out, this derivation (unlike the rest of their paper), is far from rigorous. It is, in fact, an ingenious elaboration of the derivation given by Landau and Lifshitz for the nonequilibrium entropy density of a free quantum gas [3]. The rigorous proof came few decades later [173]. In the thermodynamic limit we can evaluate the partition function in the saddle-point approximation by varying the free energy \( G[\rho,\rho_h] \) with respect to \( \rho(\lambda) \rightarrow \rho(\lambda) + \delta \rho(\lambda) \). The variation of \( \rho_h(\lambda) \) is done implicitly by means of (7.9). This leads to the saddle-point condition
\[ \ln \frac{\rho_h(\lambda)}{\rho(\lambda)} = \sum_n \beta_n \lambda^n - a_2 * \ln[1 + \rho(\lambda)/\rho_h(\lambda)]. \] (7.21)

By proceeding as usual and defining the function
\[ \varepsilon(\lambda) = \ln \frac{\rho_h(\lambda)}{\rho(\lambda)}, \] (7.22)
\(^1\)although this is strictly speaking not an energy anymore, but a dimensionless quantity
the saddle-point condition can be rewritten as

$$\varepsilon(\lambda) + a_2 \cdot \ln(1 + e^{-\varepsilon(\lambda)}) = \varepsilon_0(\lambda),$$

(7.23)

which we call the generalized TBA equation. This is a straightforward generalization of the usual TBA equations, the only difference being that the driving function $\varepsilon_0(\lambda)$ is given by the generic polynomial (7.16). One could even think of lifting the restriction of $\varepsilon_0$ to polynomial functions, and consider functions with isolated singularities. In view of the applications we have in mind, we will however not consider these more general cases here.

The equilibrium (i.e. saddle-point) state of the generalized distribution (7.19) is completely determined by (7.9) and (7.23). One can rewrite (7.9) to eliminate $\rho_h(\lambda)$ obtaining

$$\rho(\lambda) = \vartheta(\lambda) \left( \frac{1}{2\pi} + a_2 \cdot \rho(\lambda) \right),$$

(7.24)

in which $\vartheta(\lambda)$ is as usual called the Fermi weight and is defined as

$$\vartheta(\lambda) = \frac{\rho(\lambda)}{\rho(\lambda) + \rho_h(\lambda)} = \frac{1}{1 + e^{\varepsilon(\lambda)}}.$$  

(7.25)

As in the usual case, many expectation values only depend on $\rho(\lambda)$ and $\vartheta(\lambda)$ (see for instance [174, 175, 176, 177, 178]); these results can, therefore, automatically be generalized to solutions of the generalized TBA equations.

For a given set of $\beta_n$, the saddle-point state is completely determined by equations (7.23) and (7.24). Conversely, for a given $\varepsilon(\lambda)$, the Lagrange multipliers can be determined explicitly from (7.23),

$$\beta_n = \left. \frac{\partial^n}{\partial \lambda^n} \left( \varepsilon(\lambda) + a_2 \cdot \ln[1 + e^{-\varepsilon(\lambda)}] \right) \right|_{\lambda=0}.$$  

(7.26)

One can proceed in either of two ways, depending on the available data. Either for a given set $\beta_n$ one solves for $\varepsilon(\lambda)$ using (7.23) and from there finds $\rho(\lambda)$ using (7.24). This would be the procedure to follow for example in the case where the explicit values of the $\beta_n$ correspond to specific ‘user-defined’ perturbations to the original Hamiltonian [179, 180], or to situations in which (by some miracle) the generalized inverse temperatures of the GGE ensemble are known.

A dual interpretation and use of the generalized TBA equations consists of starting from a given $\rho(\lambda)$, and solving for $\varepsilon(\lambda)$. The Lagrange multipliers, which ultimately encode all characteristics of the saddle-point state, can then be computed via (7.26). While it might seem strange to expect the distribution $\rho(\lambda)$ to be given as input, this case is in fact the one which occurs when one uses (numerical) renormalization around a Bethe ansatz-solvable point [181]. This case in fact represents possibly the most immediately useful application of our equations, since the knowledge of $\rho(\lambda)$ then allows to explicitly compute GGE predictions without explicit knowledge of the set $\{\beta_j\}$, by using the generalized TBA equations to relate $\rho(\lambda)$ to the physical distribution $\varepsilon(\lambda)$ actually used in the averaging. In the case of the Lieb-Liniger model, the problems with attempting a direct implementation of the GGE according to the prescription discussed in the introduction are compounded by the fact that the conserved charges are not properly normal-ordered.
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objects [102, 103] whose expectation values can easily be computed using standard methods. We will elaborate on this in section 7.3, where we discuss interaction quenches.

7.2.1 Solving the generalized TBA equations

We can show that a solution of the generalized TBA equation (7.23) exists and can be found via iteration, in complete parallel to the traditional case, provided that two very simple conditions are fulfilled. The bare energy

\[ \varepsilon_0(\lambda) = \sum_n \beta_n \lambda^n \]  

(7.27)

should a) be bounded from below, and b) be such that \( \lim_{\lambda \to \pm \infty} \varepsilon_0(\lambda) = +\infty \).

The proof we give is essentially a repetition of the traditional one offered in [66]. Let us construct the following sequence of functions

\[ \varepsilon_{n+1}(\lambda) = \varepsilon_0(\lambda) + A[\varepsilon_n(\lambda)] \]  

(7.28)

where

\[ A[\varepsilon(\lambda)] = -\int_{-\infty}^{\infty} d\lambda' a_2(\lambda - \lambda') \ln \left(1 + e^{-\varepsilon(\lambda')}\right) \]  

(7.29)

The proof consists of two steps. First we will show that for every \( \lambda \) the sequence of functions is strictly decreasing,

\[ \varepsilon_0(\lambda) > \varepsilon_1(\lambda) > \ldots > \varepsilon_n(\lambda) > \varepsilon_{n+1}(\lambda) > \ldots \]  

(7.30)

Secondly, we will show that this sequence is bounded from below so that the limit

\[ \varepsilon(\lambda) = \lim_{n \to \infty} \varepsilon_n(\lambda) \]  

(7.31)

exists and is a solution of (7.23).

From (7.29) we see that \( A[\varepsilon(\lambda)] < 0 \) for all \( \varepsilon(\lambda) \). In order to show that \( A[\varepsilon_{n+1}(\lambda)] < A[\varepsilon_n(\lambda)] \), we consider

\[ \delta A[\varepsilon_n(\lambda)] = \int_{-\infty}^{\infty} d\lambda' a_2(\lambda - \lambda') \frac{1}{1 + e^{\varepsilon_n(\lambda')}} \delta \varepsilon_n(\lambda'). \]  

(7.32)

For \( \delta \varepsilon_n(\lambda) < 0 \) we have \( \delta A[\varepsilon_n(\lambda)] < 0 \), hence we arrive at (7.30). To prove that \( \varepsilon(\lambda) \) is bounded from below is more complicated. First, we specialize to cases in which \( \varepsilon_0(\lambda) \) is symmetric in \( \lambda \) and is monotonically increasing for positive \( \lambda \). By considering

\[ \frac{d\varepsilon_{n+1}(\lambda)}{d\lambda} = \frac{d\varepsilon_0(\lambda)}{d\lambda} + \int_{-\infty}^{\infty} d\lambda' a_2(\lambda - \lambda') \frac{1}{1 + e^{\varepsilon_n(\lambda')}} \frac{d\varepsilon_n(\lambda')}{d\lambda'}, \]  

(7.33)

we can prove by induction that \( \varepsilon_n(\lambda) \) is also symmetric in \( \lambda \) and monotonically increasing for positive \( \lambda \). From this it follows that \( A[\varepsilon_n(\lambda)] \) is monotonically increasing as a function of \( \lambda \), and goes to zero in the limit \( \lambda \to \infty \). Using this fact, we can write the following inequality

\[ \varepsilon_n(\lambda) = \varepsilon_0(\lambda) + A[\varepsilon_{n-1}(\lambda)] \geq \varepsilon_0(\lambda) - \varepsilon_0(0) + \varepsilon_n(0), \]  

(7.34)

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where the equality holds for $\lambda = 0$. Using this inequality, we can write another inequality using (7.28) and (7.32)

$$
\varepsilon_{n+1}(0) \geq \varepsilon_0(0) - \int_{-\infty}^{\infty} d\lambda' a_2(0 - \lambda') \ln(1 + e^{-(\varepsilon_0(\lambda') - \varepsilon_0(0) + \varepsilon_n(0))}).
$$

(7.35)

Next, we define the function

$$
f(x) = \varepsilon_0(0) - \int_{-\infty}^{\infty} d\lambda' a_2(0 - \lambda') \ln(1 + e^{-(\varepsilon_0(\lambda') - \varepsilon_0(0) + x)})
$$

(7.36)

$$
f(x) = \varepsilon_0(0) + x - \int_{-\infty}^{\infty} d\lambda' a_2(0 - \lambda') \ln(e^x + e^{-(\varepsilon_0(\lambda') - \varepsilon_0(0))})
$$

(7.37)

so that (7.34) can be written as $\varepsilon_{n+1}(0) \geq f(\varepsilon_n(0))$. The function $f(x)$ increases monotonically and is bounded from above, $f(x) \leq \varepsilon_0(0)$. One can also show that $f(x) - x$ decreases monotonically and that its image is $(-\infty, \infty)$. Thus, the equation $f(x_0) - x_0 = 0$ has a unique solution. For a given $\varepsilon_0(\lambda)$ we can now determine $x_0$ from the equation

$$
\varepsilon_0(0) = \int_{-\infty}^{\infty} d\lambda' a_2(0 - \lambda') \ln(e^{x_0} + e^{-(\varepsilon_0(\lambda') - \varepsilon(0))}).
$$

(7.38)

We shall now prove by induction that $\varepsilon_n(0) \geq x_0$ for all $n$. First, one notes that $\varepsilon_0(0) \geq f(x_0) = x_0$. Next, suppose that $\varepsilon_n(0) \geq x_0$. One then has from $\varepsilon_{n+1}(0) \geq f(\varepsilon_n(0))$ and the monotonicity of $f(x)$ that

$$
\varepsilon_{n+1}(0) \geq f(\varepsilon_n(0)) \geq f(x_0) = x_0.
$$

(7.39)

This proves the inequality

$$
\varepsilon_n(\lambda) \geq \varepsilon_0(\lambda) - \varepsilon_0(0) + x_0 \quad \forall \lambda.
$$

(7.40)

Combining this with (7.30), we have proved that the solution of (7.23) can be found by iteration for a symmetric $\varepsilon_0(\lambda)$, which increases monotonically for positive $\lambda$. Consider now a general $\varepsilon_0(\lambda)$ not satisfying these conditions. Since there obviously exists an $\tilde{\varepsilon}_0(\lambda)$ that is symmetric in $\lambda$, increases monotonically for positive $\lambda$ and $\tilde{\varepsilon}_0(\lambda) \leq \varepsilon_0(\lambda)$ for all $\lambda$, it follows from (7.32) that $A[\tilde{\varepsilon}_n(\lambda)] < A[\varepsilon_n(\lambda)]$ for all $n$ and $\lambda$. Hence, $\varepsilon(\lambda)$ is bounded from below as well.

### 7.2.2 Uniqueness of the solution

We can also show that a solution of (7.23) extremizes the generalized free energy, following the lines of [66]. We will also show that this solution is unique.

Consider two solutions of the Bethe equations $\rho_1$ and $\rho_2$. It is clear that $x\rho_1 + (1 - x)\rho_2$ for $0 \leq x \leq 1$ is also a solution. Using this property we can define an action $X(L, \{\beta_n\}, \rho)$ by

$$
X = L \int_{-\infty}^{\infty} d\lambda \left[ \rho(\lambda) \sum_n \beta_n \lambda^n + \rho \ln \rho + \rho_h \ln \rho_h - (\rho + \rho_h) \ln(\rho + \rho_h) \right]
$$

(7.41)
and vary it with respect to $\rho$. Consider $\rho = \rho_0 + x\rho_1$ where $\rho_0$ and $\rho_1$ are two independent solutions satisfying (7.9). The variable $x$ takes real values. We can differentiate the action $X$ with respect to $x$

$$\frac{dX}{dx} = L \int_{-\infty}^{\infty} d\rho_1 \left[ \sum_n \beta_n \lambda^n - \varepsilon(\lambda) - \int_{-\infty}^{\infty} d\lambda a_2(\lambda - \lambda') \ln(1 + e^{-\varepsilon(\lambda')}) \right].$$  \hspace{1cm} (7.42)$$

Next, using (7.24), we can compute

$$\frac{\partial\varepsilon}{\partial x} = \frac{1 + e^{-\varepsilon}}{\rho} \left( \frac{1}{1 + e^\varepsilon} \int_{-\infty}^{\infty} d\lambda a_2(\lambda - \lambda') \rho_1(\lambda') - \rho_1 \right).$$  \hspace{1cm} (7.43)$$

Now,

$$\frac{d^2X}{dx^2} = L \int_{-\infty}^{\infty} d\rho_1(\lambda) \left( -\frac{\partial\varepsilon(\lambda)}{\partial x} + \int_{-\infty}^{\infty} d\lambda' a_2(\lambda - \lambda') \frac{\partial\varepsilon(\lambda)}{\partial x} \right).$$  \hspace{1cm} (7.44)$$

By first performing the integral over $\lambda$ and then using (7.43), this can be simplified as

$$\frac{d^2X}{dx^2} = L \int_{-\infty}^{\infty} d\lambda \left( \frac{\partial\varepsilon(\lambda)}{\partial x} \right)^2 \frac{\rho(\lambda)}{1 + e^{-\varepsilon(\lambda)}} > 0.$$  \hspace{1cm} (7.45)$$

Since this is true for any $\rho$, we conclude that $X$ is convex, hence it has a unique minimum.

### 7.2.3 Thermodynamics

Now that we have established the saddle-point (equilibrium) state we can write down the standard thermodynamic relations. First we write the generalized free energy (7.19) as

$$G = L \int_{-\infty}^{\infty} \left[ \rho(\lambda)(\varepsilon_0(\lambda) - \varepsilon(\lambda)) - (\rho(\lambda) + \rho_h(\lambda)) \ln(1 + e^{-\varepsilon(\lambda)}) \right] d\lambda.$$  \hspace{1cm} (7.46)$$

At the saddle-point we use (7.23) and (7.24) to further simplify the expression

$$G = -\frac{1}{2\pi} L \int_{-\infty}^{\infty} \ln(1 + e^{-\varepsilon(\lambda)}) d\lambda.$$  \hspace{1cm} (7.47)$$

We can easily show that $G$ satisfies the following thermodynamic identities corresponding to the Hellmann-Feynman theorem [182]

$$\frac{\partial G}{\partial \beta_n} = \langle \hat{Q}_n \rangle.$$  \hspace{1cm} (7.48)$$

We first differentiate (7.23) with respect to $\beta_n$

$$\frac{\partial\varepsilon(\lambda)}{\partial \beta_n} = \lambda^n + \int_{-\infty}^{\infty} a_2(\lambda - \mu) \vartheta(\mu) \frac{\partial\varepsilon(\mu)}{\partial \beta_n} d\mu.$$  \hspace{1cm} (7.49)$$
Multiplying both sides with $\rho(\lambda)$ and integrating over $\lambda$ gives
\[
\int_{-\infty}^{\infty} \frac{\partial \epsilon(\lambda)}{\partial \beta_n} \rho(\lambda) d\lambda = \int_{-\infty}^{\infty} \lambda^n \rho(\lambda) d\lambda + \int_{-\infty}^{\infty} \left( \frac{\rho(\mu)}{\vartheta(\mu)} - \frac{1}{2\pi} \right) \frac{\partial \epsilon(\mu)}{\partial \beta_n} \frac{\partial \epsilon(\mu)}{\partial \beta_n} d\mu.
\]
(7.50)

We have used (7.24) in the second term on the right hand side to eliminate the integral over $\lambda$. From this follows the identity
\[
\frac{\partial G}{\partial \beta_n} = \frac{L}{2\pi} \int_{-\infty}^{\infty} \frac{1}{1 + e^{\epsilon(\lambda)}} \frac{\partial \epsilon(\lambda)}{\partial \beta_n} d\lambda = \langle \hat{Q}^2_n \rangle.
\]
(7.51)

For the expectation values $\langle \hat{Q}^2_n \rangle$ we can also define corresponding generalized susceptibilities as
\[
\frac{\partial^2 G}{\partial \beta_n^2} = -\left( \langle \hat{Q}^2_n \rangle - \langle \hat{Q}_n \rangle^2 \right).
\]
(7.52)

Using similar tricks as before, we obtain
\[
\frac{\partial^2 G}{\partial \beta_n^2} = -L \int_{-\infty}^{\infty} \rho(\lambda) e^{\epsilon(\lambda)} \left( \frac{\partial \epsilon(\lambda)}{\partial \beta_n} \right)^2 d\lambda < 0,
\]
(7.53)

which is essentially identical to (7.45). In summary, we can simply state that all the usual equilibrium thermodynamic equations remain unchanged as compared to the usual case, provided one uses the generalized $\epsilon(\lambda)$ and $\rho(\lambda)$ functions.

### 7.2.4 Excitations

In order to study excitations upon the saddle-point state it is instructive to first go back to a state with a finite number $N$ of particles. To a state with quantum numbers $I_j$ corresponds a set of rapidities $\lambda_j$ that satisfy the Bethe equations
\[
\lambda_j L = 2\pi I_j - \sum_{i=1}^{N} \theta(\lambda_j - \lambda_i).
\]
(7.54)

Now we consider an ‘excited’ state with quantum numbers $I_j'$ and the rapidities $\lambda_j'$ satisfying different Bethe equations
\[
\lambda_j' L = 2\pi I_j' - \sum_{i=1}^{N} \theta(\lambda_j' - \lambda_i'),
\]
(7.55)

such that $I_j = I_j'$ except when $j = n$. We make the usual assumption that for all $j \neq n$ the difference between $\lambda_j$ and $\lambda_j'$ is small. One can introduce a shift function $\chi(\lambda)$
\[
(\lambda_j' - \lambda_j)L = \chi(\lambda_j) \quad \text{for} \ j \neq n.
\]
(7.56)

Going back to the thermodynamic limit, one can show using the arguments of Lieb [57] and Yang and Yang [66] that $\chi(\lambda)$ is determined by the following integral equation
\[
\chi(\lambda) = 2\pi \int_{-\infty}^{\infty} a_2(\lambda - \mu)(\chi(\lambda) - \chi(\mu))\rho(\mu) d\mu + \theta(\lambda - \lambda_n) - \theta(\lambda - \lambda_n').
\]
(7.57)
Writing the back-flow as 
\[ g(\lambda) = \chi(\lambda)(\rho(\lambda) + \rho_h(\lambda)), \]
we obtain
\[ g(\lambda) = \int_{-\infty}^{\infty} a_2(\lambda - \mu)g(\mu)\vartheta(\mu)d\mu + \frac{1}{2\pi} (\theta(\lambda - \lambda_n) - \theta(\lambda - \lambda'_n)). \] (7.58)
The momentum difference and energy (as measured from the basic Lieb-Liniger Hamiltonian) difference between the two states are
\[ \Delta P = \sum_j (\lambda'_j - \lambda_j) = \lambda'_n - \lambda_n + \int_{-\infty}^{\infty} g(\lambda)\vartheta(\lambda)d\lambda, \] (7.59)
\[ \Delta E = \sum_j (\lambda'^2_j - \lambda^2_j) = \lambda'^2_n - \lambda^2_n + \int_{-\infty}^{\infty} 2\lambda g(\lambda)\vartheta(\lambda)d\lambda. \] (7.60)

In the case in which the density matrix Hamiltonian does not coincide with the Schrödinger Hamiltonian, we have that \( \Delta E \neq \varepsilon(\lambda'_n) - \varepsilon(\lambda_n) \), therefore \( \varepsilon(\lambda) \) cannot be interpreted as the energy of fundamental excitations anymore, as opposed to the usual case. However, if the Schrödinger Hamiltonian is by definition the generalized Hamiltonian
\[ H = H_{eff} = \sum_n \beta_n \hat{Q}_n, \]
its excitations are
\[ \Delta E_{eff} = \sum_j (\varepsilon_0(\lambda'_j) - \varepsilon_0(\lambda_j)) = \varepsilon_0(\lambda'_n) - \varepsilon_0(\lambda_n) + \int_{-\infty}^{\infty} \frac{d\varepsilon_0(\lambda)}{d\lambda} g(\lambda)\vartheta(\lambda)d\lambda \]
\[ = \varepsilon(\lambda'_n) - \varepsilon(\lambda_n). \] (7.61)

Therefore, \( \varepsilon(\lambda) \) are the excitations of the effective Hamiltonian. As in the usual case, it is straightforward to prove that a finite number of simultaneous excitations is simply the sum of the individual elementary excitations
\[ \Delta P(\{\lambda_{p_j}\}, \{\lambda_{h_j}\}) = \sum_j \Delta P(\lambda_{p_j}, \lambda_{h_j}) \] (7.63)
\[ \Delta E(\{\lambda_{p_j}\}, \{\lambda_{h_j}\}) = \sum_j \Delta E(\lambda_{p_j}, \lambda_{h_j}). \] (7.64)
this relation remaining true provided the density of excitations thus created remains zero in the thermodynamic limit. The whole bulk of knowledge about correlations of the equilibrium Lieb-Liniger gas [65] can thus be easily adapted to the generalized cases.

### 7.2.5 Expectation values

In this section we will show that for a certain class of operators their expectation value in the Generalized Gibbs Ensemble can be computed using only the state \( |\Psi_{gTBA}\rangle \) corresponding to the generalized TBA equation (7.23). More precisely, we will show that
\[ \frac{\text{Tr}\{O(x)e^{-\sum_n \mu_n \hat{Q}_n}\}}{\text{Tr}\{e^{-\sum_n \mu_n \hat{Q}_n}\}} = \frac{\langle \Psi_{gTBA}|O(x)|\Psi_{gTBA}\rangle}{\langle \Psi_{gTBA}|\Psi_{gTBA}\rangle}. \] (7.65)
Consider an eigenstate $|\Psi_N\rangle$ of a finite size system of $N$ particles. For certain operators $O(x)$ (e.g. $n$-point functions of the field operators $\Psi(x)$) one can show that the mean value $\langle \Psi_N | O(x) | \Psi_N \rangle$ in the thermodynamic limit only depends on $\rho(k)$ and $\rho_h(k)$ [65, 176, 178, 177, 183]. This allows us to write a functional integral representation for such correlations similar to the one for the generalized partition function (7.18)

$$\text{Tr}\{O(x)e^{-\sum_n \mu_n \hat{Q}_n}\} = \int D[\rho, \rho_h] \frac{\langle \Psi[\rho] | O(x) | \Psi[\rho] \rangle}{\langle \Psi[\rho] | \Psi[\rho] \rangle} e^{-G[\rho, \rho_h]}$$

When the mean value $\langle \Psi[\rho] | O(x) | \Psi[\rho] \rangle / \langle \Psi[\rho] | \Psi[\rho] \rangle$ is finite, as opposed to $G[\rho, \rho_h]$ which is proportional in $L$, the stationary point of (7.66) coincides with the one of (7.18). Hence, the equality (7.65) follows.

Recently, there has been a lot of progress in computing local correlations of the form

$$g_K = \frac{\langle (\Psi(0)\dagger K \Psi(0) \rangle}{\langle (\Psi(0)\dagger \Psi(0) \rangle^K}$$

These have been obtained as single integral representations, and only involve $\rho(k)$, so it can be applied for solutions of the generalized TBA. For $K = 1, 2, 3, 4$, closed form expressions have been derived [176, 178, 177].

### 7.3 Generalized TBA for an interaction quench

In this section we discuss the generalized TBA in case of an interaction quench (i.e. an instantaneous change of the interaction strength $c$). First, we recall the explicit form of the Hamiltonian in coordinate representation (2.18),

$$H_N = -\sum_{j=1}^N \frac{\partial^2}{\partial x_j^2} + 2c \sum_{j<k} \delta(x_j - x_k).$$

(7.69)

Consider an $N$-particle eigenfunction $\psi_N(x_1, \ldots, x_N)$. In the domain $x_1 < x_2 < \ldots < x_N$, the function $\psi_N$ is also an eigenfunction of the free Hamiltonian,

$$H_0^N = -\sum_{j=1}^N \frac{\partial^2}{\partial x_j^2}.$$  

(7.70)

In the limit when two particles with coordinates $x_j$ and $x_{j+1}$ coincide, the presence of the delta-function potential can be translated into the derivative jump condition (2.21)

$$ \left( \frac{\partial}{\partial x_{j+1}} - \frac{\partial}{\partial x_j} - c \right) \psi_N(x_1, \ldots, x_N) = 0 \quad x_{j+1} = x_j + 0^+.$$  

(7.71)

As discussed in chapter 2, (7.69) is equivalent to (7.70) combined with (7.71). In chapter 3, where we discussed the conserved charges of the Lieb-Liniger model,
we showed that the derivative jump condition (7.71) is the key to having well-defined eigenvalues for the higher conserved charges. More strictly speaking, if we consider a state $φ_N(x_1,\ldots,x_N)$ that does not satisfy the derivative jump condition (7.71), the conserved charges $Q_n$ with $n \geq 3$ are not well-defined. This has some important consequences for quantum quenches.

We prepare the system in an eigenstate $|φ(c_1)\rangle$ of the Lieb-Liniger model with interaction strength $c_1$. For convenience we will consider the ground state, although this is not necessary. We suddenly change the interaction parameter $c_1 \to c_2$ and compute the expectation value of the Hamiltonian after the quench, which we denote by $Q_2(c_2)$

$$\langle φ(c_1)|Q_2(c_2)|φ(c_1)\rangle = \langle φ(c_1)|Q_2(c_1)|φ(c_1)\rangle + (c_2 - c_1) \int_0^L \langle φ(c_1)|Ψ^\dagger(x)Ψ^\dagger(x)Ψ(x)Ψ(x)|φ(c_1)\rangle dx.$$  

(7.72)

The first term is simply the energy before the quench and is by choice a finite energy density multiplied with the volume $L$. The second term is the integrated local $g_2$ correlation function, which was discussed in chapter 6. Since $0 \leq g_2 \leq 2$, the second term is also a finite density multiplied with $L$. We therefore conclude that

$$\langle φ(c_1)|Q_2(c_2)|φ(c_1)\rangle/L = \int_{-∞}^∞ ρ(λ)λ^2 dλ < ∞,$$  

(7.73)

with $ρ(λ)$ the distribution function for the system after the quench. If we now consider expectation values of the higher conserved charges, $\langle φ(c_1)|Q_n(c_2)|φ(c_1)\rangle$, $n > 2$, these are not well-defined values. Since the jump derivative condition is not satisfied, the expectation values are diverging quantity times $L$. For example one can show that

$$\langle φ(c_1)|Q_4(c_2)|φ(c_1)\rangle/L = \int_{-∞}^∞ ρ(λ)λ^4 dλ = ∞.$$  

(7.74)

From the two equations above, we conclude that $ρ(λ) \sim 1/λ^α$ for large $λ$, with $3 < α \leq 5$. We can obtain a tighter bound by realizing that $\langle φ(c_1)|Q_3(c_2)|φ(c_1)\rangle/L$ is formally not well-defined, although one can define it to be a finite quantity, because of the parity of $Q_3$. Therefore, the integral $\int_{-∞}^∞ ρ(λ)λ^3 dλ$ is not absolutely convergent although it might be convergent. Taking this into account we obtain the bound $3 < α \leq 4$. In the case $c_2 = 0$, which is covered in chapter 6, the distribution after the quench is $ρ(k) = ⟨Ψ_k^\daggerΨ_k⟩$. We want to stress that this equation only makes sense in the thermodynamic limit and for $c_2 = 0$. From this we conclude that $α = 4$ in this particular case. Numerically studies, for finite size systems, in the general case also hinted that $α = 4$, however for the thermodynamic limit this has not been proven.

**Consequence of the fat tails**

Although the expectation values of the higher conserved charges $\hat{Q}_n$, $n \geq 3$ are not well defined, one can still have a well defined solution of the generalized TBA equations (7.23) and (7.24). For instance, the case studied in chapter 6 also suffered
from this problem, but we were able to construct a well-defined GGE by considering
the momentum occupation numbers $\Psi_k^\dagger \Psi_k$ instead. However, the algebraic decay,
opposed exponential decay for thermal states, has an important consequence. For
large $\lambda$ we have $\epsilon(\lambda) \sim \epsilon_0(\lambda)$. We also have $\epsilon(\lambda) \sim \ln(\rho(\lambda)) \sim \ln(\lambda^4)$. Therefore,$\epsilon_0(\lambda)$ cannot be a polynomial in $\lambda$ and we need an infinite number of non-zero $\beta_n$ in order to describe the saddle-point state. For this reason, finding $\rho(\lambda)$ straightaway seems the more pragmatic approach.

### 7.4 Generalized TBA for a harmonic chain

In order to illustrate the idea of the generalized TBA approach, we consider a quench for a chain of harmonic oscillators in the thermodynamic limit. In [33], the time-evolution of a 2-point function was computed exactly. By using the fact that the system can be written in terms of free bosons, the GGE could be explicitly constructed by summing over one-particles modes. The GGE was proven rigorously in this case by comparing its prediction for the 2-point function with the time-averaged one. In this section we show that, instead of computing the full trace that appears in the GGE [33], the saddle-point state predicted by the generalized TBA is sufficient to describe the the large time limit of certain correlation functions.

The diagonalized pre-quench Hamiltonian is given by

$$H_0 = \int \frac{dk}{2\pi} \Omega_k^0 A_k^0 A_k^0$$

with the commutation relation $[A_k^0, A_q^\dagger] = 2\pi \delta(k-q)$. A quench $\Omega_k^0 \to \Omega_k$ can be described via a Bogoliubov transformation [33]

$$A_k = c_k A_k^0 + d_k A_k^0 \dagger, \quad A_k^\dagger = c_k A_k^0 \dagger + d_k A_k^0$$

and the post-quench Hamiltonian is simply

$$H = \int \frac{dk}{2\pi} \Omega_k \Omega_k^\dagger A_k^\dagger A_k.$$ 

As initial state we choose the ground state $|\Psi_0\rangle$, which is defined as $A_k |\Psi_0\rangle = 0$. Post-quench expectation values can be computed easily by making use of (7.76)

$$\langle A_k A_q \rangle = c_k d_q \delta(k+q), \quad \langle A_k^\dagger A_q^\dagger \rangle = c_k d_q \delta(k+q),$$

$$\langle A_k A_q^\dagger \rangle = c_k c_q \delta(k-q), \quad \langle A_k^\dagger A_q \rangle = d_k d_q \delta(k-q),$$

where we defined the constants $c_k, d_k$ as

$$c_k = \frac{\Omega_k + \Omega_k^0}{2\sqrt{\Omega_k \Omega_k^0}}, \quad d_k = \frac{\Omega_k - \Omega_k^0}{2\sqrt{\Omega_k \Omega_k^0}}.$$ 

The time evolution after the quench is most easily computed in the Heisenberg picture. For instance, we can write the time-evolution of the field operator $\varphi(x,t)$ as

$$\varphi(x,t) = \int \frac{1}{\sqrt{\pi \Omega_k}} \left(e^{i(kx-\Omega_k t)} A_k + e^{-i(kx-\Omega_k t)} A_k^\dagger\right) dk.$$
We can now straightforwardly compute the time-evolution of the 2-point function after the quench
\[ G(x,t) = \langle \varphi(x,t)\varphi(0,0) \rangle - \langle \varphi(x,0)\varphi(0,0) \rangle = \int \frac{dk}{2\pi} e^{ikx} \left( (\Omega_0^2 - \Omega_k^2)(1 - \cos(2\Omega_k t)) \right). \] (7.82)

In the large time limit, \( t \to \infty \), the cosine averages to zero, so we are simply left with
\[ \lim_{t \to \infty} G(x,t) = \int \frac{dk}{2\pi} e^{ikx} \frac{\Omega_0^2 - \Omega_k^2}{\Omega_k^2 \Omega_0^2}. \] (7.83)

The GGE can be constructed in terms of the conserved charges \( A_k^\dagger A_k \)
\[ \rho_{GGE} = e^{-\int \beta_{eff}(k) A_k^\dagger A_k dk}. \] (7.84)
The partition function for this ensemble is
\[ Z = \prod_k \frac{1}{1 - e^{-\beta_{eff}(k)}}. \] (7.85)
see also section 6.3. The expectation value of \( A_k^\dagger A_k \) is
\[ \text{Tr}\{A_k^\dagger A_k \rho_{GGE}\} = \frac{1}{e^{\beta_{eff}(k)} - 1}. \] (7.86)
Fixing the \( \beta_{eff}(k) \) via the initial conditions \( \langle A_k^\dagger A_k \rangle \) gives
\[ \beta_{eff}(k) = \ln(1 + d_k^{-2}). \] (7.87)
By taking the Fourier-transform of (7.83) one can easily verify it agrees with the prediction of the GGE [33].

**Generalized TBA approach**

In the spirit of the TBA for the Lieb-Liniger model, we define a density function \( \rho(k) \), such that
\[ \rho(k) = \langle A_k^\dagger A_k \rangle / L. \] (7.88)
Using the density function, we can compute the density of particles and the energy density as
\[ N/L = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \rho(k), \] (7.89)
\[ E/L = \int_{-\infty}^{\infty} \frac{dk}{2\pi} \Omega_k \rho(k). \] (7.90)

The microscopic entropy for a state \( \rho(k) \) is given by
\[ S[\rho(k)] = \int_{-\infty}^{\infty} dk (\rho(k) + 1) \ln(\rho(k) + 1) - \rho(k) \ln(\rho(k)). \] (7.91)
We can simply derive this from (7.20) by taking the limit $c \to 0$ and multiplying $\rho(\lambda)$ with $2\pi$. The generalized free energy can now be defined as

$$G[\rho] = \int_{-\infty}^{\infty} dk \beta_{eff}(k) \rho(k) - S[\rho].$$  \hspace{1cm} (7.92)

The partition function can now be written as a functional integral

$$Z = \int \mathcal{D}[\rho] e^{-G[\rho]}.$$  \hspace{1cm} (7.93)

Varying the generalized free energy gives

$$\delta G[\rho] = \int_{-\infty}^{\infty} dk \left( \beta_{eff}(k) - \ln(\rho(k) + 1) + \ln(\rho(k)) \right) \delta \rho(k),$$  \hspace{1cm} (7.94)

leading to the saddle-point condition for the partition function

$$\beta_{eff}(k) = \ln \left( \frac{\rho(k) + 1}{\rho(k)} \right).$$  \hspace{1cm} (7.95)

Since $\rho(k) = d_k^2$ this results in

$$\beta_{eff}(k) = \ln(1 + d_k^{-2}).$$  \hspace{1cm} (7.96)

This agrees with the result found in the previous section, but we would like to emphasize that instead of performing the full trace in the GGE we used a single saddle-point state instead. As an example we consider a mass quench for a relativistic model: $\Omega_0 k = \sqrt{m_0^2 + k^2} \to \Omega k = \sqrt{m^2 + k^2}$. For this quench, $\rho(k)$ is in the limit of large $k$

$$\rho(k) = \frac{(m^2 - m_0^2)^2}{(2k)^4} + O\left( \frac{1}{k^6} \right).$$  \hspace{1cm} (7.97)

Note that both for this quench and the interaction quench for the Lieb-Liniger model the distribution decays algebraically.

### 7.5 Conclusion

When considering the GGE for a fully interacting system, the partition function typically does not factorize, unlike for (effectively) free models. For a finite system this implies that one has to perform the trace in the GGE by summing over all eigenstates. This summation is of the same complexity as constructing the diagonal ensemble and therefore makes the GGE superfluous. In the thermodynamic limit, as one expects from ordinary statistical mechanics, the analysis of the GGE drastically simplifies. Using the generalized TBA equations we showed that the saddle-point state is sufficient for most computations. Furthermore, one can also think of the generalized TBA as a tool to study excited states of an effective Hamiltonian, which can be constructed by a (possibly finite) set $\beta_{n}$.

Although we have concentrated on the Lieb-Liniger model and the harmonic chain, similar reasonings are (almost trivially) transportable to other models. The
generalization of generic TBA equations (with strings, nested, etc.) is straightforward since only the basic driving function (bare energy) needs to be modified. In cases other than the repulsive Lieb-Liniger model however, proving existence and uniqueness becomes even more intractable than in the traditional case, although explicit solutions can easily be found in practice.