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Master's Thesis

Exact Dynamics of Interacting Bose Gases in One Spatial Dimension

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Abstract

Ultracold atomic gases in one dimension are often described using the Lieb-Liniger model of interacting bosons. The model is exactly solvable using techniques of integrability and the Bethe Ansatz. In the repulsive regime, it describes a strongly correlated quantum gas with finite compressibility. In the attractive regime, the model exhibits additional richness in the form of bound states of constituent particles. The unique combination of experimental feasibility and exact theoretical solvability, as well as the possibility to compare the exact theory with various effective approaches, make the Lieb-Liniger model an extraordinary platform to study the many-body physics of strongly correlated systems. The thesis investigates the dynamical properties of the model in both the attractive and repulsive regimes, by constructing particular solutions of the quantum theory that are the analogue classical solitons. Therefore extensive comparisons are made between the exact results of the quantum theory and those of the related mean field theory. A detailed discussion of the ground state and the excitation spectrum of the system, using a combination of exact and effective approaches, contributes to this main objective.

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Contents

Introduction

The experimental realization of ultracold quasi-one-dimensional atomic gases in optical lattices, obtained by confining three-dimensional Bose-Einstein condensates in a long cylindrical shape (Fig. 1), see e.g. Görlitz et al. (2001); Greiner et al. (2001); Moritz et al. (2003); Paredes et al. (2004); Kinoshita et al. (2004), has renewed the interest in the rather idealized theoretical model of interacting bosons in one dimension, known as the Lieb-Liniger model (Lieb and Liniger, 1963; Lieb, 1963). Rigorous analyses of the many-body Schrödinger equation indeed show that the low-energy states of such cylindrical atomic gases are described by the Lieb-Liniger model[1] (Lieb et al., 2003; Seiringer and Yin, 2008).

Quantum physics in one dimension is very peculiar. In higher dimensions, quantum many-body systems can only be described perturbatively, namely starting from the free theory and summing a series of contributions coming from the expansion of the interaction terms, or by mean field techniques. In one dimension, there are methods for treating interacting systems in a completely non-perturbative way. The Lieb-Liniger model, in particular, belongs to a class of one-dimensional models that are exactly solvable via a technique called Bethe Ansatz, which was originally introduced by Bethe to treat exactly the nearest-neighbor interactions of the Heisenberg XXX spin chain (Bethe, 1931). These exactly solvable models have the special property that a single interaction between multiple particles can be described as multiple interaction between just two particles. In this way, the Bethe Ansatz is able to turn the time-independent Schrödinger equation into a system of algebraic equations (the Bethe equations) involving sets of complex numbers (the rapidities) which uniquely identify the eigenstates of the Hamiltonian. This property can be considered the distinctive feature of quantum integrable systems, although (unlike in the classical world) there is not yet a universally accepted definition of quantum integrability (Caux and Mossel, 2011).

The unique combination of experimental feasibility and exact theoretical solvability, as well as the possibility to compare the exact theory with various effective approaches, make the Lieb-Liniger model an extraordinary platform for studying the interplay between theory and experiment and between different theoretical descriptions. From the theory perspective, the purely one-dimensional case can also serve as a basis for the investigation of effects beyond the mean field in higher dimensions.

This thesis is centered around the study of a specific phenomenon within the Lieb-Liniger model, namely the existence of particular states representing the quantum analogue of soliton solutions in classical field theories. We will perform this study in both the attractive and repulsive interaction regimes, where the underlying physics is markedly different, and carry out extensive analyses of the relationship between the exact 'quantum' solutions of the model and the 'classical' solutions of the related mean field theory.

The contents are organized as follows. In Chapter 1 we present the Lieb-Liniger model and its exact solution via the Bethe Ansatz, following the original treatment of Lieb and Liniger, both in the attractive and repulsive cases. In Chapter 2 we study in detail the

[1] The cylinder does not have to be as narrow as the atomic diameter; it can be much wider if the excitation energy in the direction orthogonal to the axis is large compared to the energy per particle.

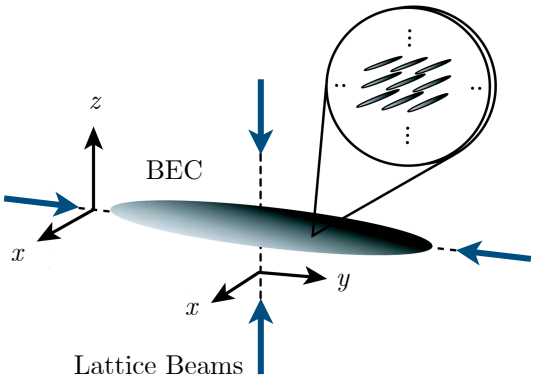


Figure 1: A 2D lattice potential is formed by overlapping two optical standing waves along the y axis and the z axis with a Bose-Einstein condensate in a magnetic trap. The condensate is then confined to an array of several thousand narrow potential tubes (inset). Adapted from Greiner et al. (2001).

ground state of the attractive model, deriving in particular its density profile, and compare the exact result with that obtained from the mean field theory. We will see that the ground state is represented by a bright soliton at rest, namely a localized density peak. In Chapter 3 we construct single and double quantum bright solitons as superpositions of exact eigenstates of the attractive model; we study their stability under time evolution and their scattering properties by exploiting general results of scattering theory in one dimension and the knowledge of the exact scattering phase shifts obtained from the Bethe Ansatz. We compare the exact results with those for the scattering of bright solitons within the mean field theory.

In Chapter 4 we turn to the repulsive model, studying the ground state and the elementary excitations using a combination of exact and effective approaches. We will show that hole-like excitations of the model can be identified (to some extent) with dark soliton solutions of the corresponding mean field theory. This motivates the search for quantum dark solitons built from superpositions of hole-like excited states. In Chapter 5 we thus present the construction of such quantum dark solitons and study their time evolution, discussing how to improve their stability.

Chapter 1

The Lieb-Liniger model

1.1 Interacting bosons in one dimension

The subject of this work is a system of N spinless bosons in one-dimensional (1D) space, interacting via an ultra-local delta function potential. The Hamiltonian is

$$H^{(N)} = -\frac{\hbar^2}{2m}\sum_{j=1}^{N}\partial_{x_j}^2 + 2c\sum_{i<j}\delta(x_i - x_j) \tag{1.1}$$

where m is the mass of the particles and c is the interaction coupling. A positive value of c denotes repulsive interaction, whereas a negative value of c corresponds to attractive interaction. As mentioned in the Introduction, such a system can be experimentally realized by applying a strong transverse confinement to a 3D ultracold atomic gas. It is then useful to relate the 1D interaction strength $g_{1\mathrm{D}} = 2c$ to that of the analogous three-dimensional model, that is $g_{3\mathrm{D}} = 4\pi\hbar^2 a_s/m$, where a_s is the s-wave scattering length (Landau and Lifshitz, 1980). The coupling c can be expressed in terms of an effective 1D scattering length $a_{1\mathrm{D}}$ as $c = -\hbar^2/ma_{1\mathrm{D}}$. Introducing the characteristic length of the transverse confinement $a_\perp = \sqrt{\hbar/m\omega_\perp}$, where $\omega_\perp$ is the frequency of the confinement, for $a_s \ll a_\perp$ one has the identification $a_{1\mathrm{D}} = -a_\perp^2/a_s$. When the above condition is not satisfied, $a_{1\mathrm{D}}$ should be properly renormalized, taking the value $a_{1\mathrm{D}} = -a_\perp(a_\perp/a_s - C)$, where $C = |\zeta(1/2)|/\sqrt{2} \simeq 1.0326$, and $\zeta(z)$ is the Riemann zeta function (Olshanii, 1998; Cazalilla et al., 2011). The resonant behavior of c as $a_\perp/a_s \to C$ is called confinement-induced resonance. Positive values of c, corresponding to negative values of $a_{1\mathrm{D}}$ and repulsive interaction, are only obtained in the interval $0 < a_s < a_\perp/C$.

The second-quantized version of the Hamiltonian (1.1) is

$$\hat{H} = \int dx \left[\hat{\psi}^\dagger(x)\left(-\frac{\hbar^2\partial_x^2}{2m}\right)\hat{\psi}(x) + c\,\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x)\right] \tag{1.2}$$

where $\hat{\psi}(x)$ and its adjoint $\hat{\psi}^\dagger(x)$ are bosonic field operators satisfying the canonical commutation relations

$$\left[\hat{\psi}(x),\, \hat{\psi}^\dagger(y)\right] = \delta(x-y), \qquad \left[\hat{\psi}(x),\, \hat{\psi}(y)\right] = 0. \tag{1.3}$$

The Heisenberg equation of motion for the field operator $\hat{\psi}(x,t) = \mathrm{e}^{-it\hat{H}/\hbar}\hat{\psi}(x)\mathrm{e}^{it\hat{H}/\hbar}$ is then

$$i\hbar\,\partial_t\hat{\psi}(x,t) = \mathrm{e}^{-it\hat{H}/\hbar}\left[\hat{\psi}(x),\, \hat{H}\right]\mathrm{e}^{it\hat{H}/\hbar} = \left(-\frac{\hbar^2\partial_x^2}{2m} + 2c\,\hat{\psi}^\dagger(x,t)\hat{\psi}(x,t)\right)\hat{\psi}(x,t). \tag{1.4}$$

The particle number and total momentum operators,

$$\hat{N} = \int dx\,\hat{\psi}^\dagger(x)\hat{\psi}(x), \qquad \hat{P} = -i\hbar\int dx\,\hat{\psi}^\dagger(x)\partial_x\hat{\psi}(x), \tag{1.5}$$

commute with the Hamiltonian, $[\hat{N}, \hat{H}] = 0$ and $[\hat{P}, \hat{H}] = 0$, giving us the two simplest conservation laws. There exist also higher-order conservation laws (Davies, 1990).

Hereafter we shall focus on the N-particle sector of the Fock space of the quantum field theory defined by Eq. (1.2). The N-particle eigenstates $|\,\Psi_N\,\rangle$ of $\hat{H}$ can be parametrized in terms of complex-valued wavefunctions $\Psi_N(x_1, \ldots, x_N)$ as

$$|\,\Psi_N\,\rangle = \int dx_1 \cdots dx_N\, \Psi_N(x_1, \ldots, x_N) \hat{\psi}^\dagger(x_1) \ldots \hat{\psi}^\dagger(x_N) |\,0\,\rangle, \tag{1.6}$$

$|\,0\,\rangle$ being the normalized Fock vacuum defined by $\hat{\psi}(x)|\,0\,\rangle = 0$. The Bose statistics imposes that the wavefunctions are completely symmetric in the exchange of positions. Projecting onto the position basis, the eigenvalue problem for $\hat{H}$ is then given by the time-independent Schrödinger equation

$$H^{(N)} \Psi_N(x_1, \ldots, x_N) = E_N \Psi_N(x_1, \ldots, x_N). \tag{1.7}$$

For convenience, from now on we choose units such that $\hbar = 1$ and $2m = 1$, thus obtaining the Lieb-Liniger Hamiltonian

$$H^{(N)} = \sum_{j=1}^{N} -\partial_{x_j}^2 + 2c \sum_{i<j} \delta\left(x_i - x_j\right). \tag{1.8}$$

In the next section we present the exact solution of the Schrödinger equation for such Hamiltonian, first obtained by Lieb and Liniger (1963), and subsequently deepened by Yang (1967, 1968) and Sutherland (1968), based on the Bethe Ansatz. Our treatment follows mainly Caux (2023).

1.2 Exact eigenstates

Let us begin with the $N = 2$ case, for which the Schrödinger equation is

$$\left[-\partial_{x_1}^2 - \partial_{x_2}^2 + 2c\,\delta(x_1 - x_2) - E_2\right] \Psi_2(x_1, x_2) = 0, \tag{1.9}$$

with $(x_1, x_2) \in \mathbb{R}^2$. For $x_1 \neq x_2$ the interaction term vanishes and the eigenfunctions should be given by plane waves. For $x_1 = x_2$, however, the delta function brings a discontinuity in the first derivative of the wavefunction $\Psi_2(x_1, x_2)$ evaluated at $x_2 - x_1 = 0^+$, so that[1]

$$\left(\partial_{x_2} - \partial_{x_1} - c\right) \Psi_2(x_1, x_2)\Big|_{x_2 - x_1 = 0^+} = 0. \tag{1.10}$$

To explicitly solve the Schrödinger equation, we restrict to a fundamental open domain $D_2 : x_1 < x_2$ with boundary $\partial D_2 : x_2 - x_1 = 0^+$. The restriction of Eq. (1.9) to D_2 is

$$\left(-\partial_{x_1}^2 - \partial_{x_2}^2 - E_2\right) \Psi_2(x_1, x_2)\Big|_{(x_1, x_2) \in D_2} = 0 \tag{1.11}$$

and is simply solved in terms of free waves, $\mathrm{e}^{i(\lambda_1 x_1 + \lambda_2 x_2)}$ and $\mathrm{e}^{i(\lambda_2 x_1 + \lambda_1 x_2)}$, for λ_1, λ_2 generic complex numbers representing quasimomenta. These plane wave solutions have total energy and total momentum

$$E_2 = \lambda_1^2 + \lambda_2^2, \qquad P_2 = \lambda_1 + \lambda_2. \tag{1.12}$$

[1] This can be seen by rewriting the Schrödinger equation (1.9) using the coordinates $x_+ = \frac{1}{2}(x_1 + x_2)$ and $x_- = x_1 - x_2$, so that $[-\partial_{x_-}^2 + 2c\,\delta(x_-) - E_2]\Psi_2 = 0$, and integrating over $x_- \in [-\epsilon, \epsilon]$ for $\epsilon \to 0^+$. This yields the condition

$$-\frac{1}{2}(\partial_{x_1} - \partial_{x_2})\Psi_2\Big|_{x_1 - x_2 = -0^+}^{x_1 - x_2 = 0^+} + c\Psi_2\Big|_{x_1 = x_2} = 0,$$

which, with the symmetry of the bosonic wavefunction, $\Psi_2(x_1, x_2) = \Psi_2(x_2, x_1)$, leads to Eq. (1.10).

Therefore we look for a solution in the form

$$\Psi_2(x_1,x_2|\lambda_1,\lambda_2)\Big|_{(x_1,x_2)\in D_2} = A_1 \mathrm{e}^{i(\lambda_1 x_1+\lambda_2 x_2)} + A_2 \mathrm{e}^{i(\lambda_2 x_1+\lambda_1 x_2)} \tag{1.13}$$

for some complex amplitudes A_1, A_2. By imposing to Eq. (1.13) the boundary condition (1.10), we obtain the following relation between the two amplitudes,

$$\frac{A_2}{A_1} = -\frac{c+i(\lambda_1-\lambda_2)}{c-i(\lambda_1-\lambda_2)} = -\mathrm{e}^{i\phi(\lambda_1-\lambda_2)}, \tag{1.14}$$

where we have defined the scattering phase shift

$$\phi(\lambda) = \frac{1}{i}\ln\left(\frac{c+i\lambda}{c-i\lambda}\right). \tag{1.15a}$$

If λ is real, ϕ takes the form

$$\phi(\lambda) = 2\arctan\left(\frac{\lambda}{c}\right). \tag{1.15b}$$

Hence we rewrite the wavefunction (up to an overall phase and a normalization factor) as

$$\Psi_2(x_1,x_2|\lambda_1,\lambda_2)\Big|_{(x_1,x_2)\in D_2} = \mathrm{e}^{i(\lambda_1 x_1+\lambda_2 x_2)-\frac{i}{2}\phi(\lambda_1-\lambda_2)} - \mathrm{e}^{i(\lambda_2 x_1+\lambda_1 x_2)+\frac{i}{2}\phi(\lambda_1-\lambda_2)}. \tag{1.16}$$

Since $\phi(-\lambda) = -\phi(\lambda)$, the wavefunction is symmetric in coordinates and antisymmetric in quasimomenta. In particular, for $\lambda_1 = \lambda_2$ it identically vanishes, and does not represent a good eigenstate. Without prejudice to this property, we may as well make our wavefunction symmetric under quasimomenta exchange by multiplying it by $\mathrm{sgn}(\lambda_2-\lambda_1)$. We can then extend the domain of validity of this form to all $(x_1,x_2)\in\mathbb{R}^2$ by imposing total symmetry under coordinate exchange. This gives

$$\begin{aligned}\Psi_2(x_1,x_2|\lambda_1,\lambda_2) &= \mathrm{sgn}(x_2-x_1)\mathrm{sgn}(\lambda_2-\lambda_1)\\ &\quad\times\sum_{Q\in\pi_2}(-1)^{[Q]}\exp\left(i\lambda_{Q_1}x_1+i\lambda_{Q_2}x_2-\frac{i}{2}\mathrm{sgn}(x_2-x_1)\phi(\lambda_{Q_1}-\lambda_{Q_2})\right),\end{aligned} \tag{1.17}$$

where π_2 is the group of permutations of two objects and $[Q]$ denotes the parity of Q.

The above construction is directly generalizable to N particles by defining the fundamental open domain $D_N : x_1 < x_2 < \cdots < x_N$ with boundaries $\partial_j D_N : x_{j+1} - x_j = 0^+$, where the Schrödinger equation (1.7) is equivalent to

$$\left(\sum_{j=1}^N -\partial_{x_j}^2 - E_N\right)\Psi_N(\mathbf{x})\Big|_{\mathbf{x}\in D_N} = 0, \qquad \left(\partial_{x_{j+1}}-\partial_{x_j}-c\right)\Psi_N(\mathbf{x})\Big|_{\mathbf{x}\in\partial_j D_N} = 0, \tag{1.18}$$

with $\mathbf{x} = (x_1,\ldots,x_N)$. In this domain, the solution is

$$\Psi_N(\mathbf{x}|\boldsymbol{\lambda})\Big|_{\mathbf{x}\in D_N} = \sum_{Q\in\pi_N} A_Q \exp\left(i\sum_{j=1}^N \lambda_{Q_j}x_j\right), \tag{1.19}$$

with $\boldsymbol{\lambda} = (\lambda_1,\ldots,\lambda_N)$, and the boundary conditions impose the relations among the A_Q's (cf. Eq. (1.14)),

$$A_{Q'} = \frac{\lambda_{Q_{j+1}}-\lambda_{Q_j}+ic}{\lambda_{Q_{j+1}}-\lambda_{Q_j}-ic}A_Q, \tag{1.20}$$

where Q' is the permutation obtained from Q by interchanging the jth and $(j+1)$th components. We can then extend this solution to the region of $\mathbb{R}^N$ in which at most two coordinates exactly coincide, obtaining the Bethe wavefunction

$$\Psi_N(\mathbf{x}|\boldsymbol{\lambda}) = \prod_{N\geq j\geq k\geq 1} \mathrm{sgn}(x_j - x_k)\mathrm{sgn}(\lambda_j - \lambda_k)$$
$$\times \sum_{Q\in\pi_N} (-1)^{[Q]} \exp\left(i\sum_{j=1}^{N} \lambda_{Q_j} x_j + \frac{i}{2} \sum_{N\geq j\geq k\geq 1} \mathrm{sgn}(x_j - x_k)\phi(\lambda_{Q_j} - \lambda_{Q_k}) \right). \quad (1.21)$$

We notice that Bethe wavefunction is a superposition of plane waves labeled by internal quasimomenta (also called rapidities), the relative amplitude of each plane wave being determined by the scattering phase shift characteristic of the two-body interaction. The rapidities obey a sort of Pauli exclusion principle, so that the wavefunction identically vanishes if two rapidities coincide.

1.3 Bethe equations

Until now we have considered our system as being defined on the whole real line. In this case the quasimomenta could in principle assume any value. In order to have a discrete set of eigenstates we introduce a finite quantization length by putting the system on an interval of length L and imposing periodic boundary conditions (equivalently, we put the system on a ring of circumference L). Starting again with the $N = 2$ case, the periodicity conditions read

$$\Psi_2(x_1 + L, x_2|\lambda_1, \lambda_2) = \Psi_2(x_1, x_2 + L|\lambda_1, \lambda_2) = \Psi_2(x_1, x_2|\lambda_1, \lambda_2). \quad (1.22)$$

Taking for instance the first of these conditions and using the symmetry of the wavefunction, we have

$$\Psi_2(x_2, x_1 + L|\lambda_1, \lambda_2) = \Psi_2(x_1, x_2|\lambda_1, \lambda_2). \quad (1.23)$$

Imposing this condition to Eq. (1.17) yields the quantization conditions for the rapidities,

$$\mathrm{e}^{i\lambda_1 L} = -\mathrm{e}^{-i\phi(\lambda_1-\lambda_2)}, \qquad \mathrm{e}^{i\lambda_2 L} = -\mathrm{e}^{i\phi(\lambda_1-\lambda_2)}, \quad (1.24)$$

or

$$\mathrm{e}^{i\lambda_1 L} = \frac{\lambda_1 - \lambda_2 + ic}{\lambda_1 - \lambda_2 - ic}, \qquad \mathrm{e}^{i\lambda_2 L} = \frac{\lambda_2 - \lambda_1 + ic}{\lambda_2 - \lambda_1 - ic}. \quad (1.25)$$

These are the Bethe equations for the two-particle Lieb-Liniger model. In view of state classification, it is more convenient to take the logarithm of Eqs. (1.24),

$$\lambda_1 + \frac{1}{L}\phi(\lambda_1 - \lambda_2) = \frac{2\pi}{L} I_1, \qquad \lambda_2 + \frac{1}{L}\phi(\lambda_2 - \lambda_1) = \frac{2\pi}{L} I_2, \quad (1.26)$$

with $I_j \in \mathbb{Z} + \frac{1}{2}$, $j = 1, 2$, taking the role of quantum numbers of the theory. Notice that taking the product of Eqs. (1.24), or equivalently, taking the sum of Eqs. (1.26), we obtain

$$\mathrm{e}^{i(\lambda_1+\lambda_2)L} = 1, \qquad \text{or} \qquad \lambda_1 + \lambda_2 = \frac{2\pi I}{L}, \qquad I \in \mathbb{Z}, \quad (1.27)$$

that is the quantization condition for the total momentum of $\Psi_2(x_1, x_2|\lambda_1, \lambda_2)$.

The above considerations generalize to an arbitrary number N of particles. The periodicity conditions, combined with the symmetry of the wavefunction, give

$$\Psi_N(x_1, \ldots, x_{j-1}, x_{j+1}, \ldots, x_N, x_j + L|\boldsymbol{\lambda}) = \Psi_N(x_1, \ldots, x_{j-1}, x_j, x_{j+1}, \ldots, x_N|\boldsymbol{\lambda}) \quad (1.28)$$

for $j = 1, \dots, N$, which lead to the Bethe equations

$$e^{i\lambda_j L} = (-1)^{N-1} e^{-i\sum_{k=1}^{N}\phi(\lambda_j-\lambda_k)} = \prod_{k\neq j} \frac{\lambda_j - \lambda_k + ic}{\lambda_j - \lambda_k - ic} \tag{1.29}$$

or in log-form

$$\lambda_j + \frac{1}{L}\sum_{k=1}^{N}\phi(\lambda_j - \lambda_k) = \frac{2\pi}{L} I_j, \qquad I_j \in \begin{cases} \mathbb{Z} + \frac{1}{2}, & N \text{ even}, \\ \mathbb{Z}, & N \text{ odd}. \end{cases} \tag{1.30}$$

Proof. We have $e^{i\lambda_j L} = (-1)^{N-1} e^{-i\sum_{k=1}^{N}\phi(\lambda_j-\lambda_k)} = e^{i\pi(N-1)-i\sum_{k=1}^{N}\phi(\lambda_j-\lambda_k)}$, that gives

$$\lambda_j L - \pi(N-1) + \sum_{k=1}^{N}\phi(\lambda_j - \lambda_k) = 2\pi n_j, \qquad n_j \in \mathbb{Z}.$$

Bringing the factor $\pi(N-1)$ to the right-hand side we obtain Eq. (1.30) with $I_j = n_j + (N-1)/2$. Therefore I_j is half-integer for N even and integer for N odd. □

A complete set of eigenstates is obtained by choosing all proper sets of quantum numbers and constructing their associated Bethe wavefunctions. As can be seen from Eq. (1.21), the eigenstate parameterized by the set of rapidities $\{\lambda_1, \dots, \lambda_N\}$ has total energy and total momentum

$$E_N = \sum_{j=1}^{N}\lambda_j^2, \qquad P_N = \sum_{j=1}^{N}\lambda_j. \tag{1.31}$$

The closure relation, orthogonality and normalizability of Bethe states has been show by Gaudin (2014, 1971a,b) and Dorlas (1993).

1.4 Attractive interaction

We now specialize the general results above to attractive interaction ($c < 0$), characterizing the ground state and the excited states of the Lieb-Liniger model in this regime.

1.4.1 String solutions

Let us introduce $\bar{c} = -c > 0$ as the interaction parameter, and rewrite Eq. (1.29) as

$$e^{i\lambda_\alpha L} = \prod_{\beta\neq\alpha} \frac{\lambda_\alpha - \lambda_\beta - i\bar{c}}{\lambda_\alpha - \lambda_\beta + i\bar{c}}. \tag{1.32}$$

for $\alpha, \beta = 1, \dots, N$. For a complex rapidity $\lambda_\alpha = \mu_\alpha + i\eta_\alpha$, where $\mu_\alpha \equiv \operatorname{Re}\lambda_\alpha$ and $\eta_\alpha \equiv \operatorname{Im}\lambda_\alpha$, the Bethe equation is

$$e^{i\mu_\alpha L - \eta_\alpha L} = \prod_{\beta\neq\alpha} \frac{\mu_\alpha + i(\eta_\alpha - \bar{c}) - \lambda_\beta}{\mu_\alpha + i(\eta_\alpha + \bar{c}) - \lambda_\beta}. \tag{1.33}$$

Now suppose to take the infinite volume limit, $L \to \infty$, while keeping the number of particles N fixed. If $\eta_\alpha > 0$, the left-hand side goes to zero as $O(e^{-\eta_\alpha L})$. The equality implies that there must be a λ_β such that $\lambda_\beta = \mu_\alpha + i(\eta_\alpha - \bar{c}) + O(e^{-\eta_\alpha L})$. On the other hand, if $\eta_\alpha < 0$ the left-hand side goes to infinity as $O(e^{|\eta_\alpha| L})$, and there must be a rapidity λ_β such that $\lambda_\beta = \mu_\alpha + i(\eta_\alpha + \bar{c}) + O(e^{-|\eta_\alpha| L})$. Thus we see that in the attractive case rapidities arrange themselves into clusters in the complex plane, the elements of each cluster being evenly spaced by $\bar{c}$ in the imaginary direction. Such clusters are called strings and represent bound states of particles.

To give a clearer physical picture, let us consider just two particles, and thus two rapidities λ_1 and λ_2. We parametrize the first one as $\lambda_1 = \mu_1 + i\eta_1$, up to deviations exponentially small in system size. Assuming for instance that $\eta_1 > 0$, the Bethe equations are solved by $\lambda_2 = \mu_1 + i(\eta_1 - \bar{c})$. To have a real energy eigenvalue $E_2 = \lambda_1^2 + \lambda_2^2$, it must be $\lambda_2 = \lambda_1^*$, that gives $\eta_1 = \bar{c}/2$. Introducing the simplified notation $\lambda = \mu_1$, the two rapidities are then

$$\lambda_1 = \lambda + i\frac{\bar{c}}{2} + O(\mathrm{e}^{-\bar{c}L/2}), \qquad \lambda_2 = \lambda - i\frac{\bar{c}}{2} + O(\mathrm{e}^{-\bar{c}L/2}). \tag{1.34}$$

Assuming that $\eta_1 < 0$ one would have found $\eta_1 = -\bar{c}/2$, which simply leads to an exchange of labels of the rapidities. Using $\lambda_1 - \lambda_2 = i\bar{c} + O(\mathrm{e}^{-\bar{c}L/2})$, we can now evaluate the relation (1.14) between the two amplitudes of the Bethe wavefunction,

$$A_1 = \frac{\lambda_1 - \lambda_2 - i\bar{c}}{\lambda_1 - \lambda_2 + i\bar{c}} A_2 = O(\mathrm{e}^{-\bar{c}L/2}) \simeq 0. \tag{1.35}$$

Hence the Bethe wavefunction in the fundamental domain $x_1 < x_2$ is

$$\Psi_2(x_1, x_2) = A_2\, \mathrm{e}^{i\lambda(x_1+x_2)} \mathrm{e}^{-\frac{\bar{c}}{2}(x_2-x_1)} \tag{1.36a}$$

and it can be extended to all $(x_1, x_2) \in \mathbb{R}^2$ by writing

$$\Psi_2(x_1, x_2) = \mathcal{N}_2\, \mathrm{e}^{i\lambda(x_1+x_2)} \mathrm{e}^{-\frac{\bar{c}}{2}|x_2-x_1|} \tag{1.36b}$$

where $\mathcal{N}_2$ is a normalization constant. The first term represents a free wave for the center of mass, while the second term brings an exponential suppression in the separation between the two particles. The wavefunction thus represents a bound state of two particles (2-string), with binding length $2/\bar{c}$. Eq. (1.27) gives $\mathrm{e}^{2i\lambda L} = 1$, which means that λ, the 'center' of the 2-string, is quantized as the total momentum P of a single 'collective' particle, with $P = 2\lambda$.

For a given number of atoms N, we can construct eigenstates with fixed string content by partitioning N into N_j strings of integer length $j \in [1, N]$, the length of a string being defined as the number of rapidities within it. Denoting the total number of strings as M_s, we have

$$N = \sum_j j N_j, \qquad M_s = \sum_j N_j. \tag{1.37}$$

We will parametrize string rapidities as

$$\lambda_\alpha^{j,a} = \lambda_\alpha^j + i\frac{\bar{c}}{2}(j + 1 - 2a) + i\delta_\alpha^{j,a} \tag{1.38}$$

where j is the string length, $\alpha = 1, \ldots, N_j$ identifies the j-string under consideration and $a = 1, \ldots, j$ is the internal index labeling rapidities within the string (Calabrese and Caux, 2007). Here $\delta_\alpha^{j,a} \sim \mathrm{e}^{-(\text{const.})L}$ are exponentially small deviations in system size. In general the string deviations $\delta_\alpha^{j,a}$ are complex numbers, and depend sensitively on the particular boundary conditions used, with the constraint that the full set of rapidities $\{\lambda_\alpha^{j,a}\}$ remains self-conjugate so that the energy eigenvalue is real. Perfect strings (i.e. with all $\delta_\alpha^{j,a} = 0$) are exact eigenstates in the limit $L \to \infty$ with $N_s/L \to 0$ for arbitrary N. It is then natural to consider the limit $L \to \infty$ at fixed N, in which the deviations can be dropped. Notice that this is different from the usual thermodynamic limit, that corresponds to taking $N, L \to \infty$ at fixed density N/L. Here, despite N remaining finite, taking $L \to \infty$ does not trivialize the physics, as the N particles remain strongly correlated and bound to one another (we will return on this in Section 1.4.5, where we discuss the norm of a string state). These string states should be viewed as individual particles of mass j, with energy and momentum of the string centered on λ_α^j given by

$$E_{(j,\alpha)} = \sum_{a=1}^{j} (\lambda_\alpha^{j,a})^2 = j(\lambda_\alpha^j)^2 - \frac{\bar{c}^2}{12} j(j^2 - 1), \qquad P_{(j,\alpha)} = \sum_{a=1}^{j} \lambda_\alpha^{j,a} = j\lambda_\alpha^j. \tag{1.39}$$

1.4.2 Bethe equations for strings

The Bethe equations (1.32) are written in terms of the string parametrization (1.38) as

$$\begin{aligned}
\mathrm{e}^{i\lambda_\alpha^{j,a}L} &= \prod_{(k,\beta,b)\neq(j,\alpha,a)} \frac{\lambda_\alpha^{j,a}-\lambda_\beta^{k,b}-i\bar{c}}{\lambda_\alpha^{j,a}-\lambda_\beta^{k,b}+i\bar{c}} \\
&= \prod_{(k,\beta,b)\neq(j,\alpha,a)} \frac{\lambda_\alpha^{j}-\lambda_\beta^{k}+i\bar{c}\big(\frac{j-k}{2}-a+b-1\big)+i\delta_\alpha^{j,a}-i\delta_\beta^{k,b}}{\lambda_\alpha^{j}-\lambda_\beta^{k}+i\bar{c}\big(\frac{j-k}{2}-a+b+1\big)+i\delta_\alpha^{j,a}-i\delta_\beta^{k,b}} \\
&= \prod_{(k,\beta)\neq(j,\alpha)} \prod_{b=1}^{k} \frac{\lambda_\alpha^{j}-\lambda_\beta^{k}+i\bar{c}\big(\frac{j-k}{2}-a+b-1\big)}{\lambda_\alpha^{j}-\lambda_\beta^{k}+i\bar{c}\big(\frac{j-k}{2}-a+b+1\big)} \prod_{\substack{a'=1\\a'\neq a}}^{j} \frac{\bar{c}(-a-a'-1)+\delta_\alpha^{j(a,a')}}{\bar{c}(-a-a'+1)+\delta_\alpha^{j(a,a')}}
\end{aligned} \tag{1.40}$$

where we have separated the product into inter-string, $(k,\beta)\neq(j,\alpha)$, and intra-string, $(k,\beta)=(j,\alpha)$, parts, dropped all string deviations for inter-string factors, and introduced the notation $\delta_\alpha^{j,(a,a')}=\delta_\alpha^{j,a}-\delta_\alpha^{j,a'}$ for the differences in the intra-string deviations. These equations can be simplified by taking the product within the string considered. The left-hand side becomes

$$\prod_{a=1}^{j} \mathrm{e}^{i\lambda_\alpha^{j,a}L} = \mathrm{e}^{i\sum_{a=1}^{j}\lambda_\alpha^{j,a}L} = \mathrm{e}^{ij\lambda_\alpha^{j}L}. \tag{1.41}$$

On the right-hand side, the intra-string part gives

$$\prod_{a=1}^{j}\prod_{\substack{a'=1\\a'\neq a}}^{j} \frac{\bar{c}(-a-a'-1)+\delta_\alpha^{j(a,a')}}{\bar{c}(-a-a'+1)+\delta_\alpha^{j(a,a')}} = (-1)^{j(j+1)} = 1, \tag{1.42}$$

while the inter-string part, writing $\lambda=\lambda_\alpha^j-\lambda_\beta^k$, gives a product over $\lambda\neq 0$ of the factors

$$\begin{aligned}
&\prod_{a=1}^{j}\prod_{b=1}^{k} \frac{\lambda_\alpha^{j}-\lambda_\beta^{k}+i\bar{c}\big(\frac{j-k}{2}-a+b-1\big)}{\lambda_\alpha^{j}-\lambda_\beta^{k}+i\bar{c}\big(\frac{j-k}{2}-a+b+1\big)} \\
&\qquad = e_{|j-k|}(\lambda)e^2_{|j-k|+2}(\lambda)e^2_{|j-k|+4}(\lambda)\dots e^2_{j+k-2}(\lambda)e_{j+k}(\lambda) \equiv E_{jk}(\lambda),
\end{aligned} \tag{1.43}$$

where

$$e_j(\lambda) = \frac{\lambda-i\bar{c}j/2}{\lambda+i\bar{c}j/2}. \tag{1.44}$$

Eqs. (1.40) have thus been reduced to the Bethe-Gaudin-Takahashi equations (Takahashi and Suzuki, 1972), that are a set of M_s coupled equations for the string centers λ_α^j,

$$\mathrm{e}^{ij\lambda_\alpha^j L} = \prod_{(k,\beta)\neq(j,\alpha)} E_{jk}(\lambda_\alpha^j-\lambda_\beta^k). \tag{1.45}$$

Defining

$$\phi_j(\lambda) = \frac{1}{i}\ln(-e_j(\lambda)) = 2\arctan\left(\frac{2\lambda}{\bar{c}j}\right), \tag{1.46}$$

these can be rewritten in the log-form

$$j\lambda_\alpha^j L - \sum_{(k,\beta)}\Phi_{jk}(\lambda_\alpha^j-\lambda_\beta^k) = 2\pi I_\alpha^j, \qquad I_\alpha^j \in \begin{cases} \mathbb{Z}+\frac{1}{2}, & N_j \text{ even}, \\ \mathbb{Z}, & N_j \text{ odd}, \end{cases} \tag{1.47}$$

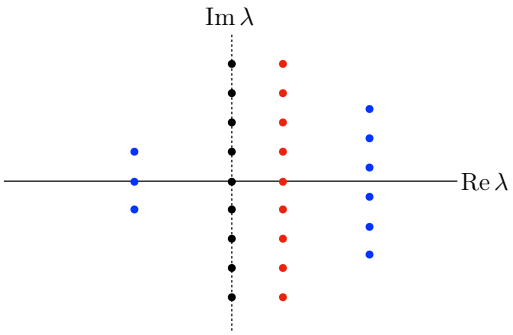


Figure 1.1: Three string states of a gas of $N = 9$ atoms. Black: the ground state consists of a single N-string centered at $\lambda_{\rm gs}^N = 0$ (zero total momentum). Red: a single-particle excited state obtained by giving momentum to the ground state N-string. Blue: a two-particle excited state obtained by splitting the ground state N-string into an M-string and an $(N-M)$-string (in this example $M = 3$).

with

$$\Phi_{jk}(\lambda) = (1-\delta_{jk})\phi_{|j-k|}(\lambda) + 2\phi_{|j-k|+2}(\lambda) + \cdots + 2\phi_{j+k-2}(\lambda) + \phi_{j+k}(\lambda) \tag{1.48}$$

representing the scattering phase shift of a j-string at a k-string, which satisfies

$$\Phi_{jk}(\lambda) = \Phi_{kj}(\lambda), \qquad \Phi_{jk}(-\lambda) = -\Phi_{jk}(\lambda). \tag{1.49}$$

In the limit $L \to \infty$, Eq. (1.47) simplifies to

$$P_{(j,\alpha)} = j\lambda_\alpha^j = \frac{2\pi I_\alpha^j}{L}, \tag{1.50}$$

which tells us that each individual string is quantized as a free particle of mass j.

1.4.3 Ground state

It is clear from Eq. (1.39) that the energy of a string state of length j is minimized for $\lambda_\alpha^j = 0$, that gives

$$E_j^{(0)} = -\frac{\bar{c}^2}{12} j(j^2-1), \qquad P_j^{(0)} = 0. \tag{1.51}$$

The lowest energy state, i.e. the ground state of the system, will thus be obtained by forming a bound state of all N particles centered on zero (McGuire, 1964) (Fig. 1.1), by choosing

$$\lambda_{\rm gs}^{N,a} = i\frac{\bar{c}}{2}(N+1-2a) + O(\delta), \qquad a = 1, \ldots, N. \tag{1.52}$$

The corresponding energy and momentum are

$$E_{\rm gs} = -\frac{\bar{c}^2}{12} N(N^2-1), \qquad P_{\rm gs} = 0. \tag{1.53}$$

Being of order N^3, the ground state energy is not extensive. It has been argued that the attractive Lieb-Linger model therefore does not have a proper thermodynamic limit (Takahashi, 1999), since in the limit of large N the energy per particle is proportional to $(\bar{c}N)^2 \to \infty$. Furthermore, it will be shown in Chapter 2 that the ground state density collapses to a linear volume of order $(\bar{c}N)^{-1} \to 0$.

We now derive the form of the Bethe wavefunction for the ground state. Substituting Eq. (1.52) into Eq. (1.19), we find that in the fundamental domain $D_N : x_1 < \cdots < x_N$,

$$\Psi_{\rm gs}(\mathbf{x})\Big|_{\mathbf{x}\in D_N} = \sum_{Q\in\pi_N} A_Q \exp\Big(-\frac{\overline{c}}{2}\sum_{a=1}^{N}(N+1-2Q_a)\,x_a\Big), \tag{1.54}$$

with the amplitudes A_Q satisfying

$$A_{Q'} = \frac{\lambda_{Q_{a+1}} - \lambda_{Q_a} - i\overline{c}}{\lambda_{Q_{a+1}} - \lambda_{Q_a} + i\overline{c}}\,A_Q = -\frac{1+(Q_{a+1}-Q_a)}{1-(Q_{a+1}-Q_a)}A_Q, \tag{1.55}$$

This implies that there is only one non-vanishing amplitude, namely the one associated to the permutation $\overline{Q}$ such that $\overline{Q}[1,2,\ldots,N-1,N] = [N,N-1,\ldots,2,1]$. In fact, $\overline{Q}_a = N+1-a$, which means that $(\overline{Q}_{a+1} - \overline{Q}_a) = -1$ for any a, and thus the amplitude of any permutation other than $\overline{Q}$ vanishes. Therefore

$$\begin{aligned}\Psi_{\rm gs}(\mathbf{x})\Big|_{\mathbf{x}\in D_N} &= A_{\overline{Q}}\exp\Big(-\frac{\overline{c}}{2}\sum_{a=1}^{N}(2a-N-1)\,x_a\Big)\\ &= A_{\overline{Q}}\exp\Big(-\frac{\overline{c}}{2}\sum_{N\geq a>b\geq 1}(x_a-x_b)\Big).\end{aligned} \tag{1.56}$$

This represents indeed a bound state of N particles, since for $x_j \ll x_{j+1}$ the wave function is exponentially small[2]. Clearly, the validity of Eq. (1.56) can be extended beyond the fundamental domain simply as

$$\Psi_{\rm gs}(\mathbf{x}) = \mathcal{N}_N \exp\Big(-\frac{\overline{c}}{2}\sum_{N\geq a>b\geq 1}|x_a-x_b|\Big) \tag{1.57}$$

where $\mathcal{N}_N$ is a normalization constant.

1.4.4 Excited states

Excitations above the ground state are obtained either by giving momentum to the ground state N-string, thus obtaining a single-particle excited state, or by partitioning it into smaller strings to which individual momenta are given (Fig. 1.1). Each of these smaller strings behaves like a collective particle; in this way we generate multi-particle excited states.

Single-particle states A single-particle excited state centered at μ is given by

$$\mu^{N,a} = \mu + i\frac{\overline{c}}{2}(N+1-2a) + O(\delta), \qquad a = 1,\ldots,N, \tag{1.58}$$

[2]We can easily convince ourselves of the equality of the two expressions above by looking at the structure of the sum

$$\begin{aligned}\textstyle\sum_{N\geq a>b\geq 1}(x_a-x_b) = {}& (x_N-x_1)+(x_{N-1}-x_1)+\cdots+(x_3-x_1)+(x_2-x_1)\\ &+(x_N-x_2)+(x_{N-1}-x_2)+\cdots+(x_3-x_2)\\ &+\quad\cdots\qquad\qquad\cdots\\ &+(x_N-x_{N-1}).\end{aligned}$$

We see that x_1 appears only in the first line, for $N-1$ times, and always with negative sign; hence its coefficient is $-(N-1) = (2a-N-1)|_{a=1}$. x_2 appears in the second line, for $N-2$ times, with negative sign, and in the first line, one time, with positive sign; hence its coefficient is $-(N-2)+1 = (2a-N-1)|_{a=2}$. The same goes for all the other x_a's.

and its energy above the ground state is

$$\omega_N(\mu) = E(\mu) - E_{\rm gs} = N\mu^2 = \frac{P(\mu)^2}{N}, \tag{1.59}$$

where $P(\mu) = N\mu$ is the total momentum of the excited state. For these states there is only one Bethe equation for the string center μ, namely $\mu = 2\pi I/NL$, with $I \in \mathbb{Z}$, hence the total momentum is quantized as for a free wave,

$$P = \frac{2\pi I}{L}, \qquad I \in \mathbb{Z}. \tag{1.60}$$

In the limit of large N, the energy of these single-particle states becomes flat and quasi-degenerate with the ground state.

The Bethe wavefunction of a single-particle excited state differs from the one of the ground state, given by (1.57), simply by a factor of $\exp(i\mu \sum_{a=1}^N x_a)$, which can be rewritten as $\exp(iPx)$, where $x = \sum_{a=1}^N x_a/N$ is the coordinate of the center of mass of the N atoms. Therefore

$$\Psi_{NP}(\mathbf{x}) = \mathcal{N}_N \exp\left(iPx - \frac{\overline{c}}{2} \sum_{N \geq a > b \geq 1} |x_a - x_b| \right). \tag{1.61}$$

Two-particle states A two-particle excited state is made of an M-string centered at μ_1 and an $(N-M)$-string centered at μ_2,

$$\mu^{M,a} = \mu_1 + i\frac{\overline{c}}{2}(M + 1 - 2a) + O(\delta), \qquad a = 1, \dots, M, \tag{1.62}$$

$$\mu^{N-M,a} = \mu_2 + i\frac{\overline{c}}{2}(N - M + 1 - 2a) + O(\delta), \qquad a = 1, \dots, N-M. \tag{1.63}$$

The energy of this state is the sum of the two string energies, and with respect to the ground state energy it is given by

$$\begin{aligned} \omega_{M:N-M}(\mu_1, \mu_2) &= \omega^0_{M:N-M} + M\mu_1^2 + (N-M)\mu_2^2 \\ &= \omega^0_{M:N-M} + \frac{P_M(\mu_1)^2}{M} + \frac{P_{N-M}(\mu_2)^2}{N-M}, \end{aligned} \tag{1.64}$$

where we have defined the rest energy

$$\omega^0_{M:N-M} = \frac{\overline{c}^2}{4} NM(N-M) > 0, \tag{1.65}$$

and $P_M(\mu_1)$, $P_{N-M}(\mu_2)$ are the two string momenta, whose sum gives the total momentum of the state,

$$P_{M:N-M}(\mu_1, \mu_2) = P_M(\mu_1) + P_{N-M}(\mu_2) = M\mu_1 + (N-M)\mu_2. \tag{1.66}$$

The Bethe equations are

$$\begin{aligned} M\mu_1 L - \Phi_{M,N-M}(\mu_1 - \mu_2) &= 2\pi I_1, \\ (N-M)\mu_2 L + \Phi_{M,N-M}(\mu_1 - \mu_2) &= 2\pi I_2, \end{aligned} \tag{1.67}$$

with I_1, $I_2 \in \mathbb{Z}$. In the limit of large L, we can ignore the scattering phase shift and take μ_1 and μ_2 as free parameters. The total momentum $k = P_{M:N-M}$ can then take on the values

$$k = \frac{2\pi(I_1 + I_2)}{L} = \frac{2\pi I}{L}, \qquad I \in \mathbb{Z} \tag{1.68}$$

while the energy is bounded from below by

$$\omega^{\ell}_{M:N-M}(k) = \omega^{0}_{M:N-M} + \frac{k^2}{N}. \tag{1.69}$$

As it can be easily seen, the bound is saturated for $\mu_1 = \mu_2$. Given the total energy ω and momentum k as external parameters, using Eqs. (1.64), (1.66) and (1.69) we find two solutions to the dynamical constraints, namely

$$\mu_1^{\pm}(k,\omega) = \frac{k}{N} \pm \left[\frac{N-M}{NM}\right]^{\frac{1}{2}} \left[\omega - \omega^{\ell}_{M:N-M}(k)\right]^{\frac{1}{2}}, \tag{1.70}$$

$$\mu_2^{\pm}(k,\omega) = \frac{k}{N} \mp \left[\frac{M}{N(N-M)}\right]^{\frac{1}{2}} \left[\omega - \omega^{\ell}_{M:N-M}(k)\right]^{\frac{1}{2}}. \tag{1.71}$$

Therefore, in the large L limit these states form a twofold-degenerate continuum beginning at $\omega^{\ell}_{M:N-M}(k)$ and extending to arbitrarily high energy, $\omega^{\ell}_{M:N-M}(k) \leq \omega < \infty$. Again, $\omega = \omega^{\ell}_{M:N-M}(k)$ for $\mu_1 = \mu_2$. For finite L, this is of course not strictly a continuum; μ_1 and μ_2 are quantized according to the Bethe equations and only discrete energy levels exist.

1.4.5 Norm of Bethe states

We complete the characterization of the eigenstates by reporting a formula for their norm. Given a set of rapidities $\{\lambda\}$ solving the Bethe equations, the norm of the corresponding Bethe eigenfunction is given by the Gaudin-Korepin formula (Gaudin et al., 1981; Korepin, 1982; Gaudin, 2014), in this case

$$\|\{\lambda\}\|^2 = |c|^N \prod_{j>k} \frac{(\lambda_j - \lambda_k)^2 + c^2}{(\lambda_j - \lambda_k)^2} \det_N \mathcal{G} \tag{1.72}$$

where $\mathcal{G}$ is the Gaudin matrix, whose entries are given by

$$\mathcal{G}_{jk}(\{\lambda\}) = \delta_{jk}\left[L + \sum_{l=1}^{N} K(\lambda_j, \lambda_l)\right] - K(\lambda_j, \lambda_k) \tag{1.73}$$

with

$$K(\lambda, \mu) = \frac{2c}{(\lambda-\mu)^2 + c^2}. \tag{1.74}$$

the Cauchy kernel. As shown by Calabrese and Caux (2007), this formula is adapted to the string parametrization (1.38) as

$$\|\{\lambda^j_\alpha\}\|^2 = (L\bar{c})^{M_s} \prod_j j^{2N_j} \prod_{(k,\beta)>(j,\alpha)} F_{jk}(\lambda^j_\alpha - \lambda^k_\beta) \tag{1.75}$$

where

$$F_{jk}(\lambda) = \frac{\lambda^2 + ((\bar{c}/2)(j+k))^2}{\lambda^2 + ((\bar{c}/2)(j-k))^2}. \tag{1.76}$$

The norm of a single N-string is thus simply

$$\|\{\lambda\}\|^2 = \bar{c} L N^2 \tag{1.77}$$

and that of an $M : N-M$ state with rapidities μ_1, μ_2 respectively for the M- and $(N-M)$-strings,

$$\|\{\mu_1, \mu_2\}\|^2 = \bar{c}^2 L^2 (N-M)^2 M^2 \frac{((\mu_1-\mu_2)/\bar{c})^2 + (N/2)^2}{((\mu_1-\mu_2)/\bar{c})^2 + (N/2-M)^2}. \tag{1.78}$$

The dependence on L of the norm of the Bethe wavefunction as L^{M_s}, M_s being the number of strings, reflects the fact that the strings are essentially independent, almost free particles. The limit $L \to \infty$ at fixed N is far from trivial, as the atoms tend to clump together in wave packets of finite extent.

1.5 Repulsive interaction

We now specialize to repulsive interaction (c $>$ 0), characterizing the ground state and the excited states of the Lieb-Liniger model in this regime. For simplicity, we shall limit our discussion to a thermodynamically large system. Useful references this section are Korepin et al. (1993); Takahashi (1999).

1.5.1 Properties of solutions of the Bethe equations

Let us start by proving some important properties of the solutions of Bethe equations in the repulsive case ($c > 0$).

1. For $c > 0$, all solutions to the Bethe equations are real.

Proof. Consider a set $\{\lambda_j\}$, $j = 1, \dots, N$, solution to the Bethe equations, and pick from this set the rapidity $\lambda_{\max}$ with maximal imaginary part, so that $\operatorname{Im}\lambda_{\max} \geq \operatorname{Im}\lambda_j$ for any j. Using the fact that, for $c > 0$,

$$\left|\frac{\lambda + ic}{\lambda - ic}\right| = \left[\frac{(\operatorname{Re}\lambda)^2 + (\operatorname{Im}\lambda + c)^2}{(\operatorname{Re}\lambda)^2 + (-\operatorname{Im}\lambda + c)^2}\right]^{1/2} = \begin{cases} \geq 1, & \operatorname{Im}\lambda \geq 0, \\ \leq 1, & \operatorname{Im}\lambda \leq 0, \end{cases}$$

the Bethe equation for $\lambda_{\max}$ gives

$$\left|e^{i\lambda_{\max} L}\right| = \left|\prod_j \frac{\lambda_{\max} - \lambda_j + ic}{\lambda_{\max} - \lambda_j - ic}\right| \geq 1.$$

On the other hand,

$$\left|e^{i\lambda L}\right| = \left|e^{iL\operatorname{Re}\lambda} e^{-L\operatorname{Im}\lambda}\right| = \left|e^{-L\operatorname{Im}\lambda}\right| = \begin{cases} \leq 1, & \operatorname{Im}\lambda \geq 0, \\ \geq 1, & \operatorname{Im}\lambda \leq 0, \end{cases}$$

which means that $\operatorname{Im}\lambda_{\max} \leq 0$, and thus $\operatorname{Im}\lambda_j \leq 0$ for any j. If instead we pick the rapidity $\lambda_{\min}$ with minimal imaginary part, we can show in the same way that $\operatorname{Im}\lambda_{\min} \geq 0$, and thus $\operatorname{Im}\lambda_j \geq 0$ for any j. Hence it must be $\operatorname{Im}\lambda_j = 0$ for any j. □

2. For $c > 0$, if $I_j > I_k$ then $\lambda_j > \lambda_k$, and if $I_j = I_k$ then $\lambda_j = \lambda_k$. On the other hand, if $\lambda_j = \lambda_k$ then $I_j = I_k$. Thus $\lambda_j = \lambda_k$ if and only if $I_j = I_k$. Since the Bethe wavefunction vanishes if two rapidities coincide, and in that case does not represent an eigenstate, a proper set of quantum numbers $\{I_j\}$ does not contain coincident I_j's.

Proof. Subtracting the Bethe equation for λ_k from the one for λ_j we get

$$\lambda_j - \lambda_k + \frac{1}{L}\sum_m \Big[\phi(\lambda_j - \lambda_m) - \phi(\lambda_k - \lambda_m)\Big] = \frac{2\pi}{L}(I_j - I_k) \tag{1.79}$$

Since the scattering phase shift (1.15b) is monotonic, the first and second terms on the left-hand side have the same sign, which then is the same sign of $I_j - I_k$. Furthermore, $I_j - I_k = 0$ implies $\lambda_j - \lambda_k = 0$. Finally, $\lambda_j - \lambda_k = 0$ obviously implies $I_j - I_k = 0$. □

3. For $c > 0$, rapidity differences are bounded by

$$\frac{2\pi}{L}\frac{|I_j - I_k|}{1 + 2n/c} \leq |\lambda_j - \lambda_k| \leq \frac{2\pi}{L}|I_j - I_k| \tag{1.80}$$

Proof. Consider the Cauchy kernel

$$\mathcal{C}(\lambda) \equiv \frac{1}{2\pi}\frac{d\phi(\lambda)}{d\lambda}\bigg|_{\lambda\in\mathbb{R}} = \frac{1}{\pi}\frac{c}{c^2 + \lambda^2}, \qquad 0 \leq \mathcal{C}(\lambda) \leq \frac{1}{\pi c}. \tag{1.81}$$

Then $\phi(\lambda_1) - \phi(\lambda_2) = 2\pi\int_{\lambda_2}^{\lambda_1} d\lambda\, \mathcal{C}(\lambda)$ satisfies $0 \leq \phi(\lambda_1) - \phi(\lambda_2) \leq (2/c)(\lambda_1 - \lambda_2)$. Substituting this into Eq. (1.79) proves the statement. □

4. For $c > 0$, given a proper set of quantum numbers $\{I_j\}$, the solution for the set $\{\lambda_j\}$ exists and is unique (Yang and Yang, 1969).

Proof. The Bethe equations are the extremum conditions for the Yang-Yang action

$$S(\{\lambda\}) = \frac{L}{2}\sum_j \lambda_j^2 + \sum_{j<k} \Phi(\lambda_j - \lambda_k) - 2\pi I_j \lambda_j, \tag{1.82}$$

where

$$\Phi(\lambda) = \int_0^\lambda d\mu\, \phi(\mu) = 2\lambda \arctan\left(\frac{\lambda}{c}\right) - c\ln\left(1 + \frac{\lambda^2}{c^2}\right). \tag{1.83}$$

In fact, equating

$$\partial_{\lambda_j} S(\{\lambda\}) = \lambda_j L + \sum_k \phi(\lambda_j - \lambda_k) - 2\pi I_j$$

to zero for all j gives the set of Bethe equations. The Hessian of the Yang-Yang action,

$$\begin{aligned} S_{jk} = \frac{\partial^2 S}{\partial\lambda_j \partial\lambda_k} &= \partial_{\lambda_j}\left[\lambda_k L + \sum_m 2\arctan\left(\frac{\lambda_k - \lambda_m}{c}\right) - 2\pi I_k\right] \\ &= \delta_{jk}\left[L + \sum_m \frac{2c}{(\lambda_j - \lambda_m)^2 + c^2}\right] - \frac{2c}{(\lambda_j - \lambda_k)^2 + c^2}, \end{aligned}$$

is positive definite, since for any $\mathbf{v} \in \mathbb{R}^N \setminus \{\mathbf{0}\}$ we have the quadratic form

$$\begin{aligned} \sum_{j,k} v_j S_{jk} v_k &= \sum_j v_j^2 L + \sum_{j,m} v_j^2 \frac{2c}{(\lambda_j - \lambda_m)^2 + c^2} - \sum_{j,k} v_j v_k \frac{2c}{(\lambda_j - \lambda_k)^2 + c^2} \\ &= \sum_j v_j^2 L + \sum_{j>k} (v_j - v_k)^2 \frac{2c}{(\lambda_j - \lambda_k)^2 + c^2}\bigg|_{c>0} > 0. \end{aligned}$$

Thus, S is a strictly convex function in $\mathbb{R}^N$, and the solution to the extremum condition for a given proper set of quantum numbers is unique. □

1.5.2 Thermodynamic limit of the Bethe equations

According to the theorems of Section 1.5.1, in the repulsive case the Bethe equations map a proper set of (integer or half-integer) quantum numbers $\{I_j\}$ to a set of real rapidities $\{\lambda_j\}$. No two quantum numbers in the set $\{I_j\}$ coincide, so they can always be ordered as $I_1 < I_2 < \cdots < I_N$, which by monotonicity implies that $\lambda_1 < \lambda_2 < \cdots < \lambda_N$. If the interaction parameter c is neither 0 nor ∞, the Bethe equations are a system of N non-linear coupled equations which cannot be solved in closed form, as changing one quantum number changes all the rapidities. Taking the thermodynamic limit allows us to make some progress. Since for a quantum number difference $I_i - I_j \sim 1$ the difference in the corresponding rapidities is $\lambda_i - \lambda_j \sim 1/L$, in the thermodynamic limit $L \to \infty$, $N \to \infty$, N/L finite, rapidities become dense on the real line.

Given a proper set of quantum numbers $\{I_j\}$, we introduce the discrete set of points $\{x_j = I_j/L\}$, and define a function $\lambda(x)$, $x \in \mathbb{R}$, such that $\lambda(x_j) = \lambda_j$, where $\{\lambda_j\}$ solves the Bethe equations with $\{I_j\}$,

$$\lambda(x_j) + \frac{1}{L}\sum_{k=1}^N \phi(\lambda(x_j) - \lambda(x_k)) = 2\pi x_j. \tag{1.84}$$

At this stage the value of $\lambda(x)$ remains arbitrary for $x \neq x_j$. However, since x_j becomes continuous as $L \to \infty$, this suggests constraining $\lambda(x)$ for any $x \in \mathbb{R}$ according to

$$\lambda(x) + \int dy\, \phi(\lambda(x) - \lambda(y))\rho(y) = 2\pi x, \tag{1.85}$$

where

$$\rho(x) = \frac{1}{L}\sum_{j=1}^{N}\delta\left(x - \frac{I_j}{L}\right) = \frac{1}{L}\sum_{n\in\{I\}}\delta\left(x - \frac{n}{L}\right) \tag{1.86}$$

is the density of occupied quantum numbers, the set of occupied quantum numbers being denoted by $\{I\}$. In a similar way we can define the density of unoccupied quantum numbers, or 'holes', ρ_h, and the total density ρ_t,

$$\rho_h(x) = \frac{1}{L}\sum_{m\in\{\widetilde{I}\}}\delta\left(x - \frac{m}{L}\right), \qquad \rho_t(x) = \rho(x) + \rho_h(x) = \frac{1}{L}\sum_{t\in\{T\}}\delta\left(x - \frac{t}{L}\right), \tag{1.87}$$

where $\{\widetilde{I}\}$ denotes the set of unoccupied quantum numbers, which is complementary to $\{I\}$ with respect to the set of all possible quantum numbers, that is $\{T\} = \mathbb{Z} + \frac{1}{2}$ for N even or $\{T\} = \mathbb{Z}$ for N odd. In the thermodynamic limit, these densities become smooth functions of x, and in particular

$$\rho_t(x) \to \int dy\, \delta(x-y) = 1. \tag{1.88}$$

The continuum Bethe equations (1.85) define a continuous differentiable mapping between the x- and λ-spaces. Thus we can rewrite the densities as function in λ-space as

$$\rho(\lambda) = \rho(x(\lambda))\frac{dx}{d\lambda}, \qquad \rho_h(\lambda) = \rho_h(x(\lambda))\frac{dx}{d\lambda}, \tag{1.89}$$

$$\rho_t(\lambda) = \rho(\lambda) + \rho_h(\lambda) = \rho_t(x(\lambda))\frac{dx}{d\lambda} = \frac{dx}{d\lambda}, \tag{1.90}$$

and we can rewrite Eq. (1.85) as

$$\lambda + \int d\lambda'\, \phi(\lambda-\lambda')\rho(\lambda') = 2\pi x(\lambda). \tag{1.91}$$

Differentiating with respect to λ, and using the definition of the Cauchy kernel $\mathcal{C}(\lambda)$ (1.81), gives

$$\rho(\lambda) + \rho_h(\lambda) = \frac{1}{2\pi} + \mathcal{C} * \rho(\lambda), \tag{1.92}$$

where $*$ denotes the convolution $f * g(\lambda) \equiv \int d\lambda'\, f(\lambda-\lambda')g(\lambda')$. Eq. (1.92) is a functional relation between $\rho(\lambda)$ and $\rho_h(\lambda)$. Thus, given any function $\rho_h(\lambda)$, it determines a function $\rho(\lambda)$ which is uniquely associated to an eigenstate of the Lieb-Liniger Hamiltonian. Once $\rho(\lambda)$ has been found, the particle, momentum, and energy densities of the corresponding eigenstate are

$$\frac{N}{L} = \int d\lambda\, \rho(\lambda), \qquad \frac{P}{L} = \int d\lambda\, \lambda\, \rho(\lambda), \qquad \frac{E}{L} = \int d\lambda\, \lambda^2 \rho(\lambda). \tag{1.93}$$

1.5.3 Ground state

For any $c > 0$, the ground state is obtained by choosing the maximally compact set of quantum numbers symmetric with respect to zero,

$$\{I_j^0\}_N = \left\{-\frac{N-1}{2}, \ldots, \frac{N-1}{2}\right\}_N = \left\{-\frac{N+1}{2} + j\right\}_N, \qquad j = 1, \ldots, N. \tag{1.94}$$

This is obviously true for $c \to \infty$, which is known as Tonks-Girardeau limit (Tonks, 1936; Girardeau, 1960). In this regime, the scattering phase shifts go to zero and $\lambda_j = (2\pi/L)I_j$,

thus $E_N = (2\pi/L)^2 \sum_{j=1}^N I_j^2$ is minimized by choosing the quantum numbers (1.94) and takes the value

$$E_{\rm gs} = \frac{\pi^2}{3L^2} N(N^2-1) \qquad (c \to \infty). \tag{1.95}$$

This is equivalent to the energy of a 1D system of non-interacting spinless fermions[3]. Any other choice of $\{I_j\}$ gives a larger energy. By the continuity and unicity of the Bethe solutions $\{\lambda_j(c)\}$ with respect to c for a given $\{I_j\}$, and the fact that the energy eigenvalues are non-degenerate, we conclude that there cannot be a level crossing, hence the same quantum numbers describe the ground state for any $c > 0$ (Yang and Yang, 1969).

Given the quantum numbers $\{I_j^0\}$, by varying c the values of the rapidities will change, but will remain ordered; in particular, since λ_N is the largest rapidity, $\sum_{k=1}^N \phi(\lambda_N - \lambda_k) > 0$, and the Bethe equation for λ_N yields $\lambda_N < (2\pi/L) I_N$. Similarly, since λ_1 is the smallest rapidity, $\lambda_1 > (2\pi/L) I_1$. Therefore for any $c > 0$,

$$\frac{2\pi}{L} I_1 < \lambda_1 < \lambda_2 < \cdots < \lambda_N < \frac{2\pi}{L} I_N. \tag{1.96}$$

In the thermodynamic limit and at arbitrary $c > 0$, to obtain the ground state we thus look for a density function $\rho(\lambda)$ that is non-zero only within a finite interval $[-\lambda_F, \lambda_F]$,

$$\rho(\lambda) = \begin{cases} \rho_t(\lambda), & |\lambda| \le \lambda_F, \\ 0, & |\lambda| > \lambda_F, \end{cases} \qquad \text{and} \qquad \rho_h(\lambda) = \rho_t(\lambda) - \rho(\lambda). \tag{1.97}$$

We immediately see from Eq. (1.93) that this state has zero momentum. This can also be seen from the fact that, since $\arctan(\lambda/c) + \arctan(-\lambda/c) = 0$, in the repulsive case

$$P_N = \sum_{j=1}^N \lambda_j = \frac{2\pi}{L} \sum_{j=1}^N I_j, \tag{1.98}$$

and therefore $P_{\rm gs} = \sum_{j=1}^N \left(-\frac{N+1}{2} + j\right) = 0$. With the ground state density function (1.97), the integral equation (1.92) becomes the Lieb equation

$$\rho(\lambda) - \int_{-\lambda_F}^{\lambda_F} d\lambda' \, \mathcal{C}(\lambda - \lambda') \rho(\lambda') = \frac{1}{2\pi}, \qquad |\lambda| \le \lambda_F. \tag{1.99}$$

The Fermi momentum λ_F can be viewed as an independent variable which (indirectly) specifies the particle density $n \equiv N/L$ according to

$$n = \int_{-\lambda_F}^{\lambda_F} d\lambda \, \rho(\lambda). \tag{1.100}$$

Eqs. (1.99) and (1.100) should be solved self-consistently for the required particle density. In the Tonks-Girardeau limit the Cauchy kernel vanishes and therefore

$$\rho(\lambda) = \frac{1}{2\pi} \theta(\lambda_F - |\lambda|), \qquad \lambda_F = \pi n \qquad (c \to \infty). \tag{1.101}$$

These correspond to the momentum distribution and the Fermi momentum of a 1D system of non-interacting spinless fermions.

[3] The wavefunction of a system of N non-interacting spinless fermions is a Slater determinant of N free waves $\exp(ikx)$, where the allowed values of k are determined by the periodic boundary conditions; $k = 2\pi j/L$, with j any integer. The single-particle energies are $\epsilon_k = k^2$. For N odd, the ground state is obtained by choosing the values of j in the Fermi interval $-\frac{1}{2}(N-1) \le j \le \frac{1}{2}(N-1)$, and has the energy

$$E_{\rm gs}^{(F)} = \sum_{j=-\frac{1}{2}(N-1)}^{\frac{1}{2}(N-1)} \left(\frac{2\pi j}{L}\right)^2 = \frac{\pi^2}{3L^2} N(N^2-1).$$

1.5.4 Elementary excitations

We now turn to the excitations. Lieb (1963) found two distinct types of excitations, which in the Tonks-Girardeau limit correspond to particle and hole excitations of the ideal Fermi gas. The two types of excitations are constructed analogously in the finite interaction case, namely by adding a particle with given rapidity to the ground state or by removing a particle from the Fermi interval. Here we present the construction and obtain the fundamental equations for the momentum and the energy of the excitations. A more detailed analysis and their numerical and analytical solutions will be presented in Chapter 4.

Type I excitations A one-particle excitation over the N-particle ground state ('Type I' excitation) is obtained by constructing the $(N+1)$-particle state with quantum numbers

$$\{I_j\}_{N+1} = \left\{-\frac{N}{2}, -\frac{N}{2}+1, \cdots, \frac{N}{2}-1, \frac{N}{2}+m\right\}_{N+1}. \tag{1.102}$$

This state is realized starting from the ground state of $N+1$ particles and moving the particle at the right edge of the Fermi interval by m steps, i.e. giving it the quantum number $I_{N+1} = N/2+m$ (alternatively, one may choose $I_1 = -N/2-m$):

The total momentum is $P = (2\pi/L)m$. Since adding a particle turns integer quantum numbers into half-integers, and vice-versa, the total momentum is produced by a rearrangement of all quantum numbers (and rapidities) with respect to the N-particle ground state.

We denote the rapidities of the new state by $\{\lambda_1, \ldots, \lambda_N, k\}$, where $k > \lambda_F$ is the rapidity of the added particle, and the rapidities of the N-particle ground state by $\{\lambda_1^0, \ldots, \lambda_N^0\}$. The Bethe equations

$$L\lambda_j^0 = 2\pi\left(-\frac{N+1}{2}+j\right) - \sum_{l=1}^{N}\phi(\lambda_j^0-\lambda_l^0), \tag{1.103a}$$

$$L\lambda_j = 2\pi\left(-\frac{N+2}{2}+j\right) - \sum_{l=1}^{N}\phi(\lambda_j-\lambda_l) - \phi(\lambda_j-k), \tag{1.103b}$$

show that the rapidities will shift by a small amount $\lambda_j - \lambda_j^0 \equiv d_j/L$, where d_j is given by

$$\begin{aligned} d_j &= -\pi - \phi(\lambda_j-k) - \sum_{l=1}^{N}\Big[\phi(\lambda_j-\lambda_l) - \phi(\lambda_j^0-\lambda_l^0)\Big] \\ &= -\pi - \phi(\lambda_j-k) - \frac{1}{L}\sum_{l=1}^{N}\frac{2c}{(\lambda_j^0-\lambda_l^0)^2+c^2}(d_j-d_l) + O(N/L^2). \end{aligned} \tag{1.104}$$

This can be rewritten as

$$d_j\left[1+\frac{1}{L}\sum_{l=1}^{N}\frac{2c}{(\lambda_j^0-\lambda_l^0)^2+c^2}\right] = -\pi-\phi(\lambda_j-k) + \frac{1}{L}\sum_{l=1}^{N}\frac{2c}{(\lambda_j^0-\lambda_l^0)^2+c^2}d_l. \tag{1.105a}$$

Introducing the density $\rho(\lambda)$ and defining the function $d(\lambda_j, k) = d_j$, we can again extend the definition of $d(\lambda, k)$ to all λ as

$$d(\lambda,k)\left[1+2\pi\int_{-\lambda_F}^{\lambda_F}d\lambda'\,\mathcal{C}(\lambda-\lambda')\rho(\lambda')\right] = -\pi-\phi(\lambda-k)+2\pi\int_{-\lambda_F}^{\lambda_F}d\lambda'\,\mathcal{C}(\lambda-\lambda')\rho(\lambda')d(\lambda',k). \tag{1.105b}$$

Making use of the Lieb equation, on the left-hand side we have the quantity $2\pi d(\lambda,k)\rho(\lambda)$. Defining the displacement function of the Type I (particle-like) excitations

$$D_p(\lambda,k) \equiv d(\lambda,k)\rho(\lambda) \tag{1.106}$$

we thus obtain

$$D_p(\lambda,k) - \int_{-\lambda_F}^{\lambda_F} d\lambda'\, \mathcal{C}(\lambda-\lambda') D_p(\lambda',k) = -\frac{1}{2\pi}\Big[\pi + \phi(\lambda-k)\Big], \qquad |\lambda| < \lambda_F, \quad k > \lambda_F. \tag{1.107}$$

The change in momentum with respect to the ground state is

$$p_{\rm I}(k) = k + \sum_{j=1}^{N} (\lambda_j - \lambda_j^0) = k + \frac{1}{L}\sum_{j=1}^{N} d_j = k + \int_{-\lambda_F}^{\lambda_F} d\lambda\, D_p(\lambda,k), \tag{1.108}$$

while the change in energy, including the chemical potential μ, is

$$\omega_{\rm I}(k) = k^2 - \mu + \sum_{j=1}^{N} (\lambda_j^2 - (\lambda_j^0)^2) = k^2 - \mu + 2\int_{-\lambda_F}^{\lambda_F} d\lambda\, \lambda\, D_p(\lambda,k). \tag{1.109}$$

These equations demonstrate the collective nature of the excitations, which cannot be simply assigned to the single particle we added. The addition of a particle with bare momentum k and bare energy k^2 produced a reorganization of the entire system, which collectively acquires momentum (1.108) and energy (1.109). This is a manifestation of the non-local nature of the excitations of a one-dimensional system and provides a concrete example of the concept that one-dimensional systems are intrinsically strongly interacting, regardless of the actual strength of the coupling constant.

In the limit $c \to 0^+$, $\mu \to 0$, $\lambda_F \to 0$, $\phi(\lambda-k) \to -\pi$, and $\mathcal{C}(\lambda-\lambda') \to 0$, thus $D_p \to 0$, $p_{\rm I} = k > 0$, and

$$\omega_{\rm I}(p_{\rm I}) = p_{\rm I}^2. \tag{1.110}$$

In the limit $c \to \infty$, $\mu = \lambda_F^2 = (\pi n)^2$ and $\phi(\lambda-k), \mathcal{C}(\lambda-\lambda') \to 0$, thus $D_p \to -\frac{1}{2}$, $p_{\rm I} = k - \lambda_F = k - \pi n > 0$, and

$$\omega_{\rm I}(p_{\rm I}) = p_{\rm I}^2 + 2\pi n p_{\rm I}. \tag{1.111}$$

Type II excitations A one-hole excitation above the N-particle ground state ('Type II' excitation) is obtained by constructing the $(N-1)$-particle state with quantum numbers

$$\{I_j\}_{N-1} = \left\{-\frac{N}{2}+1, \ldots, \frac{N}{2}-m-1, \frac{N}{2}-m+1, \ldots, \frac{N}{2}\right\}_{N-1}, \tag{1.112}$$

that is, by punching a hole in the Fermi interval:

$$\cdots \circ\circ\circ\circ \bullet\bullet\bullet \circ \bullet\bullet \circ\circ\circ\circ \cdots$$

This state also has momentum $P = (2\pi/L)m$. We have removed the quantum number $I^0 = (N-1)/2 - m$ in the Fermi interval, considering $0 < m < N/2$ (namely, the hole is on the right side of the Fermi interval). We denote by q the associated rapidity, which is such that $|q| < \lambda_F$. Following the same logic as for Type I, we therefore have

$$d_j = \pi + \phi(\lambda_j - q) - \frac{1}{L}\sum_{l=1}^{N} \frac{2c}{(\lambda_j^0 - \lambda_l^0)^2 + c^2}(d_j - d_l) + O(N/L^2), \tag{1.113}$$

which leads to the equation for the displacement of the Type II (hole-like) excitations,

$$D_h(\lambda,q)-\int_{-\lambda_F}^{\lambda_F}d\lambda'\,\mathcal{C}(\lambda-\lambda')D_h(\lambda',q)=\frac{1}{2\pi}\Big[\pi+\phi(\lambda-q)\Big],\qquad |\lambda|<\lambda_F,\quad 0<q<\lambda_F. \tag{1.114}$$

The change in momentum with respect to the ground state is

$$p_{\rm II}(q)=-q+\int_{-\lambda_F}^{\lambda_F}d\lambda\,D_h(\lambda,q), \tag{1.115}$$

while the change in energy is

$$\omega_{\rm II}(q)=-q^2+\mu+2\int_{-\lambda_F}^{\lambda_F}d\lambda\,\lambda\,D_h(\lambda,q). \tag{1.116}$$

In the limit $c\to 0^+$, $\mu\to 0$, $\lambda_F\to 0$, $\mathcal{C}(\lambda-\lambda')\to 0$, and $q<\lambda_F\to 0$, hence $\phi(\lambda-q)\to\pi\,\mathrm{sgn}(\lambda)$, $D_h\to\theta(\lambda)$, $p_{\rm II}=-q\to 0$, and

$$\omega_{\rm II}(p_{\rm II})=0. \tag{1.117}$$

In the limit $c\to\infty$, $\mu=\lambda_F^2=(\pi n)^2$ and $\phi(\lambda-q)$, $\mathcal{C}(\lambda-\lambda')\to 0$, thus $D_p\to\frac{1}{2}$, $p_{\rm II}=-q+\lambda_F=-q+\pi n\in[0,\pi n]$. Extending the definition of q to the whole interval $[-\lambda_F,\lambda_F]$ (namely, the hole can also be on the left side of the Fermi interval), we have $p_{\rm II}=-q+\pi n\in[0,2\pi n]$, and

$$\omega_{\rm II}(p_{\rm II})=-p_{\rm II}^2+2\pi n p_{\rm II},\qquad p_{\rm II}\in[0,2\pi n]. \tag{1.118}$$

Particle-hole excitations The linearity of the Eqs. (1.107) and (1.114) for the displacement functions of Type I and Type II excitations implies that we can describe more general excitations as superpositions of these two fundamental excitations. In particular, all the excitations over the physical vacuum in the zero-charge sector (i.e., excitations with the number of particles N in the excited state the same as the number of particles in the ground state) can be constructed as a superposition of equal numbers of particles and holes.

Consider for instance a single particle-hole excitation, obtained by picking out one particle with rapidity $q\in[-\lambda_F,\lambda_F]$ and giving it rapidity $k>k_F$. The rearrangement of the rapidities will be described by the displacement function $D_{ph}(\lambda,k,q)$ satisfying the integral equation

$$D_{ph}(\lambda,k,q)-\int_{-\lambda_F}^{\lambda_F}d\lambda'\,\mathcal{C}(\lambda-\lambda')D_{ph}(\lambda',k,q)=\frac{1}{2\pi}\Big[\phi(\lambda-q)-\phi(\lambda-k)\Big]. \tag{1.119}$$

By linearity, it is evident that this displacement function is equal to the sum of a single-particle and single-hole displacement functions,

$$D_{ph}(\lambda,k,q)=D_p(\lambda,k)+D_h(\lambda,q). \tag{1.120}$$

The momentum and energy of the particle-hole excitation will then be

$$\Delta P=k-q+\int_{-\lambda_F}^{\lambda_F}d\lambda\,D_{ph}(\lambda,k,q)=p_{\rm I}(k)+p_{\rm II}(q), \tag{1.121}$$

$$\Delta E=k^2-q^2+2\int_{-\lambda_F}^{\lambda_F}d\lambda\,\lambda\,D_{ph}(\lambda,k,q)=\omega_{\rm I}(k)+\omega_{\rm II}(q). \tag{1.122}$$

This construction generalizes directly to an arbitrary number of particle and hole excitations, with the constraint that the number of particles equals the number of holes if we are to describe the excitations in the zero-charge sector,

$$\Delta P = \sum_{\text{particles}} p_{\text{I}}(k) + \sum_{\text{holes}} p_{\text{II}}(q), \tag{1.123}$$

$$\Delta E = \sum_{\text{particles}} \omega_{\text{I}}(k) + \sum_{\text{holes}} \omega_{\text{II}}(q). \tag{1.124}$$

Chapter 2

Ground state in the attractive case

In the limit of a large number of particles, the ground state of the attractive Lieb-Liniger model should be well described by a Hartree mean field approximation. In this approximation, the ground state wavefunction is the solution of a nonlinear Schrödinger equation (NLSE) with cubic nonlinearity, the Gross-Pitaevskii equation (GPE). As shown by Zakharov and Shabat (1971) using the inverse scattering method, this equation admits an extensive family of analytical solutions, called n-solitons, which describe the scattering process of n bright solitons (fundamental solutions) one by another, and are such that asymptotically, i.e. for $t \to \pm\infty$, they break up in n individual solitons. In this chapter we are interested in the static problem, described by the fundamental soliton solution. We will prove that this is the only[1] non-trivial normalizable solution of the time-independent GPE. Once the solution is known, we can calculate the energy and density profile of the ground state, and compare the results of the mean field theory with the exact results obtained via the Bethe Ansatz. Moreover, we will see that giving momentum to the soliton of the ground state we obtain an approximate single-particle excited state.

2.1 Hartree mean field

The Hartree mean field approximation consists in assuming that all particles occupy the same single-particle state, $\phi(x)$, so that we can write the N-body wavefunction in the form of a product (Hartree, 1928),

$$\Psi_N(x_1, \ldots, x_n) = \prod_{j=1}^{N} \phi(x_j). \tag{2.1}$$

The expectation value of the Hamiltonian (1.1) in this state, treated as a functional of the (as yet undetermined) normalized single-particle wavefunction $\phi(x)$ and its complex conjugate $\phi^*(x)$, is the so-called Hartree functional,

$$\begin{aligned} E_N[\phi, \phi^*] &= \int dx_1 \ldots dx_N \, \Psi_N^*(x_1, \ldots, x_N) H^{(N)} \Psi_N(x_1, \ldots, x_N) \\ &= N \int dx \Big[|\partial_x \phi(x)|^2 + (N-1) c |\phi(x)|^4 \Big]. \end{aligned} \tag{2.2}$$

The variational theorem ensures that, whatever the 'trial wavefunction' $\phi(x)$, this expectation value provides a rigorous upper bound to the exact ground state energy of the system (Cohen-Tannoudji et al., 2020). To find the optimal form for $\phi(x)$, we thus minimize the Hartree functional with respect to independent variations of $\phi(x)$ and its complex conjugate $\phi^*(x)$, subject to the normalization condition $\int dx \, |\phi(x)|^2 = 1$. This constraint is conveniently taken care of by the method of Lagrange multipliers. One defines

[1] Except for the degeneracy due to the translational invariance of the GPE.

$\Omega_N[\phi,\phi^*] = E_N[\phi,\phi^*] - \mu N \int dx|\phi(x)|^2$ and imposes $\delta\Omega_N[\phi,\phi^*] = 0$ at fixed μN. This gives

$$\left[-\partial_x^2 + 2(N-1)c|\phi(x)|^2\right]\phi(x) = \mu\,\phi(x), \tag{2.3}$$

which is the time-independent Gross-Pitaevskii equation (GPE) (Gross, 1961; Pitaevskii, 1961). Multiplying both sides by $\phi^*(x)$ and integrating, we find for the Lagrange multiplier μ the expression

$$\mu = \int dx\left[|\partial_x\phi(x)|^2 + 2(N-1)c|\phi(x)|^4\right]. \tag{2.4}$$

Comparing Eqs. (2.4) and (2.2), we see that $E_N - E_{N-1} = \mu$, thus the Lagrange multiplier μ has the physical meaning of the chemical potential of the system. Moreover one can write

$$E_N[\phi,\phi^*] = N\mu - N(N-1)c\int dx\,|\phi(x)|^4. \tag{2.5}$$

Therefore the GPE is a nonlinear Schrödinger equation with cubic nonlinearity, and with the chemical potential replacing the energy eigenvalue.

It is now convenient to rescale the wavefunction $\phi(x)$ so that it is normalized to the total number of particle N. Introducing $\psi(x) = \sqrt{N}\phi(x)$, so that $\int dx\,|\psi(x)|^2 = N$, and neglecting terms of order $1/N$, Eq. (2.3) becomes

$$\left[-\partial_x^2 + 2c|\psi(x)|^2\right]\psi(x) = \mu\,\psi(x). \tag{2.6}$$

The time-dependent version of this equation is, by analogy with the standard Schrödinger equation,

$$i\partial_t\psi(x,t) = \left[-\partial_x^2 + 2c|\psi(x,t)|^2\right]\psi(x,t), \tag{2.7}$$

and an obvious solution is

$$\psi(x,t) = \psi(x)\mathrm{e}^{-i\mu t}. \tag{2.8}$$

Eq. (2.7) may be derived directly from the least action principle $\delta\int dt\,L = 0$ for the Lagrangian (Pethick and Smith, 2008)

$$\begin{aligned} L[\psi,\psi^*] &= \frac{i}{2}\int dx\,(\psi^*\partial_t\psi - \psi\partial_t\psi^*) - E_N[\psi,\psi^*] \\ &= \int dx\left[\frac{i}{2}(\psi^*\partial_t\psi - \psi\partial_t\psi^*) - |\partial_x\psi|^2 - c|\psi|^4\right], \end{aligned} \tag{2.9}$$

that is equivalent to consider Eq. (2.7) as the equation of motion of a classical field with Hamiltonian $H = E_N = \int dx\,\mathcal{H}$,

$$i\partial_t\psi(x,t) = \frac{\delta\mathcal{H}[\psi,\psi^*]}{\delta\psi^*}. \tag{2.10}$$

It may also be obtained from the Heisenberg equation of motion (1.4), by approximating the field operator $\hat\psi(x,t)$ by its expectation value in the state (2.1). Indeed, $|\,\Psi_N\,\rangle = [\hat\psi^\dagger(\phi)]^N|\,0\,\rangle = (N!)^{-1/2}\int dx_1\cdots dx_N\,\phi(x_1)\cdots\phi(x_N)\hat\psi^\dagger(x_1)\cdots\psi^\dagger(x_N)|\,0\,\rangle$, thus under the assumption that $N \gg 1$, which implies $\hat\psi(\phi)|\,\Psi_N\,\rangle \simeq \sqrt{N}\phi(x)|\,\Psi_N\,\rangle$, the average of $\hat\psi(x,t)$ is $\langle\,\Psi_N\,|\,\hat\psi(x,t)\,|\,\Psi_N\,\rangle = \sqrt{N}\phi(x,t) = \psi(x,t)$.

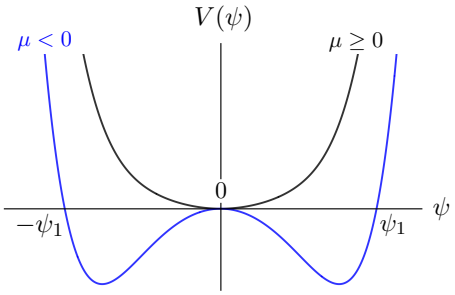


Figure 2.1: The two possible behaviors of the potential $V(\psi)$ for $\mu \geq 0$ and $\mu < 0$.

2.1.1 Bright solitons

For attractive interaction (self-focusing nonlinearity), Eq. (2.6) reads

$$-\psi''(x) - 2\bar{c}\,|\psi(x)|^2\psi(x) = \mu\,\psi(x), \tag{2.11}$$

where the primes denote derivatives with respect to x. We are interested in normalizable solutions, that must therefore vanish asymptotically. This implies that $\psi(x)$ must be real up to a constant phase factor. To show this, let us insert in Eq. (2.11) the polar representation $\psi(x) = A(x)\mathrm{e}^{i\theta(x)}$, with $A(x) > 0$ and $\theta(x)$ real. This yields the two coupled equations

$$-A''(x) + A(x)[\theta'(x)]^2 - 2\bar{c}A^3(x) = \mu A(x), \tag{2.12a}$$

$$\theta''(x)A(x) + 2\theta'(x)A'(x) = 0. \tag{2.12b}$$

The second equation can be rewritten as $\theta''(x)/\theta'(x) = -2A'(x)/A(x)$ and thus immediately integrated, yielding $\theta'(x) = \alpha[A(x)]^{-2}$ for an arbitrary real constant α. Inserting this in (2.12a) we get

$$-A''(x) + \alpha^2 A^{-3}(x) - 2\bar{c}A^3(x) = \mu A(x). \tag{2.13}$$

Considering this equation in the asymptotic region, where $A(x)$ and its derivatives are required to vanish, we conclude that it must be $\alpha = 0$ and thus $\theta(x) = \theta_0 = \text{const.}$ Hereafter we can ignore this constant phase factor and consider $\psi(x)$ as a real field. Eq. (2.11) can then be rewritten as

$$\psi''(x) = -\frac{\partial V(\psi)}{\partial \psi}, \qquad \text{with} \qquad V(\psi) = \frac{\psi^2}{2}\left(\mu + \bar{c}\,\psi^2\right). \tag{2.14}$$

Now this is a second-order differential equation that can be easily integrated by quadratures. The 1D GPE is thus a classical integrable model. If we think of x as 'time' and ψ as the coordinate of a unit-mass point particle, then (2.14) is just Newton's second law for this particle's motion in a potential given by $V(\psi)$, and $\psi(x)$ is the corresponding trajectory. Such mechanical analogues are quite common in the treatment of classical solitons (Rajaraman, 1982). The total 'energy' of the motion, conserved as x varies, is given by

$$\mathcal{E} = \frac{1}{2}(\psi')^2 + V(\psi) = \text{const.} = 0, \tag{2.15}$$

since the boundary conditions discussed above require that $V(\psi) \to 0$ and $\psi' \to 0$ for $x \to \pm\infty$. It follows that a non-trivial solution exists only for $\mu < 0$. In fact, for $\mu \geq 0$ the potential $V(\psi)$ has a unique minimum for $\psi = \psi_0 = 0$, where it takes the value zero (Fig. 2.1). The boundary conditions demand a zero-energy trajectory beginning and ending at ψ_0 in the far past and far future ($x = \pm\infty$). It is clear that in this case the only possible trajectory is the equilibrium one, namely the trivial solution $\psi(x) = \psi_0$. Instead, for $\mu < 0$

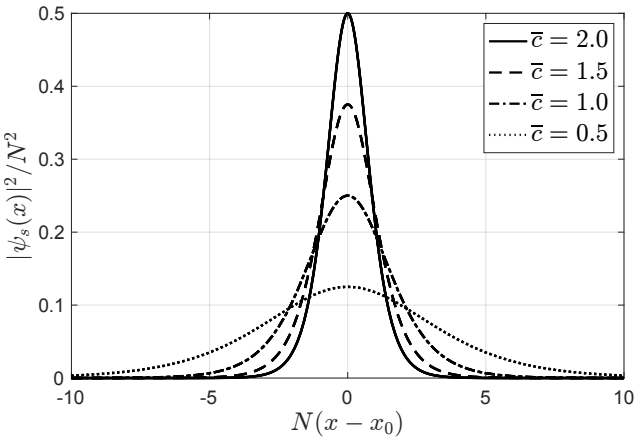


Figure 2.2: Probability density of the bright soliton $\psi_s(x)$ for different values of the interaction parameter $\overline{c}$ and arbitrary number of particles N.

the potential $V(\psi)$ has a local maximum for $\psi = \psi_0$, where it takes the value zero, and two local minima (Fig. 2.1). There are now two non-trivial zero-energy trajectories beginning and ending at ψ_0, which corresponds to the particle moving to the right (left) up to the point ψ_1 ($-\psi_1$) where the potential crosses the value zero, and coming back to ψ_0. Therefore we take $\mu = -|\mu|$. From (2.15) we get $\psi' = \pm\sqrt{-2V(\psi)}$, that gives

$$\int_{x_0}^{x} dx = \pm \int_{\psi(x_0)}^{\psi(x)} \frac{d\psi}{\sqrt{|\mu|\psi^2 - \overline{c}\,\psi^4}}. \tag{2.16}$$

We take as 'initial condition' $\psi'(x_0) = 0$, so that x_0 represents the time at which the particle inverts its motion; hence $V(\psi(x_0)) = 0$ and $\psi(x_0) = \sqrt{|\mu|/\overline{c}}$. Changing integration variable from ψ to $\zeta = \sqrt{\overline{c}/|\mu|}\psi$, we obtain

$$x - x_0 = \frac{\pm 1}{\sqrt{|\mu|}} \int_1^{\zeta(x)} \frac{d\zeta}{\zeta\sqrt{1-\zeta^2}} = \frac{\mp 1}{\sqrt{|\mu|}} \operatorname{arcsech}\zeta(x), \tag{2.17}$$

that gives $\psi(x) = \sqrt{|\mu|/\overline{c}}\,\operatorname{sech}\left[\sqrt{|\mu|}(x-x_0)\right]$. The value of μ is then fixed by imposing the normalization condition $\int dx\,|\psi(x)|^2 = N$; this yields $|\mu| = -\mu = N^2\overline{c}^2/4$ and finally

$$\psi_s(x) = \frac{N\sqrt{\overline{c}}}{2} \operatorname{sech}\left[\frac{N\overline{c}}{2}(x-x_0)\right] \mathrm{e}^{i\theta_0}, \tag{2.18}$$

where we have reintroduced the constant phase factor $\exp(i\theta_0)$. The arbitrariness of x_0 originates from the translational invariance of Eq. (2.11). This solution is called a bright soliton and the corresponding probability density is shown in Fig. 2.2. The term 'bright' refers to the fact the amplitude of $\psi_s(x)$ is positive, but we postpone the discussion of the term 'soliton' to Section 2.4.

2.1.2 Ground state energy

Substituting the solution $\psi_s(x)$ into $E_N[\psi, \psi^*]$ we obtain the estimate for the ground state energy,

$$E_{\mathrm{gs}}^{(\mathrm{GP})} = \int dx \Big[|\partial_x \psi_s(x)|^2 - \overline{c}\,|\psi_s(x)|^4 \Big] = -\frac{\overline{c}^2}{12} N^3. \tag{2.19}$$

The superscript (GP) refers to the fact that we have considered the the energy functional in the Gross-Pitaevskii approximation, where a factor of $(1 - N^{-1})$ in front of the quartic

term $|\psi(x)|^4$ is neglected (cf. Eq. (2.2))[2]. To evaluate the ground state energy in the proper Hartree approximation, it is sufficient to correct the value of $\bar{c}$ in the previous result by a factor of $(1 - N^{-1})$, i.e. $\bar{c} \to (1 - N^{-1})\bar{c}$, which yields

$$E_{\rm gs}^{\rm (H)} = -\frac{\bar{c}^2}{12} N(N-1)^2. \tag{2.20}$$

A variation of Hartree's method is proposed by Calogero and Degasperis (1975) (CD), where the expectation value of the center-of-mass Hamiltonian, $H_{\rm c.m.} = -N^{-1}\partial^2/\partial x_{\rm c.m.}^2$, $x_{\rm c.m.} = \sum_{j=1}^{N} x_j/N$, is subtracted from the expectation value of the N-body Hamiltonian. The intention of this approach is to correct (at least partially) the error introduced by the fact that the trial wavefunction (2.1) is not translationally invariant. The modified Hartree functional is

$$E_N^{\rm (CD)}[\phi, \phi^*] = N \int dx \Big[\left(1 - N^{-1}\right) |\partial_x \phi(x)|^2 - (N-1)\bar{c}|\phi(x)|^4 \Big], \tag{2.21a}$$

or in terms of $\psi(x)$, $\psi^*(x)$,

$$E_N^{\rm (CD)}[\psi, \psi^*] = \left(1 - N^{-1}\right) \int dx \Big[|\partial_x \psi(x)|^2 - \bar{c}|\psi(x)|^4 \Big]. \tag{2.21b}$$

Thus the corresponding ground state energy differs from the one obtained in the GP approximation by a factor of $(1 - N^{-1})$,

$$E_{\rm gs}^{\rm (CD)} = -\frac{\bar{c}^2}{12} N^2(N-1). \tag{2.22}$$

The comparison of these mean-field results with the exact ground state energy $E_{\rm gs}$ deduced from the Bethe Ansatz, given by Eq. (1.53), is straightforward (Fig. 2.3).

For completeness, we now show how one can perturbatively correct the mean-field results. Of course, this is not of great interest for our problem, because we already know the complete exact solution, but it may be of methodological interest for those cases where the exact solution is not known. Let us consider the standard Hartree approximation. We define the unperturbed Hamiltonian to include the mean field,

$$H_0 = \sum_{i=1}^{N} \Big[-\partial_{x_i}^2 + U(x_i) \Big], \tag{2.23}$$

where

$$U(x) = -2(1 - N^{-1})\bar{c}\,\rho^{\rm (H)}(x) = -\frac{(N-1)^2\bar{c}^2}{2} \operatorname{sech}^2 \left[\frac{(N-1)\bar{c}}{2}\, x \right], \tag{2.24}$$

and consider as a small perturbation the difference between the exact interaction potential and the mean field,

$$V = -2\bar{c} \sum_{i<j} \delta(x_i - x_j) - \sum_{i=1}^{N} U(x_i). \tag{2.25}$$

The second-order correction to ground state energy is then

$$\Delta E^{(2)} = \sum_i \frac{|\langle\, \Psi_i \,|\, \hat{V} \,|\, \Psi_{\rm gs}^{\rm (H)} \,\rangle|^2}{E_{\rm gs}^{\rm (H)} - E_i}, \tag{2.26}$$

[2]This nomenclature is not universal, and we only use it to distinguish this approximation from the one in which one retains the factor $(1 - N^{-1})$ in front of the quartic term, which we will call the Hartree approximation.

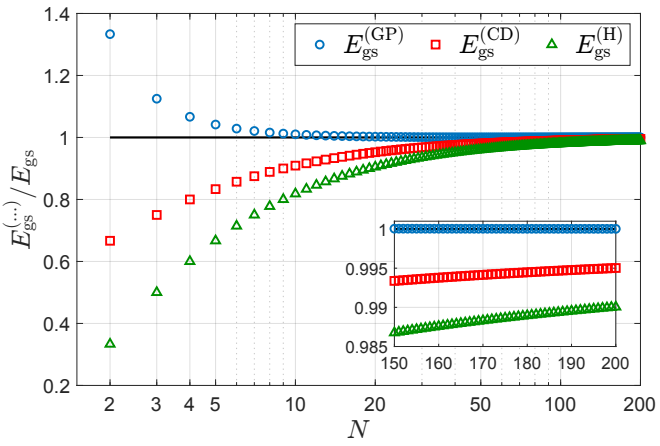


Figure 2.3: Ratio between the mean-field results $E_{\rm gs}^{(...)}$ (2.19), (2.20), (2.22), and the exact result $E_{\rm gs}$ (1.53) for the ground state energy of the attractive Lieb-Liniger gas. All these energies are negative, thus $E_{\rm gs}^{\rm (CD)}$ and $E_{\rm gs}^{\rm (H)}$, which are obtained from the minimization of the expectation value of the Hamiltonian, provide an upper bound to the exact ground state energy, according to the variational theorem. This is not true for $E_{\rm gs}^{\rm (GP)}$, since it is obtained by further approximating a term in the expectation value. Nevertheless, the latter provides the best approximation of the exact result, the error being of 1% already for $N = 10$ and of 0.25% for $N = 20$.

where $|\,\Psi_{\rm gs}^{\rm (H)}\,\rangle$ is the Hartree ground state, in which all the particles occupy the single-particle state $|\,\phi_s\,\rangle$, $E_{\rm gs}^{\rm (H)}$ is the corresponding energy (2.20), and $\{|\,\Psi_i\,\rangle\}$ is a complete set of excited eigenstates of H_0 constructed from symmetrized products of single-particle eigenfunctions satisfying (Cohen-Tannoudji et al., 2020)

$$\Big[-\partial_x^2 + U(x)\Big]\phi_k(x) = \epsilon_k \phi_k(x). \tag{2.27}$$

The energies E_i are the sums of the eigenvalues ϵ_k of the occupied single-particle states.

The potential (2.24) belongs to the class of Pöschl-Teller potentials, whose Schrödinger equation (2.27) has long been known to be exactly solvable (Pöschl and Teller, 1933; Landau and Lifshitz, 1981). With $\alpha = (N-1)\bar{c}/2$, the Schrödinger equation is

$$\phi''(x) + \left(2\alpha^2 \mathrm{sech}^2(\alpha x) + \epsilon\right)\phi(x) = 0, \tag{2.28}$$

and with the change of variables $\xi = \tanh(\alpha x) \in (-1, 1)$, $\nu = \sqrt{-\epsilon/\alpha^2}$, $\phi(\xi) = (1-\xi^2)^{\nu/2}$, and $u = (1-\xi)/2$, we obtain

$$u(1-u)w''(u) + (\nu+1)(1-2u)w'(u) - (\nu-1)(\nu+2)w(u) = 0. \tag{2.29}$$

This is an hypergeometric differential equation and its solutions are given in terms of the hypergeometric function ${}_2F_1(a, b; c; z)$[3].

For negative ϵ, $\nu \in \mathbb{R}^+$, and the finite solution for $\xi = 1$ (i.e. $x = +\infty$) is

$$\phi(\xi) = (1-\xi^2)^{\nu/2}\, {}_2F_1\left(\nu - 1,\, \nu + 2;\, \nu + 1;\, \frac{1-\xi}{2}\right). \tag{2.30}$$

For $\phi(\xi)$ to remain finite also for $\xi = -1$ (i.e. $x = -\infty$), we must have $\nu - 1 = -n$, where n is a non-negative integer[4]. Then ${}_2F_1$ is a polynomial of degree n, and the energy levels for

[3] See Olver et al. (2010), Ch. 15, for details.
[4] See Olver et al. (2010), Eq. 15.8.4.

$\epsilon < 0$ are determined by the condition $1 - \nu = n$. The only possibility is $\nu = 1$, which gives $\epsilon = -\alpha^2$ and $\phi(x) = [1 - \tanh^2(\alpha x)]^{1/2} = \mathrm{sech}(\alpha x)$, that is exactly the soliton of the GPE.

For positive ϵ, ν is imaginary, and we can set $\nu = ik$ with $\epsilon = \alpha^2 k^2$. In this case we have two independent solutions around $\xi = 0$ (i.e. $x = 0$), namely

$$\phi_1(\xi) = (1-\xi^2)^{ik/2}\, {}_2F_1\left(ik-1,\, ik+2;\, ik+1;\, \frac{1-\xi}{2}\right) = \phi_{-k}(x) \tag{2.31}$$

and

$$\phi_2(\xi) = (1-\xi^2)^{ik/2} \left(\frac{1+\xi}{2}\right)^{-ik} {}_2F_1\left(-1,\, 2;\, 1-ik;\, \frac{1-\xi}{2}\right) = \phi_k(x), \tag{2.32}$$

where

$$\phi_k(x) = 2^{ik} \mathrm{e}^{ik\alpha x}\, \frac{\tanh(\alpha x) - ik}{1 - ik}. \tag{2.33}$$

These solutions are finite for any $k \geq 0$, therefore the spectrum is continuous for positive energy. If we allow k to take on any real value, the eigenfunctions are, up to a phase factor independent of x,

$$\phi_k(x) = \mathrm{e}^{ik(N-1)\bar{c}\,x/2}\, \frac{\tanh[(N-1)\bar{c}\,x/2] - ik}{1 + ik}, \tag{2.34}$$

with eigenvalues

$$\epsilon_k = \frac{\bar{c}^2}{4}(N-1)^2 k^2. \tag{2.35}$$

Having determined the eigenfunctions and the spectrum of H_0, one can then explicitly compute the second order energy correction $\Delta E^{(2)}$, finding (Yoon and Negele, 1977)

$$\Delta E^{(2)} \simeq -0.9956\, \frac{\bar{c}^2}{12} N(N-1). \tag{2.36}$$

This correction accounts for almost half of the difference between the exact E_{gs} and the Hartree estimate $E_{\mathrm{gs}}^{(\mathrm{H})}$,

$$E_{\mathrm{gs}} - E_{\mathrm{gs}}^{(\mathrm{H})} = -\frac{\bar{c}^2}{6} N(N-1) \simeq 2.0088\, \Delta E^{(2)}. \tag{2.37}$$

2.2 Ground state density profile

Knowing both the exact and the mean-field ground state wavefunctions, we can compare the corresponding density profiles. The number density operator is

$$\hat{\rho}(x) = \sum_{i=1}^{N} \delta(x - \hat{x}_i) \tag{2.38}$$

and its average in the ground state is

$$\begin{aligned} \rho(x) &= \sum_{i=1}^{N} \int dx_1 \cdots dx_N\, \delta(x - x_i) |\Psi_N(x_1, \ldots, x_N)|^2 \\ &= N \int dx_2 \cdots dx_N\, |\Psi_N(x, x_2, \ldots, x_N)|^2. \end{aligned} \tag{2.39}$$

In the mean-field approach, the ground state wavefunction (2.1) is factorized in the product of N identical single-particle states. Within the GP and CD approximations, the normalized

single-particle states are $\phi_s(x) = N^{-1/2}\psi_s(x)$, where $\psi_s(x)$ is the bright soliton (2.18). Therefore

$$\rho^{(\mathrm{GP,\ CD})}(x) = N|\phi_s(x)|^2 = |\psi_s(x)|^2. \tag{2.40}$$

The maximum of the density occurs at $x = x_0$ and is

$$\rho^{(\mathrm{GP,\ CD})}(x_0) = \frac{\overline{c}}{4}N^2. \tag{2.41}$$

In the Hartree approximation, the value of $\overline{c}$ appearing in Eq. (2.18) is corrected by a factor of $(1 - N^{-1})$, thus

$$\rho^{(\mathrm{H})}(x) = |\psi_s(x)|^2\Big|_{\overline{c}\to(1-N^{-1})\overline{c}} \tag{2.42}$$

and

$$\rho^{(\mathrm{H})}(x_0) = \frac{\overline{c}}{4}N(N-1). \tag{2.43}$$

The exact ground state wavefunction obtained from the Bethe Ansatz is instead given by Eq. (1.57). Since it is translational invariant, i.e. $\Psi_{\mathrm{gs}}(\mathbf{x}) = \Psi_{\mathrm{gs}}(\mathbf{x} + b\mathbf{1})$ for any real b, the average density of the ground state satisfies $\rho(x) = \rho(x + b)$, and therefore is uniform and equal to

$$\rho_{\mathrm{gs}}(x) = N\int dx_2\cdots dx_N\,|\Psi_{\mathrm{gs}}(x, x_2, \ldots, x_N)|^2 = \frac{N}{L}. \tag{2.44}$$

However there is a way in which the exact ground state wavefunction can be associated with the bright soliton known from the mean field description. In fact, a bright soliton structure emerges when one measures the particles' positions, although, due to the translational invariance of the many-body ground state, in each realization of the measurement process the soliton is centered at a random position, corresponding to the center of mass position of the measured particles (Staroń et al., 2020). Therefore, the average density of the ground state in many realizations of the measurement is indeed uniform, but a single determination of the particles' positions fixes a specific position for the center of mass, and this gives rise to a bright soliton-like density profile.

To show this, the value of the normalization constant $\mathcal{N}_N$ of $\Psi_{\mathrm{gs}}(\mathbf{x})$ shall be fixed in such a way that the norm squared of the wavefunction for a fixed value x_0 of the center of mass position $x_{\mathrm{c.m.}} = \sum_{j=1}^N x_j/N$ is equal to unity (Calogero and Degasperis, 1975; Castin, 2009). Without loss of generality we can take $x_0 = 0$, that is equivalent to consider the coordinates x_j as the positions with respect to the center of mass. Thus the normalization condition reads

$$\int dx_1\cdots dx_N\,\delta(x_{\mathrm{c.m.}})|\Psi_{\mathrm{gs}}(x_1, \ldots, x_N)|^2 = 1. \tag{2.45}$$

Exploiting the bosonic symmetry of the wavefunction, the integral to compute is $N!$ times the integral over the fundamental domain $D_N : x_1 < \cdots < x_N$, where the wavefunction can be conveniently expressed in the form $\Psi_{\mathrm{gs}}(x_1, \ldots, x_N) = \mathcal{N}_N \exp(-\frac{\overline{c}}{2}\sum_{j=1}^N \alpha_j x_j)$, with $\alpha_j = 2j - N - 1$ (see Eq. (1.56)). Thus

$$N!\,|\mathcal{N}_N|^2\int_{D_N} dx_1\cdots dx_N\,\delta\left(\frac{1}{N}\sum_{j=1}^N x_j\right)\exp\left(-\overline{c}\sum_{j=1}^N \alpha_j x_j\right) = 1. \tag{2.46}$$

With the change of variables, of Jacobian equal to unity, $x_j = \sum_{k=1}^j u_k$, the condition that $(x_1, \ldots, x_N)$ is in D_N becomes that $u_2, \ldots, u_N$ are positive, and u_1 can vary over the entire real line. Using $\sum_{j=1}^N x_j = \sum_{j=1}^N\sum_{k=1}^j u_k = \sum_{k=1}^N (N + 1 - k)u_k$ and $\sum_{j=1}^N \alpha_j x_j =$

$\sum_{j=1}^{N}(2j-N-1)\sum_{k=1}^{j}u_k=\sum_{k=1}^{N}(\sum_{j=k}^{N}(2j-N-1))u_k=\sum_{k=1}^{N}(N+1-k)(k-1)u_k$, Eq. (2.46) is then

$$\begin{aligned}1&=N!\,|\mathcal{N}_N|^2\int_{\mathbb{R}}du_1\int_{(\mathbb{R}^+)^{N-1}}du_2\cdots du_N\,\delta\Big(\sum_{k=1}^{N}\frac{N+1-k}{N}u_k\Big)\exp\Big(-\overline{c}\sum_{k=2}^{N}(N+1-k)(k-1)u_k\Big)\\&=N!\,|\mathcal{N}_N|^2\prod_{k=2}^{N}\int_0^{\infty}du_k\,\mathrm{e}^{-\overline{c}(N+1-k)(k-1)u_k}\\&=N!\,|\mathcal{N}_N|^2\,\overline{c}^{1-N}\prod_{k=2}^{N}\frac{1}{(N+1-k)(k-1)}\\&=N!\,|\mathcal{N}_N|^2\,\overline{c}^{1-N}\,[(N-1)!]^{-2}.\end{aligned}\tag{2.47}$$

Therefore

$$|\mathcal{N}_N|^2=\overline{c}^{N-1}\frac{(N-1)!}{N}.\tag{2.48}$$

The average of the density operator is now

$$\rho_{\mathrm{gs}}(x)=N\int dx_1\cdots dx_N\,\delta(x_{\mathrm{c.m.}})\delta(x-x_1)|\Psi_{\mathrm{gs}}(x_1,\ldots,x_N)|^2\tag{2.49}$$

where x clearly represents the distance from the center of mass. Bringing the factor N^{-1} outside of $\delta(x_{\mathrm{c.m.}})$, we obtain

$$\rho_{\mathrm{gs}}(x)=N^2\,|\mathcal{N}_N|^2\,\overline{c}^{2-N}\,I_N(\overline{c}\,x),\tag{2.50}$$

where we have defined

$$I_N(t)=\int dt_1\cdots dt_N\,\delta\Big(\sum_{j=1}^{N}t_j\Big)\delta(t-t_1)\exp\Big(-\sum_{j>k}|t_j-t_k|\Big)=\frac{N!}{N}\sum_{n=1}^{N}I_{N,n}(t),\tag{2.51}$$

$$I_{N,n}(t)=\int_{-\infty}^{+\infty}dt_N\int_{-\infty}^{t_N}dt_{N-1}\cdots\int_{-\infty}^{t_2}dt_1\,\delta\Big(\sum_{j=1}^{N}t_j\Big)\delta(t-t_n)\exp\Big(-\sum_{j=1}^{N}\alpha_j t_j\Big).\tag{2.52}$$

Clearly $I_{N,n}(t)$ is an even function of t; hereafter we assume, for convenience, that $t>0$. Let us now consider the Fourier transform of $I_{N,n}(t)$, that is $\widetilde{I}_{N,n}(\nu)=\int dt\,\mathrm{e}^{-i\nu t}I_{N,n}(t)$. Writing $\delta(\sum_{j=1}^{N}t_j)=(2\pi)^{-1}\int d\omega\,\exp(i\omega\sum_{j=1}^{N}t_j)$, we get

$$\begin{aligned}\widetilde{I}_{N,n}(\nu)&=\int\frac{d\omega}{2\pi}\int_{-\infty}^{+\infty}dt_N\,\mathrm{e}^{(i\omega-\alpha_N)t_N}\int_{-\infty}^{t_N}dt_{N-1}\,\mathrm{e}^{(i\omega-\alpha_N)t_{N-1}}\cdots\\&\quad\cdots\int_{-\infty}^{t_{n+1}}dt_n\,\mathrm{e}^{(i\omega-i\nu-\alpha_n)t_n}\cdots\int_{-\infty}^{t_2}dt_1\,\mathrm{e}^{(i\omega-\alpha_1)t_1}\\&=\int d\omega\,\Big(\prod_{j=1}^{N-1}\sum_{k=1}^{j}\Big(i\omega-\alpha_k^{(n)}\Big)\Big)^{-1}\delta\Big(\sum_{k=1}^{N}\Big(\omega+i\alpha_k^{(n)}\Big)\Big)\\&=\Big(N\prod_{j=1}^{N-1}\sum_{k=1}^{j}\Big(A-\alpha_k^{(n)}\Big)\Big)^{-1},\end{aligned}\tag{2.53}$$

where

$$\alpha_k^{(n)}=\alpha_k+i\nu\delta_{kn},\tag{2.54}$$

$$A=\frac{1}{N}\sum_{k=1}^{N}\alpha_k^{(n)}=\frac{i\nu}{N},\tag{2.55}$$

and δ_{kn} is the Kronecker delta. Since $\sum_{k=1}^{j} \delta_{kn}$ is equal to unity if $j \geq n$ and equal to zero if $j < n$, we have

$$\begin{aligned}
&N \prod_{j=1}^{N-1} \sum_{k=1}^{j} \left(\frac{i\nu}{N} - \alpha_k - i\nu\delta_{kn} \right) \\
&= N \prod_{j=1}^{n-1} \left[j \left(\frac{i\nu}{N} + N - j \right) \right] \prod_{j=n}^{N-1} \left[(-1)(N-j) \left(\frac{i\nu}{N} - j \right) \right] \\
&= N(N-n)!(n-1)!(-1)^{N-n} \left(\frac{i}{N} \right)^{N-1} \prod_{j=1}^{n-1} \big[\nu - iN(N-j) \big] \prod_{j=n}^{N-1} \big[\nu + iNj \big]
\end{aligned} \tag{2.56}$$

and therefore

$$\widetilde{I}_{N,n}(\nu) = \frac{(-1)^n i^{N+1} N^{N-2}}{(N-n)!(n-1)!} \prod_{j=1}^{N-1} \left(\nu - \nu_j^{(n)} \right)^{-1}, \tag{2.57}$$

where

$$\nu_j^{(n)} = \begin{cases} iN(N-j), & j = 1, \ldots, n-1, \\ -iNj, & j = n, \ldots, N-1. \end{cases} \tag{2.58}$$

We can now evaluate the Fourier anti-transform

$$I_{N,n}(t) = \int \frac{d\nu}{2\pi} \, \mathrm{e}^{i\nu t} \, \widetilde{I}_{N,n}(\nu) \tag{2.59}$$

using Jordan's lemma and the residue theorem. Assuming that $t > 0$, $\mathrm{e}^{i\nu t} = \mathrm{e}^{i \operatorname{Re}(\nu) t - \operatorname{Im}(\nu) t}$ goes to zero for $\operatorname{Im}(\nu) \to +\infty$, thus we close the integration contour in the upper half-plane, and the integral is given by the sum of the residues at the poles $\nu_j = iN(N-j)$, $j = 1, \ldots, n-1$,

$$I_{N,n}(t) = i \, \frac{(-1)^n i^{N+1} N^{N-2}}{(N-n)!(n-1)!} \sum_{j=1}^{n-1} \mathrm{e}^{-N(N-j)t} \prod_{\substack{k=1 \\ k \neq j}}^{N-1} \big(\nu_j - \nu_k \big)^{-1}. \tag{2.60}$$

The product on the right-hand side is

$$\begin{aligned}
\prod_{\substack{k=1 \\ k \neq j}}^{N-1} \big(\nu_j - \nu_k \big)^{-1} &= \prod_{k=1}^{j-1} \big(\nu_j - \nu_k \big)^{-1} \prod_{k=j+1}^{n-1} \big(\nu_j - \nu_k \big)^{-1} \prod_{k=n}^{N-1} \big(\nu_j - \nu_k \big)^{-1} \\
&= (iN)^{2-N} \prod_{k=1}^{j-1} (k-j)^{-1} \prod_{k=j+1}^{n-1} (k-j)^{-1} \prod_{k=n}^{N-1} (N+k-j)^{-1} \qquad (2.61) \\
&= (iN)^{2-N} (-1)^{j+1} \frac{(N+n-j-1)!}{(j-1)!(n-j-1)!(2N-j-1)!}. \qquad (2.62)
\end{aligned}$$

Substituting this into Eq. (2.60), and the result into Eq. (2.51), we obtain

$$I_N(t) = (N-1)! \sum_{n=1}^{N} \frac{(-1)^{n+1}}{(N-n)!(n-1)!} \sum_{j=1}^{n-1} \frac{(-1)^j (N+n-j-1)! \, \mathrm{e}^{-N(N-j)t}}{(j-1)!(n-j-1)!(2N-j-1)!}. \tag{2.63}$$

It is convenient to perform the change of variables $j = N - m$, $n = N - r$, which yields

$$I_N(t) = (N-1)! \sum_{m=1}^{N-1} \frac{(-1)^{m+1} \mathrm{e}^{-mNt}}{(N+m-1)!(N-m-1)!} \sum_{r=0}^{m-1} \frac{(-1)^r (N+m-1-r)!}{r!(m-1-r)!(N-1-r)!}, \tag{2.64}$$

because now the sum over r can be performed using Saalschütz's theorem on generalized hypergeometric functions,

$$\sum_{r=0}^{n} \frac{(a)_r (b)_r (-n)_r}{r!\,(c)_r (1+a+b-c-n)_r} = \frac{(c-a)_n (c-b)_n}{(c)_n (c-a-b)_n}, \tag{2.65}$$

where $(a)_n = a(a+1)(a+2)\cdots(a+n-1) = \Gamma(a+n)/\Gamma(a)$, $n \geq 1$, $(a)_0 = 1$, is the rising factorial or Pochhammer symbol (Slater, 1966). To apply this formula to our case, we set $a = 1-N$, $n = m-1$, and $c = b+2$, and take the limit $b \to +\infty$. Eq. (2.65) then gives

$$\begin{aligned} \frac{\Gamma(N)\,\Gamma(m)}{\Gamma(N+m)} \sum_{r=0}^{m-1} \frac{(-1)^r (N+m-1-r)!}{r!(m-1-r)!(N-1-r)!} \frac{(b)_r}{(b+2)_r} \\ = \frac{\Gamma(N)\,\Gamma(m)}{\Gamma(N+m)}\, mN\, \frac{(b+1-N)_{m-1}}{(b+2)_{m-1}} \end{aligned} \tag{2.66}$$

and in the limit $b \to +\infty$ the terms containing b simplify. Therefore the sum over r in Eq. (2.64) gives mN, and

$$I_N(t) = N! \sum_{m=1}^{N-1} \frac{(-1)^{m+1} m\, \mathrm{e}^{-mNt}}{(N+m-1)!(N-m-1)!}. \tag{2.67}$$

Substituting this into Eq. (2.50) and using the expression (2.48) for $|\mathcal{N}_N|^2$, we arrive at

$$\rho_{\mathrm{gs}}(x) = \sum_{n=1}^{N-1} (-1)^{n+1} \frac{(N!)^2\, n\, \overline{c}\, \mathrm{e}^{-nN\overline{c}\,|x|}}{(N+n-1)!(N-n-1)!}, \tag{2.68}$$

a result originally obtained by Calogero and Degasperis (1975). The maximum of the density occurs at $x = 0$ (i.e. at the position of the center of mass) and is

$$\rho_{\mathrm{gs}}(0) = \sum_{n=1}^{N-1} (-1)^{n+1} \frac{(N!)^2\, n\, \overline{c}}{(N+n-1)!(N-n-1)!} = \frac{\overline{c}}{2} \frac{N^2(N-1)}{(2N-3)}. \tag{2.69}$$

We can verify that in the limit $N \to \infty$ the exact $\rho_{\mathrm{gs}}(x)$ reduces to the mean field result $|\psi_s(x)|^2$ (with $x_0 = 0$). Using Stirling's approximation,

$$\begin{aligned} \frac{(N!)^2}{(N+n-1)!(N-n-1)!} &\simeq N^2 \left(1+\frac{n}{N}\right)^{1/2-N-n} \left(1-\frac{n}{N}\right)^{1/2-N+n} \\ &\simeq N^2 \left[1 - n^2 + O(N^{-1})\right], \end{aligned} \tag{2.70}$$

and the identities $(1-n^2) = (1-N^{-1}) + N^{-1}(1-n^2)$, $\sum_{n=1}^{\infty} (-1)^{n+1} n\, \mathrm{e}^{-2nt} = \frac{1}{4}\mathrm{sech}^2(t)$, $\sum_{n=1}^{\infty} (-1)^{n+1} n (1-n^2) \mathrm{e}^{-2nt} = \frac{3}{8}\mathrm{sech}^4(t)$, we obtain indeed

$$\rho_{\mathrm{gs}}(x) \overset{N\to\infty}{\simeq} \frac{N^2\overline{c}}{4}\, \mathrm{sech}^2\left(\frac{N\overline{c}}{2}\, x\right) \left\{1 - \frac{1}{N}\left[1 - \frac{3}{2}\mathrm{sech}^2\left(\frac{N\overline{c}}{2}\, x\right)\right] + O(N^{-2})\right\}. \tag{2.71}$$

In Fig. 2.4 we compare the exact and the mean-field results for few particles. We notice the mean-field results systematically underestimate the central value of the density and therefore the sharpness of the peak. The GP and CD approximations work better than the standard Hartree approximation, and as expected, in the limit of a large number of particles the mean field results approximate increasingly better the exact result.

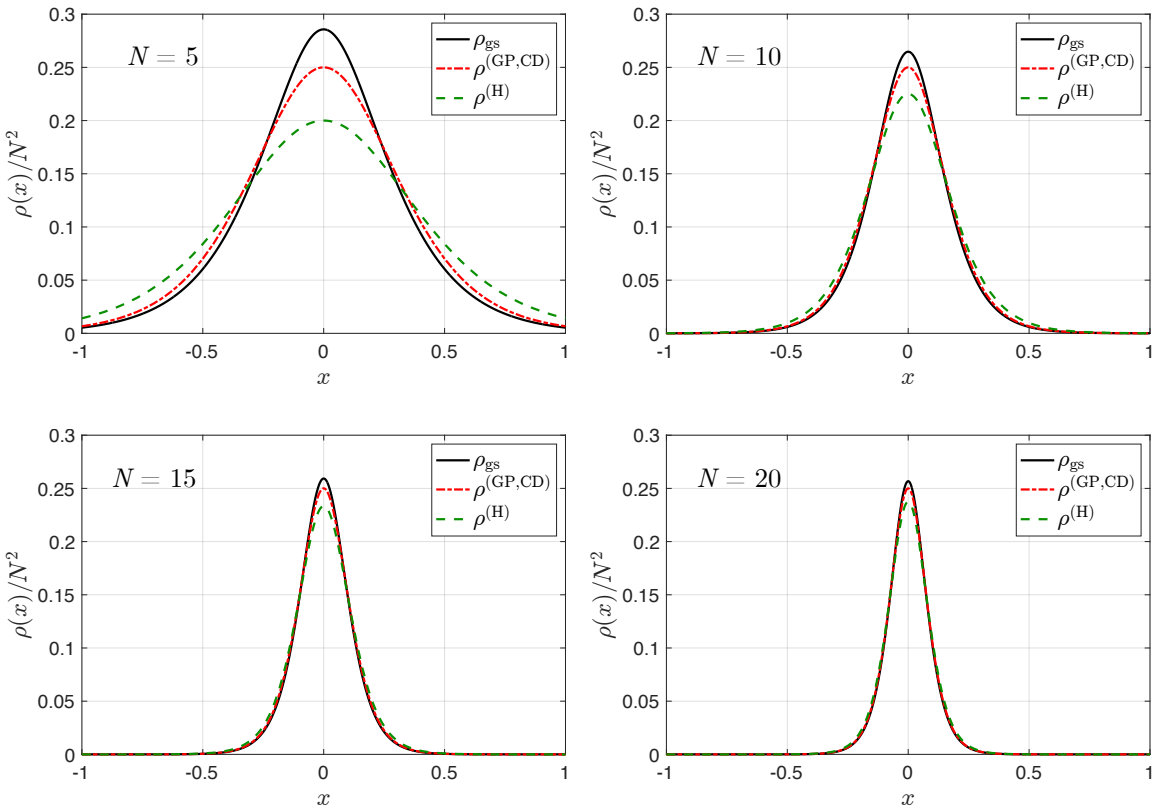


Figure 2.4: Comparison between the mean field results $\rho^{(\mathrm{GP,\ CD})}$ (2.40), $\rho^{(\mathrm{H})}$ (2.42), and the exact result $\rho_{\rm gs}$ (2.68) for the ground state density of the attractive Lieb-Liniger gas. Here the coordinate x represents the distance from the position of the center of mass. The functions are plotted for $N = 5,\ 10,\ 15,\ 20$ and $\bar{c} = 1$.

2.3 Moving soliton as a single-particle excited state

Given the stationary solution $\psi_s(x)$, a solution for the time-dependent GPE is

$$\psi_s(x,t) = \psi_s(x)\mathrm{e}^{-i\mu t}, \qquad \mu = -N^2\bar{c}^2/4. \tag{2.72}$$

Here the time dependence is contained in the overall phase factor, thus $\psi(x,t)$ still describes a bright soliton at rest. However there is an infinity of solutions of the time-dependent GPE which differ from (2.72) by a Galilean transformation, and describe a bright soliton moving at arbitrary constant velocity v. These can be obtained exploiting the Galilean invariance of the Lagrangian (2.9). Under a Galilean transformation,

$$x \to \tilde{x} = x - vt, \tag{2.73a}$$

$$\psi_s(x,t) \to \tilde{\psi}_s(\tilde{x},t) = \mathrm{e}^{i\Theta(x,t)}\psi_s(x-vt,t), \tag{2.73b}$$

and the Lagrangian is invariant provided that

$$\partial_x\Theta(x,t) = v/2, \qquad \partial_t\Theta(x,t) = -[\partial_x\Theta(x,t)]^2 = -v^2/4, \tag{2.74}$$

from which we have

$$\Theta(x,t) = \frac{1}{2}vx - \frac{1}{4}v^2t = \lambda x - \frac{1}{4}v^2t, \qquad \lambda = v/2. \tag{2.75}$$

Therefore the solution in the moving frame is

$$\psi_{N\lambda}(x,t) \equiv \tilde{\psi}_s(x-vt,t) = \exp\left[i\left(\lambda x - \frac{1}{4}v^2 t\right)\right]\psi(x-vt,t)$$
$$= \frac{N\sqrt{\bar{c}}}{2}\,\mathrm{sech}\left[\frac{N\bar{c}}{2}(x-x_0-vt)\right]\mathrm{e}^{i[\theta_0+\lambda x+(N^2\bar{c}^2-v^2)t/4]}. \quad (2.76)$$

The corresponding normalized single-particle wavefunction is $\phi_{N\lambda}(x,t) = N^{-1/2}\psi_{N\lambda}(x,t)$, in terms of which the N-body wavefunction is $\Psi_{N\lambda}(\mathbf{x},t) = \prod_{i=1}^{N}\phi_{N\lambda}(x_i,t)$, and the associated momenta and energy are

$$P_s = -i\int dx\,\psi^*_{N\lambda}(x,t)\partial_x\psi_{N\lambda}(x,t) = N\lambda, \quad (2.77)$$

$$E_s = \int dx\left[\left|\partial_x\psi_{N\lambda}(x,t)\right|^2 - \bar{c}\left|\psi_{N\lambda}(x,t)\right|^4\right] = -\frac{\bar{c}^2}{12}N^3 + \frac{P_s^2}{N}. \quad (2.78)$$

Here the energy has been calculated in the GP approximation, but can be calculated similarly in the Hartree and CD approximations using the appropriate energy functionals. The result is that E_s is given by the ground state energy (in the approximation considered) plus P_s^2/N, where $P_s = N\lambda$ is the total momentum. This is the same structure of the exact result for the energy and momentum of a single-particle excited state, constructed by giving momentum λ to the ground state N-string (see Eq. (1.59)). Therefore, just as by giving momentum to the ground state N-string we obtain an exact single-particle excited state, by giving momentum to the soliton of the GPE that approximates the ground state we obtain an approximate single-particle excited state.

2.4 Solitons and solitary waves

We are now in position to justify why we call 'soliton' the solution of the GPE. We start by clarifying the meaning of this term in the context of classical field theory, and distinguish between solitons and solitary waves, following Rajaraman (1982); Scott et al. (1973).

The names 'solitary wave' and 'soliton' refer to some special solutions of nonlinear equations of motion (or wave equations) of classical fields. The simplest wave equation is the one originally discovered by d'Alembert,

$$\partial_t^2 u(x,t) - v^2\partial_x^2 u(x,t) = 0, \quad (2.79)$$

where $u(x,t)$ is a real field in one space dimension, and v is the velocity. The properties of this equation are very well known. Its elementary solutions are the right- and left-propagating plane waves $\mathrm{e}^{\pm i(kx-\omega t)}$, satisfying the dispersion relation $\omega = vk$. Being a linear equation in the field $u(x,t)$, a linear combination of two solutions is also a solution. Therefore any function of the form $u(x-vt)$ that is sufficiently well-behaved to admit a Fourier transform $\widetilde{u}(k)$ is a solution of Eq. (2.79), since it can be written as a linear combination of the elementary solutions,

$$u(x-vt) = \int\frac{dk}{2\pi}\left[\widetilde{u}(k)\,e^{i(kx-\omega t)} + \widetilde{u}(-k)\,\mathrm{e}^{-i(kx-\omega t)}\right]. \quad (2.80)$$

These solutions have two features that are relevant to our discussion:

(i) Choosing appropriately $\widetilde{u}(k)$ (e.g. in the form of a Gaussian) we can construct a localized wave packet $u(x-vt)$ that will travel with uniform velocity v and no distortion in shape. The fact that the wave packet travels without deformation is of course due to the fact that all its plane-wave components have the same phase velocity $v = \omega/k$, i.e. that the

dispersion relation is linear in k. For this reason, a system with a linear[5] dispersion relation is said to be non-dispersive.

(ii) Thanks to the linearity of the wave equation, given two localized wave packet solutions $u_1(x-vt)$ and $u_2(x+vt)$, their sum $u_3(x,t) = u_1(x-vt)+u_2(x+vt)$ is also a solution. For $t \to -\infty$, $u_3(x,t)$ consists of the two wave packets widely separated and approaching each other essentially undistorted. Around $t = 0$, they collide, but after the collision they will asymptotically (for $t \to +\infty$) separate into the same two wave packets, retaining their original shapes and velocities.

These two features, namely (i) the shape and velocity retention of a single wave packet and (ii) the asymptotic shape and velocity retention of several wave packets after scattering with one another, hold for Eq. (2.79) because this particular equation is both linear and non-dispersive. The question is whether more complicated equations, which may contain dispersive and nonlinear terms, admit solutions that enjoy feature (i) and maybe even (ii). Solutions that enjoy feature (i) are called solitary waves. The (small) subset of these which exhibit also feature (ii) are called solitons. While all solitons are also solitary waves, the converse is clearly not true.

Generally speaking, for some equations where both dispersive and nonlinear terms are present, their effects might balance in such a way that solitary wave solutions are possible. Dispersion without nonlinearity destroys the possibility of solitary waves, because the various plane-wave components will propagate at different velocities $v(k) = \omega(k)/k$, leading to a broadening of the wave packet. On the other hand, nonlinearity without dispersion also prevents the existence of solitary waves, because the wave packet steepens to the point of breaking. This can be easily seen from the simplest example of nonlinear, non-dispersive wave equation,

$$\partial_t u(x,t) + v(u)\partial_x u(x,t) = 0, \tag{2.81}$$

where the velocity $v(u) = v_0 + \alpha u^m$, $m > 0$, depends on the amplitude u. Assuming for instance that $\alpha > 0$, the formal solution $u(x,t) = u(x - v(f)t)$ shows that the points of the wave that have grater amplitude travel faster. Thus the wave steepens and then breaks. However, with both dispersion and nonlinearity, solitary waves can again form from a balance between the tendency of the wave packet to broaden due to dispersion and to become steeper due to nonlinearity.

We shall now give a more quantitative definition of the properties (i) and (ii), in terms of the energy density (rather than the fields themselves)[6].

A solution of the equations of motion will be said localized if the corresponding energy density at fixed time is localized in space, i.e. it goes to zero at spatial infinity sufficiently rapidly as to be integrable. For a theory where $E[u] = 0$ if and only if $u(x,t) = 0$, such a localized solution also has the fields themselves localized in space.

Given localization in this sense, we define a solitary wave as a solution of the equations of motion whose energy density, as well as being localized, has a space-time dependence of the form

$$\varepsilon(x,t) = \varepsilon(x - vt) \tag{2.82}$$

where v is some constant velocity. Notice that any time-independent localized solution is automatically a solitary wave, with the velocity $v = 0$. As we have seen, assuming Galilean (or Lorentz, in high-energy context) invariance, once a static solution is known, moving

[5]Not to be confused with the (non)linearity of the wave equation, which is independent from the (non)linearity of the dispersion relation.

[6]Unfortunately there is no universal consensus on the definition of solitary waves and solitons, and different authors often adopt (slightly) different definitions. Since our definition will be given in terms if the energy density, this means that we are considering field theories that have an energy density $\varepsilon(x,t)$ which is some function of the fields $u(x,t)$, and whose space integral is the conserved total energy functional $E[u]$, i.e. the classical Hamiltonian.

solutions are trivially obtained by boosting, i.e. transforming to a moving coordinate frame. It is clear that the solution of the GPE is a solitary wave in the sense of this definition.

A soliton is a solitary wave with an additional requirement regarding its properties under scattering. Let the system have a solitary wave solution whose energy density is $\varepsilon_0(x-vt)$. Consider any other solution which in the far past consists of n such solitary waves, with arbitrary initial positions x_i and velocities v_i, $i = 1, \ldots, n$. The energy density of this solution will be

$$\varepsilon(x,t) = \sum_{i=1}^{n} \varepsilon_0(x - x_i - v_i t), \qquad t \to -\infty. \tag{2.83}$$

The solution will then evolve in time according to the equations of motion. If the evolution is such that

$$\varepsilon(x,t) = \sum_{i=1}^{n} \varepsilon_0(x - x_i - v_i t + \chi_i), \qquad t \to +\infty. \tag{2.84}$$

where χ_i are constants, this solution is called a soliton. Therefore solitons are those solitary waves whose energy densities are asymptotically (as $t \to +\infty$) restored to their original shapes and velocities. The constants χ_i account for the possibility of a bodily displacement compared with their prescattering trajectories, which should be the sole residual effect of the collisions.

It is evident that finding a soliton is much more difficult than finding a solitary wave. Assuming Galilean or Lorentz invariance, given a nonlinear and dispersive wave equation, to find a solitary wave solution it is sufficient to look for a localized static solution. In contrast, to verify that a solution is a soliton, we must find many time-dependent solutions consisting of an arbitrary number of solitary waves, and check that (2.83) and (2.84) are satisfied. Thus it is very hard to tell if a given wave equation admits soliton solutions, let alone evaluate them explicitly[7].

In the case of the GPE, Zakharov and Shabat (1971) have shown that the fundamental hyperbolic secant solution is really a soliton, according to our definition. However, it has also been shown that even a small modification of the nonlinear term of the equation, such that $i\partial_t\psi = [-\partial_x^2 + \overline{c}F(|\psi|^2)]\psi$, with $F(\xi) = -2\xi^2 + O(\xi^2)$ for $\xi \to 0$, and (2.76) is still a solution, implies that in the scattering between two such solitary waves their structure is no longer preserved after the collision (Perelman, 2011).

[7]Since condition (2.84) is very stringent, it is likely that most of the localized solutions discussed in literature are only solitary waves, although in the absence of information on all time-dependent solutions for such systems this is difficult to prove or disprove conclusively.

Chapter 3

Soliton scattering in the attractive case

Being exact eigenstates of the attractive Lieb-Liniger model, string states are stable under time evolution and thus under scattering with one another, in the sense that their energy is the same before and after the collision. This reminds us of classical solitons. However, string states are not really the quantum analogues of classical solitons, since being eigenstates of a translationally invariant system they are not localized in space. We shall see that it is possible to construct a localized bound state wave packet as a linear superposition of string states with different momenta. This wave packet will no longer be an eigenstate, and thus will not be perfectly stable, unlike its classical counterpart. However, if it is constructed in such a way that the dispersion is only relevant over very long times, it will be a quasi-soliton. In the following, we take the license to call these objects simply solitons.

Hereafter we construct spatially localized wave packets of n bound atoms as linear combinations of n-string states with Gaussian-distributed momenta (fundamental solitons). We discuss their stability in time and show how they are related to the classical solitons considered previously. We will then construct higher-order solitons and study the scattering problem exploiting the exact phase shifts obtained from the Bethe Ansatz and general results from scattering theory. In the last section of the chapter, we present the construction of soliton states and study the scattering properties within a mean field approach, and compare it with the exact approach.

3.1 General results of scattering theory

Since what we are really interested in are the asymptotic states of the solitons before and after scattering, instead of studying the whole dynamics we can make use of some general results from scattering theory, which allow us to relate the relevant observables to just the scattering phase shifts, which are known exactly from the Bethe Ansatz.

3.1.1 Scattering of two particles in one dimension

Let us consider two particles with asymptotic momenta p_1 and p_2 and dispersion relations $E_j(p_j)$, $j = 1, 2$, in an infinite volume. The statement of the Bethe Ansatz is that in the asymptotic region where the two particles are very far apart, i.e. when the distance between them is much larger than the range of interaction, the eigenfuncitons of the system are plane waves,

$$\varphi_{p_1,p_2}(x_1, x_2) = \begin{cases} \mathrm{e}^{i(p_1 x_1 + p_2 x_2)}, & x_1 \ll x_2 \\ S(p_1, p_2)\mathrm{e}^{i(p_1 x_1 + p_2 x_2)}, & x_1 \gg x_2 \end{cases} \tag{3.1}$$

where

$$S(p_1, p_2) = \mathrm{e}^{i\chi(p_1,p_2)} \tag{3.2}$$

is the scattering matrix and $\chi(p_1, p_2)$ is the scattering phase shift (Vlijm et al., 2015). At zero density, the energy of these eigenfunctions is simply

$$E(p_1, p_2) = E_1(p_1) + E_2(p_2). \tag{3.3}$$

For elementary particles, Eq. (3.1) is a consequence of the conservation of energy and momentum in one dimension, and is therefore valid for any model with sufficiently short-range interactions. Instead, if one of the particles is not elementary but is a bound state, the previous form of the post-scattering eigenfunction is not true anymore in general, since the bound state might decay, and the scattering be diffractive. Eq. (3.1) therefore assumes that the scattering process occurs without particle production. This is the case for integrable models such as Lieb-Liniger, where bound states cannot decay, but are protected by integrability. Hence the Bethe Ansatz describes a complete set of asymptotic eigenfunctions and Eq. (3.1) holds also for quasiparticles corresponding to spatially localized wave packets of bound states excitations.

Now we turn to the scattering problem. At time $t = 0$ the two quasiparticles are very far apart and have almost well defined positions $(\overline{x}_1, \overline{x}_2)$ and momenta $(\overline{p}_1, \overline{p}_2)$, and move with group velocities

$$v_j = \left.\frac{\partial E_j}{\partial p_j}\right|_{p_j=\overline{p}_j}, \qquad j = 1, 2. \tag{3.4}$$

Without loss of generality we may assume that $\overline{x}_1 \ll \overline{x}_2$. Therefore if $v_1 < v_2$ the evolution is always free, while if $v_1 > v_2$ at some time the two quasiparticles will become close and interact. With these assumptions, the initial state two-body wavefunction is factorized,

$$\psi(x_1, x_2) = \psi_1(x_1)\psi_2(x_2). \tag{3.5}$$

Its unitary time evolution is given by

$$\psi(x_1, x_2, t) = \int \frac{dp_1}{2\pi}\frac{dp_2}{2\pi}\, C(p_1, p_2) \mathrm{e}^{-it[E_1(p_1)+E_2(p_2)]} \varphi_{p_1,p_2}(x_1, x_2), \tag{3.6}$$

where

$$C(p_1, p_2) = \int dx_1\, dx_2\, \varphi^*_{p_1,p_2}(x_1, x_2)\psi_1(x_1)\psi_2(x_2). \tag{3.7}$$

To make progress, we can make the following approximations:

(i) Since the initial state $\psi_1(x_1)\psi_2(x_2)$ is sharply peaked around $\overline{x}_1$ and $\overline{x}_2$, with $\overline{x}_1 \ll \overline{x}_2$, the only relevant contribution to (3.7) comes from the regions around these two points. We may then substitute to $\varphi_{p_1,p_2}(x_1, x_2)$ the asymptotic form (3.1) valid for $\overline{x}_1 \ll \overline{x}_2$. Expressing $\psi_j(x_j)$ in terms of the Fourier transform $\widetilde{\psi}_j(p_j)$,

$$\psi_j(x_j) = \int \frac{dp_j}{2\pi}\, \widetilde{\psi}_j(p_j) \mathrm{e}^{ip_j x_j}, \tag{3.8}$$

we then obtain

$$C(p_1, p_2) \simeq \widetilde{\psi}_1(p_1)\widetilde{\psi}_2(p_2). \tag{3.9}$$

(ii) Since the functions $\widetilde{\psi}(p_j)$ in Eq. (3.9) are sharply peaked around $\overline{p}_j$, we may expand the dispersion relations $E_j(p_j)$ around these momenta in the integrand of Eq. (3.6),

$$E_j(p_j) \simeq E_j(\overline{p}_j) + v_j(p_j - \overline{p}_j) + \frac{1}{2}\delta_j(\overline{p}_j)(p_j - \overline{p}_j)^2, \tag{3.10}$$

where $\delta_j = \partial^2 E_j/\partial p_j^2$. Furthermore, for $x_1 \gg x_2$, i.e., long after the scattering, when we are again in the asymptotic region, we may substitute the asymptotic form (3.1) for $\varphi_{p_1,p_2}(x_1, x_2)$ into (3.6), and similarly expand the scattering phase shift,

$$\chi(p_1, p_2) \simeq \chi(\overline{p}_1, \overline{p}_2) + \chi_i(\overline{p}_1, \overline{p}_2)(p_i - \overline{p}_i) + \frac{1}{2}\chi_{ij}(\overline{p}_1, \overline{p}_2)(p_i - \overline{p}_i)(p_j - \overline{p}_j), \tag{3.11}$$

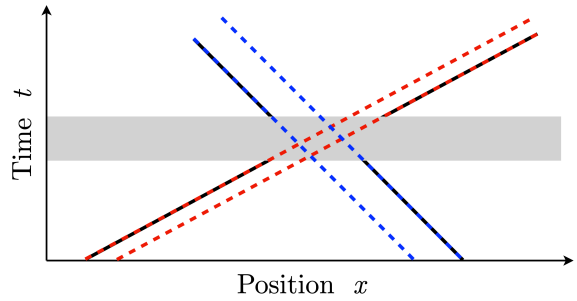


Figure 3.1: Qualitative representation of the one-dimensional scattering of two wave packets. In the asymptotic regions before and after the scattering the centers of the wave packets translate rigidly with their original velocities, but exhibit a displacement of positions. The scattering region is represented in gray; there the wave packets cannot be identified individually.

where $\chi_i = \partial\chi/\partial p_i$ and $\chi_{ij} = \partial^2\chi/\partial p_i \partial p_j$, and we sum over repeated indices.

Using these approximations, we can write the pre-scattering ($x_1 \ll x_2$) two-body wavefunction as

$$\psi(x_1, x_2, t) = \int \frac{dp_1}{2\pi}\frac{dp_2}{2\pi}\, \widetilde{\psi}_1(p_1)\widetilde{\psi}_2(p_2) \mathrm{e}^{-it[E_1(p_1)+E_2(p_2)]} \mathrm{e}^{i(p_1x_1+p_2x_2)} \tag{3.12}$$

with $E_j(p_j)$ given by (3.10), and the post-scattering ($x_1 \gg x_2$) wavefunction as

$$\psi(x_1, x_2, t) = \int \frac{dp_1}{2\pi}\frac{dp_2}{2\pi}\, \widetilde{\psi}_1(p_1)\widetilde{\psi}_2(p_2) \mathrm{e}^{-it[E_1(p_1)+E_2(p_2)]} \mathrm{e}^{i\chi(p_1,p_2)} \mathrm{e}^{i(p_1x_1+p_2x_2)} \tag{3.13}$$

with $E_j(p_j)$ given by (3.10) and $\chi(p_1, p_2)$ by (3.11).

3.1.2 Displacement, spreading, and correlation of wave packets

We are now in position to compute the motion of the center of each wave packet, which is given by

$$x_j(t) = \langle\, \hat{x}_j \,\rangle(t) = \int dx_1\, dx_2\, \psi^*(x_1, x_2, t)\, x_j\, \psi(x_1, x_2, t), \tag{3.14}$$

before and after the scattering. In the asymptotic regions the centers of the wave packets translate rigidly. However the scattering between the two quasiparticles introduces a displacement proportional to the derivative of the scattering phase shift, $\chi_j(\overline{p}_1, \overline{p}_2) = (\partial\chi/\partial p_j)|_{p_1=\overline{p}_1,\, p_2=\overline{p}_2}$ (Fig. 3.1), so that

$$x_j(t) = \begin{cases} \overline{x}_j + v_j t & \text{before scattering,} \\ \overline{x}_j + v_j t - \chi_j(\overline{p}_1, \overline{p}_2) & \text{after scattering.} \end{cases} \tag{3.15}$$

This result is independent of the specific form of the wave packets (see the proof below).

The scattering has also an effect on the width of each wave packet. To compute the spreading in time, we now assume that the functions $\psi_j(x_j)$ are normalized Gaussian wave packets centered around $\overline{x}_j$,

$$\psi_j(x_j) = \left(\frac{2}{\pi\alpha_j^2}\right)^{\frac{1}{4}} \mathrm{e}^{-\frac{(x_j-\overline{x}_j)^2}{\alpha_j^2} + i\overline{p}_j x_j}, \tag{3.16}$$

with $\int dx_j\,|\psi_j(x_j)|^2 = 1$ and $\Delta x_j^2 = \int dx_j\,(x_j - \overline{x}_j)^2 |\psi_j(x_j)|^2 = \alpha_j^2/4$. The Fourier transform of (3.16) is

$$\widetilde{\psi}_j(p_j) = \int dx_j\,\psi_j(x_j) \mathrm{e}^{-ip_j x_j} = \left(2\pi\alpha_j^2\right)^{\frac{1}{4}} \mathrm{e}^{-\frac{1}{4}\alpha_j^2 (p_j - \overline{p}_j)^2 - i(p_j - \overline{p}_j)\overline{x}_j} \tag{3.17}$$

and is normalized as $\int \frac{dp_j}{2\pi} \left|\widetilde{\psi}_j(p_j)\right|^2 = 1$. We can now evaluate explicitly

$$\Delta x_j^2(t) = \left\langle \left(\hat{x}_j - x_j\right)^2 \right\rangle (t) = \int dx_1\,dx_2\,\psi^*(x_1, x_2, t)\, x_j^2\, \psi(x_1, x_2, t) - x_j^2(t) \tag{3.18}$$

where $x_j(t)$ is given by Eq. (3.15). We find

$$\Delta x_1^2(t) = \begin{cases} \dfrac{\alpha_1^2}{4} + \dfrac{\delta_1^2 t^2}{\alpha_1^2} & \text{before scattering,} \\[2ex] \dfrac{\alpha_1^2}{4} + \dfrac{\chi_{12}^2}{\alpha_2^2} + \dfrac{(\chi_{11} - \delta_1 t)^2}{\alpha_1^2} & \text{after scattering,} \end{cases} \tag{3.19}$$

where δ_1 is evaluated in $\overline{p}_1$ and χ_{ij} in $(\overline{p}_1, \overline{p}_2)$. An analogous formula holds for $\Delta x_2^2(t)$.

Moreover, scattering builds up correlations between the (initially uncorrelated) Gaussian wave packets. The correlator

$$\begin{aligned} (\Delta x_1 \Delta x_2)(t) &= \left\langle \left(\hat{x}_1 - x_1\right)\left(\hat{x}_2 - x_2\right) \right\rangle (t) \\ &= \int dx_1\,dx_2\,\psi^*(x_1, x_2, t)\, x_1\, x_2\, \psi(x_1, x_2, t) - x_1(t) x_2(t) \end{aligned} \tag{3.20}$$

reads

$$(\Delta x_1 \Delta x_2)(t) = \begin{cases} 0 & \text{before scattering,} \\[2ex] \chi_{12} \left[\dfrac{\chi_{11} - \delta_1 t}{\alpha_1^2} + \dfrac{\chi_{22} - \delta_2 t}{\alpha_2^2} \right] & \text{after scattering,} \end{cases} \tag{3.21}$$

where δ_1 is evaluated in $\overline{p}_1$, δ_2 in $\overline{p}_2$, and χ_{ij} in $(\overline{p}_1, \overline{p}_2)$.

All the quantities above carry information about the derivatives of the scattering phase shift and the dispersion relations and can be in principle measured in scattering experiments.

Proof. Hereafter we prove Eqs. (3.15), (3.19) and (3.21). Let us start from $x_1(t)$. Using the relation $\int dx_2\,\mathrm{e}^{i(p_2 - q_2)x_2} = \delta(p_2 - q_2)$,

$$\begin{aligned} x_1(t) = \int dx_1\,dx_2\,x_1 \int \frac{dq_1}{2\pi}\frac{dq_2}{2\pi}\, \widetilde{\psi}_1^*(q_1)\widetilde{\psi}_2^*(q_2) \mathrm{e}^{it[E_1(q_1) + E_2(q_2)]} \mathrm{e}^{-i\chi(q_1, q_2)} \mathrm{e}^{-i(q_1 x_1 + q_2 x_2)} \\ \times \int \frac{dp_1}{2\pi}\frac{dp_2}{2\pi}\, \widetilde{\psi}_1(p_1)\widetilde{\psi}_2(p_2) \mathrm{e}^{-it[E_1(p_1) + E_2(p_2)]} \mathrm{e}^{i\chi(p_1, p_2)} \mathrm{e}^{i(p_1 x_1 + p_2 x_2)} \\ = \int dx_1\, x_1 \int \frac{dq_1\,dp_1\,dp_2}{(2\pi)^3}\, \widetilde{\psi}_1^*(q_1)\widetilde{\psi}_1(p_1) \left|\widetilde{\psi}_2(p_2)\right|^2 \mathrm{e}^{i(p_1 - q_1)x_1} \mathrm{e}^{-it[E_1(p_1) - E_1(q_1)]} \mathrm{e}^{i[\chi(p_1, p_2) - \chi(q_1, p_2)]}. \end{aligned}$$

Now $\int dx_1\, x_1\, \mathrm{e}^{i(p_1 - q_1)x_1} = -2\pi i \delta'(p_1 - q_1)$, where the prime denotes the distributional derivative of the δ function. Changing integration variable from p_1 to $u = p_1 - q_1$ and making use of Eqs. (3.10) and (3.11), we obtain

$$\begin{aligned} x_1(t) = -i \int \frac{dq_1\,dp_2}{(2\pi)^2}\, \widetilde{\psi}_1^*(q_1) \left|\widetilde{\psi}_2(p_2)\right|^2 \\ \times \int du\,\delta'(u)\, \widetilde{\psi}_1(q_1 + u) \mathrm{e}^{i[\chi_1 - v_1 t + \frac{1}{2}(\chi_{12} + \chi_{21})(p_2 - \overline{p}_2)]u} \mathrm{e}^{\frac{i}{2}(\chi_{11} - \delta_1 t)(u + 2q_1 - 2\overline{p}_1)u} \end{aligned}$$

and since $\int du\,\delta'(u)f(u) = -f'(0)$,

$$x_1(t) = i\int \frac{dq_1}{2\pi}\widetilde{\psi}_1^*(q_1)\widetilde{\psi}_1'(q_1) + v_1 t - \chi_1,$$

having taken into consideration the normalization of $\widetilde{\psi}_j$ and the symmetry of the integration interval. The remaining integral is

$$\begin{aligned}\int \frac{dq_1}{2\pi}\widetilde{\psi}_1^*(q_1)\widetilde{\psi}_1'(q_1) &= \int \frac{dq_1}{2\pi}\int dx\,\psi_1^*(x)\mathrm{e}^{iq_1x}\frac{d}{dq_1}\int dy\,\psi_1(y)\mathrm{e}^{-iq_1y}\\ &= -i\int dx\,dy\,\psi_1^*(x)\,y\,\psi_1(y)\int\frac{dq_1}{2\pi}\mathrm{e}^{iq_1(x-y)}\\ &= -i\int dx\,\psi_1^*(x)\,x\,\psi_1(x) = -i\,\overline{x}_1\end{aligned}$$

and therefore $x_1(t) = \overline{x}_1 + v_1 t - \chi_1$, which proves Eq. (3.15). An analogous formula holds for $x_2(t)$.

Now consider $\Delta x_1^2(t)$. Following the same procedure of the previous derivation,

$$\begin{aligned}&\Delta x_1^2(t) + x_1^2(t) =\\ &\int dx_1\,x_1^2\int\frac{dq_1\,dp_1\,dp_2}{(2\pi)^3}\,\widetilde{\psi}_1^*(q_1)\widetilde{\psi}_1(p_1)\big|\widetilde{\psi}_2(p_2)\big|^2\mathrm{e}^{i(p_1-q_1)x_1}\mathrm{e}^{-it[E_1(p_1)-E_1(q_1)]}\mathrm{e}^{i[\chi(p_1,p_2)-\chi(q_1,p_2)]}.\end{aligned}$$

In this case $\int dx_1\,x_1^2\,\mathrm{e}^{i(p_1-q_1)x_1} = -2\pi\delta''(p_1-q_2)$, thus

$$\begin{aligned}\Delta x_1^2(t) + x_1^2(t) = &-\int\frac{dq_1\,dp_2}{(2\pi)^2}\,\widetilde{\psi}_1^*(q_1)\big|\widetilde{\psi}_2(p_2)\big|^2\\ &\times\int du\,\delta''(u)\,\widetilde{\psi}_1(q_1+u)\mathrm{e}^{i[\chi_1-v_1t+\frac{1}{2}(\chi_{12}+\chi_{21})(p_2-\overline{p}_2)]u}\mathrm{e}^{\frac{i}{2}(\chi_{11}-\delta_1t)(u+2q_1-2\overline{p}_1)u}\end{aligned}$$

and since $\int du\,\delta''(u)f(u) = f''(0)$, calculating explicitly the derivatives of $\widetilde{\psi}_1$ from Eq. (3.17), taking into consideration the normalization of $\widetilde{\psi}_j$ and the symmetry of the integration interval, and performing the Gaussian integrations, we obtain

$$\Delta x_1^2(t) + x_1^2(t) = \frac{\alpha_1^2}{4} + \frac{(\chi_{12}+\chi_{21})^2}{4\alpha_2^2} + \frac{(\chi_{11}-\delta_1 t)^2}{\alpha_1^2} + (\overline{x}_1 + v_1 t - \chi_1)^2.$$

Exploiting the symmetry of second derivatives (Schwarz's theorem) this reduces to (3.19). An analogous formula holds for $\Delta x_2^2(t)$.

Now consider $\Delta x_1(t)\Delta x_2(t)$. Following the same procedure,

$$\begin{aligned}&(\Delta x_1\Delta x_2)(t) + x_1(t)x_2(t) =\\ &\int dx_1\,dx_2\,x_1\,x_2\int\frac{dq_1}{2\pi}\frac{dq_2}{2\pi}\,\widetilde{\psi}_1^*(q_1)\widetilde{\psi}_2^*(q_2)\mathrm{e}^{it[E_1(q_1)+E_2(q_2)]}\mathrm{e}^{-i\chi(q_1,q_2)}\mathrm{e}^{-i(q_1x_1+q_2x_2)}\\ &\qquad\times\int\frac{dp_1}{2\pi}\frac{dp_2}{2\pi}\,\widetilde{\psi}_1(p_1)\widetilde{\psi}_2(p_2)\mathrm{e}^{-it[E_1(p_1)+E_2(p_2)]}\mathrm{e}^{i\chi(p_1,p_2)}\mathrm{e}^{i(p_1x_1+p_2x_2)}.\end{aligned}$$

Now $\int dx_1\,x_1\,\mathrm{e}^{i(p_1-q_1)x_1}\int dx_2\,x_2\,\mathrm{e}^{i(p_2-q_2)x_2} = -(2\pi)^2\delta'(p_1-q_1)\delta'(p_2-q_2)$. Changing integration variables from p_1 to $u = p_1 - q_1$ and from p_2 to $s = p_2 - q_2$ and making use of Eqs. (3.10) and (3.11), we obtain

$$\begin{aligned}&(\Delta x_1\Delta x_2)(t) + x_1(t)x_2(t) =\\ &-\int\frac{dq_1}{2\pi}\frac{dq_2}{2\pi}\,\widetilde{\psi}_1^*(q_1)\widetilde{\psi}_2^*(q_2)\int du\,\delta'(u)\,\widetilde{\psi}_1(q_1+u)\mathrm{e}^{i[\chi_1-v_1t+\frac{1}{2}(\chi_{12}+\chi_{21})(q_2-\overline{p}_2)]u}\mathrm{e}^{\frac{i}{2}(\chi_{11}-\delta_1t)(u+2q_1-2\overline{p}_1)u}\\ &\times\int ds\,\delta'(s)\,\widetilde{\psi}_2(q_2+s)\mathrm{e}^{i[\chi_2-v_2t+\frac{1}{2}(\chi_{12}+\chi_{21})(q_1-\overline{p}_1)]s}\mathrm{e}^{\frac{i}{2}(\chi_{22}-\delta_2t)(s+2q_2-2\overline{p}_2)s}\mathrm{e}^{\frac{i}{2}(\chi_{12}+\chi_{21})us}\\ &=\int\frac{dq_1}{2\pi}\frac{dq_2}{2\pi}\,\widetilde{\psi}_1^*(q_1)\widetilde{\psi}_2^*(q_2)\int du\,\delta'(u)\,\widetilde{\psi}_1(q_1+u)\mathrm{e}^{i[\chi_1-v_1t+\frac{1}{2}(\chi_{12}+\chi_{21})(q_2-\overline{p}_2)]u}\mathrm{e}^{\frac{i}{2}(\chi_{11}-\delta_1t)(u+2q_1-2\overline{p}_1)u}\\ &\times\left[\frac{i}{2}(\chi_{12}+\chi_{21})\widetilde{\psi}_2(q_2)u + \frac{d}{ds}\Big(\widetilde{\psi}_2(q_2+s)\mathrm{e}^{i[\chi_2-v_2t+\frac{1}{2}(\chi_{12}+\chi_{21})(q_1-\overline{p}_1)]s}\mathrm{e}^{\frac{i}{2}(\chi_{22}-\delta_2t)(s+2q_2-2\overline{p}_2)s}\Big)\Big|_{s=0}\right]\end{aligned}$$

$$= -\frac{i}{2}(\chi_{12}+\chi_{21}) - \int \frac{dq_1}{2\pi}\frac{dq_2}{2\pi}\,\widetilde{\psi}_1^*(q_1)\widetilde{\psi}_2^*(q_2)$$
$$\times \frac{d}{du}\Big(\widetilde{\psi}_1(q_1+u)\mathrm{e}^{i[\chi_1-v_1t+\frac{1}{2}(\chi_{12}+\chi_{21})(q_2-\overline{p}_2)]u}\mathrm{e}^{\frac{i}{2}(\chi_{11}-\delta_1 t)(u+2q_1-2\overline{p}_1)u}\Big)\Big|_{u=0}$$
$$\times \frac{d}{ds}\Big(\widetilde{\psi}_2(q_2+s)\mathrm{e}^{i[\chi_2-v_2t+\frac{1}{2}(\chi_{12}+\chi_{21})(q_1-\overline{p}_1)]s}\mathrm{e}^{\frac{i}{2}(\chi_{22}-\delta_2 t)(s+2q_2-2\overline{p}_2)s}\Big)\Big|_{s=0}.$$

Calculating explicitly the derivatives of $\widetilde{\psi}_j$ from Eq. (3.17), taking into consideration the normalization of $\widetilde{\psi}_j$ and the symmetry of the integration interval, and performing the Gaussian integrations, we arrive at

$$(\Delta x_1\Delta x_2)(t) + x_1(t)x_2(t) = \frac{\chi_{12}+\chi_{21}}{2}\left[\frac{\chi_{11}-\delta_1 t}{\alpha_1^2}+\frac{\chi_{22}-\delta_2 t}{\alpha_2^2}\right] + (\overline{x}_1+v_1t-\chi_1)(\overline{x}_2+v_2t-\chi_2).$$

Exploiting the symmetry of second derivatives this reduces to Eq. (3.21). □

3.2 *n*-string states

Consider the n-particle sector of the Fock space, and let $\{\lambda^{(n)}\}$ denote the set of rapidities of an n-string centered at $\lambda^{(n)} = p/n$, where p is the total momentum of the string. We will denote by $|\,n,p\,\rangle$ the corresponding eigenstate, which in the position basis is represented by a Bethe wavefunction of the form (1.61),

$$\Psi_n(\mathbf{x}|\{\lambda^{(n)}\}) \equiv \Psi_{np}(\mathbf{x}) = \mathcal{N}_n \exp\left(ipx - \frac{\overline{c}}{2}\sum_{n\geq j>k\geq 1}|x_j-x_k|\right), \tag{3.22}$$

where $\mathbf{x}=(x_1,\ldots,x_n)$, $\mathcal{N}_n$ is a normalization constant and $x=\sum_{j=1}^n x_j/n$ is the position of the center of mass of the n atoms. Thus

$$|\,n,p\,\rangle = \frac{1}{\sqrt{n!}}\int dx_1\cdots dx_n\,\Psi_{np}(x_1,\ldots,x_n)\,\hat{\psi}^\dagger(x_1)\cdots\hat{\psi}^\dagger(x_n)|\,0\,\rangle. \tag{3.23}$$

These are simultaneous eigenstates of the Hamiltonian, the momentum operator and the total number operator,

$$\hat{H}|\,n,p\,\rangle = \left(-\frac{\overline{c}}{12}n(n^2-1)+\frac{p^2}{n}\right)|\,n,p\,\rangle, \tag{3.24}$$
$$\hat{P}|\,n,p\,\rangle = p|\,n,p\,\rangle, \tag{3.25}$$
$$\hat{N}|\,n,p\,\rangle = n|\,n,p\,\rangle, \tag{3.26}$$

and can be normalized in such a way that

$$\langle\,n',p'\,|\,n,p\,\rangle = n\,\delta_{nn'}\delta(p-p'). \tag{3.27}$$

In fact, if $n'\neq n$ then $\langle\,n',p'\,|\,n,p\,\rangle = 0$, because states of different n involve a different number of field operators. For equal n's, using the same change of variables as in Eq. (2.47), we get

$$\langle\,n,p'\,|\,n,p\,\rangle = n!\,|\mathcal{N}_n|^2\int_{D_N} dx_1\cdots dx_n\,\exp\left(-\overline{c}\sum_{j=1}^n(2j-n-1)x_j+\frac{i}{n}(p-p')\sum_{j=1}^n x_j\right)$$
$$= n!\,|\mathcal{N}_n|^2\int_{\mathbb{R}}du_1\int_{(\mathbb{R}^+)^{n-1}}du_2\cdots du_N\,\exp\left[-\overline{c}\sum_{k=2}^n(n+1-k)\left(k-1+\frac{i}{n\overline{c}}(p-p')\right)u_k\right]$$
$$= n!\,|\mathcal{N}_n|^2\prod_{k=2}^n\int_0^\infty du_k\,\mathrm{e}^{-\overline{c}(n+1-k)(k-1+i(p-p')/n\overline{c})u_k}\int_{-\infty}^{+\infty}du_1\,\mathrm{e}^{-i(p-p')u_1}$$
$$= n!\,|\mathcal{N}_n|^2\,\overline{c}^{1-n}[(n-1)!]^{-2}\,2\pi\delta(p-p'), \tag{3.28}$$

hence the normalization condition (3.27) is obtained by fixing

$$|\mathcal{N}_n|^2 = \overline{c}^{n-1}\frac{(n-1)!}{2\pi}. \tag{3.29}$$

Naturally we will take $\mathcal{N}_n = |\mathcal{N}_n|$.

3.2.1 Matrix elements

It is useful to compute the matrix elements of the field operator and the density operator between two string states.

Field operator The matrix elements of the field operator $\hat{\psi}(z)$ between an n-string and an $(n+1)$-string state are

$$\begin{aligned}
&\langle\, n, p' \,|\, \hat{\psi}(z) \,|\, n+1, p \,\rangle \\
&= \frac{1}{\sqrt{n!(n+1)!}} \int dx'_1 \cdots dx'_n \, dx_1 \cdots dx_{n+1} \, \Psi^*_{np'}(x'_1, \ldots, x'_n) \Psi_{n+1,p}(x_1, \ldots, x_{n+1}) \\
&\qquad\qquad \times \langle\, 0 \,|\, \hat{\psi}(x'_1) \cdots \hat{\psi}(x'_n) \hat{\psi}(z) \hat{\psi}^\dagger(x_1) \cdots \hat{\psi}^\dagger(x_{n+1}) \,|\, 0 \,\rangle \\
&= \frac{(n+1)!}{\sqrt{n!(n+1)!}} \int dx_1 \cdots dx_n \, \Psi^*_{n,p'}(x_1, \ldots, x_n) \Psi_{n+1,p}(x_1, \ldots, x_n, z),
\end{aligned} \tag{3.30}$$

where in the last step we have used the symmetry of the wavefunction. By the same property, the integration over $\mathbb{R}^n$ is equal to $n!$ times the integration over the domain of ordered positions $\bigcup_{m=0}^{n} \{x_1 < \cdots < x_m < z < x_{m+1} < \cdots < x_n\}$. Denoting the strings' centers as $\lambda = p/(n+1)$ and $\lambda' = p'/n$, we get[1,2]

$$\begin{aligned}
&\langle\, n, p' \,|\, \hat{\psi}(z) \,|\, n+1, p \,\rangle \\
&= \sqrt{n+1}\, \mathcal{N}^*_n \mathcal{N}_{n+1}\, n! \sum_{m=0}^{n} \int_{-\infty}^{z} dx_m \cdots \int_{-\infty}^{x_2} dx_1 \int_{z}^{+\infty} dx_{m+1} \cdots \int_{x_{n-1}}^{+\infty} dx_n \\
&\times \exp\left[i(\lambda - \lambda') \sum_{j=1}^{n} x_j + i\lambda z - \overline{c} \sum_{j=1}^{n} (2j - n - 1) x_j - \frac{\overline{c}}{2}(2m - n) z + \frac{\overline{c}}{2} \sum_{j=1}^{m} x_j - \frac{\overline{c}}{2} \sum_{j=m+1}^{n} x_j \right] \\
&= \sqrt{n+1}\, \mathcal{N}^*_n \mathcal{N}_{n+1}\, n!\, (2/\overline{c})^n \mathrm{e}^{i[\lambda + n(\lambda - \lambda')]z} \sum_{m=0}^{n} \frac{1}{m!(n-m)!} \\
&\times \prod_{j=1}^{m} \frac{1}{2(n-j) + 1 + i(2/\overline{c})(\lambda - \lambda')} \prod_{j=1}^{n-m} \frac{1}{2(n-j) + 1 - i(2/\overline{c})(\lambda - \lambda')}.
\end{aligned} \tag{3.31}$$

[1] The summations in the exponential are obtained as follows. We let $\{x_1, \ldots, x_m, z, x_{m+1}, \ldots, x_n\} = \{x_1, \ldots, x_s, x_{s+1}, x_{s+2}, \ldots, x_l\}$, write $\sum_{j=1}^{l}(2j-l-1)x_j = \sum_{j=1}^{s}(2j-l-1)x_j + [2(s+1)-l-1]x_{s+1} + \sum_{j=s+2}^{l}(2j-l-1)x_j$, reparametrize the last summation as $\sum_{j=s+1}^{l-1}(2j-l+1)x_j$, and finally substitute $x_{s+1} \to z$, $s \to m$, $l \to n+1$. We thus get $(2m-n)z + \sum_{j=1}^{m}(2j-n-2)x_j + \sum_{j=m+1}^{n}(2j-n)$, which we reexpress as $\sum_{j=1}^{n}(2j-n-1)x_j + (2m-n)z - \sum_{j=1}^{m} x_j + \sum_{j=m+1}^{n} x_j$.

[2] To compute the integrals, notice that $\int_{-\infty}^{x_{j+1}} dx_j \, \exp(a_j x_j)$ yields a_j^{-1} times $\exp(a_j x_{j+1})$, which enters in the integration over x_{j+1}; therefore $a_j = \sum_{k=1}^{j} a_k$, for $j = 1, \ldots, m$. For the integrals over $x_{m+1}, \ldots, x_n$, it is convenient to change labels as $j \to j-m$, so that $\sum_{j=m+1}^{n}(2j-n-1)x_j \to \sum_{j=1}^{n-m}(2j-n+2m-1)x_j$. Then $\int_{x_{j-1}}^{+\infty} dx_j \, \exp(-a_j x_j)$ gives a_j^{-1} times $\exp(-a_j x_{j-1})$, which enters in the integration over x_{j-1}; therefore $a_j = \sum_{k=j}^{n-m} a_k$, for $j = 1, \ldots, n-m$.

Now the sum over m can be rewritten as

$$\begin{aligned}
&\left[\prod_{j=1}^{n}\frac{1}{(2n-2j+1)^2+(4/\bar{c}^2)(\lambda-\lambda')^2}\right]\sum_{m=0}^{n}\frac{1}{m!(n-m)!}\\
&\times\prod_{j=m+1}^{n}[2(n-j)+1+i(2/\bar{c})(\lambda-\lambda')]\prod_{j=n-m+1}^{n}[2(n-j)+1-i(2/\bar{c})(\lambda-\lambda')]\\
&=2^n\prod_{j=1}^{n}\frac{1}{(2n-2j+1)^2+(4/\bar{c}^2)(\lambda-\lambda')^2}\\
&=2^n\prod_{j=1}^{n}\frac{1}{(2j-1)^2+(4/\bar{c}^2)(\lambda-\lambda')^2},
\end{aligned}\tag{3.32}$$

where we have used the identity

$$\sum_{m=0}^{n}\frac{1}{m!(n-m)!}\prod_{j=1}^{n-m}(2j-1+ia)\prod_{j=1}^{m}(2j-1-ia)=2^n,\tag{3.33}$$

and, in the last step, relabeled $j\to n-j+1$. Substituting (3.32) and (3.29) into Eq. (3.31), we arrive at

$$\begin{aligned}
\langle\, n',p'\,|\,\hat{\psi}(z)\,|\,n+1,p\,\rangle=\delta_{nn'}\sqrt{n(n+1)}n!(n-1)!\frac{2^{2n}}{2\pi\sqrt{\bar{c}}}\mathrm{e}^{i(p-p')z}\\
\times\prod_{j=1}^{n}\frac{1}{(2j-1)^2+(4/\bar{c}^2)[\,p/(n+1)-p'/n\,]^2},
\end{aligned}\tag{3.34}$$

in agreement with Nohl (1976); Wadachi and Sakagami (1984). The same result may be obtained from the Algebraic Bethe Ansatz (Calabrese and Caux, 2007). Using the identities

$$\prod_{j=1}^{n}\frac{1}{(2j-1)^2+x^2}=\frac{1}{[(2j-1)!!]^2}\prod_{j=1}^{n}\frac{(2j-1)^2}{(2j-1)^2+x^2},\tag{3.35}$$

$$\lim_{n\to\infty}\prod_{j=1}^{n}\frac{(2j-1)^2}{(2j-1)^2+x^2}=\operatorname{sech}\left(\frac{\pi x}{2}\right),\tag{3.36}$$

$$\lim_{n\to\infty}\frac{1}{n}\frac{2^{2n}(n!)^2}{[(2n-1)!!]^2}=\lim_{n\to\infty}\frac{1}{n}\left[\frac{(2n)!!}{(2n-1)!!}\right]^2=\pi,\tag{3.37}$$

in the limit $n\to\infty$ the matrix elements (3.34) reduce to

$$\langle\, n',p'\,|\,\hat{\psi}(z)\,|\,n+1,p\,\rangle\overset{n\to\infty}{\simeq}\delta_{nn'}\sqrt{\frac{n(n+1)}{4\bar{c}}}\mathrm{e}^{i(p-p')z}\operatorname{sech}\left[\frac{\pi}{\bar{c}}\left(\frac{p}{n+1}-\frac{p'}{n}\right)\right].\tag{3.38}$$

Density operator We can compute in a similar way the matrix elements of the density operator $\hat{\rho}(z)=\hat{\psi}^\dagger(z)\hat{\psi}(z)$,

$$\langle\, n,p'\,|\,\hat{\rho}(z)\,|\,n,p\,\rangle=n\int dx_1\cdots dx_{n-1}\,\Psi^*_{np'}(x_1,\ldots,x_{n-1},z)\Psi_{np}(x_1,\ldots,x_{n-1},z).\tag{3.39}$$

We remark that for $p-p'=0$ this matrix element does not reduce to the static density (2.49) that we considered in Section 2.2, because here we are not fixing the position of the

center of mass; in fact $\langle\, n,p' \,|\, \hat\rho(z) \,|\, n,p \,\rangle|_{p-p'=0}$ is not localized in space. As before, we have

$$\begin{aligned}
&\langle\, n,p' \,|\, \hat\rho(z) \,|\, n,p \,\rangle \\
&= n\,|\mathcal{N}_n|^2(n-1)!\sum_{m=0}^{n-1}\int_{-\infty}^{z}dx_m\cdots\int_{-\infty}^{x_2}dx_1\int_{z}^{+\infty}dx_{m+1}\cdots\int_{x_{n-2}}^{+\infty}dx_{n-1} \\
&\times\exp\biggl[i(\lambda-\lambda')\Bigl(\sum_{j=1}^{n-1}x_j+z\Bigr)-\overline{c}\sum_{j=1}^{n-1}(2j-n)x_j-\overline{c}(2m-n+1)z+\overline{c}\sum_{j=1}^{m}x_j-\overline{c}\sum_{j=m+1}^{n-1}x_j\biggr] \\
&= n\,|\mathcal{N}_n|^2(n-1)!\,\overline{c}^{1-n}\mathrm{e}^{i(p-p')z}\sum_{m=0}^{n-1}\frac{1}{m!(n-1-m)!} \\
&\times\prod_{j=1}^{m}\frac{1}{n-j+(i/\overline{c})(\lambda-\lambda')}\prod_{j=1}^{n-1-m}\frac{1}{n-j-(i/\overline{c})(\lambda-\lambda')}.
\end{aligned}\tag{3.40}$$

With the identity

$$\sum_{m=0}^{n-1}\frac{1}{m!(n-1-m)!}\prod_{j=1}^{n-1-m}(j+ia)\prod_{j=1}^{m}(j-ia)=n,\tag{3.41}$$

the sum over m reduces to

$$n\prod_{j=1}^{n-1}\frac{1}{(n-j)^2+(\lambda-\lambda')^2/\overline{c}^2}=n\prod_{j=1}^{n-1}\frac{1}{j^2+(1/\overline{c}^2)(\lambda-\lambda')^2},\tag{3.42}$$

and we thus obtain

$$\langle\, n',p' \,|\, \hat\rho(z) \,|\, n,p \,\rangle=\delta_{nn'}\frac{(n!)^2}{2\pi}\mathrm{e}^{i(p-p')z}\prod_{j=1}^{n-1}\frac{1}{j^2+(1/n\overline{c})^2(p-p')^2}.\tag{3.43}$$

Using the identities

$$\prod_{j=1}^{n-1}\frac{1}{j^2+x^2}=\frac{1}{[(n-1)!]^2}\prod_{j=1}^{n-1}\frac{j^2}{j^2+x^2},\tag{3.44}$$

$$\lim_{n\to\infty}\prod_{j=1}^{n-1}\frac{j^2}{j^2+x^2}=\pi x\,\mathrm{csch}(\pi x),\tag{3.45}$$

in the limit $n\to\infty$ the matrix elements (3.43) reduce to

$$\langle\, n',p' \,|\, \hat\rho(z) \,|\, n,p \,\rangle\overset{n\to\infty}{\simeq}\delta_{nn'}\frac{n}{2\overline{c}}\,\mathrm{e}^{i(p-p')z}(p-p')\,\mathrm{csch}\biggl[\frac{\pi}{n\overline{c}}(p-p')\biggr].\tag{3.46}$$

3.3 Bound state wave packets

3.3.1 Building the fundamental soliton

To create, at a reference time $t=0$, a localized wave packet $|\,\psi(0)\,\rangle$ of n bound atoms with almost well-defined momentum $\overline{p}$ and well-defined position $\overline{x}$, we sum over many n-string states with momenta p taken from a Gaussian distribution around $\overline{p}$,

$$g(p)=(2\pi\alpha^2)^{\frac{1}{4}}\mathrm{e}^{-\frac{1}{4}\alpha^2(p-\overline{p})^2-i(p-\overline{p})\overline{x}}.\tag{3.47}$$

The parameter α is related to the width of the distribution, a larger α corresponding to a more sharply peaked Gaussian. The n-string wave packet (fundamental soliton) is thus

$$|\,\psi(0)\,\rangle = \int \frac{dp}{2\pi}\, g(p)|\,n,p\,\rangle \tag{3.48}$$

and depends on the free parameters $\overline{x}$, $\overline{p}$ and α.

Although not strictly necessary, we can also sum over string states with different n, obtaining a wave packet with an average number of particles $\overline{n}$. Because of the phase-number uncertainty relation, this makes our bound state wave packet to also have almost well-defined phase (Auletta et al., 2009). We will thus consider

$$|\,\psi(0)\,\rangle = \sum_n a_n \int \frac{dp}{2\pi}\, g(p)|\,n,p\,\rangle, \tag{3.49}$$

with $\sum_n |a_n|^2 = 1$. The natural choice for a_n is

$$a_n = \frac{\zeta^n}{\sqrt{n!}}\,\mathrm{e}^{-|\zeta|^2/2}, \qquad |\zeta|^2 = \overline{n}, \tag{3.50}$$

so that the overlaps of $|\,\psi(0)\,\rangle$ with the n-string states $|\,n,p\,\rangle$ are

$$\frac{1}{n^2}|\langle\, n,p\,|\,\psi(0)\,\rangle|^2 = g^2(p)|a_n|^2 = g^2(p)\,\frac{\overline{n}^{\,n}}{n!}\mathrm{e}^{-\overline{n}}. \tag{3.51}$$

That is, the probability amplitude (normalized to n^2) of finding n particles in the bound state wave packet follows a Poisson distribution with expectation value $\overline{n}$.

In terms of wavefunctions,

$$\psi(\mathbf{x},0) = \int \frac{dp}{2\pi}\,(2\pi\alpha^2)^{\frac{1}{4}}\mathrm{e}^{-\frac{1}{4}\alpha^2(p-\overline{p})^2 - i(p-\overline{p})\overline{x}} \sum_n a_n \Psi_{np}(\mathbf{x}). \tag{3.52}$$

Substituting to $\Psi_{np}(\mathbf{x})$ its expression (3.22) and performing the integration over p, we obtain the n-string wave packet in real space,

$$\psi(\mathbf{x},0) = \left(\frac{2}{\pi\alpha^2}\right)^{\frac{1}{4}} \mathrm{e}^{-\frac{(x-\overline{x})^2}{\alpha^2} + i\overline{p}x}\,\Upsilon(\mathbf{x}), \tag{3.53}$$

where $\Upsilon(\mathbf{x}) = \sum_n a_n \mathcal{N}_n\,\mathrm{e}^{-(\overline{c}/2)\sum_{j>k}^n |x_j - x_k|}$ represents the suppression in the separation among the atoms constituting the bound state. The effective binding length is $\xi = 2/\overline{c}$. Thus the shape of the bound state wave packet in real space is that of a Gaussian centered around $\overline{x}$, $g(x) = (2/\pi\alpha^2)^{\frac{1}{4}}\mathrm{e}^{-(x-\overline{x})^2/\alpha^2 + i\overline{p}x}$, of width

$$\Delta x(0) = \sqrt{\int dx\,(x-\overline{x})^2 |g(x)|^2} = \frac{\alpha}{2}, \tag{3.54}$$

and whose amplitude is modulated by an exponential decay with characteristic length ξ. This average distance between the constituent atoms provides a lower bound on how localized the wave packets can be, since for $\alpha < \xi$ the wave packet will begin to lose its Gaussian shape in real space in favor of a simple exponential decay around $\overline{x}$.

3.3.2 Stability of the fundamental soliton

The wave packet (3.49) prepared at $t = 0$ evolves unitarily in time according to

$$|\,\psi(t)\,\rangle = \mathrm{e}^{-it\hat{H}}|\,\psi(0)\,\rangle = \sum_n a_n \int \frac{dp}{2\pi}\, g(p,t)|\,n,p\,\rangle, \tag{3.55}$$

where

$$g(p,t) = (2\pi\alpha^2)^{\frac{1}{4}}\mathrm{e}^{-\frac{1}{4}\alpha^2(p-\overline{p})^2 - i(p-\overline{p})\overline{x}}\mathrm{e}^{-itE^{(n)}(p)} \tag{3.56}$$

and $E^{(n)}(p)$ is the energy of the n-string eigenstate $|\,n,p\,\rangle$, given by Eq. (3.24). Correspondingly, the Gaussian profile in real space at time $t > 0$ will be

$$g(x,t) = (2\pi\alpha^2)^{\frac{1}{4}}\int \frac{dp}{2\pi}\,\mathrm{e}^{-\frac{1}{4}\alpha^2(p-\overline{p})^2 - i(p-\overline{p})\overline{x}}\mathrm{e}^{-itE^{(n)}(p)}\mathrm{e}^{ipx}. \tag{3.57}$$

Let us consider the equation of motion for the center of mass of the wave packet. This is given by $x(t) = \langle\,\hat{x}\,\rangle_{\psi(t)}$, where $\hat{x}$ is the center-of-mass' position operator and $\langle\cdots\rangle_{\psi(t)}$ is the quantum average

$$\langle\,\mathcal{O}\,\rangle_{\psi(t)} \equiv \frac{\langle\,\psi(t)\,|\,\mathcal{O}\,|\,\psi(t)\,\rangle}{\langle\,\psi(t)\,|\,\psi(t)\,\rangle} \tag{3.58}$$

for a generic operator $\mathcal{O}$ in the Schrödinger picture. We have[3]

$$x(t) = \sum_n |a_n|^2 \int dx\, g^*(x,t)\, x\, g(x,t) = \overline{x} + \left(\sum_n |a_n|^2\, v(n,\overline{p})\right)t, \tag{3.59}$$

where

$$v(n,\overline{p}) = \left.\frac{\partial E^{(n)}(p)}{\partial p}\right|_{p=\overline{p}} = \frac{2\overline{p}}{n} \tag{3.60}$$

is the group velocity of an n-string wave packet. Since we are summing over different n's, the group velocity of our fundamental soliton is the average of the $v(n,\overline{p})$ with Poissonian weights $|a_n|^2$,

$$v(\overline{n},\overline{p}) = \sum_n |a_n|^2\, v(n,\overline{p}) = C(\overline{n})\frac{2\overline{p}}{\overline{n}}, \tag{3.61}$$

where

$$C(\overline{n}) = \overline{n}\sum_n \frac{|a_n|^2}{n} = \overline{n}\,\mathrm{e}^{-\overline{n}}\int_0^{\overline{n}} dt\,\frac{\sinh t + \cosh t - 1}{t} \tag{3.62}$$

is a $O(1)$ correction, which takes the maximum value $C_{\max} \simeq 1.29436$ for $\overline{n} = 4$ and tends monotonically to 1^+ for $\overline{n} \to \infty$.

As anticipated, the wave form of the bound state wave packet is not constant in time. Two effects contribute to the spreading of the wave packet. The first is related to the fact that the wave packet is constructed from string states having different momenta. Since $E^{(n)}(p)$ has constant positive curvature $\delta(n) = \partial^2 E^{(n)}(p)/\partial p^2 = 2/n$, the width of the Gaussian profile would increase over time according to Eq. (3.19). Moreover, we are summing over many n-string Gaussian wave packets with different string lengths; each of these n-string wave packets moves at a different group velocity (3.60), further favoring the spreading. The width thus increases over time as

$$\Delta x(t) = \sqrt{\sum_n |a_n|^2 \int dx\, g^*(x,t)\, x^2\, g(x,t) - x(t)^2} = \sqrt{\frac{\alpha^2}{4} + D(\overline{n})\frac{\delta^2(\overline{n})t^2}{\alpha^2}}, \tag{3.63}$$

[3]For details on the calculations of $x(t)$ and other averages of interest for a Gaussian wave packet, see the proofs of Section 3.1.2.

where the factor

$$D(\overline{n}) = \overline{n}^2 \sum_n \frac{|a_n|^2}{n^2} = \overline{n}^3 \mathrm{e}^{-\overline{n}}\, {}_3F_3(1,1,1;\, 2,2,2;\, \overline{n}) \tag{3.64}$$

accounts for the effect of the different string lengths. Here ${}_3F_3$ is a generalized hypergeometric function[4]. $D(\overline{n})$ takes the maximum value $D_{\max} \simeq 2.47802$ for $\overline{n} = 4$ and tends monotonically to 1^+ for $\overline{n} \to \infty$. The broadening of the bound state wave packet of initial width $\Delta x(0) = \alpha/2$ is thus slower the larger the product $\overline{n}\alpha$. In particular, for the same number $\overline{n}$ of atoms, an initially very localized wave packet (in real space) widens more rapidly than an initially less localized one.

3.3.3 Classical limit

In the previous section we have constructed spatially localized bound state wave packets from a linear combination of n-string eigenstates. We now might ask what the relation is between these wave packets and the classical solitons considered in Section 2.3. In general, the relation between a (nonrelativistic, bosonic) quantum field theory and the corresponding classical field theory is obtained by showing that, taking the expectation value of the field operator in a the limit of a large number of particles, one obtains a classical solution, i.e.

$$\langle\, \alpha \,|\, \hat{\psi}(z) \,|\, \alpha \,\rangle \overset{n\to\infty}{\longrightarrow} \psi_\alpha(z). \tag{3.65}$$

In our case, $\langle \hat{\psi}(z) \rangle_{\psi(t)} \equiv \langle\, \psi(t) \,|\, \hat{\psi}(z) \,|\, \psi(t) \,\rangle$ is

$$\begin{aligned}
\langle \hat{\psi}(z) \rangle_{\psi(t)} &= \sum_n a_n^* a_{n+1} \int \frac{dp'}{2\pi} \frac{dp}{2\pi}\, g^*(p',t) g(p,t) \langle\, n, p' \,|\, \hat{\psi}(z) \,|\, n+1, p \,\rangle \\
&\simeq \sum_n a_n^* a_{n+1} \mathrm{e}^{in(n+1)\bar{c}^2 t/4} \sqrt{\frac{n(n+1)}{4\bar{c}}} \int \frac{dp'}{2\pi} \frac{dp}{2\pi}\, g_r^*(p') g_r(p) \\
&\quad \times \mathrm{e}^{-i[p^2/(n+1) - p'^2/n]t} \mathrm{e}^{i(p-p')(z-\overline{x})} \mathrm{sech}\left[\frac{\pi}{\bar{c}} \left(\frac{p}{n+1} - \frac{p'}{n} \right) \right],
\end{aligned} \tag{3.66}$$

where $g_r(p) = (2\pi\alpha^2)^{\frac{1}{4}} \mathrm{e}^{-\alpha^2(p-\overline{p})^2/4}$ (cf. Eq. (3.47)), having used in the second line Eq. (3.38) for the large n limit of the matrix elements. Here it is convenient to consider, instead of the total momenta p and p', the corresponding string centers $\lambda = p/(n+1)$ and $\lambda' = p'/n$. The integrand then reads

$$g_r^*(\lambda') g_r(\lambda)\, \mathrm{e}^{-i[(n+1)\lambda^2 - n\lambda'^2]t} \mathrm{e}^{i[(n+1)\lambda - n\lambda'](z-\overline{x})} \mathrm{sech}\left[\frac{\pi}{\bar{c}} (\lambda - \lambda') \right], \tag{3.67}$$

where

$$g_r^*(\lambda') g_r(\lambda) \simeq (2\pi\alpha^2)^{\frac{1}{2}} \mathrm{e}^{-(\alpha^2/4)[(n\lambda - \overline{p})^2 + (n\lambda' - \overline{p})^2]}. \tag{3.68}$$

Changing variables to $\lambda_1 = \frac{1}{2}(\lambda - \lambda')$ and $\lambda_2 = \frac{1}{2}(\lambda + \lambda')$, in terms of which $\lambda = \lambda_1 + \lambda_2$ and $\lambda' = \lambda_2 - \lambda_1$, Eq. (3.66) becomes

$$\begin{aligned}
\langle \hat{\psi}(z) \rangle_{\psi(t)} &\simeq \sum_n a_n^* a_{n+1} \mathrm{e}^{in(n+1)\bar{c}^2 t/4} \frac{n(n+1)}{\sqrt{\bar{c}}} (2\pi\alpha^2)^{\frac{1}{2}} \int \frac{d\lambda_1}{2\pi} \frac{d\lambda_2}{2\pi}\, \mathrm{e}^{-(\alpha^2/2)[(n\lambda_1)^2 + (n\lambda_2 - \overline{p})^2]} \\
&\quad \times \mathrm{e}^{i[(2n+1)\lambda_1(z-\overline{x}) + \lambda_2(z-\overline{x}) - \lambda_1^2 t - \lambda_2^2 t - (4n+2)\lambda_1\lambda_2 t]} \mathrm{sech}\left[\frac{2\pi\lambda_1}{\bar{c}} \right].
\end{aligned} \tag{3.69}$$

[4] See Olver et al. (2010), Ch. 16, for details.

With two further assumptions, namely (i) $\bar{c}^2 t \ll 1$, so that we can ignore the term $i\lambda_1^2 t$ in the phase, and (ii) $\Delta\lambda \sim (n\alpha)^{-1} \gg \bar{c}$, so that we can neglect the exponential term $\mathrm{e}^{-(\alpha n)^2\lambda_1^2/2}$, we can carry out the integration over λ_1, which gives the Fourier transform of the hyperbolic secant. Renaming λ_2 as λ, and multiplying by an overall factor of 2π in order to adjust the normalization, we thus get

$$\langle\hat{\psi}(z)\rangle_{\psi(t)} \simeq \sum_n a_n^* a_{n+1} \frac{n\alpha}{\sqrt{2\pi}} \int d\lambda\, \mathrm{e}^{-(\alpha^2/2)(n\lambda-\overline{p})^2} \times \frac{(n+1)\sqrt{\bar{c}}}{2} \operatorname{sech}\left[\frac{(n+\frac{1}{2})\bar{c}}{2}(z-\overline{x}-2\lambda t)\right] \mathrm{e}^{i[\lambda(z-\overline{x})+(n(n+1)\bar{c}^2-4\lambda^2)t/4]}. \tag{3.70}$$

Approximating one last time $n+1 \simeq n+\frac{1}{2} \simeq n$, and recognizing that $2\lambda = 2p/n = v$, the group velocity, the final result is

$$\langle\hat{\psi}(z)\rangle_{\psi(t)} \simeq \sum_n |a_n|^2 \frac{n\alpha}{\sqrt{2\pi}} \int d\lambda\, \mathrm{e}^{-(\alpha^2/2)(n\lambda-\overline{p})^2} \times \frac{n\sqrt{\bar{c}}}{2} \operatorname{sech}\left[\frac{n\bar{c}}{2}(z-\overline{x}-v(\lambda)t)\right] \mathrm{e}^{i[\lambda(z-\overline{x})+(n^2\bar{c}^2-v^2(\lambda))t/4]}. \tag{3.71}$$

In the last line we have precisely the classical soliton of Eq. (2.76). This shows that in the large n limit, the expectation value of the quantum field in the bound state wave packet is the average of a set of classical soliton solutions with Gaussian-distributed momenta and Poissonian-distributed number of particles (Lai and Haus, 1989b). The difference in phase velocity and group velocity among the classical solitons implies a spreading of the phase and the amplitude of the quantum average. With a simple change of variables, we can shift the time dependence from the argument of the hyperbolic secant to the Gaussian factor; then we see that the width of the momenta distribution is doubled after a period $t_{\mathrm{dis}} \sim 2/n\bar{c}\,\Delta\lambda$. The dispersion effect is thus proportional to the 'bandwidth' $\Delta\lambda$ of momenta. Comparing t_{dis} with the soliton period $t_s \sim 2\pi/n^2\bar{c}^2/4$, we have $t_{\mathrm{dis}}/t_s \sim n\bar{c}/4\pi\Delta\lambda$. In order to localize the soliton in Eq. (3.70), we imposed the condition $\bar{c} \ll \Delta\lambda$. Here we see that if $\bar{c} \ll \Delta\lambda \ll n\bar{c}$, then the soliton is localized and the dispersion effect is relevant only after many soliton periods. This also means that the width of the hyperbolic secant pulse is much smaller than the inverse of the momentum bandwidth[5].

3.4 Scattering of bound state wave packets

3.4.1 Higher-order soliton states and scattering phase shifts

Consider the (n_1+n_2)-particle sector of the Fock space. To construct a two-soliton state we start from a two-particle excited state, i.e. an eigenstate whose rapidities are partitioned into two strings of length n_1 and n_2,

$$\lambda_j = \frac{p_1}{n_1} + i\frac{\bar{c}}{2}(n_1+1-2j), \qquad j = 1,\ldots,n_1, \tag{3.72a}$$

$$\lambda_{n_1+j} = \frac{p_2}{n_2} + i\frac{\bar{c}}{2}(n_2+1-2j), \qquad j = 1,\ldots,n_2. \tag{3.72b}$$

[5]Compare this with the case of a linear wave function, where a bandwidth of order $1/\Delta x$ is necessary to construct a pulse of width Δx, because the distribution of momenta is the Fourier transform of the pulse in real space.

The two-particle excited state is

$$
\begin{aligned}
|\, n_1, p_1;\, n_2, p_2 \,\rangle &= \int dx_1 \cdots dx_{n_1+n_2} \Psi_{\{n_j p_j\}}(x_1, \ldots, x_{n_1+n_2}) \hat{\psi}^\dagger(x_1) \cdots \hat{\psi}^\dagger(x_{n_1+n_2}) |\, 0 \,\rangle \\
&= (n_1+n_2)! \int_{D_{n_1+n_2}} d\mathbf{x}\, \Psi_{\{n_j p_j\}}(\mathbf{x}) \hat{\psi}^\dagger(x_1) \cdots \hat{\psi}^\dagger(x_{n_1+n_2}) |\, 0 \,\rangle
\end{aligned}
\tag{3.73}
$$

where $D_{n_1+n_2} : x_1 < \cdots < x_{n_1+x_2}$ and, in this domain,

$$
\begin{aligned}
\Psi_{\{n_j p_j\}}(\mathbf{x})\big|_{\mathbf{x}\in D_{n_1+n_2}} = \sum_{Q\in\pi_{n_1+n_2}} A_Q \exp\Bigg(\frac{ip_1}{n_1} \sum_{j=1}^{n_1} x_{Q_j^{-1}} - \frac{\overline{c}}{2} \sum_{n_1 \geq j > k \geq 1} (x_{Q_j^{-1}} - x_{Q_k^{-1}}) \Bigg) \\
\times \exp\Bigg(\frac{ip_2}{n_2} \sum_{j=n_1+1}^{n_1+n_2} x_{Q_j^{-1}} - \frac{\overline{c}}{2} \sum_{n_1+n_2 \geq j > k \geq n_1+1} (x_{Q_j^{-1}} - x_{Q_k^{-1}}) \Bigg).
\end{aligned}
\tag{3.74}
$$

Here we have converted the permutation over λ's into the permutation over x's. The sum is extended to all permutations of $[n_1+n_2, \ldots, n_1+1, n_1, \ldots, 1]$ such that the order of $[n_1+n_2, \ldots, n_1+1]$ and $[n_1, \ldots, 1]$ is unchanged, otherwise the amplitude A_Q vanishes for the same reason we discussed in Section 1.4.3. As always, the ratios between non-vanishing A_Q's are then fixed by the Bethe equations.

The two-soliton state $|\, \psi^{(2)}(0) \,\rangle$ is prepared at the reference time $t = 0$ as two Gaussian wave packets with initial average positions and momenta $(\overline{x}_j, \overline{p}_j)$, $j = 1, 2$, constructed separately at large distances from the n_1-string and n_2-string within a two-particle excited state,

$$
|\, \psi^{(2)}(0) \,\rangle = \int \frac{dp_1}{2\pi} \frac{dp_2}{2\pi}\, g(p_1) g(p_2) |\, n_1, p_1;\, n_2, p_2 \,\rangle,
\tag{3.75}
$$

where

$$
g(p_j) = (2\pi\alpha_j^2)^{\frac{1}{4}}\, \mathrm{e}^{-\frac{1}{4}\alpha_j^2 (p_j - \overline{p}_j)^2 - i(p_j - \overline{p}_j)\overline{x}_j}.
\tag{3.76}
$$

depends on the free parameters $\overline{x}$, $\overline{p}$ and α. The unitary time evolution is then

$$
|\, \psi^{(2)}(t) \,\rangle = \mathrm{e}^{-i[E^{(n_1)}(p_1) + E^{(n_2)}(p_2)]t} |\, \psi^{(2)}(0) \,\rangle.
\tag{3.77}
$$

For simplicity, in this case we do not sum over different n's, but consider n-string wave packets with fixed particle content. As can be deduced from the discussion in Section 3.3, this does not significantly change the physics. The results for wave packets constructed by summing over n are obtained from those for wave packets with fixed n by averaging the dependencies on n according to the probability distribution chosen for n. Of course the indeterminacy of n introduces variances in the results, which can be calculated.

Since the n_1- and n_2-string wave packets are initially localized and well-separated, the two-soliton state at $t = 0$ is composed of two well-separated fundamental solitons, with $\{x_{Q_j^{-1}} : j = 1, \ldots, n_1\}$ grouped together and $\{x_{Q_j^{-1}} : j = n_1+1, \ldots, n_2\}$ grouped together. Thus the wavefunction $\Psi_{\{n_j p_j\}}$ in Eq. (3.75) factorizes into the product $\Psi_{n_1 p_1} \Psi_{n_2 p_2}$. The time evolution then makes the two solitons collide, and long after the collision they are again well-separated. For $t \to +\infty$ the wavefunction differs from the one at $t = 0$ just for a phase factor $-\exp(-i\Phi_{n_1 n_2}(p_1, p_2))$, that is equal to the ratio between $A_{\text{out}} = A_{[n_1, \ldots, 1, n_1+n_2, \ldots, n_1+1]}$ and $A_{\text{in}} = A_{[n_1+n_2, \ldots, n_1+1, n_1, \ldots, 1]}$,

$$
\begin{aligned}
&\Psi_{\{n_j p_j\}}(x_1, \ldots, x_{n_1+n_2}) \\
&= \begin{cases}
\Psi_{n_1 p_1}(x_1, \ldots, x_{n_1}) \Psi_{n_2 p_2}(x_{n_1+1}, \ldots, x_{n_1+n_2}), & \text{before collision,} \\
-\mathrm{e}^{-i\Phi_{n_1 n_2}(p_1, p_2)} \Psi_{n_1 p_1}(x_1, \ldots, x_{n_1}) \Psi_{n_2 p_2}(x_{n_1+1}, \ldots, x_{n_1+n_2}), & \text{after collision.}
\end{cases}
\end{aligned}
\tag{3.78}
$$

The scattering phase shifts of two strings of arbitrary length is obtained from the scattering kernel $\Phi_{n_1 n_2}$ (1.48) of the Bethe-Gaudin-Takahashi equations, which can be rewritten more explicitly as

$$\Phi_{n_1 n_2}(\lambda) = 2(1-\delta_{n_1 n_2}) \arctan\left[\frac{2\lambda}{\bar{c}\,|n_1-n_2|}\right] + 2\arctan\left[\frac{2\lambda}{\bar{c}\,(n_1+n_2)}\right] + 4\sum_{j=1}^{\min(n_1,n_2)-1} \arctan\left[\frac{2\lambda}{\bar{c}\,(|n_1-n_2|+2j)}\right]. \tag{3.79}$$

3.4.2 Displacement of trajectories

Analytic expressions for the displacement of the trajectory of each wave packet, as function of the interaction strength $\bar{c}$ and the incoming momenta $\bar{p}_1$, $\bar{p}_2$, are obtained by taking derivatives of the Bethe Ansatz scattering kernel, according to Eq. (3.15). For the scattering of an n_1-string wave packet with a n_2-string wave packet, the displacements are given by

$$\chi_j^{(n_1,n_2)}(\bar{p}_1,\bar{p}_2) = -\frac{\partial \Phi_{n_1 n_2}\left(\lambda^{(n_1)}(p_1) - \lambda^{(n_2)}(p_2)\right)}{\partial p_j}\bigg|_{p_1=\bar{p}_1,\, p_2=\bar{p}_2} \tag{3.80}$$

where $\lambda^{(n_j)}(p_j) = p_j/n_j$. Eq. (1.49) implies that they satisfy

$$\chi_1^{(n,n)}(\bar{p}_1,\bar{p}_2) = -\chi_2^{(n,n)}(\bar{p}_1,\bar{p}_2), \qquad \chi_1^{(n,m)}(\bar{p}_1,\bar{p}_2) = -\chi_2^{(m,n)}(\bar{p}_2,\bar{p}_1). \tag{3.81}$$

Explicitly,

$$\chi_j^{(n_1,n_2)}(\bar{p}_1,\bar{p}_2) = \frac{(-1)^j}{n_j}\Bigg[(1-\delta_{n_1 n_2})\frac{\bar{c}\,|n_1-n_2|}{(\bar{p}_1/n_1-\bar{p}_2/n_2)^2+[(\bar{c}/2)|n_1-n_2|]^2} + \frac{\bar{c}\,(n_1+n_2)}{(\bar{p}_1/n_1-\bar{p}_2/n_2)^2+[(\bar{c}/2)(n_1+n_2)]^2} + 2\sum_{l=1}^{\min(n_1,n_2)-1}\frac{\bar{c}\,(|n_1-n_2|+2l)}{(\bar{p}_1/n_1-\bar{p}_2/n_2)^2+[(\bar{c}/2)(|n_1-n_2|+2l)]^2}\Bigg]. \tag{3.82}$$

Notice that, in terms of the group velocities, $(\bar{p}_1/n_1 - \bar{p}_2/n_2) = \frac{1}{2}(v_1 - v_2)$. The displacements as functions of n_1, n_2 for fixed $v_1 - v_2$ have the trend shown in Fig. 3.2. At fixed n_1, n_2, the displacements are given by a summation of Lorentzian functions of $(\bar{p}_1/n_1 - \bar{p}_2/n_2)$. They are maximized for $\bar{p}_1/n_1 \to \bar{p}_2/n_2$, or $v_1 \to v_2$, i.e. in the limit of an infinitely slow scattering process, where

$$\max \chi_j^{(n_1,n_2)} = \frac{(-1)^j 4}{n_j \bar{c}}\left[(1-\delta_{n_1 n_2})\frac{1}{|n_1-n_2|} + \frac{1}{n_1+n_2} + 2\sum_{l=1}^{\min(n_1,n_2)-1}\frac{1}{|n_1-n_2|+2l}\right]. \tag{3.83}$$

Given n_1, n_2, the absolute value of the maximal displacement is larger the smaller $\bar{c}$ is. On the other hand, given $\bar{c}$, a larger total number of particles $n_1 + n_2$ generally produces a smaller maximal displacement (Fig. 3.3).

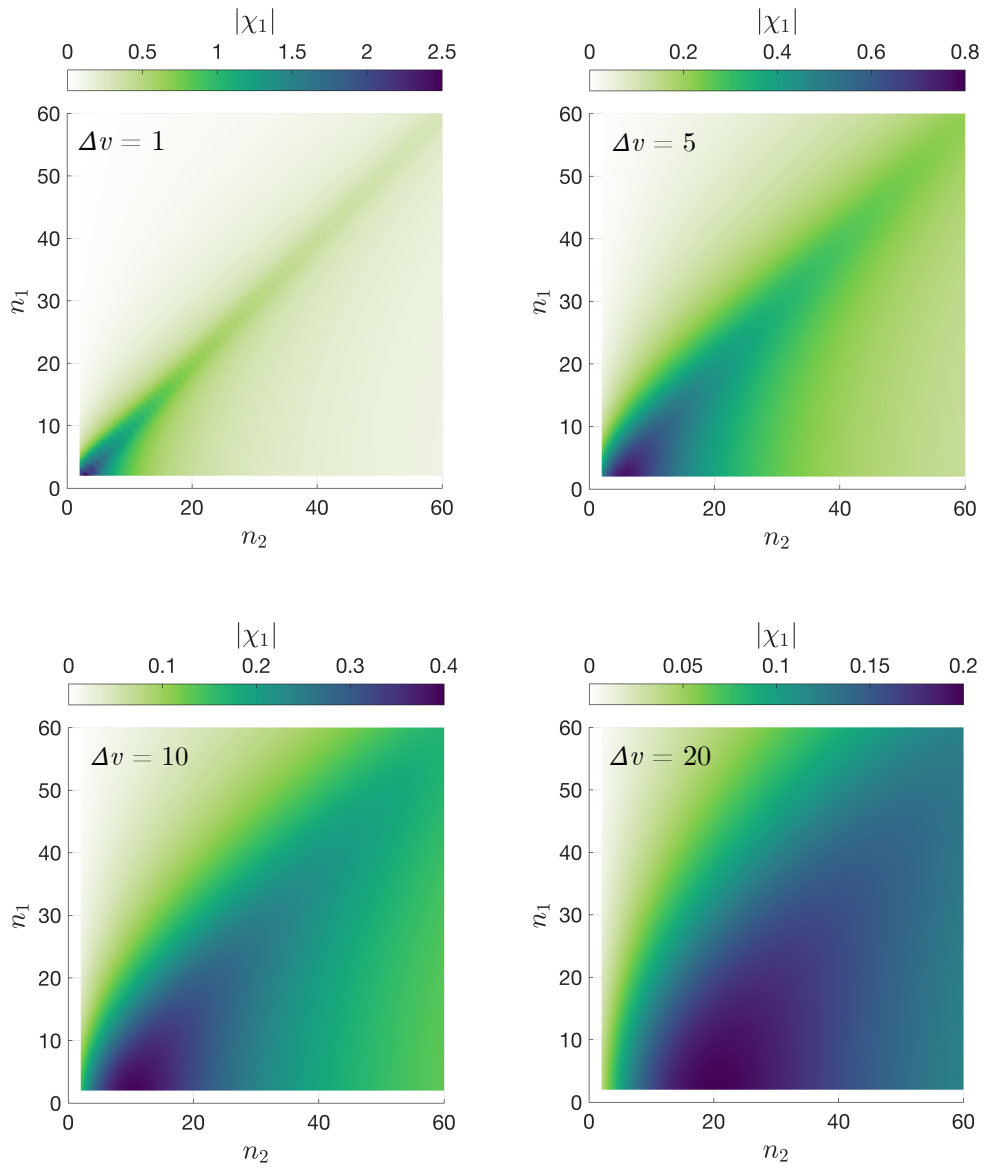


Figure 3.2: Pseudocolor plots of the absolute value of the displacement of the first soliton, $|\chi_1|$, as a function of n_1, n_2, for $\Delta v = v_1 - v_2 = 1$, 5, 10, 20 and $\overline{c} = 1$. Notice that the colorbar limits are different for each plot.

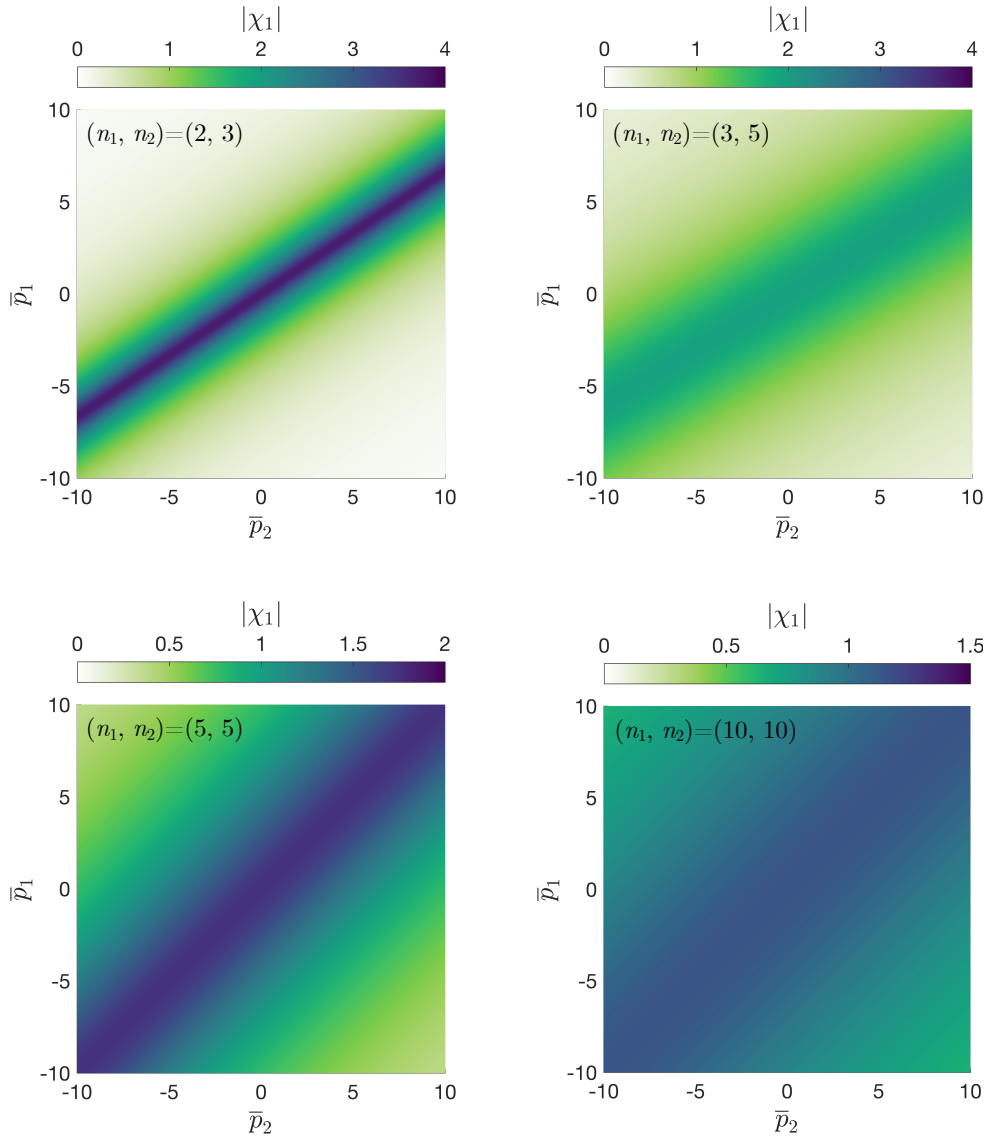


Figure 3.3: Pseudocolour plots of the absolute value of the displacement of the first soliton, $|\chi_1|$, as function of $\overline{p}_1$, $\overline{p}_2$, for $(n_1, n_2) = (2,3), (3,5), (5,5), (10,10)$ and $\overline{c} = 1$. Notice that the colorbar limits are equal for the first two plots, and different for the last two plot.

By way of illustration, we give below the explicit expressions of the displacements for some few-particle cases,

$$\chi_1^{(1,1)}(\overline{p}_1,\overline{p}_2) = -\frac{2\overline{c}}{\overline{c}^2+(\overline{p}_1-\overline{p}_2)^2},$$

$$\chi_1^{(2,2)}(\overline{p}_1,\overline{p}_2) = -8\overline{c}\left[\frac{1}{4\overline{c}^2+(\overline{p}_1-\overline{p}_2)^2}+\frac{1}{16\overline{c}^2+(\overline{p}_1-\overline{p}_2)^2}\right],$$

$$\chi_1^{(3,3)}(\overline{p}_1,\overline{p}_2) = -6\overline{c}\left[\frac{2}{9\overline{c}^2+(\overline{p}_1-\overline{p}_2)^2}+\frac{4}{36\overline{c}^2+(\overline{p}_1-\overline{p}_2)^2}+\frac{3}{81\overline{c}^2+(\overline{p}_1-\overline{p}_2)^2}\right],$$

$$\chi_1^{(4,4)}(\overline{p}_1,\overline{p}_2) = -16\overline{c}\left[\frac{1}{16\overline{c}^2+(\overline{p}_1-\overline{p}_2)^2}+\frac{2}{64\overline{c}^2+(\overline{p}_1-\overline{p}_2)^2}+\frac{3}{144\overline{c}^2+(\overline{p}_1-\overline{p}_2)^2}+\frac{2}{256\overline{c}^2+(\overline{p}_1-\overline{p}_2)^2}\right],$$

$$\chi_1^{(1,2)}(\overline{p}_1,\overline{p}_2) = -4\overline{c}\left[\frac{1}{\overline{c}^2+(2\overline{p}_1-\overline{p}_2)^2}+\frac{3}{9\overline{c}^2+(2\overline{p}_1-\overline{p}_2)^2}\right],$$

$$\chi_2^{(1,2)}(\overline{p}_1,\overline{p}_2) = 2\overline{c}\left[\frac{1}{\overline{c}^2+(2\overline{p}_1-\overline{p}_2)^2}+\frac{3}{9\overline{c}^2+(2\overline{p}_1-\overline{p}_2)^2}\right],$$

$$\chi_1^{(1,3)}(\overline{p}_1,\overline{p}_2) = -4\overline{c}\left[\frac{1}{4\overline{c}^2+\frac{2}{9}(3\overline{p}_1-\overline{p}_2)^2}+\frac{1}{4\overline{c}^2+\frac{1}{9}(3\overline{p}_1-\overline{p}_2)^2}\right],$$

$$\chi_2^{(1,3)}(\overline{p}_1,\overline{p}_2) = \frac{4\overline{c}}{3}\left[\frac{1}{2\overline{c}^2+\frac{2}{9}(3\overline{p}_1-\overline{p}_2)^2}+\frac{1}{4\overline{c}^2+\frac{1}{9}(3\overline{p}_1-\overline{p}_2)^2}\right].$$

3.4.3 Spreading and correlations

Second order derivatives of the scattering kernel,

$$\chi_{ij}^{(n_1,n_2)}(\overline{p}_1,\overline{p}_2) = -\frac{\partial^2\Phi_{n_1n_2}\left(\lambda^{(n_1)}(p_1)-\lambda^{(n_2)}(p_2)\right)}{\partial p_i\partial p_j}\bigg|_{p_1=\overline{p}_1,\,p_2=\overline{p}_2}, \tag{3.84}$$

allow us to evaluate the spreading of the wave packets and their correlation after scattering according to Eqs. (3.19) and (3.21). Explicitly,

$$\begin{aligned}\chi_{ij}^{(n_1,n_2)}(\overline{p}_1,\overline{p}_2) = {}& \frac{(-1)^{i+j}}{n_in_j}2(\overline{p}_1/n_1-\overline{p}_2/n_2)\\ &\times\Bigg[(1-\delta_{n_1n_2})\frac{\overline{c}\,|n_1-n_2|}{[(\overline{p}_1/n_1-\overline{p}_2/n_2)^2+((\overline{c}/2)|n_1-n_2|)^2]^2}\\ &+\frac{\overline{c}\,(n_1+n_2)}{[(\overline{p}_1/n_1-\overline{p}_2/n_2)^2+((\overline{c}/2)(n_1+n_2))^2]^2}\\ &+2\sum_{l=1}^{\min(n_1,n_2)-1}\frac{\overline{c}\,(|n_1-n_2|+2l)}{[(\overline{p}_1/n_1-\overline{p}_2/n_2)^2+((\overline{c}/2)(|n_1-n_2|+2l))^2]^2}\Bigg].\end{aligned} \tag{3.85}$$

In particular,

$$\chi_{ij}^{(n_1,n_2)}(\overline{p}_1,\overline{p}_2) = 0 \qquad \text{for} \qquad \overline{p}_1/n_1 = \overline{p}_2/n_2. \tag{3.86}$$

3.5 Mean-field soliton scattering

Similarly to the static case, where the Hartree mean field approximation (or its variations) approximates well the exact ground state for a large number of particles, we expect also

the scattering of quasi-solitons to be well described by a mean field approximation if the number of particles composing each wave packet is large.

The fundamental soliton state in the mean field approach is given by an Hartree product with all the particles having the same classical soliton wavefunction (2.76),

$$|\,\psi_s(t)\,\rangle = \frac{1}{\sqrt{n!}}\left[\int dx\,\phi_{n\lambda}(x,t)\hat{\psi}^\dagger(x)\right]^n |\,0\,\rangle. \tag{3.87}$$

Notice that the wavefunction is $\phi_{n\lambda}(x,t) = n^{-1/2}\psi_{n\lambda}(x,t)$, so that $|\,\psi_s(t)\,\rangle$ is normalized to unity[6]. This the mean field analogue of the n-string state defined by Eq. (3.23). However, since $\phi_{n\lambda}(x,t)$ already localized in space, there is no need to sum over different momenta to obtain a localized wave packet. In the limit of large n,

$$\langle\,\psi_s(t)\,|\,\hat{\psi}(z)\,|\,\psi_s(t)\,\rangle \overset{n\to\infty}{\simeq} \psi_{n\lambda}(z,t), \tag{3.88}$$

that is the mean field analogue of Eq. (3.71).

A two-soliton state is constructed in the same way, now taking as single-particle wavefunction a two-soliton solution of the time-dependent GPE,

$$i\partial_t\phi_{n_1n_2\lambda}(x,t) = \left[-\partial_x^2 - 2(n_1+n_2)\bar{c}|\phi_{n_1n_2\lambda}(x,t)|^2\right]\phi_{n_1n_2\lambda}(x,t). \tag{3.89}$$

The structure of the general n-soliton solution is discussed by Zakharov and Shabat (1971), and the explicit expression for the two-soliton solution can be found in Yoon and Negele (1977); Dolan (1976). The total wavefunction is thus

$$\Psi^{(c)}_{n_1n_2}(x_1,\ldots,x_{n_1+n_2},t) = \prod_{j=1}^{n_1+n_2}\phi_{n_1n_2\lambda}(x_j,t) \tag{3.90}$$

and the two-soliton state is

$$|\,\psi^{(2)}_s(t)\,\rangle = \frac{1}{\sqrt{(n_1+n_2)!}}\int dx_1\cdots dx_{n_1+n_2}\Psi^{(c)}_{n_1n_2}(x_1,\ldots,x_{n_1+n_2},t)\hat{\psi}^\dagger(x_1)\cdots\hat{\psi}^\dagger(x_{n_1+n_2})|\,0\,\rangle. \tag{3.91}$$

As before, the actual expression of the two-soliton wavefunction is unnecessary, since long before and long after the scattering it factorizes into the product of two well-separated fundamental solitons. That is, the total wavefunction (3.90) is asymptotic to

$$\Psi^{(0)}_{n_1n_2}(x_1,\ldots,x_{n_1+n_2},t) = \sum_Q\prod_{j=1}^{n_1}\phi_{n_1\lambda_1}(x_{Q_j},t)\prod_{j=n_1+1}^{n_1+n_2}\phi_{n_2\lambda_2}(x_{Q_j},t) \tag{3.92}$$

where Q are the permutations of $[1,\ldots,n_1,n_1+1,\ldots,n_1+n_2]$ with the grouping of bosons into $[1,\ldots,n_1]$ and $[n_1+1,\ldots,n_1+n_2]$ unchanged. The corresponding two-soliton state is

$$\begin{aligned}|\,\psi^{(2)}_s(t)\,\rangle &= \mathcal{N}_{n_1n_2}\int dx_1\cdots dx_{n_1+n_2}\Psi^{(0)}_{n_1n_2}(x_1,\ldots,x_{n_1+n_2},t)\hat{\psi}^\dagger(x_1)\cdots\hat{\psi}^\dagger(x_{n_1+n_2})|\,0\,\rangle\\ &= \frac{1}{\sqrt{n_1!n_2!}}\left[\int dx\,\phi_{n_1\lambda_1}(x,t)\hat{\psi}^\dagger(x)\right]^{n_1}\left[\int dx\,\phi_{n_2\lambda_2}(x,t)\hat{\psi}^\dagger(x)\right]^{n_2}|\,0\,\rangle\end{aligned} \tag{3.93}$$

The connection between $\phi_{n_1n_2\lambda}$ and $\phi_{n_1\lambda_1}$, $\phi_{n_2\lambda_2}$ is (Zakharov and Shabat, 1971)

$$\phi_{n_1n_2\lambda}(x,t) = \begin{cases}\mathcal{N}_1\phi_{n_1\lambda_1}(x,t) + \mathcal{N}_2\phi_{n_2\lambda_2}(x,t), & \text{before collision,}\\ \mathcal{N}_1 e^{i\delta\theta_1}\phi_{n_1\lambda_1}(x-\delta x_1,t) + \mathcal{N}_2 e^{i\delta\theta_2}\phi_{n_2\lambda_2}(x-\delta x_2,t), & \text{after collision,}\end{cases} \tag{3.94}$$

[6]Here we consider the wavefunction in the GP or CD approximation; as usual, the result in the Hartree approximation is recovered by setting $\bar{c}\to(1-n^{-1})\bar{c}$.

where $\mathcal{N}_j = \sqrt{n_j/(n_1+n_2)}$ ensures the correct normalization, and the phase shifts and position displacements are (Lai and Haus, 1989a)

$$\delta\theta_1 = -2\arctan\left[\frac{2(\lambda_1-\lambda_2)}{\bar{c}\,|n_1-n_2|}\right] + 2\arctan\left[\frac{2(\lambda_1-\lambda_2)}{\bar{c}\,(n_1+n_2)}\right], \tag{3.95a}$$

$$\delta\theta_2 = -\delta\theta_1, \tag{3.95b}$$

$$\delta x_1 = \frac{2}{n_1\bar{c}}\ln\left[\frac{(\lambda_1-\lambda_2)^2+(\bar{c}^2/4)(n_1-n_2)^2}{(\lambda_1-\lambda_2)^2+(\bar{c}^2/4)(n_1+n_2)^2}\right], \tag{3.95c}$$

$$\delta x_2 = -\frac{2}{n_2\bar{c}}\ln\left[\frac{(\lambda_1-\lambda_2)^2+(\bar{c}^2/4)(n_1-n_2)^2}{(\lambda_1-\lambda_2)^2+(\bar{c}^2/4)(n_1+n_2)^2}\right]. \tag{3.95d}$$

We can verify that the displacement obtained from the Bethe Ansatz approaches the mean field result in the limit of large n_1,

$$\begin{aligned}
\chi_1^{(n_1,n_2)} &= -\frac{1}{n_1}\frac{\partial\Phi_{n_1n_2}(\lambda_1-\lambda_2)}{\partial\lambda_1} \\
&= -\frac{1}{n_1}\left[(1-\delta_{n_1n_2})\frac{\bar{c}\,|n_1-n_2|}{(\lambda_1-\lambda_2)^2+[(\bar{c}/2)|n_1-n_2|]^2} + \frac{\bar{c}\,(n_1+n_2)}{(\lambda_1-\lambda_2)^2+[(\bar{c}/2)(n_1+n_2)]^2}\right. \\
&\qquad \left. + 2\sum_{l=1}^{\min(n_1,n_2)-1}\frac{\bar{c}\,(|n_1-n_2|+2l)}{(\lambda_1-\lambda_2)^2+[(\bar{c}/2)(|n_1-n_2|+2l)]^2}\right] \\
&\overset{n_1\to\infty}{\simeq} -\frac{1}{n_1}\int_{|n_1-n_2|}^{n_1+n_2} dx\,\frac{\bar{c}\,x}{(\lambda_1-\lambda_2)^2+(\bar{c}^2/4)x^2} = \delta x_1.
\end{aligned} \tag{3.96}$$

In Figs. 3.4 and 3.5 we compare the Bethe Ansatz and mean field results for the displacement of the first soliton as a function of the incoming momenta or group velocities. The first observation is that the mean field result has a pathological behavior for $n_1 = n_2$ and any finite $\bar{c}$ in the limit of a zero collision velocity, since it diverges logarithmically. For $n_1 \neq n_2$, the mean field approach approximates quite well the Bethe Ansatz already for a relatively small total number of particles, such as $n_1 + n_2 = 10$. In general, the approximation works better for larger collision velocities.

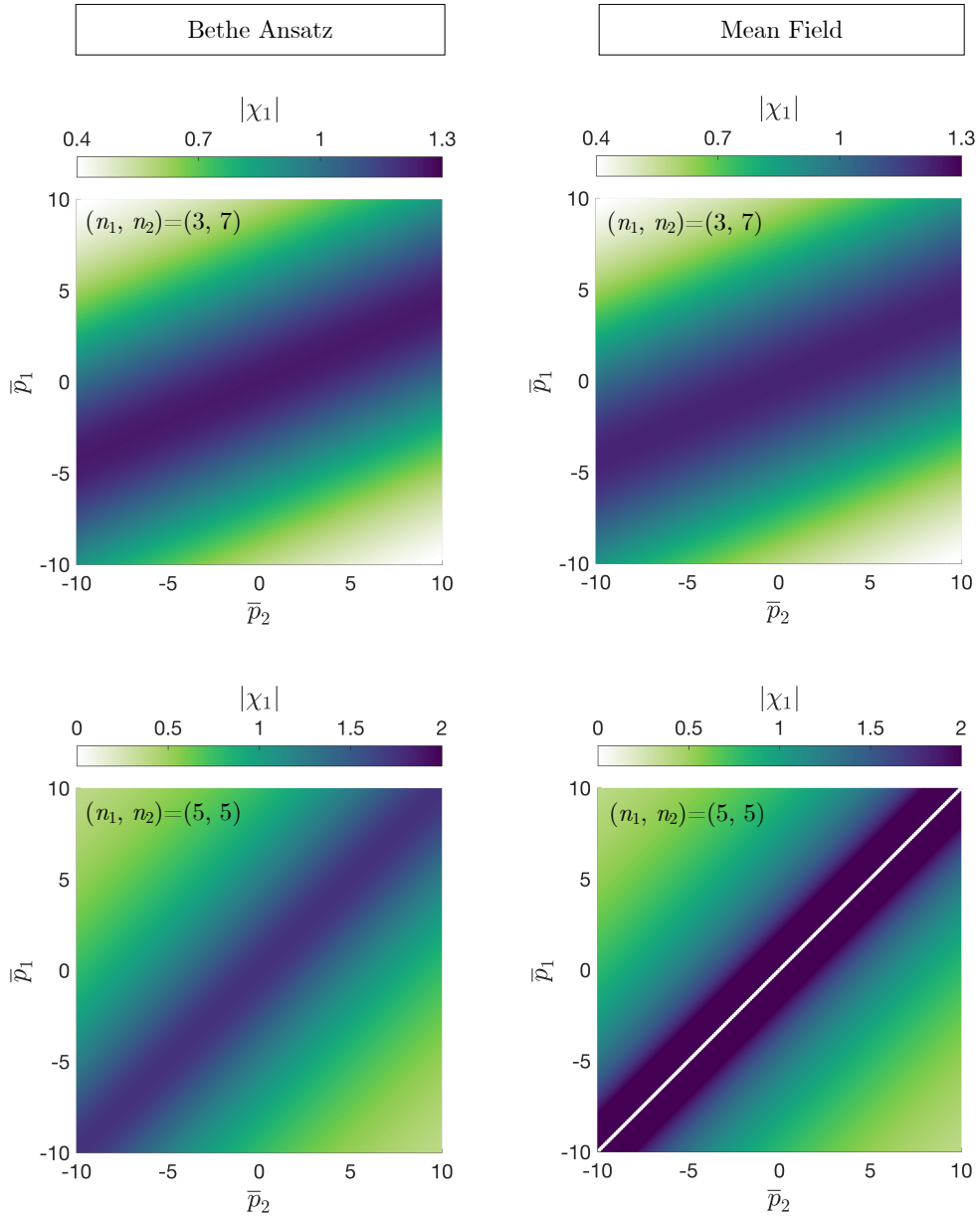


Figure 3.4: Pseudocolour plots of the absolute value of the displacement of the first soliton, $|\chi_1|$, as function of $\overline{p}_1$, $\overline{p}_2$, for $(n_1, n_2) = (3, 7), (5, 5)$ and $\overline{c} = 1$, obtained from the Bethe Ansatz (left column) and the mean field approach (right column). The white line cut in the mean field plot represents the divergence for $n_1 = n_2$ and $p_1 \to p_2$.

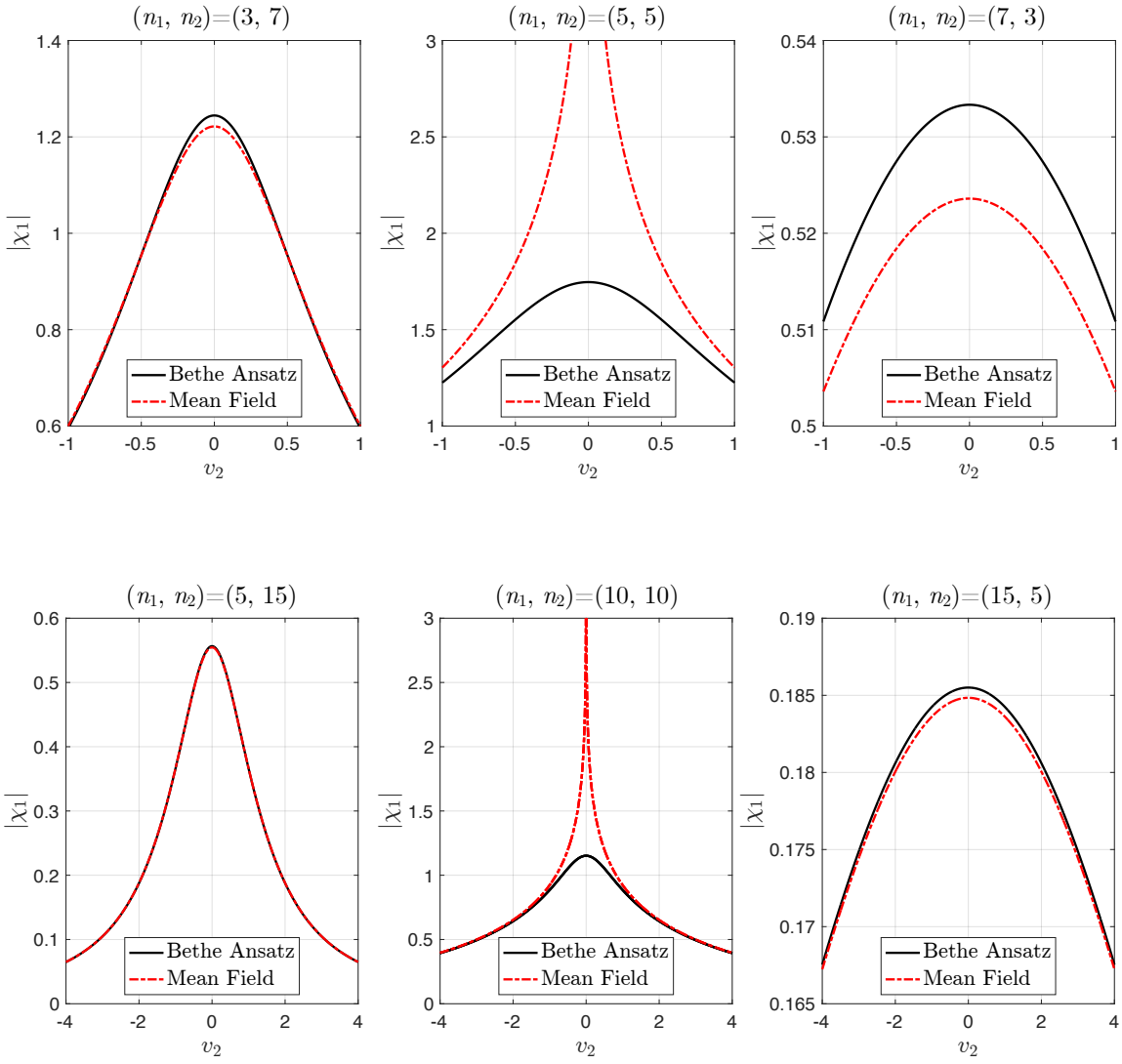


Figure 3.5: Absolute value of the displacement of the first soliton as a function of v_2, for several values of (n_1, n_2) and $\bar{c} = 1$, along the line $p_1 = -(n_2/n_1)p_2$, orthogonal to the line $p_1/n_1 = p_2/n_2$ (i.e. $v_1 = v_2$) where the displacement is maximal. The mean field result diverges logarithmically for $v_2 \to 0$ when $n_1 = n_2$.

Chapter 4

Ground state and excitations in the repulsive case

In the repulsive case, the excitation spectrum of the Lieb-Liniger model has two distinct branches, corresponding to particle-like (Type I) and hole-like (Type II) excitations. The coexistence of these two types of elementary excitations leads to a significant broadening of the dynamical response functions, clearly visible for strong interactions (Caux et al., 2007; Meinert at al., 2015). Particle-like excitations, which exist also in 2D and 3D, are of the same nature of Bogoliubov modes, which represent their weakly interacting limit. Hole-like excitations, instead, have no counterpart in Bose systems in higher dimensions. They cannot be obtained directly in the framework of Bogoliubov or mean field theories, however their dispersion relation can be identified with that of dark soliton solutions of the mean field theory.

In this chapter we discuss in detail the energetics of the repulsive model, comparing the exact results with various effective approaches, and we investigate the correspondence between classical dark solitons and Lieb's Type II excitation, which motivates the search for quantum dark solitons we will consider in the next chapter.

4.1 Thermodynamic Bethe Ansatz

The dispersion relations of Type I and Type II excitations depend on the corresponding displacement functions, which quantify how the rapidity of the additional particle or hole influences all the other rapidities of the system. They can be written in a more explicit form by using the Thermodynamic Bethe Ansatz, that is a formulation of the thermodynamics of the system in terms of the densities of rapidities which define Bethe eigenstates, and taking eventually $T = 0$.

The equilibrium thermodynamics of our system is encoded in the partition function. In the grand canonical ensemble, this is given by

$$Z = \mathrm{Tr}\, \exp\left(-\frac{\hat{H} - \mu\hat{N}}{T}\right) = \sum_{N=0}^{\infty} \sum_{\{I\}_N} \exp\left(-\frac{E_{\{I\}_N} - \mu N}{T}\right), \tag{4.1}$$

where μ is the chemical potential, T is the absolute temperature, and $\{I\}_N$ represents a proper set of quantum numbers at fixed number of particles N.

In the thermodynamic limit, we can transform the explicit summation over all possible configurations of quantum numbers into a functional integral. In order to do so, we partition the real line for $x = I/L$ into 'boxes' $B_\alpha = [x_\alpha, x_\alpha + \Delta x_\alpha \equiv x_{\alpha+1}]$, $\alpha \in \mathbb{Z}$, with the condition $L^{-1} \ll \Delta x_\alpha \ll 1$. In each such box, for each individual eigenstate specified by the densities $\rho(x_\alpha)$, $\rho_h(x_\alpha)$, and $\rho_t(x_\alpha)$, there are $L\rho_t(x_\alpha)\Delta x_\alpha$ allowed quantum numbers, $L\rho(x_\alpha)\Delta x_\alpha$

particles, and $L\rho_h(x_\alpha)\Delta x_\alpha$ holes. We can then rewrite the sum over quantum number configurations as

$$\sum_{N=0}^{\infty}\sum_{\{I\}_N}\Big(\dots\Big) = \prod_{\alpha=-\infty}^{\infty}\sum_{n_\alpha}^{L\Delta x_a}\sum_{\{\frac{I}{L}\}_{n_\alpha}\in B_\alpha}\Big(\dots\Big), \tag{4.2}$$

i.e. we take the product over all boxes, and for a given box we sum over the possible occupations and over the sets of occupied quantum numbers given the occupation. In the thermodynamic limit, 'in-box' rearrangements of quantum numbers do not affect the result to leading order, i.e. $(\dots)$ is insensitive to the choice of $\{I/L\}_{n_\alpha}\in B_\alpha$. Thus we factor out

$$\sum_{\{\frac{I}{L}\}_{n_\alpha}\in B_\alpha} 1 \;=\; \frac{(L\rho_t(x_\alpha)\Delta x_\alpha)!}{(L\rho(x_\alpha)\Delta x_\alpha)!(L\rho_h(x_\alpha)\Delta x_\alpha)!}. \tag{4.3}$$

By assumption, $L\Delta x_\alpha \gg 1$, so all these factorials are very large and we can use Stirling's approximation, $\ln n! \simeq n\ln n - n$, to write

$$\sum_{\{\frac{I}{L}\}_{n_\alpha}\in B_\alpha} 1 \;=\; \mathrm{e}^{L\Delta x_\alpha S_\alpha(x_\alpha)}, \tag{4.4}$$

where

$$S_\alpha(x_\alpha) \equiv \Big[(\rho+\rho_h)\ln(\rho+\rho_h) - \rho\ln\rho - \rho_h\ln\rho_h\Big](x_\alpha). \tag{4.5}$$

This leads us to rewrite the partition function as a functional integral weighted by an entropy functional,

$$Z = \int \mathcal{D}[\rho(x)]\,\mathrm{e}^{S[\rho(x)]-\frac{1}{T}(E[\rho(x)]-\mu N[\rho(x)])}, \tag{4.6}$$

where $\int\mathcal{D}[\rho(x)](\dots) = \prod_{\alpha=-\infty}^{\infty}\int_0^1 d\rho(x_\alpha)(\dots)$ and the entropy functional is

$$S[\rho(x)] \equiv L\int_{-\infty}^{+\infty} dx\,\Big[(\rho+\rho_h)\ln(\rho+\rho_h) - \rho\ln\rho - \rho_h\ln\rho_h\Big](x). \tag{4.7}$$

Since it is more convenient to work with densities in rapidity space rather than quantum number space, we formally perform the functional transformation

$$\rho(x),\,\rho_h(x)\,\Big|_{\rho(x)+\rho_h(x)=1} \longrightarrow \rho(\lambda),\,\rho_h(\lambda)\,\Big|_{\rho(\lambda)+\rho_h(\lambda)=\frac{1}{2\pi}+\mathcal{C}*\rho(\lambda)} \tag{4.8}$$

and rewrite Z as the functional integral of a Gibbs weight $G[\rho,\rho_h]$ (from now on, except if explicitly stated otherwise, $\rho=\rho(\lambda)$ and $\rho_h=\rho_h(\lambda)$),

$$Z = \int \mathcal{D}[\rho,\rho_h]\,\mathrm{e}^{-G[\rho,\rho_h]/T}, \tag{4.9}$$

where $\int\mathcal{D}[\rho,\rho_h](\dots) = \int\mathcal{D}[\rho(\lambda)]\mathcal{D}[\rho_h(\lambda)]\,\det\Big[\frac{\delta\rho(x)}{\delta\rho(\lambda)}\Big]\,\delta(\rho(\lambda)+\rho_h(\lambda)-C*\rho(\lambda)-\frac{1}{2\pi})(\dots)$ and

$$G[\rho,\rho_h] = E[\rho] - TS[\rho,\rho_h] - \mu N[\rho], \tag{4.10}$$

with

$$\begin{aligned} E[\rho] &= L\int_{-\infty}^{+\infty} d\lambda\,\lambda^2\rho(\lambda), \qquad N[\rho] = L\int_{-\infty}^{+\infty} d\lambda\,\rho(\lambda) \\ S[\rho,\rho_h] &= L\int_{-\infty}^{+\infty} d\lambda\,\Big[(\rho+\rho_h)\ln(\rho+\rho_h) - \rho\ln\rho - \rho_h\ln\rho_h\Big](\lambda). \end{aligned} \tag{4.11}$$

In the limit $L \to \infty$, the functional integral can be evaluated in a saddle-point approximation, i.e. at the minimum of G. Imposing $\delta G = 0$ for arbitrary variations $\delta\rho$ (the variations $\delta\rho$ and $\delta\rho_h$ are related by the Bethe equations, $\delta\rho - \mathcal{C} * \delta\rho = -\delta\rho_h$) yields the Yang-Yang equilibrium condition (Yang and Yang, 1969),

$$\epsilon(\lambda) = \lambda^2 - \mu - \mathcal{C} * T \ln\left[1 + \mathrm{e}^{-\epsilon(\lambda)/T}\right], \tag{4.12}$$

where $\epsilon(\lambda)$ is the function defined by

$$\epsilon(\lambda) \equiv T \ln\left[\frac{\rho_h(\lambda)}{\rho(\lambda)}\right]. \tag{4.13}$$

Substituting this into the expression of G we finally obtain the grand canonical potential of the system,

$$\frac{G(\mu, T, L)}{L} = -T \int_{-\infty}^{+\infty} \frac{d\lambda}{2\pi} \ln\left[1 + \mathrm{e}^{-\epsilon(\lambda)/T}\right]. \tag{4.14}$$

Eqs. (4.12)–(4.14) encode all the equilibrium thermodynamics of the system.

4.1.1 Lieb and Yang-Yang equations

Let us now consider the ϵ function for the ground state, which we shall denote ϵ_g. The Yang-Yang equation (4.12) for ϵ_g is

$$\epsilon_g(\lambda) = \lambda^2 - \mu + \mathcal{C} * T \ln\left(\frac{\rho_{g,h}}{\rho_g + \rho_{g,h}}\right) \tag{4.15}$$

where ρ_g and $\rho_{g,h}$ are the densities of particles and holes of the ground state, respectively. The former satisfies the Lieb equation (1.99). Introducing the Cauchy kernel restricted to the Fermi interval,

$$\mathcal{C}^{(F)}(\lambda, \lambda') \equiv \theta(\lambda_F - |\lambda|)\, \mathcal{C}(\lambda - \lambda')\, \theta(\lambda_F - |\lambda'|), \tag{4.16}$$

and its inverse $\mathcal{L}^{(F)}$, such that

$$\left(1 + \mathcal{L}^{(F)}\right) * \left(1 - \mathcal{C}^{(F)}\right)(\lambda, \lambda') = \delta(\lambda - \lambda'), \qquad \lambda, \lambda' \in \mathbb{R}, \tag{4.17}$$

the Lieb equation can be rewritten in a form that is valid for all λ,

$$\left(1 - \mathcal{C}^{(F)}\right) * \rho_g(\lambda) = \frac{\theta(\lambda_F - |\lambda|)}{2\pi}, \tag{4.18}$$

and solved as

$$\rho_g(\lambda) = \frac{1}{2\pi}\left(1 + \mathcal{L}^{(F)}\right) * \theta(\lambda_F - |\lambda|) = \frac{\theta(\lambda_F - |\lambda|)}{2\pi} + \frac{1}{2\pi}\int_{-\lambda_F}^{\lambda_F} d\lambda'\, \mathcal{L}^{(F)}(\lambda, \lambda'). \tag{4.19}$$

Since $\rho_g = 0$ outside the Fermi interval, and $\rho_{g,h} = 0$ inside it, in the limit $T \to 0$ the Yang-Yang equation becomes

$$\epsilon_g(\lambda) - \int_{-\lambda_F}^{\lambda_F} d\lambda'\, \mathcal{C}(\lambda - \lambda')\epsilon_g(\lambda') = \epsilon_0(\lambda), \qquad \lambda \in \mathbb{R}, \tag{4.20}$$

where $\epsilon_0(\lambda) \equiv \lambda^2 - \mu$. The chemical potential μ is fixed by the condition

$$\epsilon_g(\pm\lambda_F) = 0. \tag{4.21}$$

Let us now define a function $\epsilon^{(-)}(\lambda)$ such that

$$\Big(1-\mathcal{C}^{(F)}\Big)*\epsilon^{(-)}(\lambda)=\epsilon_0(\lambda),\qquad \text{i.e.}\qquad \epsilon^{(-)}(\lambda)=\Big(1+\mathcal{L}^{(F)}\Big)*\epsilon_0(\lambda). \tag{4.22}$$

Clearly this function is equal to $\epsilon_g(\lambda)$ inside the Fermi interval, while it is equal to $\epsilon_0(\lambda)$ outside the Fermi interval. Therefore, we can rewrite Eq. (4.20) as

$$\epsilon_g(\lambda)=\epsilon_0(\lambda)+\int_{-\lambda_F}^{\lambda_F}d\lambda'\,\mathcal{C}(\lambda-\lambda')\epsilon^{(-)}(\lambda'),\qquad \lambda\in\mathbb{R}. \tag{4.23}$$

This is the solution of the zero temperature Yang-Yang equation, and it is determined once the function $\epsilon^{(-)}(\lambda)$ inside the Fermi interval is known[1]. The function $\epsilon_g(\lambda)$ satisfies the following properties:

$$\begin{aligned}
\epsilon_g(\lambda)&=\epsilon_g(-\lambda), && && \text{(4.24a)}\\
\partial_\lambda\epsilon_g(\lambda)&>0, && \text{for} \quad \lambda\ &>0, && \text{(4.24b)}\\
\epsilon_g(\lambda)&<0, && \text{for} \quad |\lambda|\ &<\lambda_F, && \text{(4.24c)}\\
\epsilon_g(\lambda)&>0, && \text{for} \quad |\lambda|\ &>\lambda_F, && \text{(4.24d)}\\
\epsilon_g(\lambda)&\to\epsilon_0(\lambda)+O(\lambda^{-2}), && \text{for} \quad \lambda\ &\to\pm\infty. && \text{(4.24e)}
\end{aligned}$$

Finally, notice that using Eqs. (4.19) and (4.22) we can rewrite the total ground state energy $E_0-\mu N$, which includes the contribution from the microcanonical ensemble, $E_0=L\int_{-\lambda_F}^{\lambda_F}d\lambda\,\lambda^2\rho_g(\lambda)$, and from the chemical potential, $-\mu N=-\mu L\int_{-\lambda_F}^{\lambda_F}d\lambda\,\rho_g(\lambda)$, as

$$E_0-\mu N=L\int_{-\lambda_F}^{\lambda_F}d\lambda\,\epsilon_0(\lambda)\rho_g(\lambda)=\frac{L}{2\pi}\int_{-\lambda_F}^{\lambda_F}d\lambda\,\epsilon_g(\lambda). \tag{4.25}$$

4.1.2 Dispersion relations of particle and hole excitations

Eq. (1.107) for the displacements of Type I excitations is written in terms of the restricted kernel $\mathcal{C}^{(F)}$ as

$$\Big(1-\mathcal{C}^{(F)}\Big)*D_p(\lambda,k)=-\frac{\theta(\lambda_F-|\lambda|)}{2\pi}\Big[\mathrm{sgn}(k)\pi+\phi(\lambda-k)\Big],\qquad |k|>\lambda_F. \tag{4.26}$$

The formal solution is

$$\begin{aligned}
D_p(\lambda,k)&=-\frac{1}{2\pi}\int_{-\lambda_F}^{\lambda_F}d\lambda''\,\Big[\delta(\lambda-\lambda'')+\mathcal{L}^{(F)}(\lambda,\lambda'')\Big]\,\Big[\mathrm{sgn}(k)\pi+\phi(\lambda''-k)\Big]\\
&=-\int_{k}^{\mathrm{sgn}(k)\infty}d\lambda'\int_{-\lambda_F}^{\lambda_F}d\lambda''\,\Big[\delta(\lambda-\lambda'')+\mathcal{L}^{(F)}(\lambda,\lambda'')\Big]\,\mathcal{C}(\lambda''-\lambda').
\end{aligned} \tag{4.27}$$

The momentum (1.108) of a Type I excitation can then be written

$$p_{\mathrm{I}}(k)=k-\frac{1}{2\pi}\int_{-\lambda_F}^{\lambda_F}d\lambda''\int_{-\lambda_F}^{\lambda_F}d\lambda\,\Big[\delta(\lambda-\lambda'')+\mathcal{L}^{(F)}(\lambda,\lambda'')\Big]\,\Big[\mathrm{sgn}(k)\pi+\phi(\lambda''-k)\Big], \tag{4.28}$$

and using the Lieb equation to perform the integration over λ we obtain

$$p_{\mathrm{I}}(k)=k+\int_{-\lambda_F}^{\lambda_F}d\lambda\,\Big[\phi(k-\lambda)-\mathrm{sgn}(k)\pi\Big]\rho_g(\lambda)\equiv p(k),\qquad |k|>\lambda_F. \tag{4.29}$$

[1] Notice that $\epsilon_g(\lambda)$ is a smooth function, and it is different for $\epsilon_0(\lambda)$ outside the Fermi interval, since $\int_{-\lambda_F}^{\lambda_F}d\lambda'\,\mathcal{C}(\lambda-\lambda')\epsilon^{(-)}(\lambda')$ gives a finite contribution. Consequently, $\epsilon^{(-)}(\lambda)$ is discontinuous in $|\lambda|=\lambda_F$.

The energy (1.109) of a Type I excitation can be written

$$\omega_{\rm I}(k) = \epsilon_0(k) + \int_{-\lambda_F}^{\lambda_F} d\lambda \, \frac{d\epsilon_0(\lambda)}{d\lambda} \, D_p(\lambda, k), \tag{4.30}$$

and since $D_p(\lambda, k)$ vanishes identically for $|\lambda| > \lambda_F$, we can equivalently write

$$\begin{aligned}
\omega_{\rm I}(k) &= \epsilon_0(k) + \int_{-\infty}^{+\infty} d\lambda \, \frac{d\epsilon_0(\lambda)}{d\lambda} \, D_p(\lambda, k) \\
&= \epsilon_0(k) - \int_k^{\mathrm{sgn}(k)\infty} d\lambda' \int_{-\lambda_F}^{\lambda_F} d\lambda'' \int_{-\infty}^{+\infty} d\lambda \, \frac{d\epsilon_0(\lambda)}{d\lambda} \Big[\delta(\lambda - \lambda'') + \mathcal{L}^{(F)}(\lambda, \lambda'')\Big] \, \mathcal{C}(\lambda'' - \lambda') \\
&= \epsilon_0(k) - \int_k^{\mathrm{sgn}(k)\infty} d\lambda \left[\frac{d\epsilon_g(\lambda)}{d\lambda} - \frac{d\epsilon_0(\lambda)}{d\lambda}\right].
\end{aligned} \tag{4.31}$$

Finally, using property (4.24e) to simplify the last integral, we obtain

$$\omega_{\rm I}(k) = \epsilon_g(k), \qquad |k| > \lambda_F. \tag{4.32}$$

Thus the function $\epsilon_g(k)$ represents the energy of a fundamental particle-like excitation above the ground state.

The same considerations applied to Type II excitations lead to similar equations,

$$p_{\rm II}(q) = -q - \int_{-\lambda_F}^{\lambda_F} d\lambda \, \Big[\phi(q - \lambda) - \mathrm{sgn}(q)\pi\Big] \rho_g(\lambda) = -p(q), \tag{4.33}$$

$$\omega_{\rm II}(q) = -\epsilon_g(q), \qquad |q| < \lambda_F. \tag{4.34}$$

Then for a generic number of particle and hole excitations,

$$\Delta P = \sum_{\text{particles}} p(k) - \sum_{\text{holes}} p(q), \tag{4.35}$$

$$\Delta E = \sum_{\text{particles}} \epsilon_g(k) - \sum_{\text{holes}} \epsilon_g(q). \tag{4.36}$$

4.1.3 Sound velocity and effective masses

At small momenta, and for arbitrary interaction strength, the dispersion relations of Type I and Type II excitations may be expanded in series of p as

$$\omega(p) = vp + \frac{p^2}{2m^*} + O(p^3), \tag{4.37}$$

where

$$v = \left.\frac{\partial \omega(p)}{\partial p}\right|_{p\to 0} \qquad \text{and} \qquad \frac{1}{m^*} = \left.\frac{\partial^2 \omega(p)}{\partial p^2}\right|_{p\to 0} \tag{4.38}$$

are respectively the group velocity and the inverse effective mass of the elementary excitations. From Eqs. (4.29), (4.32), (4.33), and (4.34) it is clear that

$$v \equiv v_{\rm I} = v_{\rm II} \qquad \text{and} \qquad m^* \equiv m^*_{\rm I} = -m^*_{\rm II}. \tag{4.39}$$

Let us first consider the group velocity. We have

$$v = \left.\frac{\partial \omega(p)}{\partial p}\right|_{p\to 0} = \left.\frac{\partial \omega(k)}{\partial k}\left(\frac{\partial p(k)}{\partial k}\right)^{-1}\right|_{k\to\lambda_F} \tag{4.40}$$

and from Eq. (4.29),

$$\left.\frac{\partial p(k)}{\partial k}\right|_{k\to\lambda_F} = 1 + 2\pi \int_{-\lambda_F}^{\lambda_F} d\lambda\, \mathcal{C}(\lambda_F - \lambda)\rho_g(\lambda) = 2\pi\rho_g(\lambda_F). \tag{4.41}$$

Therefore

$$v = \frac{1}{2\pi\rho_g(\lambda_F)} \left.\frac{\partial \epsilon_g(k)}{\partial k}\right|_{k=\lambda_F}. \tag{4.42}$$

This group velocity is actually the sound velocity in the Lieb-Liniger gas.

By a well-known macroscopic argument, the sound velocity v_s is related to the isoentropic compressibility κ_S of the system,

$$\frac{1}{\kappa_S} = -L\left(\frac{\partial P}{\partial L}\right)_S = n\left(\frac{\partial P}{\partial n}\right)_S, \tag{4.43}$$

by the Newton-Laplace equation

$$v_s = \sqrt{\frac{1}{\varrho\kappa_S}}, \tag{4.44}$$

where $\varrho = mn$ is the mass density. In our units, where $2m = 1$, we thus have

$$v_s = \sqrt{-\frac{2L}{n}\left(\frac{\partial P}{\partial L}\right)_S} = \sqrt{2\left(\frac{\partial P}{\partial n}\right)_S}. \tag{4.45}$$

By definition, the pressure is the derivative of the internal energy at fixed entropy and number of particles. At zero temperature, $P = -\partial E_0/\partial L$, where E_0 is the ground state energy. Introducing the dimensionless coupling constant (Lieb parameter)

$$\gamma \equiv \frac{c}{n}, \tag{4.46}$$

we may parametrize the ground state energy as $E_0(\gamma) = Nn^2(\gamma)e(\gamma)$, where $e(\gamma)$ represents the dimensionless ground state energy per particle. Substituting the definition of the pressure into Eq. (4.45) and writing $\partial^2 E_0/\partial L^2 = (c^2/N^2)\partial^2 E_0/\partial\gamma^2$, we then obtain the exact thermodynamic relation (Lieb, 1963; Lang et al., 2017)

$$v_s = 2n\sqrt{3e(\gamma) - 2\gamma\frac{\partial e}{\partial\gamma}(\gamma) + \frac{\gamma^2}{2}\frac{\partial^2 e}{\partial\gamma^2}(\gamma)}. \tag{4.47}$$

In the Lieb-Liniger model,

$$e(\gamma) = \frac{\int_{-\lambda_F}^{\lambda_F} d\lambda\, \lambda^2\rho_g(\lambda)}{[\int_{-\lambda_F}^{\lambda_F} d\lambda\, \rho_g(\lambda)]^3}, \tag{4.48}$$

but remarkably, one does not need to compute $e(\gamma)$ to find v_s, as the latter can be expressed simply in terms of the ground state density evaluated in $\lambda = \lambda_F$:

$$v_s = \frac{v_F}{[2\pi\rho_g(\lambda_F)]^2}, \tag{4.49}$$

where $v_F = 2\pi n$ is the Fermi velocity in the Tonks-Girardeau regime. This equality, which is proved in Appendix A, is based on the fact that the pressure is also the derivative of the grand canonical potential (4.14) with respect to the volume at fixed temperature,

$$P = -\left(\frac{\partial G(\mu,T,L)}{\partial L}\right)_T = T\int_{-\infty}^{+\infty}\frac{d\lambda}{2\pi}\ln\left[1+\mathrm{e}^{-\epsilon(\lambda)/T}\right] \overset{T\to 0}{\longrightarrow} -\frac{1}{2\pi}\int_{-\lambda_F}^{\lambda_F} d\lambda\,\epsilon_g(\lambda), \tag{4.50}$$

and on the properties of the functions $\epsilon_g(\lambda)$ and $\rho_g(\lambda)$. Eq. (4.49) also establishes the identity between the macroscopic definition of the sound velocity in terms of pressure variations, and the microscopic definition as group velocity of the elementary excitations. In fact, as shown in Appendix A, Eqs. (4.49) and (4.42) are identical.

The inverse effective mass is

$$\frac{1}{m^*} = \frac{\partial^2\omega(p)}{\partial p^2}\bigg|_{p\to 0} = \left(\frac{\partial p(k)}{\partial k}\right)^{-2}\left[\frac{\partial^2\omega(k)}{\partial k^2} - \frac{\partial\omega(k)}{\partial k}\left(\frac{\partial p(k)}{\partial k}\right)^{-1}\frac{\partial^2 p(k)}{\partial k^2}\right]\bigg|_{k\to\lambda_F}. \tag{4.51}$$

We compute it explicitly in Appendix A, showing that it can be written as

$$\frac{1}{m^*} = \frac{v_s}{K}\frac{\partial}{\partial\mu}\left(v_s\sqrt{K}\right), \tag{4.52}$$

or equivalently

$$\frac{1}{2m^*} = \left(1 - \gamma\frac{\partial}{\partial\gamma}\right)\frac{1}{\sqrt{K}}, \tag{4.53}$$

where the parameter $\sqrt{K}$ is defined as

$$\sqrt{K} = 2\pi\rho_g(\lambda_F) = \sqrt{\frac{v_F}{v_s}}. \tag{4.54}$$

We notice that m^* is positive; therefore Type I excitations have positive effective mass, corresponding to upward curvature of the dispersion relation, while Type II excitations have negative effective mass, corresponding to downward curvature.

4.2 Numerical solutions

By integrating the Lieb equation, one can easily verify that $p_{\rm I}(\pm\lambda_F) = 0$. Moreover $\epsilon_g(\pm\lambda_F) = 0$. We can use these properties to reexpress Eqs. (4.29), (4.32), (4.33), and (4.34) in the unitary form

$$p(k) = 2\pi\left|\int_{\lambda_F}^{k} d\lambda\,\rho_g(\lambda)\right|, \qquad \omega(k) = \left|\int_{\lambda_F}^{k} d\lambda\,\frac{d\epsilon_g(\lambda)}{d\lambda}\right|, \tag{4.55}$$

where $|k| \geq \lambda_F$ ($|k| \leq \lambda_F$) for the Type I (Type II) excitations[2], and λ_F is fixed by

$$n \equiv \frac{N}{L} = \int_{-\lambda_F}^{\lambda_F} d\lambda\,\rho_g(\lambda). \tag{4.56}$$

We notice that the momentum p of Type II excitations takes value in the interval $[0, 2\pi n]$. The associated energy is zero at the endpoints of this interval. The upper endpoint $p = 2\pi n$ (which is equal to twice the Fermi momentum in the Tonks-Girardeau limit) corresponds to a hole rapidity $k = -\lambda_F$, and is called 'umklapp point'. The maximal energy associated with the Type II excitations lies at $k = 0$, corresponding to $p = \pi n$. Since for $|k| \leq \lambda_F$, $p(-k) = 2\pi n - p(k)$ and $\omega(-k) = \omega(k)$, we have $\omega_{\rm II}(p) = \omega_{\rm II}(2\pi n - p)$, therefore the dispersion curve of Type II excitations is symmetric with respect to $p = \pi n$, exacly as in the Tonks-Girardeau regime.

We can now conveniently switch to dimensionless variables, obtaining

$$p(k) = 2\pi\lambda_F\left|\int_1^{k/\lambda_F} dx\, f_e(x)\right|, \qquad \omega(k) = 2\lambda_F^2\left|\int_1^{k/\lambda_F} dx\, f_o(x)\right|, \tag{4.57}$$

[2]Notice that in Eq. (4.55), $\rho_g(\lambda)$ is not strictly the ground state particle density in λ-space, because that vanishes outside the Fermi interval, but is the solution of the Lieb equation (1.99) for $\lambda \in \mathbb{R}$. Outside the Fermi interval, $\rho_g(\lambda)$ corresponds to the ground state hole density in λ-space.

where $f_e(x) \equiv \frac{1}{2}[f(x)+f(-x)]$ and $f_o(x) \equiv \frac{1}{2}[f(x)-f(-x)]$ are, respectively, the even and the odd part of the function $f(x)$ solving the Fredholm integral equation of the second kind

$$\begin{aligned} f(x) &= g(x) + \int_{-1}^{1} dy\, \mathcal{K}(x-y) f(y), \\ g(x) &= \frac{1}{2\pi} + x, \qquad \mathcal{K}(x) = \frac{\alpha}{\pi(\alpha^2+x^2)}, \qquad \alpha \equiv \frac{c}{\lambda_F} > 0. \end{aligned} \tag{4.58}$$

The value of $f(x)$ for any real x is thus determined once $f(x)$ is known in the interval $[-1,1]$. The Fermi momentum is

$$\lambda_F = n\left(\int_{-1}^{1} dx\, f_e(x)\right)^{-1}, \tag{4.59}$$

the ground state density of rapidities is

$$\rho_g(\lambda/\lambda_F) = f_e(x), \qquad x \in [-1,1], \tag{4.60}$$

and the ground state energy is $E_0 = Nn^2 e(\gamma)$, where

$$e(\gamma) = \frac{\int_{-1}^{1} dx\, x^2 f_e(x)}{[\int_{-1}^{1} dx\, f_e(x)\,]^3}. \tag{4.61}$$

Fredholm integral equations have been widely studied in mathematics for many years. There is therefore a well-developed theory, of which Farina et al. (2022) review the fundamental points. Eq. (4.58) has exactly one solution, which although not known in closed form, can be constructed via the convergent iterative process

$$f_0(x) = g(x), \qquad f_n(x) = g(x) + \int_{-1}^{1} dy\, \mathcal{K}(x-y) f_{n-1}(y). \tag{4.62}$$

This is equivalent to the Liouville-Neumann expansion

$$f(x) = g(x) + \sum_{n=0}^{\infty} \int_{-1}^{1} dy\, \mathcal{K}_n(x-y) g(x), \tag{4.63}$$

where the iterated kernels $\mathcal{K}_n$ are defined by $\mathcal{K}_0 = \mathcal{K}$ and

$$\mathcal{K}_n(x-y) = \int_{-1}^{1} ds\, \mathcal{K}(x-s)\mathcal{K}_{n-1}(s-y). \tag{4.64}$$

To solve Eq. (4.58) numerically, a convenient route is offered by Nyström's method, which consists of discretizing the integral with a quadrature scheme

$$\int_{-1}^{1} dx\, h(x) \simeq \sum_{j=1}^{M} w_j h(x_j), \tag{4.65}$$

with weights w_j and the quadrature points ('nodes') x_j such that $x_1 = -1$, $x_M = 1$ and $x_j < x_{j+1}$. Collocation at $x = x_i$ then gives the $M \times M$ linear system

$$f(x_i) - \sum_{j=1}^{M} w_j \mathcal{K}(x_i - x_j) f(x_j) = g(x_i), \qquad i = 1, \ldots, M. \tag{4.66}$$

Having solved this system, the solution of Eq. (4.58) for any real x is given by Nyström's natural interpolant

$$f(x) \simeq g(x) + \sum_{j=1}^{M} w_j \mathcal{K}(x - x_j) f(x_j). \tag{4.67}$$

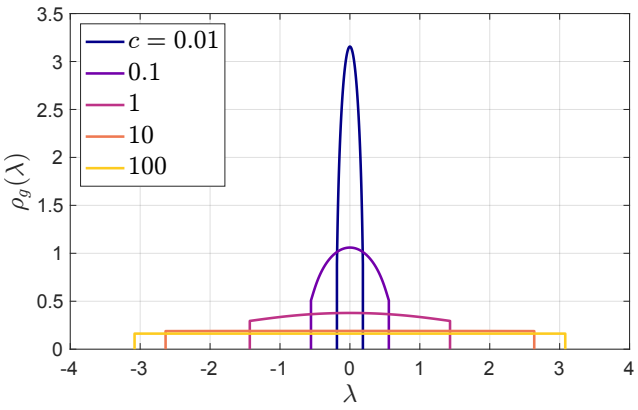


Figure 4.1: Ground state density of rapidities for different values of the interaction parameter c at unit filling.

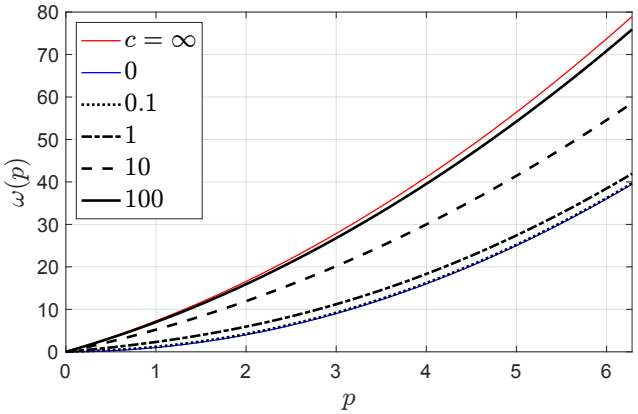


Figure 4.2: Spectrum of Type I excitations for different values of the interaction parameter c at unit filling. For comparison, the finer red line represents the dispersion relation in the Tonks-Girardeau limit, $\omega = 2\pi p + p^2$, while the finer blue line corresponds to the dispersion relation of non-interacting bosons, $\omega = p^2$.

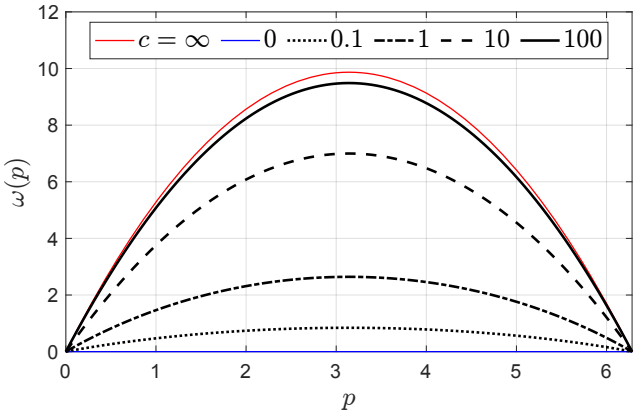


Figure 4.3: Spectrum of Type II excitations for different values of the interaction parameter c at unit filling. For comparison, the finer red line represents the dispersion relation in the Tonks-Girardeau limit, $\omega = 2\pi p - p^2$, while the finer blue line corresponds to non-interacting bosons, which do not have hole-like excitations.

An implementation of Nyström's method in MATLAB is provided by the `Fie` package developed by Atkinson and Shampine (2008). In Figs. 4.1-4.3 we show the numerical solutions for the ground state density function and the spectra of Type I and Type II excitations at unit filling ($n = 1$) for different values of the interaction strength c, obtained using `Fie`[3]. The ground state energy is plotted in Fig. 4.5, where the exact result is compared with various effective approaches that we will discuss shortly.

Over the years there have been many efforts to obtain analytical approximations of the ground state energy in the weak and strong interaction regimes. Relevant works on weak interaction are the ones by Tracy and Widom (2016); Prolhac (2017); Mariño and Reis (2019); Ristivojevic (2019). In particular, the latter provides an expansion of $e(\gamma)$ in powers of γ up to the order γ^5. Relevant works on strong interaction are the ones by Ristivojevic (2014); Lang et al. (2017). The latter provides an expansion of $e(\gamma)$ in powers of $1/\gamma$ up to the order $1/\gamma^{20}$. Such high-precision results on the ground state energy, namely on the ground state density of rapidities, are relevant also for the excitation spectrum, as the energy of the excitations can also be written (Petković and Ristivojevic, 2018)

$$\omega(k) = \left| \int_{\lambda_F}^{|k|} d\lambda \, \frac{\rho_g(k,\lambda)\tilde{n}(\lambda)}{\rho_g^2(\lambda,\lambda)} \right|, \tag{4.68}$$

where $\tilde{n}(\lambda) = \int_{-\lambda}^{\lambda} d\lambda' \, \rho_g(\lambda',\lambda)$, and

$$\rho(k,\lambda) = \frac{1}{2\pi} + \int_{-\lambda}^{\lambda} dk' \, \mathcal{C}(k-k')\rho(k',\lambda). \tag{4.69}$$

This remarkable result shows that knowing the ground state density of rapidities one can directly infer the whole excitation spectrum, and therefore the spectrum at arbitrary momentum is fully determined by the properties of the ground state.

We will not go into the details of the sophisticated analytical approximations mentioned above. For moderate to strong interaction, we present below a relatively simple result obtained from the first step in the iterative solution of Eq. (4.58). In the next section, the case of weak interaction is addressed through effective theories, in particular the Bogoliubov theory and the hydrodynamic (or Luttinger liquid) approach, which are independent from the exact Bethe Ansatz solution.

4.2.1 Moderate to strong coupling expansion

Since the kernel $\mathcal{K}(x)$ is at most $1/\pi\alpha$, for moderate to strong interaction the first few terms of the expansion (4.63) should provide a sufficiently accurate approximation of $f(x)$. In particular, if we limit ourselves to just the first step of the iterative procedure, we get

$$f_e(x) = \frac{1}{2\pi}\left[1 + \frac{\alpha}{\arctan\alpha}\frac{1}{(x^2+\alpha^2)}\right], \tag{4.70}$$

$$f_o(x) = x\left[1 + \frac{1}{\pi}\arctan\left(\frac{2\alpha}{\alpha^2+x^2-1}\right)\right] + \frac{\alpha}{2\pi}\ln\left[\frac{(x-1)^2+\alpha^2}{(x+1)^2+\alpha^2}\right]. \tag{4.71}$$

Substituting the first equation into Eq. (4.61), we obtain the dimensionless ground state energy per particle

$$e = \frac{(2\arctan\alpha)^3}{\pi}\left[\frac{1}{3} + \frac{\alpha}{\arctan\alpha}\left(1 - \alpha\arctan\frac{1}{\alpha}\right)\right]. \tag{4.72}$$

[3]The unit filling fixes $\lambda_F^{(\mathrm{TG})} \equiv \lambda_F(c=\infty) = \pi$ and $p \in [0, 2\lambda_F^{(\mathrm{TG})}] = [0, 2\pi]$, but does not entail a loss of generality. The results for generic γ can be obtained from the results for $(c = \gamma,\, n = 1)$ by rescaling the momenta as $p \to np$ and energies as $\omega \to n^2\omega$.

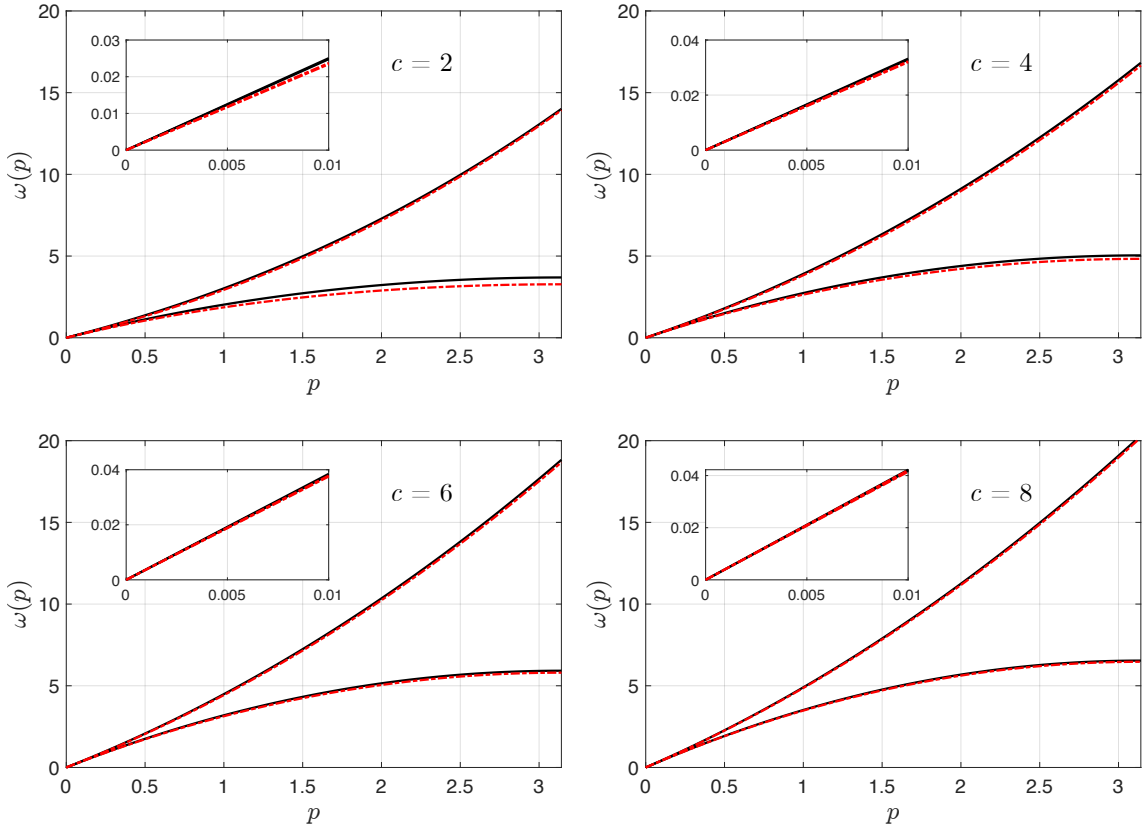


Figure 4.4: Comparison between exact numerical results and the analytical expressions (4.73a)-(4.73e) of the dispersion relations of Type I and Type II excitations at unit filling. The insets show the very small-momentum region.

In the Tonks-Girardeau limit $e(\gamma)$ tends to the constant value $\pi^2/3$, consistently with Eq. (1.95) in the thermodynamic limit. The comparison of Eq. (4.72) with the exact result is shown in Fig. 4.5.

Substituting Eqs. (4.70) and (4.71) into Eqs. (4.55) and (4.59), we obtain

$$\lambda_F = 2n \arctan \alpha, \tag{4.73a}$$

$$p_{\rm I} = k - \lambda_F \frac{\arctan(\alpha/\chi)}{\arctan \alpha}, \tag{4.73b}$$

$$\begin{aligned}\omega_{\rm I} = {} & \left(k^2 - \lambda_F^2\right)\left[1 + \frac{1}{\pi}\arctan\left(\frac{2\alpha}{\chi^2+\alpha^2-1}\right)\right] \\ & + \frac{c^2}{\pi}\left\{\arctan\left[\frac{2\chi^2-2}{\alpha(\chi^2+\alpha^2+3)}\right] + \frac{1}{\alpha}\ln\left(1+\frac{4}{\alpha^2}\right) + \frac{\chi}{\alpha}\ln\left[\frac{(\chi-1)^2+\alpha^2}{(\chi+1)^2+\alpha^2}\right]\right\},\end{aligned} \tag{4.73c}$$

$$p_{\rm II} = k + \lambda_F\left[1 + \frac{\arctan\left(\frac{\alpha(\chi+1)}{\alpha^2-\chi}\right)}{\arctan \alpha}\right], \tag{4.73d}$$

$$\omega_{\rm II} = |\omega_{\rm I}|, \tag{4.73e}$$

where $\chi \equiv k/\lambda_F \in [1, +\infty)$ for Type I and $\chi \in [-1, 1]$ for Type II excitations. Eq. (4.73a) is the self-consistent equation for $\lambda_F = \lambda_F(c)$, and once λ_F is known the last four equations allow us to determine the dispersion relations parametrically as $\omega(k)[p(k)]$, with k in the appropriate interval. It is worth mentioning that in the limit of large momenta

($p \gg p_0^* \equiv n\gamma$, for finite γ), the Type I dispersion relation simplifies to

$$\omega(p) = p^2 + 4n^2\gamma - \pi^2 n^2 + O(p^{-2}). \tag{4.74}$$

As can be seen in Fig. 4.4, the analytical expressions (4.73a)-(4.73e) approximate quite well the exact dispersion relations already for $\gamma \sim 4$. For such value of γ, the sound velocity is underestimated by about 3% and the maximum energy of Type II excitations is underestimated by about 4%. In principle, a better approximation could be obtained with an additional step in the iterative procedure, but in practice it is a huge challenge to express $p(k)$ and $\omega(k)$ in closed form, so one has to resort to more sophisticated methods (Lang et al., 2017).

4.3 Effective approaches for weak interaction

In this section we discuss some effective approaches that allow to determine the ground state energy and the excitation spectrum in the weak interaction regime independently from the exact solution obtained via the Bethe Ansatz. We emphasize that these effective approaches can reproduce only the Type I dispersion relation.

4.3.1 Bogoliubov approach

Expressing the bosonic field operators occurring in the Lieb-Liniger Hamiltonian (1.2) in terms of the operators that create and destroy a particle with well-defined momentum via the Fourier transform[4]

$$\hat{\psi}(x) = \frac{1}{\sqrt{L}} \sum_p \hat{a}_p e^{ipx}, \tag{4.75}$$

where $\hat{a}_p$ and $\hat{a}_p^\dagger$ satisfy the canonical commutation relations $[\hat{a}_p, \hat{a}_{p'}^\dagger] = \delta_{p,p'}$, $[\hat{a}_p, \hat{a}_{p'}] = 0$, Eq. (1.2) becomes

$$\hat{H} = \sum_p p^2 \hat{a}_p^\dagger \hat{a}_p + \frac{c}{L} \sum_{p\,p'\,q} \hat{a}_{p+q}^\dagger \hat{a}_{p'-q}^\dagger \hat{a}_{p'} \hat{a}_p. \tag{4.76}$$

Assuming that at zero temperature the zero-momentum mode is macroscopically occupied[5], i.e. $\langle \hat{a}_0^\dagger \hat{a}_0 \rangle = N_0 \sim O(N)$, we can treat perturbatively the quartic interaction term in Eq. (4.76) following Bogoliubov's theory for quasi-degenerate Bose gases. The key observation is that in the thermodynamic limit

$$\hat{a}_0 |\, N_0, \{N_{p\neq 0}\}\,\rangle = \sqrt{N_0}\,|\, N_0 - 1, \{N_{p\neq 0}\}\,\rangle \overset{N_0 \sim O(N)}{\simeq} \sqrt{N_0}\,|\, N_0, \{N_{p\neq 0}\}\,\rangle, \tag{4.77}$$

and similarly for $\hat{a}_0^\dagger$. These operators may therefore be regarded as ordinary c-numbers, equal to $\sqrt{N_0}$ (Bogoliubov, 1947). In terms of the field operator, this means that

$$\hat{\psi}(x) = \psi_0 + \frac{1}{\sqrt{L}} \sum_{p\neq 0} \hat{a}_p e^{ipx} = \psi_0 + \delta\hat{\psi}(x), \tag{4.78}$$

where $\psi_0 = \sqrt{N_0/L}$. Since $\delta\hat{\psi}(x)$ is assumed to be small, one retains in Eq. (4.76) only those terms that are no more than quadratic in $\hat{a}_p$ and $\hat{a}_p^\dagger$ for $p \neq 0$, finding

$$\hat{H}_{\text{Bog}} = \frac{cN^2}{L} + \sum_{p\neq 0} \left[\left(p^2 + 2cn\right) \hat{a}_p^\dagger \hat{a}_p + cn \left(\hat{a}_p \hat{a}_{-p} + \hat{a}_p^\dagger \hat{a}_{-p}^\dagger \right) \right]. \tag{4.79}$$

[4] Notice that with our conventions, $\hat{a}_p$ is the Fourier transform of $\hat{\psi}(x)/\sqrt{L}$.

[5] We will return on the validity of this assumption at the end of Section 4.4.1.

Clearly such approximation can only be valid for weak interaction. This Hamiltonian can be diagonalized by a Bogoliubov transformation (see Appendix B), which leads to

$$\hat{H}_{\rm Bog} = E_0 + \sum_{p\neq 0} \omega_{\rm Bog}(p)\hat{b}_p^\dagger \hat{b}_p, \tag{4.80}$$

where $\hat{b}_p$ and $\hat{b}_p^\dagger$ are bosonic operators,

$$\omega_{\rm Bog}(p) = \sqrt{p^2(p^2+4cn)} \tag{4.81}$$

is the spectrum of elementary excitations, and

$$E_0 = \frac{cN^2}{L} + \frac{1}{2}\sum_{p\neq 0}\left[\omega_{\rm Bog}(p) - p^2 - 2cn\right] \tag{4.82}$$

is the ground state energy. (The first term represents the ground state energy at tree-level or zeroth-order in perturbation theory).

These results demonstrate that, within the assumptions made, the original system of interacting bosons can be described by the Hamiltonian for non-interacting quasiparticles, having the dispersion relation $\omega_{\rm Bog}(p)$ and bosonic nature. The operators $\hat{b}_p$ and $\hat{b}_p^\dagger$ represent the annihilation and creation operators of these quasiparticles. From this perspective, a physical particle created by $\hat{a}_p^\dagger$ is described as a superposition of quasiparticles, according to $\hat{a}_p^\dagger = u_p\hat{b}_p^\dagger + v_p\hat{b}_{-p}$ (see Appendix B). At small momenta, $u_p \sim n\sqrt{\gamma}/p \gg 1$ and $v_p \sim -u_p$, therefore $\hat{a}_p^\dagger \sim n\sqrt{\gamma}\,p^{-1}(\hat{b}_p^\dagger - \hat{b}_{-p})$ and a physical particle is described by a very large number of quasiparticles. This is equivalent to say that a single quasiparticle excitation corresponds to a collective excitation of many physical particles. Instead, at high momenta $u_p \sim 1$ and $v_p \sim 0$, so that $\hat{a}_p^\dagger \sim \hat{b}_p^\dagger$ and the quasiparticles become indistinguishable from the real particles.

Going to the continuum limit, the ground state energy reads

$$E_0 = cn^2L + \frac{L}{2\pi}\int_0^\infty dp\,\left[\sqrt{p^2(p^2+4cn)} - p^2 - 2cn\right] = Nn^2\gamma\left(1 - \frac{4}{3\pi}\sqrt{\gamma}\right). \tag{4.83}$$

This is the analogue in one dimension of the well-known Lee-Huang-Yang result for the ground state energy of a 3D weakly interacting Bose gas (Lee and Yang, 1957; Lee et al., 1957). The zero-temperature chemical potential is

$$\mu = \frac{\partial E_0}{\partial N} = 2n^2\gamma\left(1 - \frac{1}{\pi}\sqrt{\gamma}\right) \tag{4.84}$$

and the dimensionless ground state energy per particle is

$$e(\gamma) = \gamma\left(1 - \frac{4}{3\pi}\sqrt{\gamma}\right). \tag{4.85}$$

The latter is compared with the exact result in Fig. 4.5. Substituting Eq. (4.85) into the thermodynamic relation (4.47), we obtain for the sound velocity

$$v_s = 2n\sqrt{\gamma - \frac{1}{2\pi}\gamma^{3/2}}. \tag{4.86}$$

This is different from the 'bare' sound velocity occurring in the Bogoliubov spectrum (4.81), that is instead

$$u = \left.\frac{\partial\omega_{\rm Bog}(p)}{\partial p}\right|_{p\to 0} = 2n\sqrt{\gamma}, \tag{4.87}$$

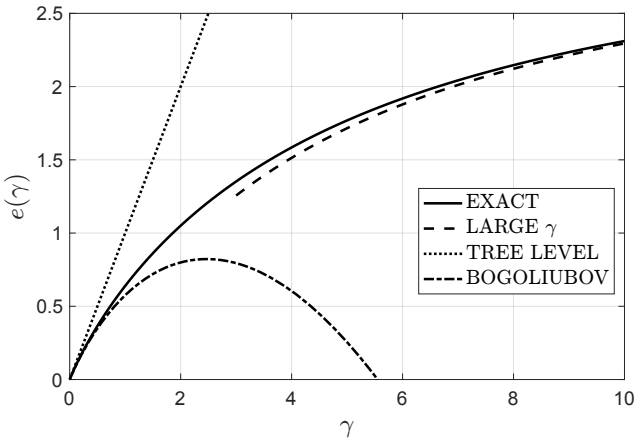


Figure 4.5: Dimensionless ground state energy per particle as a function of γ. The exact result is obtained numerically from Eq. (4.61). The large γ approximation is given by Eq. (4.72). The prediction of Bogoliubov's theory is Eq. (4.85), while the tree-level result is $e(\gamma) = \gamma$. In the Tonks-Girardeau limit, the exact $e(\gamma)$ approaches $\pi^2/3 \simeq 3.29$.

and provides a much better approximation of the exact result, accurate up to the remarkable value of $\gamma \sim 10$ (Fig. 4.6). Using Eq. (4.86) in Eq. (4.53) we then get an approximation for the effective mass valid in the same range of γ,

$$\frac{1}{2m^*} = \frac{12\pi\gamma - 5\gamma^{3/2}}{[2^{13/3}\pi(2\pi\gamma - \gamma^{3/2})]^{3/4}}. \tag{4.88}$$

4.3.2 Hydrodynamic approach

The collective nature of elementary excitation motivates a field theoretic description in terms of collective fields, which is known as 'hydrodynamic approach' or 'bosonization' (Haldane, 1981a; Giamarchi, 2003; Cazalilla et al., 2011). Appendix C provides a summary of the bosonization method, where all the results necessary for the purposes of this section are obtained. In the case of the repulsive Lieb-Liniger model,

$$\hat{H} = \int dx \left[\partial_x\hat{\psi}^\dagger(x)\partial_x\hat{\psi}(x) + c\,\hat{\psi}^\dagger(x)\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}(x)\right], \qquad c > 0, \tag{4.89}$$

the collective fields are the density $\hat{\rho}(x)$ and the phase $\hat{\theta}(x)$, in terms of which the field operator is written

$$\hat{\psi}(x) = \sqrt{\hat{\rho}(x)}\mathrm{e}^{i\hat{\theta}(x)}. \tag{4.90}$$

The canonical commutation relations of the field operator impose

$$\left[\hat{\rho}(x), \mathrm{e}^{-i\hat{\theta}(x')}\right] = \delta(x - x')\mathrm{e}^{-i\hat{\theta}(x')}, \tag{4.91}$$

which is satisfied by

$$\left[\hat{\rho}(x), \hat{\theta}(x')\right] = i\delta(x - x'). \tag{4.92}$$

In a translationally invariant system, the ground-state density is constant and equal to $\rho_0 = n = N/L$. At small excitation energies, we can account for small density fluctuations consistently with Eq. (4.92) by writing the density operator as

$$\hat{\rho}(x) \simeq n - \frac{1}{\pi}\partial_x\hat{\phi}(x), \tag{4.93}$$

with the fields $\hat{\theta}$ and $\hat{\phi}$ satisfying the commutation relation $[\partial_x\hat{\phi}(x), \hat{\theta}(x')] = -i\pi\delta(x-x')$. Eq. (4.93) is only valid in the weak interaction regime, characterized by $\gamma \ll 1$, since this is only the $p = 0$ component of the density, which in general contains an infinite series of harmonics of $2[\pi\rho_0 x - \hat{\phi}(x)]$ (Cazalilla et al., 2011). In this regime, the Lieb-Liniger Hamiltonian is thus

$$\hat{H} \simeq \int dx \left[\left(n - \frac{1}{\pi}\partial_x\hat{\phi}(x) \right) (\partial_x\hat{\theta}(x))^2 + \frac{1}{4\pi^2 n}(\partial_x^2\hat{\phi}(x))^2 + \frac{c}{\pi^2}(\partial_x\hat{\phi}(x))^2 \right]. \tag{4.94}$$

$\hat{H}$ contains two operators of scaling dimension two, $(\partial_x\hat{\theta})^2$ and $(\partial_x\hat{\phi})^2$, one operator of scaling dimension three, $(\partial_x\hat{\phi})(\partial_x\hat{\theta})^2$, and one operator of scaling dimension four, $(\partial_x^2\hat{\phi})^2$. At lowest momenta, the excitation spectrum is determined by the most relevant[6] operators, namely those with scaling dimension two. Retaining only these operators, we obtain the effective Hamiltonian

$$\hat{H}_0 = \int dx \left[n(\partial_x\hat{\theta}(x))^2 + \frac{c}{\pi^2}(\partial_x\hat{\phi}(x))^2 \right], \tag{4.95}$$

describing a Luttinger liquid with renormalized velocity $u = 2n\sqrt{\gamma} = (\sqrt{\gamma}/\pi)v_F$, and Luttinger parameter $K = \pi/\sqrt{\gamma} = v_F/u$ (see Appendix C). Therefore the excitation spectrum is linear, with the sound velocity u,

$$\omega_0(p) = up, \qquad u = 2n\sqrt{\gamma}. \tag{4.96}$$

This sound velocity coincides with that of Bogoliubov, Eq. (4.87). Notice that since a Luttinger liquid exactly describes both the excitations of free bosons and of fermions with linear spectrum, $\hat{H}_0$ does not uniquely determine the statistics of quasiparticle excitations.

At lowest momenta, the first correction to the effective theory $\hat{H}_0$ comes from the leading irrelevant operator, namely the one of scaling dimension three, which gives the Hamiltonian

$$\hat{H}_F = \hat{H}_0 - \frac{1}{\pi}\int dx\, \partial_x\hat{\phi}(x)(\partial_x\hat{\theta}(x))^2. \tag{4.97}$$

This is the Hamiltonian of a Luttinger liquid with a band curvature term and can be mapped to a basis of free fermionic quasiparticles having the spectrum $\omega = up + p^2/2m^*$, where the effective mass m^* is related to the Luttinger parameters by $m^{*-1} = \pi^{-1}\partial(u\sqrt{K})/\partial n$ (see Appendix C and in particular Eq. (C.60)). Therefore $\hat{H}_F$ yields the fermionic excitation spectrum

$$\omega_F(p) = up + \frac{p^2}{2m^*}, \qquad m^* = 2\sqrt{\pi}/3\gamma^{1/4}. \tag{4.98}$$

We notice that the relation $u = 2\pi n/K$ between the Luttinger parameters for the Lieb-Liniger model allows us to rewrite Eq. (C.60) for the effective mass in the form

$$\frac{1}{2m^*} = \left(1 - \gamma\frac{\partial}{\partial\gamma}\right)\sqrt{\frac{u}{v_F}}, \tag{4.99}$$

which coincides with the exact relation (4.53). This is a very significant result. It tells us that for the Lieb-Liniger model, the phenomenological relation between the effective mass and the sound velocity in the Luttinger theory, which is an effective description for weak interaction and small momenta, actually holds for arbitrary interaction strength. This means that the effective description correctly captures the degrees of freedom of the system even at strong interaction, although the Luttinger parameter must be properly 'renormalized' to agree with

[6] An operator is more relevant, in the sense of the renormalization group, the smaller its scaling dimension is. Relevant operators determine the low-energy properties of the theory.

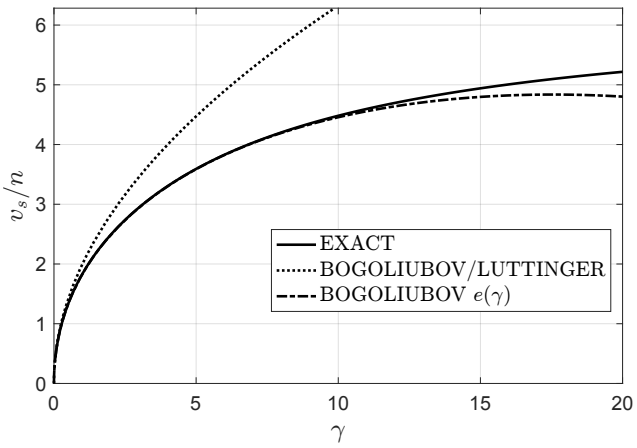


Figure 4.6: Sound velocity as a function of γ. The exact result is obtained numerically from Eq. (4.49). The sound velocity of the Bogoliubov spectrum, which coincides with the sound velocity in the Luttinger liquid theory, is given by Eqs. (4.87) and (4.96). The sound velocity obtained from the macroscopic compressibility using Bogoliubov's $e(\gamma)$, Eq. (4.86), is indistinguishable from the exact result up to $\gamma \sim 10$. In the Tonks-Girardeau limit, the exact v_s/n approaches 2π.

the exact value. Both in the effective and exact descriptions, the dispersion relation up to order p^2 is thus completely characterized by the sound velocity $v_s = v_F/K$ (Matveev and Pustilnik, 2016); in the effective theory $K = \pi/\sqrt{\gamma}$, while for arbitrary interaction strength $K = [2\pi\rho_g(\lambda_F)]^2$. As expected, the former relation agrees with the exact one in the limit of weak interaction (Fig. 4.6), see also Pustilnik and Matveev (2014).

At larger momenta, we expect the operator of scaling dimension four to be more important than the one of scaling dimension three. The first correction to $\hat{H}_0$ will then be

$$\hat{H}_B = \hat{H}_0 + \frac{1}{4\pi^2 n}\int dx\,(\partial_x^2\hat{\phi}(x))^2. \tag{4.100}$$

The excitation spectrum of this theory is most easily obtained in a functional integral approach. The Euclidean action

$$S_B = \int d\tau\,dx\,\left[\psi^\dagger(x,\tau)\partial_\tau\psi(x,\tau) + H_B\right] = \frac{T}{L}\sum_{\mathbf{q}}\begin{pmatrix}\theta_{-\mathbf{q}} & \phi_{-\mathbf{q}}\end{pmatrix} G_{\mathbf{q}}^{-1}\begin{pmatrix}\theta_{\mathbf{q}}\\ \phi_{\mathbf{q}}\end{pmatrix}, \tag{4.101a}$$

where $\mathbf{q} = (p, \omega_\ell)$, is Gaussian, with

$$G_{\mathbf{q}}^{-1} = \begin{pmatrix} np^2 & \frac{i\omega_\ell p}{2\pi} \\ \frac{i\omega_\ell p}{2\pi} & \frac{cp^2}{\pi^2} + \frac{p^4}{4\pi^2 n}\end{pmatrix}. \tag{4.101b}$$

The single-particle Green's function is simply $G_{\mathbf{q}}$, and the excitation spectrum is given by its poles, which are the solutions of $\det G_{\mathbf{q}}^{-1} = \omega_\ell^2 + p^2(p^2+u^2) = 0$. Rotating to real frequencies by $i\omega_\ell \to \omega$, we thus obtain that $\hat{H}_B$ describes bosonic quasiparticles with the Bogoliubov spectrum

$$\omega_B(p) = \sqrt{p^2(p^2+u^2)} = up\sqrt{1+\frac{p^2}{u^2}}. \tag{4.102}$$

Below and above the crossover momentum $p_0 \equiv u = 2n\sqrt{\gamma}$, the Bogoliubov spectrum simplifies to

$$\omega_B(p) \simeq \begin{cases} up + p^3/2u, & p \lesssim p_0, \\ u^2/2 + p^2, & p \gtrsim p_0, \end{cases} \tag{4.103}$$

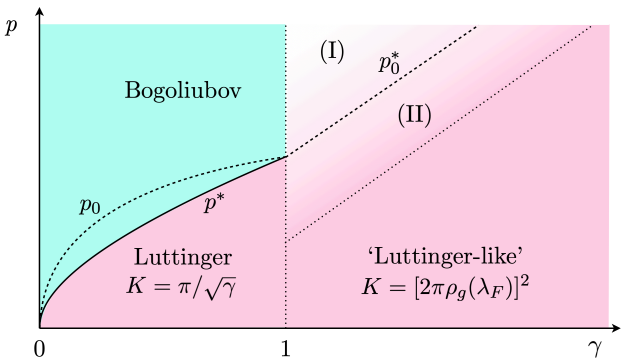


Figure 4.7: Particle-like excitations in different regions of the momentum-interaction plane. In the pink regions elementary excitations are fermionic quasiparticles, while in the cyan region they are bosonic. The crossover momenta are $p^* \sim \gamma^{3/4}$, $p_0 \sim \sqrt{\gamma}$, and $p_0^* \sim \gamma$, while the value of the Lieb parameter separating the weak and strong interaction regimes is $\gamma \sim 1$. For weak interaction and small momenta, we have the Luttinger dispersion relation (4.98). Above the crossover momentum p^*, the Bogoliubov spectrum (4.102). For strong interaction and small momenta, the 'Luttinger-like' dispersion relation given by Eq. (4.37), with Eqs. (4.49) and (4.53). In region I the dispersion relation is given by Eq. (4.74), while in region II terms of order p^3 and higher are important (for $\gamma \gtrsim 4$ Eqs. (4.73a)-(4.73c) provide a quite accurate approximation). The separation (dotted line) between the regions II and 'Luttinger-like' is just qualitative.

and $\omega_F(p)$ and $\omega_B(p \lesssim p_0)$ cross at $p^* \equiv (3n/\sqrt{\pi})\gamma^{3/4}$.

We can thus distinguish the excitation spectrum of the repulsive Lieb-Liniger model in different regions of the momentum-interaction plane (Fig. 4.7). For weak interaction and small momenta, the system is described by the Luttinger liquid paradigm. Elementary excitations are fermionic quasiparticles characterized by a linear dispersion with sound velocity $v_s = u$ and a quadratic correction controlled by the effective mass m^*, which is related to v_s by Eq. (4.99). At larger momenta, between the values $p^* \sim \gamma^{3/4}$ and $p_0 \sim \sqrt{\gamma}$, the cubic correction in the spectrum becomes dominant with respect to the quadratic one, and fermionic quasiparticles transform into Bogoliubov phonons. Finally, above p_0 the Bogoliubov spectrum is quadratic up to a constant term $2n^2\gamma$, with the effective mass equal to the physical mass of the particles.

For moderate and strong interaction, the Bethe Ansatz shows that for small momenta the dispersion relation is still 'Luttinger-like', i.e. it is linear with a quadratic correction controlled by the effective mass, which is related to the sound velocity by the same relation valid at weak interactions. Ristivojevic (2014) has shown that the next term in the expansion in powers of p, of order p^3, is controlled by a coefficient $\sigma(\gamma) \sim \gamma^{-3}$, therefore the momentum interval in which the dispersion is Luttinger-like increases with the interaction strength. In fact, in the Tonks-Girardeau limit the exact dispersion relation is Luttinger-like with $v_s = v_F$ and $m^* = m$. Instead, at finite γ and momenta larger than $p_0^* \sim \gamma$, according to Eq. (4.74) the dispersion relation is quadratic up to the constant $4n^2\gamma - \pi n^2$, with the effective mass equal to the physical mass. This is qualitatively similar to the large-momenta limit of the Bogoliubov spectrum, however the constant terms are different; the one for strong interaction is larger than that for weak interaction. This is consistent with a picture of fermionic quasiparticles at strong interaction, which due to the Pauli principle are expected to have higher energy than bosonic ones for a given momentum. Indeed, we have just seen that a change in the nature of quasiparticles is signaled by the fact that the cubic correction becomes dominant over the quadratic one. Since the cubic correction is

$\sigma(\gamma)p^3$, with $\sigma(\gamma) \sim \gamma^{-3}$ to leading order, the crossover momentum would be $p^*_> \sim \gamma^3$, which however for $\gamma \gg 1$ is higher than $p^*_0 \sim \gamma$. We see from the Eq. (4.74) that at such large momenta the cubic correction is not present at all. Therefore, at strong interaction we do not have a change in the statistics of quasiparticles, as there is simply no room for bosonic quasiparticles to develop.

4.4 Mean field approaches and dark solitons

In addition to Bogoliubov's perturbative approach and the hydrodynamic approach, some relevant physical aspects of the model in the weak interaction regime are captured by the Hartree mean field approach, which we have already used previously in the attractive case.

4.4.1 Gross-Pitaevskii equation

As discussed in Section 2.1, in the mean field approach the many-body wavefunction is assumed to be a product of single-particle wavefunctions satisfying the Gross-Pitaevskii equation (GPE)

$$i\partial_t \psi(x,t) = \left[-\partial_x^2 + 2c|\psi(x,t)|^2\right]\psi(x,t). \tag{4.104}$$

To ensure consistency between the time-dependent GPE and the time-independent one, under stationary conditions $\psi(x,t)$ must evolve in time as

$$\psi(x,t) = \psi(x)\mathrm{e}^{-i\mu t}. \tag{4.105}$$

The underlying assumption of is that there is (at least approximately, for weak interaction) a macroscopic occupation of the state described by $\psi(x,t)$, in the same spirit of Bogoliubov's approach. The validity of this assumption will be addressed shortly. It is then not surprising that if one considers small-amplitude oscillations over the stationary and spatially-uniform solution, $\psi(x,t) = [\psi_0 + \delta\psi(x,t)]\mathrm{e}^{-i\mu t}$, and linearizes the GPE in $\delta\psi(x,t)$, one obtains exactly the Bogoliubov spectrum of elementary excitations (Pethick and Smith, 2008).

In the attractive case, the GPE admits a class of analytical solutions describing bright solitons, i.e. localized and shape-invariant density peaks over a uniform zero-density background. A similar class of analytical solutions exists in the repulsive case, but this time it describes dark solitons, i.e. localized and shape-invariant density depressions over a uniform constant-density background. Here we discuss just the fundamental (one-soliton) solution; the n-soliton solution was obtained by Zakharov and Shabat (1973) using the inverse scattering method, similarly to the attractive case. However, in contrast to the attractive case, where a bright soliton can be observed even in the ground state, a dark soliton always represents a collective excitation imprinted on the uniform ground state, for a dark soliton with non-vanishing amplitude necessarily has non-zero momentum (see the discussion below).

For repulsive interaction (self-defocusing nonlinearity), the time-independent GPE reads

$$-\psi''(x) + 2c|\psi(x)|^2\psi(x) = \mu\,\psi(x), \qquad c > 0, \tag{4.106}$$

where the primes denote derivatives with respect to x. Let us look for a real solution with the properties that $\psi'(x) \to 0$ and $|\psi(x)| \to \psi_0 = \text{const.}$ (non-zero) for $x \to \pm\infty$. The analogue mechanical problem is

$$\psi''(x) = -\frac{\partial V(\psi)}{\partial \psi}, \qquad \text{with} \qquad V(\psi) = \frac{\psi^2}{2}\left(\mu - c\,\psi^2\right). \tag{4.107}$$

The potential $V(\psi)$ is sketched in Fig. 4.8, and it is clear that a non-trivial solution with the required properties exists only for $\mu > 0$. In particular, it must be $\partial V(\psi_0)/\partial\psi = 0$,

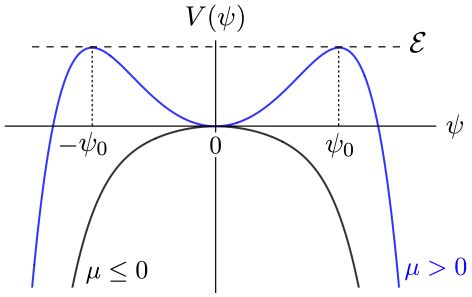


Figure 4.8: The two possible behaviors of the potential $V(\psi)$ for $\mu \leq 0$ and $\mu > 0$.

that gives $\mu = 2c\psi_0^2$, and the total 'energy' of the motion must be

$$\mathcal{E} = \frac{1}{2}(\psi')^2 + V(\psi) = V(\psi_0) = \frac{c}{2}\psi_0^4. \tag{4.108}$$

We can now integrate Eq. (4.107) by quadratures. We have $\psi' = \pm\sqrt{c(\psi_0^2 - \psi^2)^2}$, hence

$$\int_{x_0}^{x} dx = \frac{\pm 1}{\sqrt{c}} \int_{\psi(x_0)}^{\psi(x)} \frac{d\psi}{\psi_0^2 - \psi^2}. \tag{4.109}$$

Taking as 'initial condition' $\psi'(x_0) = \sqrt{2\mathcal{E}}$, so that $V(\psi(x_0)) = 0$ and $\psi(x_0) = 0$, we obtain

$$x - x_0 = \frac{1}{\sqrt{c}} \int_0^{\psi(x)} \frac{d\psi}{\psi_0^2 - \psi^2} = \frac{1}{\psi_0\sqrt{c}} \operatorname{arctanh}\left(\frac{\psi(x)}{\psi_0}\right), \tag{4.110}$$

and therefore

$$\psi_s(x) = \sqrt{\frac{\mu}{2c}} \tanh\left[\sqrt{\frac{\mu}{2}}(x - x_0)\right] = \sqrt{n} \tanh\left(\frac{x - x_0}{\sqrt{2}\xi}\right). \tag{4.111}$$

Here we have used the fact that the chemical potential is related to the amplitude of the wavefunction for $x \to \pm\infty$ by $\mu = 2c\psi_0^2$, but according to Eq. (4.84) it is also (to leading order) $\mu = 2cn$, where n is the background density. We thus have the identification $\psi_0^2 = n$. In the last step, we have introduced the quantity

$$\xi = \frac{1}{\sqrt{2cn}}, \tag{4.112}$$

which is called the coherence (or healing) length. It represents the distance over which the wavefunction tends to its bulk value (ψ_0, in our case) from a localized variation. Eq. (4.111) describes a black soliton, namely a localized density depression which reaches the value zero in $x = x_0$ (Fig. 4.9).

The GPE also possesses solutions for which the associated density depends on the spatial coordinate x and the time t through the combination $x - vt$. These represent propagating dark solitons, and have the form

$$\psi_s(x, t) = \psi_s(x - vt)\mathrm{e}^{-i\mu t}. \tag{4.113}$$

Substituting this expression into Eq. (4.104), we get

$$-iv\psi_s'(\tilde{x}) + \mu\psi_s(\tilde{x}) = -\psi_s''(\tilde{x}) + 2c|\psi_s(\tilde{x})|^2\psi_s(\tilde{x}), \tag{4.114}$$

where the primes denote derivatives with respect to $\tilde{x} = x - vt$. We separate $\psi_s(\tilde{x})$ into real and imaginary parts by writing

$$\psi_s(\tilde{x}) = \psi_0\Big[f(\tilde{x}) + ig(\tilde{x})\Big], \tag{4.115}$$

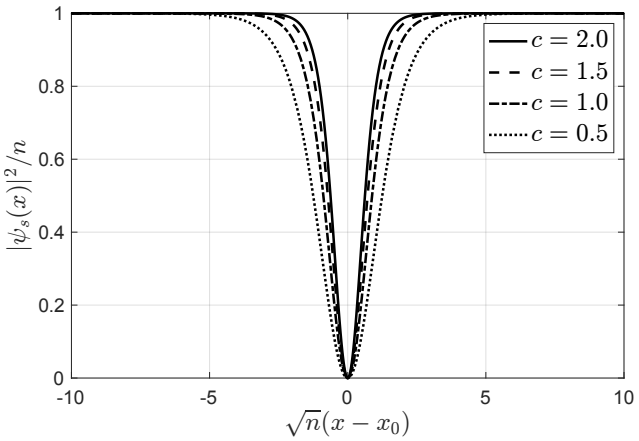


Figure 4.9: Probability density of the black soliton $\psi_s(x)$ for different values of the interaction parameter c and arbitrary background density n.

with the condition that $f^2(\tilde{x}) + g^2(\tilde{x}) = 1$ for $\tilde{x} \to \pm\infty$. Let us consider the case for which the imaginary part is a constant, $g(\tilde{x}) = g_0$. Substituting Eq. (4.115) into Eq. (4.114) then yields the two equations

$$f''(\tilde{x}) = \mu \left(f^2(\tilde{x}) + g_0^2 - 1\right) f(\tilde{x}), \tag{4.116a}$$

$$f'(\tilde{x}) = -\frac{\mu}{v} \left(f^2(\tilde{x}) + g_0^2 - 1\right) g_0. \tag{4.116b}$$

We notice that the first equation is formally equivalent to Eq. (4.106) upon the substitutions $x \to \tilde{x}$, $\mu \to \mu(1 - g_0^2)$, and $2c \to \mu$. Its solution is therefore

$$f(\tilde{x}) = \sqrt{1 - g_0^2} \tanh\left[\sqrt{\frac{\mu(1 - g_0^2)}{2}}(\tilde{x} - x_0)\right]. \tag{4.117}$$

We then have to ensure consistency between the Eqs. (4.116a) and (4.116b). Multiplying the first one by $f'(\tilde{x})$ and integrating gives $2[f'(\tilde{x})]^2 = \mu(f^2(\tilde{x}) + g_0^2 - 1)^2$. The comparison with the second equation yields the condition

$$g_0^2 = \frac{v^2}{2\mu}. \tag{4.118}$$

As one last step, we can relate the chemical potential to the velocity of Bogoliubov phonons by $u = \sqrt{2\mu}$. Putting things together, the soliton wavefunction is (Tsuzuki, 1971)

$$\psi_s(x,t) = \sqrt{n}\left[i\frac{v}{u} + \sqrt{1 - \frac{v^2}{u^2}} \tanh\left(\frac{x - x_0 - vt}{\sqrt{2}\xi_v}\right)\right] \mathrm{e}^{-iu^2t/2}, \tag{4.119}$$

with $\xi_v = \xi/\sqrt{1 - v^2/u^2}$. The associated density is

$$\begin{aligned} |\psi_s(x,t)|^2 &= n\left[\frac{v^2}{u^2} + \left(1 - \frac{v^2}{u^2}\right) \tanh^2\left(\frac{x - x_0 - vt}{\sqrt{2}\xi_v}\right)\right] \\ &= n - (n - n_{\mathrm{min}}) \operatorname{sech}^2\left(\frac{x - x_0 - vt}{\sqrt{2}\xi_v}\right), \end{aligned} \tag{4.120}$$

where $n_{\mathrm{min}} \equiv |\psi_s(x = x_0 + vt, t)|^2 = nv^2/u^2$ is the minimal value of the density, corresponding to the bottom of the soliton dip. The integrated density is

$$\int dx\, |\psi_s(x,t)|^2 = N - 2\sqrt{\frac{1 - v^2/u^2}{\gamma}} = N - 2\sqrt{\frac{n - n_{\mathrm{min}}}{c}}. \tag{4.121}$$

Since $u^2 = 4cn$, the propagation velocity v of the soliton is given by $v = 2\sqrt{cn_{\min}}$, that is the bulk sound velocity evaluated at the density $n_{\min}$. The latter is zero when the soliton is stationary (black soliton), while for non-zero v the minimum density is grater than zero, and we call $\psi_s(x,t)$ a gray soliton. In Fig. 4.10 we present the time evolution of the density of dark soliton for different propagation velocities. It is worth emphasizing that the velocity of gray solitons cannot exceed the bulk sound velocity, while there is no similar limitation on the velocity of bright solitons in the attractive Bose gas, as the height and width of a bright soliton are independent from the velocity at which it propagates.

The density notch is associated to a flip of the phase of the wavefunction. The phase is

$$\theta(x,t) = \arctan\left[\frac{v}{\sqrt{u^2-v^2}}\coth\left(\frac{x-x_0-vt}{\sqrt{2}\xi_v}\right)\right] \tag{4.122}$$

for $x > x_0 + vt$, and $\theta(x,t) + \pi$ for $x < x_0 + vt$. The change of phase along the soliton is therefore

$$\Delta\theta = \theta(+\infty,t) - \theta(-\infty,t) = 2\arctan\left(\frac{v}{\sqrt{u^2-v^2}}\right) - \pi = -2\arccos\left(\frac{v}{u}\right). \tag{4.123}$$

For a gray soliton moving in the positive x direction the phase change is negative. In the case of a black soliton ($v = 0$), one observes a single phase flip $\Delta\theta = -\pi$ at the position of the density dip.

The energy associated to the soliton can be obtained by substituting the expression of $\psi_s(x,t)$ into the Gross-Pitaevskii energy functional $E = \int dx \left(|\partial_x\psi|^2 + c|\psi|^4\right)$, which we introduced in Section 2.1. Actually, to allow for the deficit of particles in the soliton, we consider the quantity $E - \mu N = \int dx \left(|\partial_x\psi|^2 + c|\psi|^4 - \mu|\psi^2|\right)$, namely the zero-temperature grand canonical potential, rather than the energy E itself (Pethick and Smith, 2008)[7]. In the absence of the soliton, assuming the background density to be uniform, $(E-\mu N)_{\text{unif}} = cn^2 - \mu n$. The difference $\Delta(E-\mu N)$ between the grand canonical potential with and without the soliton is thus

$$E_s = \Delta(E-\mu N) = \int dx \left[|\partial_x\psi_s(x,t)|^2 + c\left(|\psi_s(x,t)|^2 - n\right)^2\right], \tag{4.124}$$

which yields the soliton energy

$$E_s = \frac{4}{3}nu\left(1-\frac{v^2}{u^2}\right)^{3/2}. \tag{4.125}$$

Identification of the soliton momentum requires a more careful discussion, as one needs to take into account two separate contributions (Syrwid, 2021). The first is of course the 'local momentum' associated to the field $\psi_s(x,t)$,

$$P_1 = -i\int dx\, \psi_s^*(x,t)\partial_x\psi_s(x,t) = -2n\frac{v}{u}\sqrt{1-\frac{v^2}{u^2}}, \tag{4.126}$$

which is produced in a region of the order of ξ_v around the density dip. The second contribution is related to the asymptotic change of phase of the soliton. This effect is well understood if one consider the system on a ring with circumference much larger than the soliton width; then the requirement of a single-valued wavefunction enforces the appearance of a counterflow at large distances, which compensates the phase difference (4.123). Concretely, in the hydrodynamic formulation of the Gross-Pitaevskii equation, the space-dependent phase

[7] For a direct derivation of the dark soliton energy using a limiting procedure that conserves the number of particles, see Zhao et al. (2020).

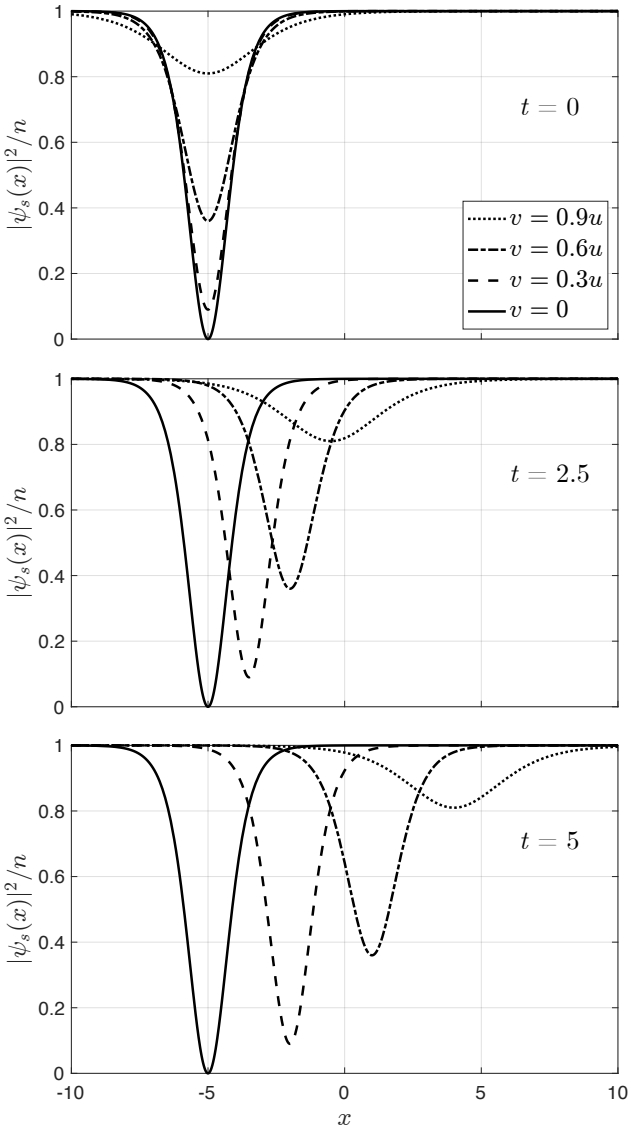


Figure 4.10: Time evolution of the probability density of dark solitons with different propagation velocities. We set $cn = 1$ (thus $u = 2$) and $x_0 = -5$.

$\theta(x)$ of the wavefunction is identified with the particles' velocity field $V(x)$ according to $V(x) = (\hbar/m)\partial_x\theta(x)$ (Pethick and Smith, 2008). This is associated to a momentum density $p(x) = mnV(x) = \hbar n\partial_x\theta(x)$ and a total momentum $P = \hbar n \int dx\, \partial_x\theta(x) = \hbar n\Delta\theta$. To compensate the phase difference as required by periodic boundary conditions, we thus need a counterflow carrying opposite momentum, which in our units ($\hbar = 1$) reads

$$\Delta P = -n\Delta\theta = 2n \arccos\left(\frac{v}{u}\right). \tag{4.127}$$

The total momentum of the soliton is then

$$P_s = P_1 + \Delta P = 2n\left[\arccos\left(\frac{v}{u}\right) - \frac{v}{u}\sqrt{1 - \frac{u^2}{v^2}}\right]. \tag{4.128}$$

One can easily check that P_s satisfies the relation $v = dE_s/dP_s$, or $P_s = \int \frac{dv}{v}\frac{dE_s(v)}{dv}$, and therefore is the canonical momentum of the soliton.

Due to its localization and stability, a simple description of the dark soliton is that it behaves as a mass defect (a 'hole') moving with velocity v and momentum P_1. The

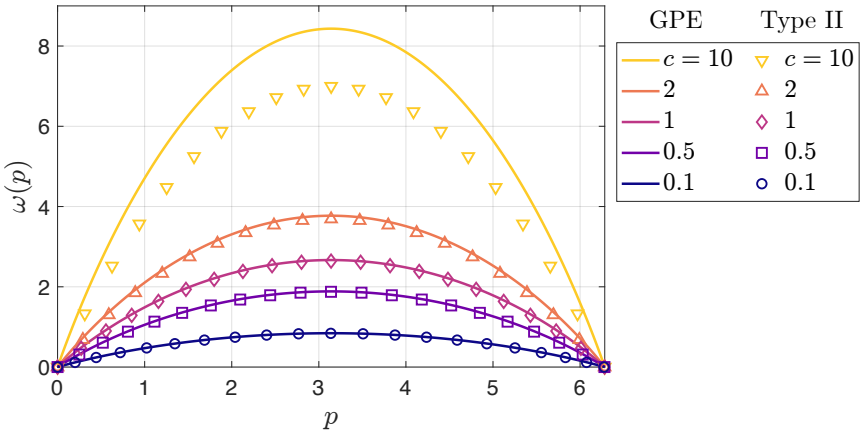


Figure 4.11: Dispersion relation of dark solitons of the Gross-Pitaevskii equation (continuous lines) compared with the dispersion relation of Lieb's Type II excitations (discrete markers), for different values of the interaction parameter c at unit filling.

additional counterflow momentum ΔP can be interpreted as contribution accounting for the reorganization of particles around the moving soliton. This description sounds quite similar to the definition of Lieb's Type II excitations. Indeed, as first noted by Kulish et al. (1976), the dispersion relation of a classical dark soliton closely follows that of Type II excitations. Evident clues to this correspondence are that P_s takes values in the interval $[0, 2\pi n]$ ($P_s = 0$ for $v = u$ and $P_s = 2\pi n$ for $v = -u$), exactly as the momentum of Type II excitations, and that E_s has downward curvature, thus negative effective mass, and vanishes at the endpoints of the momentum interval. The correspondence becomes exact in the weakly interacting limit (Ishikawa and Takayama, 1980). We can prove it analytically by using the expansions for $\alpha \ll 1$ of the functions $f_e(x)$ and $f_o(x)$ occurring in Eq. (4.57), obtained by Popov (1977) and Reichert et al. (2019), respectively:

$$f_e(x) = \frac{\sqrt{1-x^2}}{2\pi\alpha} + \frac{1 + \ln\left(\frac{16\pi}{\alpha}\right) - x\ln\left(\frac{1+x}{1-x}\right)}{4\pi^2\sqrt{1-x^2}} + O(\alpha), \tag{4.129a}$$

$$f_o(x) = \frac{x\sqrt{1-x^2}}{\alpha} + \frac{x\left[1 + \ln\left(\frac{16\pi}{\alpha}\right)\right] + (1-2x^2)\ln\left(\frac{1+x}{1-x}\right)}{4\pi\sqrt{1-x^2}} + O(\alpha). \tag{4.129b}$$

Retaining only the first term of each expansion, Eqs. (4.57) and (4.59) give

$$\lambda_F = 4\alpha n, \tag{4.130a}$$

$$p_{\mathrm{II}} = 2\pi\lambda_F \frac{1}{4\pi\alpha}\left(\arccos\chi - \chi\sqrt{1-\chi^2}\right), \tag{4.130b}$$

$$\omega_{\mathrm{II}} = 2\lambda_F^2 \frac{(1-\chi^2)^{3/2}}{3\alpha}, \tag{4.130c}$$

with $\chi = k/\lambda_F \in [-1, 1]$. Eq. (4.130a) fixes $\lambda_F = 2\sqrt{cn}$, and the dispersion curve $\omega_{\mathrm{II}}(\chi)[p_{\mathrm{II}}(\chi)]$ obtained parametrically from Eqs. (4.130b) and (4.130c) is identical to the dispersion curve $E_s(v/u)[P_s(v/u)]$ obtained from Eqs. (4.125) and (4.128). In Fig. 4.11 we compare the dispersion relation of dark solitons with the Type II dispersion relation obtained numerically. Rather surprisingly, this correspondence remains quite good well beyond the range of c within which the mean field is expected to provide an accurate description of the system.

Our discussion has focused on the zero-temperature case, however further insights into the correspondence between dark solitons and Type II excitations of the Lieb-Liniger model come from exploring the statistical distribution excitations at finite temperature (Karpiuk et al., 2015). Let us just give an idea of how to proceed. The equilibrium properties of the system can be described in terms of a gas of two kinds of quasiparticles, corresponding to Type I and Type II excitations. The total energy of the system is

$$\mathcal{E}(\{n_{p_{\rm I}}, \tilde{n}_{p_{\rm II}}\}) = \sum_{p_{\rm I}} n_{p_{\rm I}} \omega_{\rm I}(p_{\rm I}) + \sum_{p_{\rm II}} \tilde{n}_{p_{\rm II}} \omega_{\rm II}(p_{\rm II}), \tag{4.131}$$

where $n_{p_{\rm I}}$ and $\tilde{n}_{p_{\rm II}}$ are the number of Type I excitations with momentum $p_{\rm I}$ and the number of Type II excitations with momentum $p_{\rm II}$, respectively, and $\omega_{\rm I}(p_{\rm I})$ and $\omega_{\rm II}(p_{\rm II})$ are the corresponding spectra, which are obtained based on the Yang-Yang equation (4.12). The quasiparticles' states are populated according to the probability distribution

$$\mathcal{P}(\{n_{p_{\rm I}}, \tilde{n}_{p_{\rm II}}\}) = \frac{1}{Z} \mathrm{e}^{-\mathcal{E}(\{n_{p_{\rm I}}, \tilde{n}_{p_{\rm II}}\})/T}, \tag{4.132}$$

where Z is the partition function, and then one can compute the average number of Type II excitations at a given temperature as a function of the momentum. This number should be compared with the statistical distribution of dark solitons within the mean field approach. The latter can obtained with the following method. Using a Monte Carlo algorithm (Witowska et al., 2010), one prepares an ensemble of classical fields corresponding to a given temperature, in which the density $\rho(x,t)$ associated to a classical field is a sum of regularized dark soliton densities,

$$\rho(x,t) = \sum_j \rho_s(x - x_j - v_j t), \tag{4.133}$$

where $\rho_s(x,t) = |\psi_s(x,t)|^2 - n$, and x_j and v_j are the initial position and the velocity of the jth soliton, respectively. The Fourier transform of the density in both position and time is[8]

$$\widetilde{\rho}(k,\omega) = \sum_j \mathrm{e}^{-ikx_j} \widetilde{\rho}_s(k; v_j) \delta(\omega - v_j k), \tag{4.134}$$

where $\widetilde{\rho}_s(k; v_j)$ is the Fourier transform of a single solitonic density, which depends on the soliton velocity as a parameter. The square of $\widetilde{\rho}(k,\omega)$ is then

$$\begin{aligned} |\widetilde{\rho}(k,\omega)|^2 &= \sum_j A_j \, |\widetilde{\rho}_s(k; v_j)|^2 \, \delta(\omega - v_j k), \\ A_j &= N_j + 2 \sum_{j_1 > j_2} \cos[k(x_{j_1} - x_{j_2})], \end{aligned} \tag{4.135}$$

where N_j is the number of solitons with velocity v_j. Since in the thermal ensemble the initial positions of solitons are random, averaging Eq. (4.135) over many realizations one obtains

$$\langle |\widetilde{\rho}(k,\omega)|^2 \rangle = \sum_j N_j \, |\widetilde{\rho}_s(k; v_j)|^2 \, \delta(\omega - v_j k). \tag{4.136}$$

It follows that the ratio $\langle |\widetilde{\rho}(k,\omega)|^2 \rangle / \, |\widetilde{\rho}_s(k; \omega/k)|^2$ yields the number of solitons with velocity $v = \omega/k$. Implementing this soliton-counting procedure (and introducing a phenomenological correction at higher temperatures to take into account soliton collisions), Karpiuk et

[8] Explicitly, $\widetilde{\rho}(k,\omega) = \sum_j \int dx\, dt\, \rho_s(x - x_j - v_j t) \mathrm{e}^{-ikx} \mathrm{e}^{i\omega t}$. Introducing the variable $\tilde{x} = x - x_j - x_j t$, this can be written as $\widetilde{\rho}(k,\omega) = \sum_j \mathrm{e}^{-ikx_j} (\int d\tilde{x}\, \rho_s(\tilde{x}) \mathrm{e}^{-ik\tilde{x}}) \int dt\, \mathrm{e}^{i(\omega - v_j k)t}$, which gives the result.

al. (2015) have matched the thermal distribution of dark solitons with that of Type II excitation, providing further evidence that Type II excitations are solitonic in nature.

The question remains whether the relationship between dark solitons and Type II excitations is valid also for stronger interactions. In order to address this problem, in the next section we present a generalized mean field approach, leading to nonlinear Schrödinger equations (NLSEs) with different nonlinearities depending on the interaction strength, and which reduce to the usual Gross-Pitaveskii equation (GPE), namely a NLSE with cubic nonlinearity, in the limit $c \to 0$. The hope is that this approach can extend the effectiveness of the mean field theory to the moderate and strong interaction regimes. However, that is probably too optimistic[9]. The main concern is that mean field theory relies on the introduction of an 'order parameter', i.e. a single-particle wavefunction which is assumed to be able to collectively describe the bosonic system. While this is typically the case in 3D, at temperatures below the critical temperature of Bose-Einstein condensation (BEC), whose occurrence is signaled by the presence of off-diagonal-long-range-order (ODLRO) in the one-body density matrix $\rho(x, y) = \langle \hat{\psi}^\dagger(x)\hat{\psi}(y)\rangle$ (Penrose and Onsager, 1956; Pitaevskii and Stringari, 2016), in 1D the situation is more delicate. In 1D, ODLRO is absent at any $T \geq 0$ and for any $c > 0$, and therefore we never have true BEC. However, for small interaction, at $T = 0$ we have a mesoscopic condensation (or quasi-condensation) characterized by a finite condensate fraction, a phenomenon that, for all practical purposes, can be considered as an ordinary condensation (Colcelli et al., 2018, 2020). For this reason, the mean field approach works reasonably well for weak interaction even in 1D. For stronger interaction, however, we do not even have mesoscopic condensation. It is therefore difficult to base the generalized mean field approach on solid ground. We will discuss its effectiveness by comparing it with the exact result, but we can already expect, for instance, that the agreement between the dispersion relation of mean-field solitons and Type II excitations in the strong interaction regime will not be as good as the agreement we observe for weak interaction.

4.4.2 Generalized Gross-Pitaevskii equation

A modified GPE in 1D was first introduced by Kolomeisky et al. (2000) for the Tonks-Girardeau regime. Despite initial criticisms by Girardeau and Wright (2000)[10], the idea was soon after generalized by Dunjko et al. (2001); Öhberg and Santos (2002) and successfully applied to the problem of an expanding 1D cloud, and was later used by Lieb et al. (2003) to study the 3D to 1D dimensional crossover. The idea is the following. The standard mean field approach starts from the Gross-Pitaevskii energy functional,

$$E_{\rm GP}[\psi, \psi^*] = \int dx \left[|\partial_x \psi(x)|^2 + c|\psi(x)|^4 \right], \tag{4.137}$$

where the nonlinear term $c|\psi(x)|^4$ corresponds to the tree-level approximation of the ground state energy density, $E_0/L = cn^2$ (for a uniform system, the energy is minimized by $|\psi(x)| = \sqrt{n} = \text{const.}$). Minimization of the associated action leads to the GPE. In the generalized mean field approach, we conserve the relationship between the nonlinear term and the ground state energy density, but instead of using the tree-level result for the latter, we use the exact ground state energy density of the Lieb-Liniger model, that is $E_0/L = n^3 e_{\rm LL}(\gamma)$.

[9] See also the next footnote.

[10] Girardeau and Wright pointed out that if a 1D atomic cloud in the ground state of a harmonic trap is split and later recombined, the mean field treatment of Kolomeisky et al. predicts interference, whereas the exact analysis does not. Thus the mean field approach endows the order parameter with phase information that is beyond the real degree of coherence present in the system. This is consistent with the lack of off-diagonal-long-range-order in the 1D Bose gas, which instead is normally required for the introduction of an order parameter (macroscopic occupation). This is a problem that also affects the 1D Gross-Pitaevskii approximation, although, as we have discussed, we expect it to be less severe for weak interaction.

This leads to the energy functional

$$E_{\mathrm{GGP}}[\psi,\psi^*] = \int dx \left[|\partial_x \psi(x)|^2 + |\psi(x)|^6 \, e_{\mathrm{LL}}\left(\frac{c}{|\psi(x)|^2}\right)\right]. \tag{4.138}$$

Applying the least action principle in the usual way (see Section 2.1), one obtains the generalized Gross-Pitaevskii equation (GGPE)

$$i\partial_t \psi(x,t) = \left[-\partial_x^2 + 3|\psi|^4 e_{\mathrm{LL}}\left(\frac{c}{|\psi|^2}\right) - c|\psi|^2 e'_{\mathrm{LL}}\left(\frac{c}{|\psi|^2}\right)\right]\psi(x,t). \tag{4.139}$$

Similarly to what is done with the standard GPE, we can determine the spectrum of the elementary excitations of the GGPE by linearizing on small amplitude oscillations over the stationary and spatially uniform solution $\psi_0 = \sqrt{n}$. Thus we consider

$$\psi(x,t) = \left[\sqrt{n} + \delta(x,t)\right] \mathrm{e}^{-i\mu t}, \tag{4.140}$$

where $\mu_{\mathrm{LL}} = \partial E_0/\partial N = 3n^2 e_{\mathrm{LL}}(\gamma) - cne'_{\mathrm{LL}}(\gamma)$ is the exact chemical potential. Substituting this expression into the GGPE we obtain

$$i\partial_t \delta\psi(x,t) = \left[-\partial_x^2 + \frac{v_{\mathrm{LL}}^2}{2}\right]\delta\psi(x,t) + \frac{v_{\mathrm{LL}}^2}{2}\delta\psi^*(x,t), \tag{4.141}$$

where v_{LL} is the exact sound velocity (4.47). Taking the Fourier transform of Eq. (4.141) and its complex conjugate yields the homogeneous linear system

$$\begin{pmatrix} -\omega + p^2 + \frac{v_{\mathrm{LL}}^2}{2} & \frac{v_{\mathrm{LL}}^2}{2} \\ \frac{v_{\mathrm{LL}}^2}{2} & \omega + p^2 + \frac{v_{\mathrm{LL}}^2}{2} \end{pmatrix} \begin{pmatrix} \widetilde{\delta\psi}(p,\omega) \\ \widetilde{\delta\psi}^*(p,\omega) \end{pmatrix} = \mathbf{0}, \tag{4.142}$$

which has non-trivial solution only if the the determinant of the matrix of coefficients is zero. This gives the excitation spectrum of the GGPE,

$$\omega(p) = \sqrt{p^2(p^2 + v_{\mathrm{LL}}^2)}, \tag{4.143}$$

which differs from the Bogoliubov spectrum just by having the exact sound velocity of the Lieb-Liniger model v_{LL} in place of $u = 2n\sqrt{\gamma}$.

In the limit $\gamma \ll 1$, Eq. (4.139) reduces either to the GPE (using the tree-level result $e(\gamma) \simeq \gamma$) or, by using the Bogoliubov result $e(\gamma) \simeq \gamma - 4\gamma^{3/2}/3\pi$, to

$$i\partial_t \psi(x,t) = \left[-\partial_x^2 + 2c|\psi|^2 - \frac{2c^{3/2}}{\pi}|\psi|\right]\psi(x,t), \tag{4.144}$$

that is a NLSE with quadratic-cubic nonlinearity. In the Tonks-Girardeau limit, instead, where e_{LL} approaches the constant value $\pi^2/3$, Eq. (4.139) coincides with the equation originally proposed by Kolomeisky et al. (2000),

$$i\partial_t \psi(x,t) = \left[-\partial_x^2 + \pi^2|\psi|^4\right]\psi(x,t), \tag{4.145}$$

that is a NLSE with quintic nonlinearity. Since our next discussion will focus on the construction of quantum dark solitons in the Tonks-Girardeau limit, we now consider this specific equation, which should represent a sort of classical limit of the strong interaction regime. For brevity, in the following we shall refer to it as the Kolomeisky equation.

The sound velocity and the chemical potential in the Tonks-Girardeau limit are $v_{\mathrm{LL}} = 2\pi n$ and $\mu_{\mathrm{LL}} = \pi^2 n^2$, respectively. As usual, we look for a solution of the form $\psi_s(x,t) = \psi_s(x - vt)\mathrm{e}^{-i\mu_{\mathrm{LL}}t}$. Substituting this into Eq. (4.145), we obtain

$$-iv\psi'_s(\tilde{x}) = -\psi''_s(\tilde{x}) + \pi^2\left(|\psi_s(\tilde{x})|^4 - n^2\right)\psi_s(\tilde{x}), \tag{4.146}$$

where the primes denote derivatives with respect to $\tilde{x} = x - vt$. We can parametrize $\psi(\tilde{x})$ in polar coordinates as

$$\psi_s(\tilde{x}) = \sqrt{n} A(\tilde{x}) \mathrm{e}^{i\theta(\tilde{x})}, \tag{4.147}$$

with the assumptions that $|A(\tilde{x})| \to 1$ and $\theta'(\tilde{x}) \to 0$ for $\tilde{x} \to \pm\infty$. This yields the two coupled equations

$$vA\theta' = -A'' + A(\theta')^2 + \frac{v_{\mathrm{LL}}^2}{4}(A^4 - 1)A, \tag{4.148a}$$

$$vA' = 2A'\theta' + A\theta''. \tag{4.148b}$$

The second one is a linear first-order differential equation for θ', which can be integrated to obtain $\theta' = (v/2)(1 - A^{-2})$. With some work, one can then integrate the first equation to finally obtain

$$A^2(x,t) = 1 - \frac{3(1 - v^2/v_{\mathrm{LL}}^2)}{2 + \sqrt{1 + 3v^2/v_{\mathrm{LL}}^2}\cosh\left[2\pi n\sqrt{1 - v^2/v_{\mathrm{LL}}^2}(x - x_0 - vt)\right]} \tag{4.149a}$$

$$\theta(x,t) = \frac{1}{2}\arccos\left[\frac{(3v^2/v_{\mathrm{LL}}^2)/A^2 - 1}{\sqrt{1 + 3v^2/v_{\mathrm{LL}}^2}}\right] \tag{4.149b}$$

These equations describe a gray soliton propagating with velocity v, which bears some similarities with the gray soliton of the GPE. The density $|\psi_s(x,t)|^2 = nA^2(x,t)$ takes the minimal value

$$n_{\min} = |\psi_s(x = x_0 + vt, t)|^2 = n\left(\sqrt{1 + 3v^2/v_{\mathrm{LL}}^2} - 1\right), \tag{4.150}$$

which goes to zero for zero propagation velocity (black soliton). The density notch is associated to a flip of the phase of the wavefunction, whose total change along the soliton is

$$\Delta\theta = \arccos\left[\frac{3v^2/v_{\mathrm{LL}}^2 - 1}{\sqrt{1 + 3v^2/v_{\mathrm{LL}}^2}}\right], \tag{4.151}$$

and takes value between $-\pi$ (for $v = 0$) and zero (for $v = v_{\mathrm{LL}}$). Following the same procedure of Section 4.4.1, we can then compute the energy and momentum of the dark soliton of the Kolomeisky equation, which are given by

$$E_s = \sqrt{3}\pi n^2\left(1 - \frac{v^2}{v_{\mathrm{LL}}^2}\right)\ln\left[\frac{2 + \sqrt{3(1 - v^2/v_{\mathrm{LL}}^2)}}{\sqrt{1 + 3v^2/v_{\mathrm{LL}}^2}}\right], \tag{4.152a}$$

$$P_s = -\frac{v/v_{\mathrm{LL}}}{(1 - v^2/v_{\mathrm{LL}}^2)}\frac{E_s}{\pi n} + n\arccos\left[\frac{3v^2/v_{\mathrm{LL}}^2 - 1}{\sqrt{1 + 3v^2/v_{\mathrm{LL}}^2}}\right], \qquad \text{for } 0 \le v \le v_{\mathrm{LL}}. \tag{4.152b}$$

The dispersion relation, which is determined parametrically as $E_s(v/v_{\mathrm{LL}})[P_s(v/v_{\mathrm{LL}})]$, is compared with the exact dispersion relation of Type II excitation in the Tonks-Girardeau regime, $\omega(p) = 2\pi np - p^2$, in Fig. 4.12. As we can see, the agreement is only qualitative at moderate and large momenta, however for $p \ll 1$ the two dispersion relations have the same linear behavior. This is ensured by construction in the generalized mean field approach, since we use the exact value of the sound velocity v_{LL}.

Using different expansions for $e_{\mathrm{LL}}(\gamma)$, the GGPE takes on various particular forms that might be more or less appropriate for describing the system in a given interaction regime.

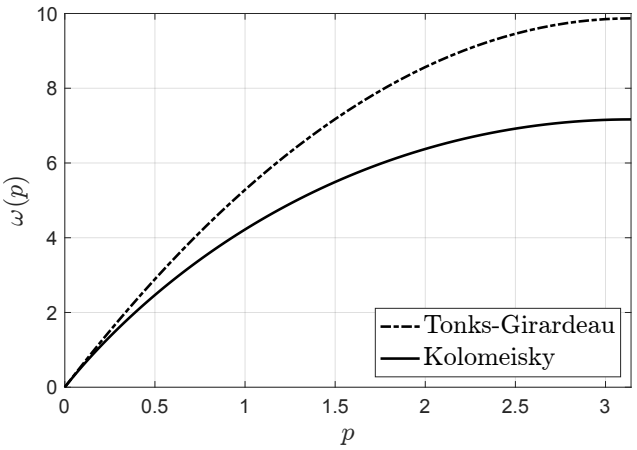


Figure 4.12: Dispersion relation of dark solitons of the Kolomeisky equation (continuous line) compared with the dispersion relation of Lieb's Type II excitations (dashed-dotted line) in the Tonks-Girardeau regime at unit filling.

The corresponding dark soliton solutions will likely have to be found numerically, as recently discussed by Kopyciński et al. (2022). The agreement between such classical solitons and quantum dark solitons in the same interaction regime remains to be investigated. In the next chapter we begin the construction of quantum dark solitons and propose a new way to search for wave packets that enjoy the stability of classical solitons while remaining sufficiently well localized.

Chapter 5

Quantum solitons in the repulsive case

The correspondence between the dispersion relations of classical dark solitons and Lieb's Type II excitations (which is exact in the limit of weak interaction and arguably only qualitative for moderate and strong interactions) motivates the search for quantum dark solitons built from a superposition of Type II excited states. This has been subject of intense research in recent years (Sato et al., 2016; Shamailov and Brand, 2019; Golletz et al., 2020; Kaminishi et al., 2020; Ishiguro et al., 2022; Kinjo et al., 2022, 2023). Current literature has mainly focused on the construction of localized wave packets from a superposition all possible one-hole states, weighted in various ways (for instance, according to a uniform or a Gaussian distribution). Such wave packets, although well localized, do not enjoy the stability under time evolution that one would like to find in the quantum analogue of a classical soliton. In this chapter we will analyze these aspects in detail and propose a possible solution to the above mentioned difficulty, based on the inclusion of a selective superposition of multi-hole states. Unlike the previous chapters, the results of the present one are based on the algebraic formulation of the Bethe Ansatz, which we present in the first section.

5.1 Algebraic Bethe Ansatz

Although the Coordinate Bethe Ansatz provides a convenient framework for finding the eigenstates of the Lieb-Liniger model, it is not suited for computing overlaps between states or matrix elements in a tractable way. We have seen in previous chapters that already in the attractive case, even though the Bethe wavefunctions are quite simple, since the rapidities are organized in string clusters, the explicit computation of matrix elements of the field operator or the density operator is rather cumbersome. In the repulsive case, where the wavefunctions are more complicated, similar computations are totally infeasible. To this end, a different approach has been developed, which we refer to as the Algebraic Bethe Ansatz (Sklyanin et al., 1979; Korepin et al., 1993).

Rather than starting from a given Hamiltonian and finding its eigentstates, the purpose of the Algebraic Bethe Ansatz is to start from an Hilbert space $\mathcal{H}$ and construct a complete set of operators $\{\hat{Q}_n\}$ which are in involution, i.e. satisfy $[\hat{Q}_n, \hat{Q}_m] = 0$ for any n, m. One of this operator will be identified with the Hamiltonian of the model, ensuring that $\{\hat{Q}_n\}$ is a complete set of conserved charges. Instead of constructing the charges one at a time, one looks for a generating function for them all. This is called the transfer matrix, and is an operator-valued function taking as argument a spectral parameter λ, of the form

$$\tau(\lambda) = \exp\left(\sum_{n=0}^{\infty} \frac{\alpha_n}{n!} \hat{Q}_n \lambda^n\right). \tag{5.1}$$

The problem of finding a complete set of operators in involution is then equivalent to the

problem of finding a transfer matrix satisfying

$$[\tau(\lambda), \tau(\mu)] = 0 \qquad \text{for any } \lambda, \mu. \tag{5.2}$$

To solve this problem, one introduces an auxiliary space $\mathcal{A}$ along with a new operator-valued function $T(\lambda)$ acting on the tensor product space $\mathcal{A} \otimes \mathcal{H}$, called the monodromy matrix, such that

$$\tau(\lambda) = \mathrm{Tr}_{\mathcal{A}}\, T(\lambda). \tag{5.3}$$

Then Eq. (5.2) is satisfied provided that

$$[\mathrm{Tr}_{\mathcal{A}_1} T_1(\lambda), \mathrm{Tr}_{\mathcal{A}_2} T_2(\mu)] = \mathrm{Tr}_{\mathcal{A}_1 \otimes \mathcal{A}_2} [T_1(\lambda) T_2(\mu) - T_2(\mu) T_1(\lambda)] = 0, \tag{5.4}$$

where the indices denote on which auxiliary space the operators act[1]. By the cyclicity of the trace, we can satisfy Eq. (5.4) by finding an intertwining operator for the monodromy matrix, i.e. an invertible operator-valued function $R_{12}(\lambda, \mu)$ acting on $\mathcal{A}_1 \otimes \mathcal{A}_2$, called the R-matrix, such that

$$R_{12}(\lambda, \mu) T_1(\lambda) T_2(\mu) = T_2(\mu) T_1(\lambda) R_{12}(\lambda, \mu). \tag{5.5}$$

Consistency of the intertwining relations for three monodromy matrices is ensured by the condition that the R-matrix satisfies the Yang-Baxter equation

$$R_{12}(\lambda, \mu) R_{13}(\lambda, \nu) R_{23}(\mu, \nu) = R_{23}(\mu, \nu) R_{13}(\lambda, \nu) R_{12}(\lambda, \mu). \tag{5.6}$$

This automatically guarantees that all higher products are also consistently defined. Thus the problem of constructing a quantum integrable model reduces to defining a monodromy matrix $T(\lambda)$ and finding a corresponding R-matrix satisfying the Yang-Baxter equation.

For the Lieb-Liniger model, the auxiliary space $\mathcal{A}$ is isomorphic to $\mathbb{C}^2$. The monodromy matrix is represented as the 2×2 matrix

$$T(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}, \tag{5.7}$$

whose elements A, B, C, and D are operators depending on a spectral parameter λ and acting on the Hilbert space. Their commutation relations are fixed by the intertwining relation (5.5) with the R-matrix

$$R(\lambda, \mu) = \begin{pmatrix} f(\mu, \lambda) & 0 & 0 & 0 \\ 0 & g(\mu, \lambda) & 0 & 0 \\ 0 & 0 & g(\mu, \lambda) & 0 \\ 0 & 0 & 0 & f(\mu, \lambda) \end{pmatrix}, \tag{5.8a}$$

in which

$$f(\lambda, \mu) = \frac{\lambda - \mu + ic}{\lambda - \mu} \qquad \text{and} \qquad g(\lambda, \mu) = \frac{ic}{\lambda - \mu}. \tag{5.8b}$$

The operators A, B, C, and D are used to construct the states in Hilbert space. We first notice that the transfer matrix is

$$\tau(\lambda) = \mathrm{Tr}_{\mathcal{A}}\, T(\lambda) = A(\lambda) + D(\lambda). \tag{5.9}$$

Simultaneous eigenstates of all conserved charges are obtained by seeking eigenstates of the transfer matrix itself, i.e. the operator $A(\lambda) + D(\lambda)$. We assume the existence of a pseudovacuum $|\,0\,\rangle$ that is an eigenstate of $A(\lambda)$ and $D(\lambda)$,

$$A(\lambda)|\,0\,\rangle = a(\lambda)|\,0\,\rangle \qquad \text{and} \qquad D(\lambda)|\,0\,\rangle = d(\lambda)|\,0\,\rangle, \tag{5.10}$$

[1] More precisely, $T_1(\lambda) = T(\lambda) \otimes \mathbb{1}_2$ and $T_2(\mu) = \mathbb{1}_1 \otimes T(\lambda)$ are operators acting on $\mathcal{A}_1 \otimes \mathcal{A}_2 \otimes \mathcal{H}$, and $T_1(\lambda) T_2(\mu)$ is a shorthand notation for $T_1(\lambda) \otimes T_2(\mu)$

with $a(\lambda) = \mathrm{e}^{-iL\lambda/2}$ and $d(\lambda) = \mathrm{e}^{iL\lambda/2}$, while $B(\lambda)$ and $C(\lambda)$ act respectively as creation and annihilation operators,

$$\langle\, 0\,|B(\lambda) = 0 \qquad \text{and} \qquad C(\lambda|\, 0\,\rangle = 0. \tag{5.11}$$

Repeatedly applying $B(\lambda)$ to the pseudovaccum then gives rise to new states,

$$|\,\{\lambda\}_N\,\rangle = \prod_{j=1}^{N} B(\lambda_j)|\,0\,\rangle, \tag{5.12}$$

which are eigenstates of the transfer matrix provided that the set of rapidities $\{\lambda\}_N$ solves the Bethe equations

$$\mathrm{e}^{i\lambda_j L} = \prod_{l\neq j} \frac{\lambda_j - \lambda_l + ic}{\lambda_j - \lambda_l - ic}, \qquad j = 1, \ldots, N. \tag{5.13}$$

Once the Bethe equations are solved for the rapidities, the eigenstate is fully characterized. Its norm is given by the Gaudin-Korepin formula (1.72),

$$\|\{\lambda\}_N\|^2 = c^N \prod_{j>k} \frac{\lambda_{jk}^2 + c^2}{\lambda_{jk}^2} \det_N \Big[\delta_{jk}\Big(L + \sum_l K_{jl}\Big) - K_{jk}\Big], \qquad K_{jk} = \frac{2c}{\lambda_{jk}^2 + c^2}, \tag{5.14}$$

which can be proven by using the commutation relations between B and C operators. (Here and in the following sections, we use the shorthand notation λ_{jk} to denote the difference $\lambda_j - \lambda_k$, and the absence of limits in a sum or a product means that it extends from 1 to N). Based on this algebraic description of the eigenstates, a crucial theorem by Slavnov (1989) provides a formula for the overlaps between two states of the form (5.12), in which at least one satisfies the Bethe equations. This theorem underpins the matrix element expressions that we discuss in the following section.

5.2 Density matrix elements

We are interested in the matrix elements of the density operator $\hat\rho(x) = \hat\psi^\dagger(x)\hat\psi(x)$ between two arbitrary Bethe states $|\,\{\mu\}_N\,\rangle$ and $|\,\{\lambda\}_N\,\rangle$. These are clearly related to the matrix elements of the integrated density

$$\hat Q_1(x) = \int_0^x dy\, \hat\rho(y), \tag{5.15}$$

representing the number of particles in the interval $[0, x]$. We thus consider the form factor

$$F_N(\{\mu\},\{\lambda\}) = \frac{\langle\,\{\mu\}_N\,|\,\hat Q_1(x)\,|\,\{\lambda\}_N\,\rangle}{\|\{\mu\}_N\|\;\|\{\lambda\}_N\|}. \tag{5.16}$$

The matrix elements of $\hat Q_1(x)$ obtained from the Algebraic Bethe Ansatz are (Izergin and Korepin, 1984; Slavnov, 1990)

$$\langle\,\{\mu\}_N\,|\,\hat Q_1(x)\,|\,\{\lambda\}_N\,\rangle = \big(\mathrm{e}^{i\mathcal{P}x} - 1\big)\,\Omega(\{\mu\},\{\lambda\}), \tag{5.17}$$

where $\mathcal{P} = \sum_j(\lambda_j - \mu_j)$ is the difference in momenta between $|\,\{\lambda\}_N\,\rangle$ and $|\,\{\mu\}_N\,\rangle$, and

$$\Omega(\{\mu\},\{\lambda\}) = \prod_j (V_j^+ - V_j^-) \prod_{j,k}\left(\frac{\lambda_{jk} + ic}{\mu_j - \lambda_k}\right) \frac{\det_N(\delta_{jk} + U_{jk}(\lambda_p))}{V_p^+ - V_p^-}. \tag{5.18}$$

Here λ_p is an arbitrary element of the set $\{\lambda\}_N$, and the quantities $V_j^{\pm}$, U_{jk} are defined by

$$V_j^{\pm} = \prod_m \frac{\mu_m - \lambda_j \pm ic}{\lambda_{mj} \pm ic}, \tag{5.19}$$

$$U_{jk}(\lambda_p) = \frac{i(\mu_j - \lambda_j)}{V_j^+ - V_j^-} \prod_{m \neq j} \left(\frac{\mu_m - \lambda_j}{\lambda_{mj}} \right) (K_{jk} - K_{pk}). \tag{5.20}$$

In particular, the matrix elements of $\hat{\rho}(x)$ are

$$\rho(x) = \frac{\partial}{\partial x} F_N(\{\mu\}, \{\lambda\}) = \mathrm{e}^{i\mathcal{P}x} \rho(0), \tag{5.21}$$

where

$$\rho(0) = \frac{i\mathcal{P}\,\Omega(\{\mu\}, \{\lambda\})}{\|\{\mu\}_N\|\ \|\{\lambda\}_N\|}. \tag{5.22}$$

Strong coupling expansions In the limit of large c, we can simplify the above result by expanding the various quantities up to the order $1/c$.

* *Expansion of rapidities.* Substituting $\phi(\lambda) = 2\arctan(\frac{\lambda}{c}) = \frac{2\lambda}{c} + O(c^{-3})$ into the Bethe equations (1.30), we obtain

$$\lambda_j = \frac{2\pi I_j^{\lambda}}{L} - \frac{1}{L} \sum_k \phi(\lambda_j - \lambda_k) = \frac{2\pi I_j^{\lambda}}{L} \left(1 - \frac{2N}{cL} \right) + \frac{2P_{\{\lambda\}}}{cL} + O(c^{-2}), \tag{5.23}$$

  where $P_{\{\lambda\}} = \frac{2\pi}{L} \sum_k I_k^{\lambda}$ is the momentum of the state $|\,\{\lambda\}_N\,\rangle$.

* *Expansion of K_{jk}.* We have

$$K_{jk} = \frac{2c}{\lambda_{jk}^2 + c^2} = \frac{2}{c} - \frac{2\lambda_{jk}^2}{c^3} + O(c^{-5}) \tag{5.24a}$$

  and thus

$$K_{jk} - K_{pk} = -\frac{2}{c^3} \lambda_{jp} (\lambda_{jk} + \lambda_{pk}) + O(c^{-5}). \tag{5.24b}$$

* *Expansion of $V_j^{\pm}$.* We have

$$\begin{aligned} V_j^{\pm} &= \prod_m \frac{\mu_m - \lambda_j \pm ic}{\lambda_{mj} \pm ic} = \prod_m \left[1 \mp \frac{i}{c} (\mu_m - \lambda_m) + O(c^{-2}) \right] \\ &= 1 \mp \frac{i}{c} \sum_m (\mu_m - \lambda_m) + O(c^{-2}) = 1 \pm \frac{i\mathcal{P}}{c} + O(c^{-2}), \end{aligned} \tag{5.25a}$$

  where $\mathcal{P} = P_{\{\lambda\}} - P_{\{\mu\}}$, and thus

$$\prod_j (V_j^+ - V_j^-) = \left(\frac{2i\mathcal{P}}{c} \right)^N + O(c^{-2N}). \tag{5.25b}$$

* *Expansion of U_{jk}.* Inserting the expansions (5.23), (5.24b), and (5.25a) into (5.20), we get

$$\begin{aligned} U_{jk} = &-\frac{1}{L} \left[(I_j^{\mu} - I_j^{\lambda}) \frac{\pi}{\mathcal{P}} \left(c - \frac{2N}{L} \right) - 1 \right] \\ &\times \prod_{m \neq j} \frac{I_m^{\mu} - I_j^{\lambda} - \frac{\mathcal{P}}{\pi} (c - \frac{2N}{L})^{-1}}{I_m^{\lambda} - I_j^{\lambda}} \left[\frac{2}{c^3} \lambda_{jp} (\lambda_{jk} + \lambda_{pk}) \right] + \cdots = O(c^{-2}). \end{aligned} \tag{5.26}$$

* *Expansion of* Ω. According to (5.26), to leading order $\det_N(\delta_{jk}+U_{jk}) \simeq 1$, and since λ_{jk} is at most $O(1)$, $\prod_{j,k}(\lambda_{jk}+ic) \simeq (ic)^{N^2}$. Using also (5.25a) and (5.25b) we thus obtain

$$\Omega = \frac{i^{N^2+N-1} c^{N^2-N+1} (2\mathcal{P})^{N-1}}{\prod_{j,k}(\mu_j - \lambda_k)} + \cdots \tag{5.27}$$

* *Expansion of the norm.* To leading order the determinant is simply L^N, and since $\prod_{j>k}(\lambda_{jk}^2 + c^2) \simeq \prod_{j>k} c^2 = c^{N^2-N}$, we obtain

$$\|\{\lambda\}_N\|^2 = \frac{c^{N^2} L^N}{\prod_{j>k} \lambda_{jk}^2} + \cdots \tag{5.28a}$$

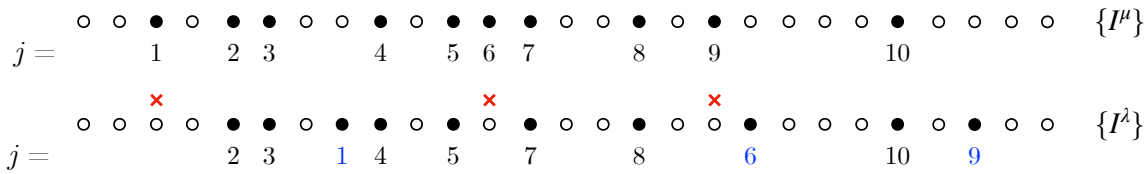
Therefore

$$\frac{1}{\|\{\mu\}_N\| \|\{\lambda\}_N\|} = \frac{\prod_{j>k} |\mu_{jk}||\lambda_{jk}|}{c^{N^2} L^N} + \cdots \tag{5.28b}$$

From (5.27) and (5.28b) we obtain the expansion for large c of the density matrix element,

$$\rho(0) = \frac{i^{N(N+1)} \mathcal{P}^N}{L} \left(\frac{2}{cL}\right)^{N-1} \frac{\prod_{j>k} |\mu_{jk}||\lambda_{jk}|}{\prod_{j,k}(\mu_j - \lambda_k)} + \cdots \tag{5.29}$$

Let us look more carefully at the relationship between the quantum numbers of the states $|\{\mu\}_N\rangle$ and $|\{\lambda\}_N\rangle$. State $|\{\lambda\}_N\rangle$ can be obtained from state $|\{\mu\}_N\rangle$ by punching n holes, with n an integer between 1 and N, and adding an equal number of particles. In other words, the set of quantum numbers $\{I^\lambda\}$ differs from the set $\{I^\mu\}$ by n elements. We parametrize the quantum numbers $\{I^\mu\}$ in increasing order, so that $I_1^\mu < I_2^\mu < \cdots < I_N^\mu$. To minimize the number of I_j^λ's that are different from I_j^μ's for the same value of j, we parameterize $\{I^\lambda\}$ so as to keep unchanged the indices of the quantum numbers that remain occupied, while we parameterize in increasing order the new quantum numbers. For example,



We will denote by $\mathscr{H}$ the set of indices j corresponding to the new quantum numbers. The number of elements in $\mathscr{H}$ is n. In the example above, $n = 3$ and $\mathscr{H} = \{1, 6, 9\}$.

With this convention, several terms in the product on the right-hand side of Eq. (5.29) simplify. We can write the product in the denominator as

$$\prod_{j,k}(\mu_j - \lambda_k) = \prod_j (\mu_j - \lambda_j) \prod_{j<k} (\mu_j - \lambda_k) \prod_{j>k} (\mu_j - \lambda_k). \tag{5.30}$$

We compute each of these three factors separately, splitting the product over j or k into the product over $\{1, \ldots, N\} \setminus \mathscr{H}$ and $\mathscr{H}$. Recalling that

$$\mu_j - \lambda_k = \frac{2\pi}{L}(I_j^\mu - I_k^\lambda) - \frac{2N}{cL}\left[\frac{2\pi}{L}(I_j^\mu - I_k^\lambda) + \frac{\mathcal{P}}{N}\right] + O(c^{-2}), \tag{5.31}$$

we see that for $j \notin \mathscr{H}$ or $k \notin \mathscr{H}$, (i) if $j = k$, then $I_k^\mu - I_k^\lambda = 0$ and $\mu_k - \lambda_k = -2\mathcal{P}/cL + O(c^{-2})$; (ii) if $j \neq k$, then $\mu_j - \lambda_k = \lambda_j - \lambda_k + O(c^{-1})$. Therefore

$$\prod_j (\mu_j - \lambda_j) = \left(-\frac{2\mathcal{P}}{cL}\right)^{N-n} \prod_{j\in\mathscr{H}} (\mu_j - \lambda_j), \tag{5.32a}$$

$$\begin{aligned}\prod_{j<k} (\mu_j - \lambda_k) &= (-1)^{N(N-1)/2} \prod_{j>k} (\lambda_j - \mu_k) \\ &= (-1)^{N(N-1)/2} \prod_{\substack{j>k \\ k\notin\mathscr{H}}} (\mu_j - \mu_k) \prod_{\substack{j>k \\ k\in\mathscr{H}}} (\lambda_j - \mu_k) + O(c^{-1}) \\ &= (-1)^{N(N-1)/2} (-1)^\ell \prod_{\substack{j>k \\ k\notin\mathscr{H}}} (\mu_j - \mu_k) \prod_{\substack{j<k \\ j\in\mathscr{H}}} (\mu_j - \lambda_k) + O(c^{-1}),\end{aligned} \tag{5.32b}$$

$$\prod_{j>k} (\mu_j - \lambda_k) = \prod_{\substack{j>k \\ j\notin\mathscr{H}}} (\lambda_j - \lambda_k) \prod_{\substack{j>k \\ j\in\mathscr{H}}} (\mu_j - \lambda_k) + O(c^{-1}), \tag{5.32c}$$

where ℓ is the number of elements in the product $\prod_{j>k,\, k\in\mathscr{H}} (\lambda_j - \mu_k)$. Substituting these expressions into (5.29), and noting that $i^{N(N+1)}(-1)^{N(3-N)/2} = 1$, we thus obtain

$$\rho(0) = \frac{(-\mathcal{P})^n}{L} \left(\frac{2}{cL}\right)^{n-1} (-1)^\ell \mathrm{sgn}\left(\prod_{\substack{j>k \\ k\notin\mathscr{H}}} \mu_{jk} \prod_{\substack{j>k \\ j\notin\mathscr{H}}} \lambda_{jk}\right) \frac{\prod_{\substack{j>k \\ k\in\mathscr{H}}} |\mu_{jk}| \prod_{\substack{j>k \\ j\in\mathscr{H}}} |\lambda_{jk}|}{\prod_{\substack{j,k \\ j\in\mathscr{H}}} (\mu_j - \lambda_k)}. \tag{5.33}$$

One-hole differences Consider for instance the simplest case $n = 1$, when the states $|\{\lambda\}_N\rangle$ and $|\{\mu\}_N\rangle$ differ by only one quantum number. We can always take this quantum number to be the one of index N, i.e. $\mathscr{H} = \{N\}$, and the other quantum numbers parameterized in increasing order. Then the products on the right-hand side of Eq. (5.33) simplify to[2] $(\mu_N - \lambda_N)^{-1} = (-\mathcal{P})^{-1}$, and the density matrix elements, which we denote as $\rho_1(0)$, read

$$\rho_1(0) = \frac{1}{L} \mathrm{sgn}\Big(\textstyle\prod_{j>k} \mu_{jk}\lambda_{jk}\Big) = \frac{1}{L} \mathrm{sgn}\Big(\textstyle\prod_{k=1}^{N-1} I_{Nk}^\mu I_{Nk}^\lambda\Big) = \frac{(-1)^{|C_{h,h'}|}}{L}, \tag{5.34}$$

where $|C_{h,h'}|$ is the number of particles (i.e. occupied quantum numbers) between the two holes' quantum numbers, $\widetilde{I}_h = I_N^\lambda$ and $\widetilde{I}_{h'} = I_N^\mu$, in agreement with Sarvi (2023).

Multi-hole differences We can treat in a similar fashion the cases $n > 1$, by taking $\mathscr{H} = \{N, N-1, \ldots, N-n+1\}$. Then

$$\rho(0) = \frac{(-\mathcal{P})^n}{L} \left(\frac{2}{cL}\right)^{n-1} (-1)^{n(n-1)/2} \mathrm{sgn}\left(\prod_{\substack{j>k \\ k\notin\mathscr{H}}} \mu_{jk}\lambda_{jk}\right) \left.\frac{\prod_{j>k} |\mu_{jk}||\lambda_{jk}|}{\prod_{j,k}(\mu_j - \lambda_k)}\right|_{j,k\in\mathscr{H}}. \tag{5.35}$$

[2] We use the fact that

$$\begin{aligned}&\mathrm{sgn}\left(\prod_{\substack{j>k \\ k\notin\mathscr{H}}} \mu_{jk} \prod_{\substack{j>k \\ j\notin\mathscr{H}}} \lambda_{jk}\right) \frac{\prod_{\substack{j>k \\ k\in\mathscr{H}}} |\mu_{jk}| \prod_{\substack{j>k \\ j\in\mathscr{H}}} |\lambda_{jk}|}{\prod_{\substack{j,k \\ j\in\mathscr{H}}} (\mu_j - \lambda_k)} \\ &\qquad = \mathrm{sgn}\left(\prod_{\substack{j>k \\ k\notin\mathscr{H}}} \mu_{jk}\lambda_{jk}\right) \frac{\prod_{\substack{j>k \\ k\in\mathscr{H}}} |\mu_{jk}| \prod_{\substack{j>k \\ k\in\mathscr{H}}} |\lambda_{jk}|}{\prod_{j\in\mathscr{H}} (\mu_j - \lambda_j) \prod_{\substack{j<k \\ j\in\mathscr{H}}} (\mu_j - \lambda_k) \prod_{\substack{j>k \\ k\in\mathscr{H}}} (\mu_j - \lambda_k)}.\end{aligned}$$

Notice that the factors $\mu_j - \lambda_k$ in the denominator are always non-zero, therefore the matrix elements are well-behaved. The equation implies that in the Tonks-Girardeau regime the density matrix elements between Bethe states differing by more than one quantum number are zero.

5.3 Type II wave packets

We now wish to construct a localized wave packet out of many Type II states. Let us begin by setting some conventions. We call 'n-hole Type II state' a Bethe state in the N-particle sector, constructed from the ground state of the N-particle system, e.g.

by removing one particle and adding it to the first empty slot to the right of the Fermi edge, and repeating the process for n distinct hole positions, e.g.

The N-particle ground state is specified by the quantum numbers

$$\{I_j^0\} = \left\{ -\frac{N+1}{2} + j \right\}_N, \qquad j = 1, \ldots, N. \tag{5.36}$$

The quantum numbers of the n holes in the ground state interval are

$$\{\widetilde{I}_j^h\} = \left\{ \frac{N+1}{2} - h_j \right\}_n, \qquad j = 1, \ldots, n, \tag{5.37}$$

with $h_j \in \{1, \ldots, N\}$, and the quantum numbers of the resulting n particles to the right of the ground state interval are

$$\{I_j^p\} = \left\{ \frac{N-1}{2} + j \right\}_n, \qquad j = 1, \ldots, n. \tag{5.38}$$

The quantum numbers of the n-hole Type II state are thus

$$\{I\}_N = \{I^0\}_N \cup \{I^p\}_n \setminus \{\widetilde{I}^h\}_n, \tag{5.39}$$

and according to Eq. (1.98) the corresponding momentum is

$$P_n^{\mathbf{h}} = \frac{2\pi}{L} \sum_{j=1}^{N} I_j = \frac{2\pi}{L} \left[\frac{n(n-1)}{2} + \sum_{j=1}^{n} h_j \right], \tag{5.40}$$

where $\mathbf{h}$ denotes the set $\{h_1, \ldots, h_n\}$. For finite interaction strength, the energy of the state is $E_n^{\mathbf{h}} = \sum_{j=1}^{N} \lambda_j^2$, where $\{\lambda_j\}$ is the set of rapidities to which the Bethe equations map the set of quantum numbers $\{I_j\}$. In the Tonks-Girardeau regime, this simplifies to

$$\begin{aligned} E_n^{\mathbf{h}} &= \left(\frac{2\pi}{L}\right)^2 \sum_{j=1}^{N} I_j^2 \qquad (c \to \infty) \\ &= E_{\mathrm{gs}} + \left(\frac{2\pi}{L}\right)^2 \sum_{j=1}^{n} \big[j(j-1) - h_j(h_j-1) + N(j+h_j-1) \big], \end{aligned} \tag{5.41}$$

where $E_{\rm gs}$ is the ground-state energy (1.95).

We can construct a spatially localized 'Type II wave packet' $|\,\psi(t)\,\rangle$ as a linear superposition of n-hole Type II states $|\,P_n^{\mathbf{h}}\,\rangle$, according to

$$|\,\psi(t)\,\rangle = \frac{1}{\sqrt{\mathfrak{S}}} \sum_{\{\widetilde{I}^h\}_n} A_n^{\mathbf{h}}\, \mathrm{e}^{-iE_n^{\mathbf{h}}t} |\,P_n^{\mathbf{h}}\,\rangle, \tag{5.42}$$

where $\mathfrak{S}$ is the number of Type II states in the superposition and the coefficients $A_n^{\mathbf{h}} \equiv \langle\, P_n^{\mathbf{h}}\,|\,\psi(0)\,\rangle$ should be tuned in order to obtain the desired density profile at $t=0$. The density profile is given by $\rho(x,t) = \langle\,\psi(t)\,|\,\hat{\rho}(x)\,|\,\psi(t)\,\rangle$, and since by translational invariance $\hat{\rho}(x) = \mathrm{e}^{-i\hat{P}x}\hat{\rho}(0)\mathrm{e}^{i\hat{P}x}$,

$$\rho(x,t) = \frac{1}{\mathfrak{S}} \sum_{\mathbf{h},\mathbf{h}'} (A_n^{\mathbf{h}'})^* A_n^{\mathbf{h}}\, \mathrm{e}^{-i[(P_n^{\mathbf{h}'}-P_n^{\mathbf{h}})x - (E_n^{\mathbf{h}'}-E_n^{\mathbf{h}})t]} \langle\, P_n^{\mathbf{h}'}\,|\,\hat{\rho}(0)\,|\,P_n^{\mathbf{h}}\,\rangle. \tag{5.43}$$

In the logic of a 'flat summation', we take the coefficients $A_n^{\mathbf{h}}$ to be simply $A_n^{\mathbf{h}} = \mathrm{e}^{-iP_n^{\mathbf{h}}x_0}$, where x_0 is a constant position. This results in the density profile

$$\rho(x,t) = \frac{1}{\mathfrak{S}} \sum_{\mathbf{h},\mathbf{h}'} \mathrm{e}^{-i[(P_n^{\mathbf{h}'}-P_n^{\mathbf{h}})(x-x_0) - (E_n^{\mathbf{h}'}-E_n^{\mathbf{h}})t]} \langle\, P_n^{\mathbf{h}'}\,|\,\hat{\rho}(0)\,|\,P_n^{\mathbf{h}}\,\rangle, \tag{5.44}$$

which is centered around $L/2 - x_0$.

In addition to the choice of the number n of holes and the sum weights $A_n^{\mathbf{h}}$, there is further freedom that comes from the possibility of choosing which subset of the n-hole Type II states to include in the superposition that defines $|\,\psi(t)\,\rangle$. The standard choice is to include in the summation all possible states, the number of which is $\binom{N}{n}$ in a system of N particles. We will call this a 'flat superposition' of states. This choice endows the wave packet with two properties that are of contrasting utility in the search for soliton-like robustness. On the one hand, summing over states with the widest distribution of momenta produces a maximally localized wave packet. On the other hand, the large energy difference between these states leads to a rapid dephasing and decay of the wave packet, which seriously compromise the correspondence with a classical soliton.

The pseudo-parabolic form of the Type II dispersion relation offers an enticing opportunity to build very long-lived wave packets, exploiting the singularity of the density of states which occurs for hole rapidities close to zero, i.e. for hole quantum numbers close to the center of the Fermi interval. To see this, let us consider first a 1-hole state with hole rapidity λ, and expand the dispersion relation around $\lambda = 0$: $\omega(\lambda) \simeq \omega(0) - \frac{\alpha}{2}\lambda^2$, where $\alpha = -d^2\omega(0)/d\lambda^2 > 0$. In the thermodynamic limit, the number of states with hole rapidity within λ and $\lambda + d\lambda$ is $dI = g(\lambda)d\lambda$, where $g(\lambda)$ is the density of states (in the Tonks-Girardeau regime, $g(\lambda)$ is simply $L/2\pi$). The number of states with energy between ω and $\omega + d\omega$ is then

$$dI = \frac{dI}{d\omega}d\omega = g(\lambda)\left(\frac{d\omega}{d\lambda}\right)^{-1} d\omega \propto \frac{d\omega}{\sqrt{\omega(0)-\omega}}. \tag{5.45}$$

For $\lambda \to 0$ the density of states is indeed divergent, exhibiting a Van Hove singularity. This provides us with a large number of states with closely spaced energies, and thus with the possibility of constructing a very long-lived wave packet. In order to do so, we will restrict the summation to hole quantum numbers close to zero, creating a 'selective superposition' of states. While restricting the distribution of momenta will necessarily lead to a wider (less localized) wave packet, the idea is to compensate for this problem by considering multi-hole states. In this case, denoting by $\lambda_1, \ldots, \lambda_n$ the holes' rapidities, the Type II dispersion

relation $\omega = \omega(\lambda_1, \ldots, \lambda_n)$ is represented by a n-dimensional pseudo-paraboloid, and a small energy interval at the maximum of this hyper-surface contains more states than the equivalent interval in the 1-hole case.

In the following, we start implementing this program in the Tonks-Girardeau regime, where Eq. (5.34) is all we need to compute the expectation value of the density operator in the wave packets, and some analytical results can be obtained. These will serve as a useful benchmark for numerical results that may be obtained more generally by calculating all matrix elements directly from the Algebraic Bethe Ansatz and which will allow to extend the construction of wave packets to finite interaction strength.

5.3.1 One-hole Type II wave packets

Consider a wave packet constructed from a flat superposition of 1-hole Type II states $|\, P_1^h \,\rangle$, which have momentum $P_1^h = (2\pi/L)h$ and energy $E_1^h - E_{\rm gs} = (2\pi/L)^2 h(N+1-h)$. The density matrix elements are given by $\langle\, P_1^{h'} \,|\, \hat\rho(0) \,|\, P_1^h \,\rangle = (-1)^{|C_{h,h'}|}/L$, where $|C_{h,h'}|$ (the number of particles between the holes h and h') is simply $|C_{h,h'}| = |\widetilde I^h - \widetilde I^{h'}| - 1 = |h - h'| - 1$. Therefore $\langle\, P_1^{h'} \,|\, \hat\rho(0) \,|\, P_1^h \,\rangle = -\mathrm{e}^{i\pi(h-h')}/L$. Substituting these expressions into Eq. (5.44), we get

$$\rho_1(x,t) = \frac{N}{L} - \frac{1}{NL} \sum_{h \neq h'} \exp\left\{ -i \frac{2\pi}{L}(h'-h) \left[x - x_0 + \frac{L}{2} - \frac{2\pi}{L}(N+1-h-h')t \right] \right\}, \tag{5.46}$$

where $\sum_{h\neq h'}(\cdots)$ means $\sum_{h'=1}^{N}[\sum_{h=1}^{h'-1}(\cdots) + \sum_{h=h'+1}^{N}(\cdots)]$. In particular, at $t = 0$ we have (taking for convenience $x_0 = L/2$),

$$\rho_1(x,0) = \frac{N+1}{L} - \frac{1}{NL} \sum_{h,h'} \mathrm{e}^{-i(2\pi/L)(h-h')x} = \frac{N+1}{L} - \frac{1}{NL} \frac{\sin^2(N\pi x/L)}{\sin^2(\pi x/L)}, \tag{5.47}$$

which coincides with the expression obtained by Sato et al. (2016) through a mapping to free fermions. In the thermodynamic limit, the quantity $z \equiv h/L$ becomes continuous and takes values in the interval $[0, n]$, where n is the particle density. Therefore

$$\rho_1(x,t) \overset{\text{Th.Lim.}}{=} n - \frac{1}{n} \int_0^n dz \int_0^n dz' \, \exp\left\{ -2\pi i (z-z')[x - 2\pi(n - z - z')t] \right\}. \tag{5.48}$$

At $t = 0$, we get

$$\rho_1(x,0) \overset{\text{Th.Lim.}}{=} n - \frac{\sin^2(n\pi x)}{n\pi^2 x^2}, \tag{5.49}$$

which coincides with the thermodynamic limit of Eq. (5.47).

Some comments are in order:

i. As expected, the 'flat' 1-hole Type II wave packet describes a single localized density depression, of width (measured at the base) equal to $2/n$. The density takes values between $1/L$ and $(N+1)/L$, and thus between zero and n in the thermodynamic limit (Fig. 5.1). This is physically clear if we think that what we are actually doing is removing a particle at a given position x_0 and adding it back with a fixed momentum, hence delocalized in space. Then, similarly to what happens in a liquid, a localized depletion causes the overall level of the liquid to rise.

ii. There is decent qualitative agreement between the density profile of the 1-hole Type II wave packet at $t = 0$ and that of the black soliton solution of the Kolomeisky equation (NLSE with quintic nonlinearity), given by Eq. (4.149a). In particular, the widths of the two profiles are quantitatively close. However, the mean field approach predicts a smooth density profile, whereas $\rho_1(x,0)$ is characterized by long-range oscillations of wavelength

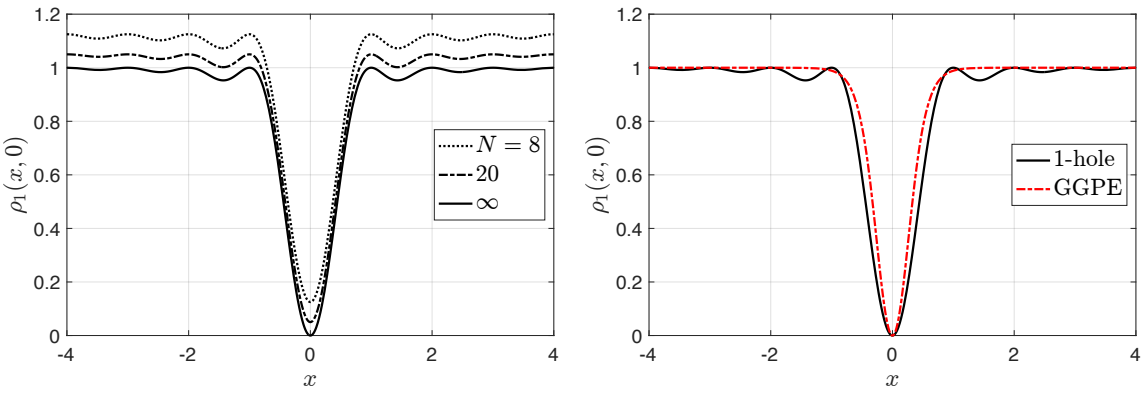


Figure 5.1: 'Flat' 1-hole density profiles $\rho_1(x,0)$ for $N = L = 8$, 20, and in the thermodynamic limit, in the Tonks-Girardeau regime (left panel). On the right panel, $\rho_1(x,0)$ in the thermodynamic limit (labeled '1-hole') is compared with the black soliton solution of the generalized Gross-Pitaevskii equation in the Tonks-Girardeau regime, Eq. (4.149a).

$\pi/\lambda_F = n^{-1}$, whose amplitude decays with the inverse square of $x - x_0$ (Friedel oscillations), which are yet another sign of the fermionization of the 1D Bose system in the Tonks-Girardeau regime. There are at least two reasons for this difference. The first is that the GGPE is an effective bosonic theory, while the system is essentially fermionic. The second is is to be found in the failure of the assumptions underlying the mean field description in the strong interaction regime. In addition to the difficulty related to the introduction of an order parameter, which we have already discussed, there is the fact that a mean field or hydrodynamic approach is founded on the assumption of local equilibrium, i.e. on the possibility of describing collectively a group of many atoms distributed over a length much shorter than the length scale of density variations. In the present case, such length scale is of the order of the soliton width, i.e. $n^{-1} = L/N$. But due to the fermionization which occurs in the Tonks-Girardeau regime, the average interparticle distance is also L/N. In this situation, where the average interparticle distance is of the same order of the length scale of density variations, we cannot expect the mean field to go beyond a merely qualitative description of the system.

iii. Concerning the dynamical evolution of the wave packet, we first notice that since we are summing over h, h' in the full interval $[1, N]$, the density profile remains symmetric with respect to $x = x_0$ for any t. Therefore, the density depletion is produced at rest. What we observe is that, under time evolution, the initial depletion at $x = x_0$ is soon redistributed throughout the whole system. The time t^* it takes for the depletion to disappear depends only on the particle density n, with a higher density corresponding to a shorter lifetime. In the thermodynamic limit, this can be seen by evaluating Eq. (5.48) for $x = x_0 = 0$, which gives

$$\rho_1(0,t) = n + \frac{\mathrm{erf}\left[(-1)^{1/4}\pi n\sqrt{t}\,\right]\mathrm{erf}\left[(-1)^{3/4}\pi n\sqrt{t}\,\right]}{4\pi n t}, \tag{5.50}$$

where erf is the error function. For $n = 1$, for instance, the disappearance time, identified as the value of $t > 0$ for which $\rho_1(0,t)$ has its first local maximum, is $t^* \simeq 0.5815$.

At finite size, however, the disappearance of the initial depletion is not definitive, because the time evolution shows a recurrence, called quantum revival[3] (Fig. 5.2). The revival time t_{rev} can be identified as the smallest value of $t > 0$ such that $\exp(iE_1^h t) = 1$ for any

[3] See e.g. Robinett (2004) and Zhao and Wu (2019) for discussions of the concept of quantum revival.

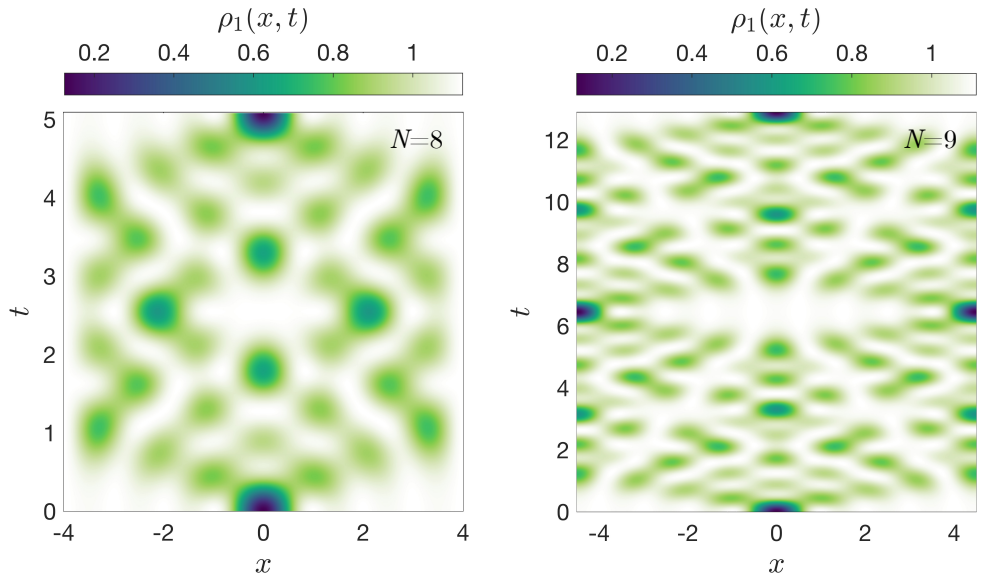


Figure 5.2: 'Flat' 1-hole density profiles $\rho_1(x,t)$ for $N = L = 8$ (left panel) and $N = L = 9$ (right panel) in the Tonks-Girardeau regime, plotted for $-L/2 \leq x \leq L/2$ and $0 \leq t \leq t_{\rm rev}$. The recursion time is $t_{\rm rec} = L^2/4\pi \simeq 5.09$ for $L = 8$ and $t_{\rm rev} = L^2/2\pi \simeq 12.89$ for $L = 9$.

$h \in [1, N]$, that is

$$t_{\rm rev} = \frac{L^2}{2\pi\,\gcd[h(N+1-h)]} = \begin{cases} \frac{L^2}{4\pi} & \text{for } N \text{ even}, \\ \frac{L^2}{2\pi} & \text{for } N \text{ odd}. \end{cases} \tag{5.51}$$

Since $t_{\rm rev}$ scales with L^2, in the thermodynamic limit we will have no revival.

Let us now discuss an example of a selective wave packet at finite size and in the thermodynamic limit. In the first case, we construct the wave packet restricting the summation over h, h' between $\lceil (N+3)/4 \rceil$ and $\lfloor (3N+1)/4 \rfloor$. For N even, this is exactly one-half of the original interval $[1, N]$. The normalization constant $\mathfrak{S}$ should be adjusted accordingly to $N/2$. In the thermodynamic limit, we construct the wave packet restricting the integration over z, z' between to $[2n/5,\, 3n/5]$, which corresponds to one-fifth of the original interval, and appropriately adjusting the normalization constant to $n/5$. The wave packets thus constructed are compared with the corresponding flat wave packets in Fig. 5.3. As anticipated, selective wave packets are wider (and therefore shallower) and longer-lived. Halving the intervals available for hole positions produces a wave packet twice as wide and with four times the disappearance time. We remark that as long as the interval available for hole positions is symmetric with respect to the midpoint $(N+1)/2$, the depletion will still be produced at rest.

5.3.2 Multi-hole Type II wave packets

Consider instead a wave packet constructed from a flat superposition of 2-hole Type II states $|\, P_2^{h,\bar{h}} \,\rangle$, which have momentum $P_2^{h,\bar{h}} = (2\pi/L)(h + \bar{h} + 1)$ and energy $E_2^{h,\bar{h}} - E_{\rm gs} = (2\pi/L)^2[h(N+1-h) + (1+\bar{h})(N+2-\bar{h})]$. In the Tonks-Girardeau regime, the hole $\bar{h}$ must be common to all the states in the superposition. The density matrix elements are then given by $\langle\, P_2^{h',\bar{h}} \,|\, \hat{\rho}(0) \,|\, P_2^{h,\bar{h}} \,\rangle = (-1)^{|C_{h,h',\bar{h}}|}/L$, where $|C_{h,h',\bar{h}}|$ (the number of particles between the holes h and h') is $|C_{h,h',\bar{h}}| = |h - h'| - 1$ if $\bar{h}$ is not between h and h', whereas $|C_{h,h',\bar{h}}| = |h - h'| - 2$ if $\bar{h}$ is between h and h'. The difference amounts to a global

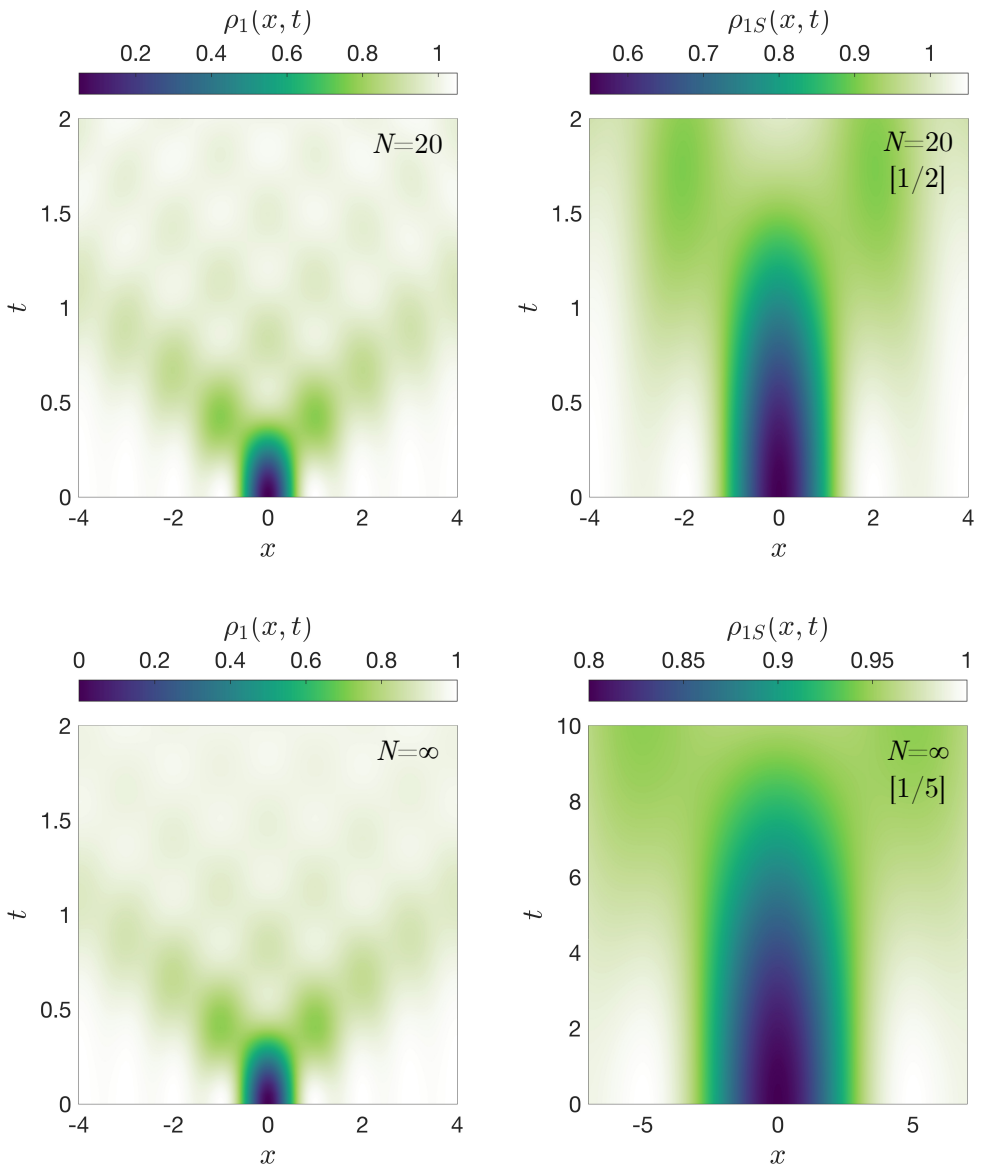


Figure 5.3: Comparison between the 'flat' and 'selective' 1-hole density profiles $\rho_1(x,t)$ for $N = L = 20$ (upper panels) and in the thermodynamic limit (lower panels), in the Tonks-Girardeau regime. The selective wave packets are obtained restricting the summation over h, h' between $\lceil (N+3)/4 \rceil$ and $\lfloor (3N+1)/4 \rfloor$ in the case $N = 20$, which corresponds to $1/2$ of the original interval, and restricting the integration over z, z' between to $[0.4n,\, 0.6n]$ (with $n = 1$) in the thermodynamic limit, which corresponds to $1/5$ of the original interval.

change of sign of the matrix elements (that is a signal of the fermionic nature of the Lieb-Liniger model in the Tonks-Girardeau regime), which are thus given in the two cases by $\langle\, P_2^{h',\bar{h}} \,|\, \hat{\rho}(0) \,|\, P_2^{h,\bar{h}} \,\rangle = \mp e^{i\pi(h-h')}/L$. Beside the crucial difference in the matrix elements, since $|\, P_2^{h',\bar{h}} \,\rangle$ and $|\, P_2^{h,\bar{h}} \,\rangle$ still differ by just one hole, the constitutive exponential carrying the space-time dependence of the $\rho(x,t)$ is the same as in the 1-hole case, namely

$$\mathcal{F}_{h,h'}(x,t) \equiv \exp\left\{-i\frac{2\pi}{L}(h'-h)\left[x - x_0 + \frac{L}{2} - \frac{2\pi}{L}(N+1-h-h')t\right]\right\}. \tag{5.52}$$

The density is therefore

$$\rho_2(x,t) = \frac{N}{L} + \frac{1}{\mathfrak{S}L}\sum_{\bar{h},h,h'}{}' (\mp\mathcal{F}_{h,h'})(x,t), \qquad \mathfrak{S} = \binom{N}{2}, \tag{5.53}$$

where the summation is, according the above discussion,

$$\begin{aligned}\textstyle\sum'_{\bar{h},h,h'} \mp\mathcal{F} = \sum_{\bar{h}=1}^{N}\{\, &\textstyle\sum_{h>\bar{h}}[\,\sum_{h'>h}(-\mathcal{F}) + \sum_{\bar{h}<h'<h}(-\mathcal{F}) + \sum_{h'<\bar{h}}(+\mathcal{F})\,] \\ &+ \textstyle\sum_{h<\bar{h}}[\,\sum_{h'<h}(-\mathcal{F}) + \sum_{h<h'<\bar{h}}(-\mathcal{F}) + \sum_{h'>\bar{h}}(+\mathcal{F})\,]\,\}.\end{aligned}$$

In the thermodynamic limit, the constitutive exponential becomes

$$\mathcal{F}_{z,z'}(x,t) \equiv \exp\left\{-2\pi i(z-z')[x - 2\pi(n-z-z')t]\right\} \tag{5.54}$$

and the density is

$$\rho_2(x,t) \overset{\text{Th.Lim.}}{=} n + \frac{2}{n^2}\int_D d\bar{z}\, dz\, dz'\, (\mp\mathcal{F}_{z,z'})(x,t), \tag{5.55}$$

where the integration is the continuous version of the summation above,

$$\begin{aligned}\textstyle\int_D d\bar{z}\, dz\, dz' \,\mp\mathcal{F} = \int_0^n d\bar{z}\,\{\, &\textstyle\int_{\bar{z}}^n dz\,[\,\int_{\bar{z}}^n dz'\,(-\mathcal{F}) + \int_0^{\bar{z}} dz'\,(+\mathcal{F})\,]\} \\ &+ \textstyle\int_0^{\bar{z}} dz\,[\,\int_0^{\bar{z}} dz'\,(-\mathcal{F}) + \int_{\bar{z}}^n dz'\,(+\mathcal{F})\,]\,\}.\end{aligned}$$

The density profiles at $t = 0$ of flat 2-hole and 1-hole wave packets are compared in Fig. 5.4. Instead of a single density depletion centered at $x = x_0 = 0$, we now have a double depletion. The dynamical evolution of a flat and a selective 2-hole wave packet in the thermodynamic limit is compared in Fig. 5.5. The comments made for 1-hole wave packets also apply here.

It is clear that the above construction can be generalized to n-hole Type II wave packets with arbitrary number of holes n. The density in the Tonks-Girardeau regime will be given by

$$\rho_n(x,t) = \frac{N}{L} + \frac{1}{\mathfrak{S}L}\sum_{\substack{\bar{h}_1,\ldots,\bar{h}_{n-1},\\ h,h'}}{}' (\mp\mathcal{F}_{h,h'})(x,t), \qquad \mathfrak{S} = \binom{N}{n}, \tag{5.56}$$

where $\bar{h}_1,\ldots,\bar{h}_{n-1}$ are the $n-1$ holes that must be common between $|\, P_n^{\mathbf{h}} \,\rangle$ and $|\, P_n^{\mathbf{h}'} \,\rangle$ in order for $\langle\, P_n^{\mathbf{h}'} \,|\, \hat{\rho}(0) \,|\, P_n^{\mathbf{h}} \,\rangle$ to be non-vanishing. As in the 2-hole case, the matrix element leads to the contribution $-\mathcal{F}$ (respectively, $+\mathcal{F}$) if the number of $\bar{h}$'s between h and h' is even (respectively, odd).

In the thermodynamic limit, we have the possibility to consider a very large number of holes. We expect that this, combined with the selection of hole positions around the center of the Fermi interval, should produce very long-lived wave packets. Further investigations are ongoing in this direction.

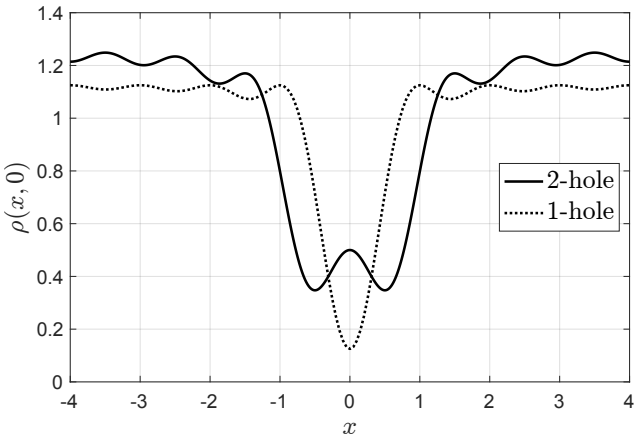


Figure 5.4: Comparison between the 'flat' 2-hole and 1-hole density profiles, $\rho_2(x,0)$ and $\rho_1(x,0)$, for $N = L = 8$ in the Tonks-Girardeau regime.

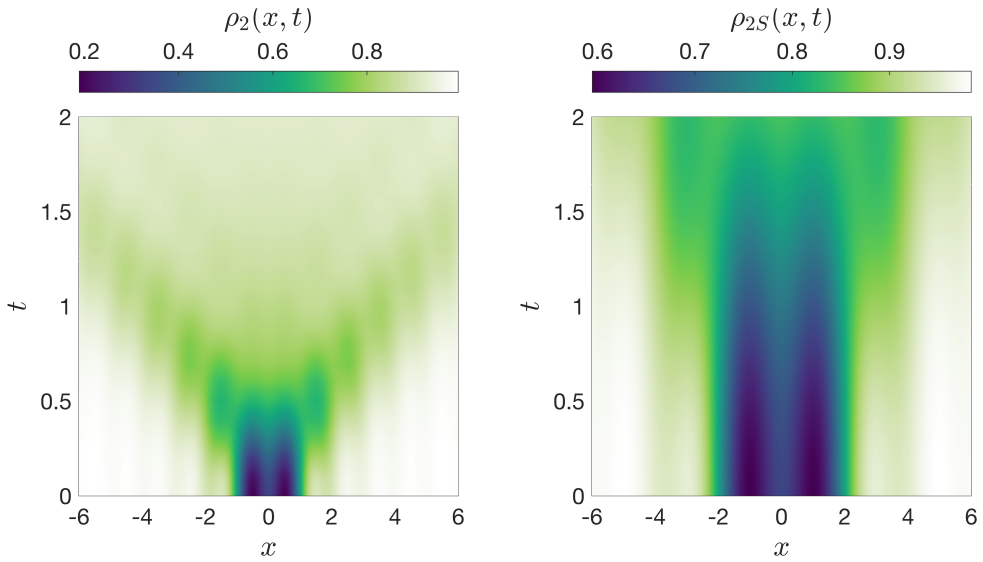


Figure 5.5: Comparison between the 'flat' and 'selective' 2-hole density profiles $\rho_2(x,t)$ in the thermodynamic limit, in the Tonks-Girardeau regime. The selective wave packet is obtained restricting the integration over $\bar{z}$, z, z' to the interval $[n/4,\, 3n/4]$ (with $n = 1$), which corresponds to $1/2$ of the original interval.

Conclusions and outlook

In this thesis we have discussed the construction of quantum bright solitons and quantum dark solitons in the Lieb-Liniger model, in the attractive and repulsive regimes, respectively. A detailed analysis of the ground state and the excitations using a combination of exact and efficient techniques has been helpful for this purpose.

In the attractive case, rapidities are organized in strings in the complex plane, which greatly simplifies the form of the Bethe wavefunctions. This has allowed us to proceed analytically using the Coordinate Bethe Ansatz, and to study the soliton scattering by exploiting general results from scattering theory and the knowledge of the exact scattering phase shifts appearing in the Bethe equations. We have found that in the limit of a large number of particles, the density profile of quantum bright solitons reduces to that of bright solitons of the Hartree mean field theory. The results for the scattering within the mean field theory are in good agreement with those of the Bethe Ansatz even for a moderate number of particles in each soliton, and the agreement is better for higher collision velocities. However, the Bethe Ansatz is able to cure a non-physical divergence of the displacement of trajectories predicted by the mean field approach in the limit of a very slow scattering of two identical solitons.

In the repulsive case, things are much more complicated, and we had to resort to the Algebraic Bethe Ansatz. The exact correspondence between the dispersion relation of hole-like (Type II) excitations and that of the dark solitons of the Gross-Pitaveskii mean field theory in the weak interaction limit, and the existence of a similar correspondence, although only qualitative, with a generalized mean field theory for strong interaction, prompted us to try to construct Type II wave packets that enjoy the robustness of classical solitons. We showed that the procedure usually considered in the literature is not satisfactory from this point of view, and we suggested how this difficulty could be solved by the inclusion of multi-hole states with quasi-degenerate energies exploiting the Van Hove singularity that characterizes the Type II dispersion relation. The first steps in this direction have been presented in the last chapter, with the derivation of some analytical results in the Tonks-Girardeau limit. Looking ahead, we intend to continue the implementation of this improved procedure by considerably increasing the number of holes and by extending the treatment to the case of finite interaction strength, which will necessarily have to be treated numerically, due to the extremely large number of matrix elements entering the computations. An important simplification of this process would be provided by finding semi-analytic relations for the ratio of matrix elements involving states differing by a few quantum numbers. Some preliminary results in this direction are reported in Appendix D. The analytical results in the Tonks-Girardeau limit that we have already obtained will serve as benchmark for this numerical treatment. Soliton scattering in the repulsive regime could then be studied numerically by directly simulating the dynamics of multi-solitons, in the same way we simulated the dynamics of a single soliton.

Appendix A

Sound velocity and effective masses

In the first part of this appendix we prove Eq. (4.49) for the macroscopically-defined sound velocity and its equivalence to the microscopic definition given by Eq. (4.42). In the second part we derive Eqs. (4.52) and (4.53) for the effective mass.

Sound velocity The sound velocity is defined macroscopically as

$$v_s = \sqrt{\frac{2}{n\kappa_S}}, \tag{A.1}$$

where κ_S is the compressibility. Its inverse is given by

$$\frac{1}{\kappa_S} = n\frac{\partial P}{\partial n} = n\frac{\partial \mu}{\partial n}\frac{\partial P}{\partial \mu} = -\frac{n}{2\pi}\frac{\partial \mu}{\partial n}\int_{-\lambda_F}^{\lambda_F} d\lambda\, \frac{\partial \epsilon_g(\lambda)}{\partial \mu}, \tag{A.2}$$

where for the last equality we have used Eq. (4.50). We compute this as follows.

* From Eq. (4.20) we have

$$\frac{\partial \epsilon_g(\lambda)}{\partial \mu} - \int_{-\lambda_F}^{\lambda_F} d\lambda'\, \mathcal{C}(\lambda-\lambda')\frac{\partial \epsilon_g(\lambda')}{\partial \mu} = -1, \qquad \lambda \in \mathbb{R}, \tag{A.3}$$

  where we have used the fact that the boundary terms involve $\epsilon_g(\pm\lambda_F) = 0$. Comparing this with the Lieb equation (1.99) immediately gives

$$\frac{\partial \epsilon_g(\lambda)}{\partial \mu} = -2\pi\rho_g(\lambda), \qquad |\lambda| < \lambda_F. \tag{A.4}$$

* From Eq. (1.100) we have

$$\frac{\partial n}{\partial \mu} = \frac{\partial}{\partial \mu}\int_{-\lambda_F}^{\lambda_F} d\lambda\, \rho_g(\lambda) = 2\rho_g(\lambda_F)\frac{\partial \lambda_F}{\partial \mu} + \int_{-\lambda_F}^{\lambda_F} d\lambda\, \frac{\partial \rho_g(\lambda)}{\partial \mu}. \tag{A.5}$$

  The quantity $\partial\lambda_F/\partial\mu$ can be rewritten starting again from Eq. (4.20),

$$\frac{\partial \epsilon_g(\lambda)}{\partial \lambda_F} - \int_{-\lambda_F}^{\lambda_F} d\lambda'\, \mathcal{C}(\lambda-\lambda')\frac{\partial \epsilon_g(\lambda')}{\partial \lambda_F} = -\frac{\partial \mu}{\partial \lambda_F}. \tag{A.6}$$

  The right-hand side is independent of λ, therefore we can invoke the Lieb equation to get

$$\frac{\partial \mu}{\partial \lambda_F} = -\frac{1}{2\pi\rho_g(\lambda)}\frac{\partial \epsilon_g(\lambda)}{\partial \lambda_F}, \tag{A.7}$$

  where the right-hand side is the same constant for any λ in the Fermi interval.

It remains to compute $\partial\rho_g(\lambda)/\partial\mu$. From the Lieb equation we have

$$\frac{\partial\rho_g(\lambda)}{\partial\mu} = \rho_g(\lambda_F)\big[\mathcal{C}(\lambda-\lambda_F)+\mathcal{C}(\lambda+\lambda_F)\big]\frac{\partial\lambda_F}{\partial\mu} + \int_{-\lambda_F}^{\lambda_F} d\lambda'\,\mathcal{C}(\lambda-\lambda')\frac{\partial\rho_g(\lambda')}{\partial\mu}. \tag{A.8}$$

This can be solved by using the inverse kernel $\mathcal{L}^{(F)}(\lambda,\lambda')$, yielding

$$\frac{\partial\rho_g(\lambda)}{\partial\mu} = \rho_g(\lambda_F)\frac{\partial\lambda_F}{\partial\mu}\left[\mathcal{L}^{(F)}(\lambda,\lambda_F)+\mathcal{L}^{(F)}(\lambda,-\lambda_F)\right], \tag{A.9}$$

and in particular, using Eq. (4.19),

$$\int_{-\lambda_F}^{\lambda_F} d\lambda\,\frac{\partial\rho_g(\lambda)}{\partial\mu} = 2\rho_g(\lambda_F)\frac{\partial\lambda_F}{\partial\mu}\Big[2\pi\rho_g(\lambda_F)-1\Big]. \tag{A.10}$$

Substituting Eqs. (A.7) and (A.10) into Eq. (A.5) we thus obtain

$$\frac{\partial\mu}{\partial n} = -\frac{1}{8\pi^2\rho_g^3(\lambda_F)}\frac{\partial\epsilon_g(\lambda)}{\partial\lambda_F}\bigg|_{\lambda=\lambda_F} \tag{A.11}$$

and from this, together with Eq. (A.4), the inverse compressibility

$$\frac{1}{\kappa_S} = -\frac{n^2}{8\pi^2\rho_g^3(\lambda_F)}\frac{\partial\epsilon_g(\lambda)}{\partial\lambda_F}\bigg|_{\lambda=\lambda_F}. \tag{A.12}$$

∗ To further simplify the last result, we consider the following equalities. For $|\lambda|<\lambda_F$, deriving Eq. (4.22) with respect to λ we obtain

$$2\lambda = \frac{\partial}{\partial\lambda}\left(1-\mathcal{C}^{(F)}\right)*\epsilon_g(\lambda) = \left(1-\mathcal{C}^{(F)}\right)*\frac{\partial\epsilon_g}{\partial\lambda}(\lambda) \tag{A.13}$$

(the last equality follows from an integration by parts and the fact that the boundary terms vanish), hence

$$\frac{\partial\epsilon_g(\lambda)}{\partial\lambda} = 2\lambda + \int_{-\lambda_F}^{\lambda_F} d\lambda'\,2\lambda'\,\mathcal{L}^{(F)}(\lambda,\lambda'). \tag{A.14}$$

Similarly, for $\rho_g(\lambda)$ we have

$$0 = \frac{\partial}{\partial\lambda}\left(1-\mathcal{C}^{(F)}\right)*\rho_g(\lambda) = \left(1-\mathcal{C}^{(F)}\right)*\frac{\partial\rho_g}{\partial\lambda}(\lambda)+\rho_g(\lambda_F)\big[\mathcal{C}(\lambda-\lambda_F)-\mathcal{C}(\lambda+\lambda_F)\big] \tag{A.15}$$

and therefore

$$\frac{\partial\rho_g(\lambda)}{\partial\lambda} = \rho_g(\lambda_F)\left[-\mathcal{L}^{(F)}(\lambda,\lambda_F)+\mathcal{L}^{(F)}(\lambda,-\lambda_F)\right]. \tag{A.16}$$

On the other hand, the particle density can be written

$$n = \int_{-\lambda_F}^{\lambda_F} d\lambda\,\rho_g(\lambda) = \int_{-\lambda_F}^{\lambda_F} d\lambda\left[\frac{\partial}{\partial\lambda}(\lambda\rho_g(\lambda)) - \lambda\frac{\partial\rho_g(\lambda)}{\partial\lambda}\right] = 2\lambda_F\rho_g(\lambda_F) - \int_{-\lambda_F}^{\lambda_F} d\lambda\,\lambda\frac{\partial\rho_g(\lambda)}{\partial\lambda}. \tag{A.17}$$

Thus Eqs. (A.14) and (A.16) yield the useful relation

$$n = \rho_g(\lambda_F)\frac{\partial\epsilon_g(\lambda)}{\partial\lambda}\bigg|_{\lambda=\lambda_F}. \tag{A.18}$$

∗ Since we obviously have

$$-\frac{\partial\epsilon_g(\lambda)}{\partial\lambda_F}\bigg|_{\lambda=\lambda_F} = \frac{\partial\epsilon_g(\lambda)}{\partial\lambda}\bigg|_{\lambda=\lambda_F}, \tag{A.19}$$

Eq. (A.18) allows us to rewrite the inverse compressibility in the equivalent forms

$$\frac{1}{\kappa_S} = \frac{n}{8\pi^2\rho_g^2(\lambda_F)}\left(\frac{\partial\epsilon_g(\lambda)}{\partial\lambda}\bigg|_{\lambda=\lambda_F}\right)^2 = \frac{n^3}{8\pi^2\rho_g^4(\lambda_F)}. \tag{A.20}$$

The sound velocity is then

$$v_s = \frac{1}{2\pi\rho_g(\lambda_F)}\frac{\partial\epsilon_g(\lambda)}{\partial\lambda}\bigg|_{\lambda=\lambda_F} = \frac{n}{2\pi\rho_g^2(\lambda_F)}. \tag{A.21}$$

This concludes the proof of Eq. (4.49), where n is expressed in terms of the Fermi velocity $v_F = 2\pi n$, and of the equivalence between Eqs. (4.49) and (4.42). It is worth noting that Eq. (A.7) is then equal to

$$\frac{\partial\mu}{\partial\lambda_F} = v_s. \tag{A.22}$$

Effective mass We now look at the inverse effective mass

$$\frac{1}{m^*} = \frac{\partial^2\omega(p)}{\partial p^2}\bigg|_{p\to 0} = \left(\frac{\partial p(\lambda)}{\partial\lambda}\right)^{-2}\left[\frac{\partial^2\omega(\lambda)}{\partial\lambda^2} - \frac{\partial\omega(\lambda)}{\partial\lambda}\left(\frac{\partial p(\lambda)}{\partial\lambda}\right)^{-1}\frac{\partial^2 p(\lambda)}{\partial\lambda^2}\right]\bigg|_{\lambda\to\lambda_F}, \tag{A.23}$$

where $\omega(\lambda) = \epsilon_g(\lambda)$ (Eq. (4.32)). From Eq. (4.41) we have $\partial p/\partial\lambda|_{\lambda\to\lambda_F} = 2\pi\rho_g(\lambda_F)$ and

$$\frac{\partial^2 p(\lambda)}{\partial\lambda^2}\bigg|_{\lambda\to\lambda_F} = 2\pi\frac{\partial\rho_g(\lambda)}{\partial\lambda}\bigg|_{\lambda\to\lambda_F} = 2\pi\rho_g(\lambda_F)\mathcal{L}^{(F)}(\lambda_F, -\lambda_F), \tag{A.24}$$

having used for the last equality Eq. (A.16). From Eq. (A.18) we have $\partial\epsilon_g/\partial\lambda|_{\lambda\to\lambda_F} = n/\rho_g(\lambda_F)$, and then from Eq. (A.13),

$$\frac{\partial^2\epsilon_g(\lambda)}{\partial\lambda^2} = 4\pi\rho_g(\lambda) - \frac{n}{\rho_g(\lambda_F)}\left[\mathcal{L}^{(F)}(\lambda,\lambda_F) + \mathcal{L}^{(F)}(\lambda,-\lambda_F)\right]. \tag{A.25}$$

It follows that

$$\frac{1}{m^*} = \frac{1}{[\,2\pi\rho_g(\lambda_F)\,]^2}\left[4\pi\rho_g(\lambda_F) - \frac{2n}{\rho_g(\lambda_F)}\mathcal{L}^{(F)}(\lambda_F,-\lambda_F)\right]. \tag{A.26}$$

To express this in terms of physical quantities, let us consider the total derivative of the sound velocity v_s with respect to λ_F, i.e. the derivative with respect to λ_F with λ thought of as depending on λ_F in such a way that $\partial\lambda/\partial\lambda_F|_{\lambda=\lambda_F} = 1$. Then

$$\begin{aligned}\frac{dv_s}{d\lambda_F} = {}& \frac{1}{2\pi\rho_g(\lambda_F)}\left[\frac{\partial^2\epsilon_g(\lambda)}{\partial\lambda^2}\bigg|_{\lambda=\lambda_F} + \frac{\partial^2\epsilon_g(\lambda)}{\partial\lambda_F\partial\lambda}\bigg|_{\lambda=\lambda_F}\right] \\ & - \frac{1}{2\pi\rho_g^2(\lambda_F)}\frac{\partial\epsilon_g(\lambda)}{\partial\lambda}\bigg|_{\lambda=\lambda_F}\left[\frac{\partial\rho_g(\lambda)}{\partial\lambda}\bigg|_{\lambda=\lambda_F} + \frac{\partial\rho_g(\lambda)}{\partial\lambda_F}\bigg|_{\lambda=\lambda_F}\right].\end{aligned} \tag{A.27}$$

Using Eq. (A.22) to write $\partial/\partial\lambda_F = v_s\partial/\partial\mu$, and exploiting the previous results for the various derivative quantities, we obtain

$$\frac{dv_s}{d\lambda_F} = 2 - \frac{2n}{\pi\rho_g^2(\lambda_F)}\mathcal{L}^{(F)}(\lambda_F,-\lambda_F) = 2 + 2\frac{\partial v_s}{\partial\lambda_F}. \tag{A.28}$$

Defining $\sqrt{K} = 2\pi\rho_g(\lambda_F)$, this can also be written as

$$\frac{dv_s}{d\lambda_F} = 2 - 2\frac{v_s}{\sqrt{K}}\frac{d\sqrt{K}}{d\lambda_F} = 2 - 4\frac{v_s}{\sqrt{K}}\frac{\partial\sqrt{K}}{\partial\lambda_F}. \tag{A.29}$$

The inverse effective mass is then

$$\frac{1}{m^*} = \frac{1}{4\pi\rho_g(\lambda_F)}\left(2 + \frac{dv_s}{d\lambda_F}\right) = \frac{v_s}{K}\frac{d}{d\mu}\big(v_s\sqrt{K}\big). \tag{A.30}$$

Exploiting Eqs. (A.11) and (A.19), which give

$$\frac{\partial\mu}{\partial n} = \frac{\pi v_s}{K}, \tag{A.31}$$

Eq. (A.30) becomes

$$\frac{1}{m^*} = \frac{1}{\pi}\frac{d}{dn}\big(v_s\sqrt{K}\big), \tag{A.32}$$

and writing $\partial/\partial n = (-\gamma^2/c)\partial/\partial\gamma$, this is equivalent to

$$\frac{1}{2m^*} = \left(1 - \gamma\frac{d}{d\gamma}\right)\frac{1}{\sqrt{K}}. \tag{A.33}$$

Appendix B

Bogoliubov theory

In this appendix we show how to arrive at the Hamiltonian (4.79) using the Bogoliubov prescription $\hat{a}_0^\dagger$, $\hat{a}_0 \to \sqrt{N_0}$, and how to diagonalize it with a Bogoliubov transformation, leading to Eqs. (4.80)-(4.82) (Landau and Lifshitz, 1980).

With the Bogoliubov prescription, the interaction term in Eq. (4.76) becomes

$$\sum_{p\,p'\,q} \hat{a}^\dagger_{p+q}\hat{a}^\dagger_{p'-q}\hat{a}_{p'}\hat{a}_p = N_0^2 + N_0 \sum_{p\neq 0}\left(\hat{a}_p\hat{a}_{-p} + \hat{a}^\dagger_p\hat{a}^\dagger_{-p} + 4\,\hat{a}^\dagger_p\hat{a}_p\right) + O(\hat{a}^3). \tag{B.1}$$

Notice that terms containing a single $\hat{a}_p$ operator with $p \neq 0$ are ruled out by momentum conservation. Since the original Hamiltonian conserves the total number of particles N, we prefer to express N_0 in terms of N by using the relation

$$\hat{N} = N_0 + \sum_{p\neq 0}\hat{a}^\dagger_p\hat{a}_p. \tag{B.2}$$

To quadratic order, $N_0^2 \simeq N^2 - 2N\sum_{p\neq 0}\hat{a}^\dagger_p\hat{a}_p$, while $N_0 \simeq N$ in the second term of Eq. (B.1), so that

$$\sum_{p\,p'\,q} \hat{a}^\dagger_{p+q}\hat{a}^\dagger_{p'-q}\hat{a}_{p'}\hat{a}_p = N^2 + N \sum_{p\neq 0}\left(\hat{a}_p\hat{a}_{-p} + \hat{a}^\dagger_p\hat{a}^\dagger_{-p} + 2\,\hat{a}^\dagger_p\hat{a}_p\right) + O(\hat{a}^3). \tag{B.3}$$

The Hamiltonian then becomes the one of Eq. (4.79),

$$\hat{H}_{\rm Bog} = \frac{cN^2}{L} + \sum_{p\neq 0}\left[\left(p^2 + 2cn\right)\hat{a}^\dagger_p\hat{a}_p + cn\left(\hat{a}_p\hat{a}_{-p} + \hat{a}^\dagger_p\hat{a}^\dagger_{-p}\right)\right]. \tag{B.4}$$

The reduction of the coefficient of $\hat{a}^\dagger_p\hat{a}_p$ from $p^2 + 4cn_0$ to $p^2 + 2cn \simeq p^2 + 2cn_0$, is due to the condition that the total number of particles be fixed. In the grand canonical treatment this corresponds to the subtraction of the chemical potential, since for a uniform Bose gas at zero temperature the chemical potential (at tree level) is $\mu = 2cn_0$.

Eq. (B.4) can be written in the symmetrical form

$$\hat{H}_{\rm Bog} = \frac{cN^2}{L} + \sum_{p>0}\left[\left(p^2 + 2cn\right)\left(\hat{a}^\dagger_p\hat{a}_p + \hat{a}^\dagger_{-p}\hat{a}_{-p}\right) + 2cn\left(\hat{a}_p\hat{a}_{-p} + \hat{a}^\dagger_p\hat{a}^\dagger_{-p}\right)\right] \tag{B.5}$$

and can be diagonalized by an appropriate canonical transformation. We introduce new operators $\hat{b}_p$ and $\hat{b}^\dagger_p$ by the transformation

$$\hat{a}_p = u_p\hat{b}_p + v_p\hat{b}^\dagger_{-p}, \qquad \hat{a}_{-p} = u_p\hat{b}_{-p} + v_p\hat{b}^\dagger_p, \tag{B.6}$$

where u_p and v_p are real coefficients to be determined. Requiring that the new operators satisfy canonical commutation relations, $[\hat{b}_p, \hat{b}^\dagger_{p'}] = \delta_{p,p'}$ and $[\hat{b}_p, \hat{b}_{p'}] = 0$, imposes that

$$u_p^2 - v_p^2 = 1. \tag{B.7}$$

We notice, parenthetically, that such condition allows us to write the inverse transformation corresponding to Eq. (B.6) as

$$\hat{b}_p = u_p \hat{a}_p - v_p \hat{a}^\dagger_{-p}, \qquad \hat{b}_{-p} = u_p \hat{a}_{-p} - v_p \hat{a}^\dagger_p. \tag{B.8}$$

Substituting Eq. (B.6) into Eq. (B.5), and introducing the shorthand notations $\epsilon_0 \equiv p^2 + 2cn$ and $\epsilon_1 \equiv 2cn$, we obtain

$$\begin{aligned}\hat{H}_{\text{Bog}} = \frac{cN^2}{L} + \sum_{p>0}\Big[2v_p^2\epsilon_0 + 2u_p v_p \epsilon_1 + \left[(u_p^2 + v_p^2)\epsilon_0 + 2u_p v_p \epsilon_1\right]\left(\hat{b}^\dagger_p \hat{b}_p + \hat{b}^\dagger_{-p}\hat{b}_{-p}\right) \\ + \left[(u_p^2 + v_p^2)\epsilon_1 + 2u_p v_p \epsilon_0\right]\left(\hat{b}_p \hat{b}_{-p} + \hat{b}^\dagger_p \hat{b}^\dagger_{-p}\right)\Big].\end{aligned} \tag{B.9}$$

The non diagonal term proportional to $(\hat{b}_p\hat{b}_{-p} + \hat{b}^\dagger_p\hat{b}^\dagger_{-p})$ can be made to vanish by imposing

$$(u_p^2 + v_p^2)\epsilon_1 + 2u_p v_p \epsilon_0 = 0. \tag{B.10}$$

If we choose to parametrize u_p and v_p as

$$u_p = \cosh\theta_p, \qquad v_p = -\sinh\theta_p, \tag{B.11}$$

which is consistent with Eq. (B.7), condition (B.10) becomes

$$\frac{\epsilon_1}{\epsilon_0} = \tanh 2\theta_p. \tag{B.12}$$

This gives $\theta_p = \frac{1}{2}\text{arctanh}(\epsilon_1/\epsilon_0) > 0$, and

$$u^2 = \frac{1}{2}\left(\frac{\epsilon_0}{\epsilon} + 1\right), \qquad v^2 = \frac{1}{2}\left(\frac{\epsilon_0}{\epsilon} - 1\right), \qquad \epsilon = \sqrt{\epsilon_0^2 - \epsilon_1^2}. \tag{B.13}$$

In particular,

$$u_p^2 + v_p^2 = \frac{\epsilon_0}{\epsilon} \qquad \text{and} \qquad 2u_p v_p = -\frac{\epsilon_1}{\epsilon}, \tag{B.14}$$

which substituted into Eq. (B.9) yield

$$\hat{H}_{\text{Bog}} = \frac{cN^2}{L} + \sum_{p>0}\left[\epsilon - \epsilon_0 + \epsilon\left(\hat{b}^\dagger_p \hat{b}_p + \hat{b}^\dagger_{-p}\hat{b}_{-p}\right)\right]. \tag{B.15}$$

This corresponds to Eqs. (4.80)-(4.82).

Appendix C

Luttinger liquids

This appendix provides a brief review of the bosonization method, which allows mapping a low-energy effective theory of 1D interacting fermions (Luttinger liquid) to massless, non-interacting bosons. The paradigm of the Luttinger liquid is actually a universal low-energy theory of interacting quantum particles in one dimension. The excitations in this theory are phonons, i.e. bosonic quasiparticles representing particle density waves propagating with constant velocity. When including the effect of the curvature of the spectrum of physical fermions, the bosonized theory is no longer free. However, by performing a Bogoliubov transformation and following the bosonization procedure in reverse, we can map the system of interacting bosons to a basis of (almost) free fermionic quasiparticles ('fermionization'). This last mapping is our main point of interest and is what is needed to justify the results of Section 4.3.2. Throughout this chapter $\hbar = 1$, and to simplify the notation we omit to write a hat above operators.

C.1 Bosonization without band curvature

We begin by reviewing standard bosonization (i.e. without band curvature effects), following Giamarchi (2003); Haldane (1981b); Fradkin (2013). Let us consider a system of non-interacting (spinless) fermions on a line segment $x \in [0, L]$. The single-particle energy is given as function of the momentum p (possibly taking discrete values due to finite size quantization) by

$$\epsilon(p) = \frac{p^2}{2m} - \epsilon_F = \frac{(p - p_F)^2}{2m} + v_F(p - p_F), \tag{C.1}$$

where p_F is the Fermi momentum, $v_F = p_F/m$ is the Fermi velocity and $\epsilon_F = p_F^2/2m$ is the Fermi energy. The Fermi momentum is determined by an external chemical potential μ through the condition $\epsilon_F = \mu$, or $\epsilon(p_F) = 0$. The ground state of the systems consists of a compact set of symmetrically-distributed occupied levels up to the Fermi surface, which is composed of two disconnected points at $\pm p_F$.

To construct an effective low-energy theory we focus on the sector spanned by states sufficiently close to the Fermi points, for which we can neglect band curvature effects and write the energy as

$$\epsilon(p) \simeq v_F(|p| - p_F). \tag{C.2}$$

We thus identify two types of modes, some living around momentum p_F (right-movers) and some others around $-p_F$ (left-movers). These two branches can be treated as two separate types of fermions, whose dispersion relation is simplified to a purely linear form. This leads to the Luttinger liquid model. To formalize this construction, let us consider the fermionic field operator

$$\psi(x) = \frac{1}{\sqrt{L}} \sum_p c_p \mathrm{e}^{ipx}, \tag{C.3}$$

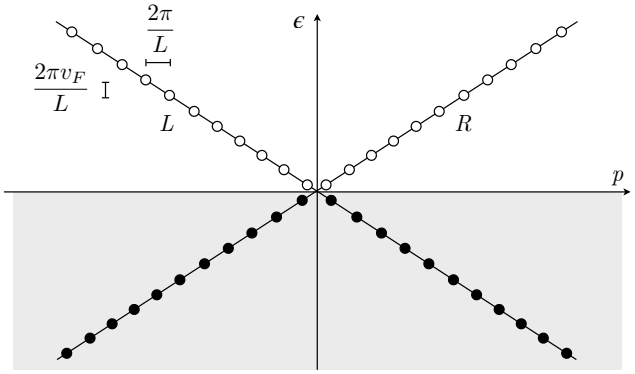


Figure C.1: The spectrum of left- and right-movers in the Luttinger model. The slope of the dispersion relation is $\pm v_F$ and remains constant at all momenta. The ground state is obtained by filling the right-moving states with negative momentum and filling the left-moving states with positive momentum.

where the destruction operator c_p is related to the Fourier component ψ_p by $c_p = \psi_p/\sqrt{L}$. These operators satisfy the canonical anticommutation relations

$$\left\{c_p, c_{p'}^\dagger\right\} = \delta_{p,p'}, \qquad \left\{c_p, c_{p'}\right\} = 0, \tag{C.4a}$$

$$\left\{\psi(x), \psi^\dagger(x')\right\} = \delta(x'-x), \qquad \left\{\psi(x), \psi(x')\right\} = 0. \tag{C.4b}$$

In Eq. (C.3), only the Fourier components close to $\pm p_F$ describe low-energy states. This suggests that we restrict the summation to momentum modes in a neighborhood of $\pm p_F$ introducing a momentum cutoff Λ, so that

$$\begin{aligned}\psi(x) &\simeq \frac{1}{\sqrt{L}} \sum_{-\Lambda<p-p_F<\Lambda} c_p \mathrm{e}^{ipx} + \frac{1}{\sqrt{L}} \sum_{-\Lambda<p+p_F<\Lambda} c_p \mathrm{e}^{ipx} \\ &= \frac{1}{\sqrt{L}} \sum_{-\Lambda<p<\Lambda} \left[c_{R,p} \mathrm{e}^{i(p+p_F)x} + c_{L,p} \mathrm{e}^{i(p-p_F)x}\right] \\ &= \mathrm{e}^{ip_F x}\psi_R(x) + \mathrm{e}^{-ip_F x}\psi_L(x),\end{aligned} \tag{C.5}$$

where we have defined $c_{R,p} = c_{p+p_F}$, $c_{L,p} = c_{p-p_F}$ and the right- and left-moving fields

$$\psi_r(x) = \frac{1}{\sqrt{L}} \sum_{-\Lambda<p<\Lambda} c_{r,p} \mathrm{e}^{ipx}, \qquad r = R, L, \tag{C.6}$$

splitting off the rapidly oscillating pieces $\mathrm{e}^{\pm ip_F x}$. These new operators satisfy the canonical anticommutation relations

$$\left\{c_{r,p}, c_{r',p'}^\dagger\right\} = \delta_{r,r'}\delta_{p,p'}, \qquad \left\{c_{r,p}, c_{r',p'}\right\} = 0, \tag{C.7a}$$

$$\left\{\psi_r(x), \psi_{r'}^\dagger(x')\right\} = \delta_{r,r'}\delta(x'-x), \qquad \left\{\psi_r(x), \psi_{r'}(x')\right\} = 0, \tag{C.7b}$$

with the convention that $r = +1$ for $r = R$ and $r = -1$ for $r = L$ when used in mathematical expressions. The free-electron Hamiltonian then becomes

$$H_0 = \sum_p \epsilon(p) c_p^\dagger c_p \simeq \sum_{-\Lambda<p<\Lambda} v_F p \left(c_{R,p}^\dagger c_{R,p} - c_{L,p}^\dagger c_{L,p}\right). \tag{C.8}$$

We can formally remove the momentum cutoff Λ, extending the energy spectrum of Luttinger model to $\pm\infty$. The ground state $|\,0\,\rangle$ of the Hamiltonian (C.8) is then a Fermi sea

of right- and left-movers built on the vacuum $|\,\mathrm{vac}\,\rangle$ of the $c_{r,p}$ operators, and is defined by the relations

$$|\,0\,\rangle = \prod_{p<0} c^\dagger_{R,p} \prod_{p>0} c^\dagger_{L,p} |\,\mathrm{vac}\,\rangle,$$
$$c_{R,p}|\,0\,\rangle = 0, \quad p>0, \qquad c_{L,p}|\,0\,\rangle = 0, \quad p<0. \tag{C.9}$$

The removal of the cutoff comes at the cost of having an infinite number of occupied states and thus an infinite ground state energy. To make sense of this, we define the Hamiltonian via normal ordering[1],

$$\begin{aligned} H_0 &= \sum_p v_F p \left(: c^\dagger_{R,p} c_{R,p} : - : c^\dagger_{L,p} c_{L,p} : \right) \\ &= -iv_F \int dx \left[: \psi^\dagger_R(x) \partial_x \psi_R(x) : - : \psi^\dagger_L(x) \partial_x \psi_L(x) : \right], \end{aligned} \tag{C.10}$$

where $: \cdots :$ represents normal ordering with respect to the ground state $|\,0\,\rangle$, so that the ground state energy is zero.

The densities of right- and left-movers are

$$\rho_r(x) = \psi^\dagger_r(x)\psi_r(x) = \frac{1}{L} \sum_p \rho_r(p)\, \mathrm{e}^{ipx}, \tag{C.11}$$

where the Fourier component $\rho_r(p)$ is

$$\rho_r(p) = \int dx\, \psi^\dagger_r(x)\psi_r(x)\, \mathrm{e}^{-ipx} = \sum_k c^\dagger_{r,k} c_{r,k+p}. \tag{C.12}$$

The number operators are therefore

$$N_r = \sum_k c^\dagger_{r,k} c_{r,k} = \rho_r(p)\Big|_{p=0} \tag{C.13}$$

and since $\rho(x)$ is real, $\rho^\dagger_r(p) = \rho_r(-p)$. Let us now look at the commutator of the density operators. Using the canonical anticommutation relations (C.7a),

$$\begin{aligned} \left[\rho_r(p), \rho^\dagger_r(p')\right] &= \sum_{k_1,k_2} \left[c^\dagger_{r,k_1} c_{r,k_1+p},\, c^\dagger_{r,k_2} c_{r,k_2-p'}\right] \\ &= \sum_{k_1,k_2} \left(c^\dagger_{r,k_1} c_{r,k_2-p'} \delta_{k_1+p,k_2} - c^\dagger_{r,k_2} c_{r,k_1+p} \delta_{k_1,k_2-p'} \right) \\ &= \sum_{k_2} \left(c^\dagger_{r,k_2-p} c_{r,k_2-p'} - c^\dagger_{r,k_2} c_{r,k_2+p-p'} \right). \end{aligned} \tag{C.14}$$

Naively one would perform a change of variables in the second term of Eq. (C.14) and find that the commutator is zero. However, because of the infinite number of occupied states, the bare density operators contain infinity and Eq. (C.14) is in fact the subtraction of two

[1] In a normal ordered product, the destruction operators (with respect to the vacuum $|\,0\,\rangle$) are put on the right and creation operators on the left. For two operators A and B that are linear combinations of creation and destruction operators, normal ordering the operators is equivalent to subtracting the average value in the vacuum,

$$: AB := AB - \langle\, 0\,|\, AB\,|\,0\,\rangle.$$

such infinities. We can only make a change of variable in the normal ordered densities, obtaining

$$\begin{aligned}\left[\rho_r(p), \rho_r^\dagger(p')\right] &= \sum_{k_2} \left(: c^\dagger_{r,k_2-p} c_{r,k_2-p'} : - : c^\dagger_{r,k_2} c_{r,k_2+p-p'} : \right) \\ &+ \sum_{k_2} \left(\langle\, 0 \,|\, c^\dagger_{r,k_2-p} c_{r,k_2-p'} \,|\, 0 \,\rangle - \langle\, 0 \,|\, c^\dagger_{r,k_2} c_{r,k_2+p-p'} \,|\, 0 \,\rangle \right) \\ &= \delta_{p,p'} \sum_{k_2} \left(\langle\, 0 \,|\, c^\dagger_{r,k_2-p} c_{r,k_2-p} \,|\, 0 \,\rangle - \langle\, 0 \,|\, c^\dagger_{r,k_2} c_{r,k_2} \,|\, 0 \,\rangle \right). \end{aligned} \tag{C.15}$$

$\langle\, 0 \,|\, c^\dagger_{r,k} c_{r,k} \,|\, 0 \,\rangle$ is equal to one if the state with momentum k is occupied and zero otherwise. Depending on whether we are considering right- or left-movers, we have

$$\langle\, 0 \,|\, c^\dagger_{r,k} c_{r,k} \,|\, 0 \,\rangle = \theta(-rk) = \begin{cases} 1 & \text{for } rk \leq 0, \\ 0 & \text{for } rk > 0. \end{cases} \tag{C.16}$$

The momentum k_2 is quantized as $k_2 = 2\pi n/L$ for integer n (taking, for instance, periodic boundary conditions), therefore $\sum_{k_2}[\theta(rp - rk_2) - \theta(-rk_2)] = rpL/2\pi$, which leads to

$$\left[\rho_r(p), \rho_{r'}^\dagger(p')\right] = \delta_{r,r'}\delta_{p,p'} \frac{rpL}{2\pi}. \tag{C.17}$$

This fundamental relation, together with $\rho_R(p > 0)|\, 0 \,\rangle = 0$, $\rho_L(p < 0)|\, 0 \,\rangle = 0$, shows that we can define canonical bosonic destruction and creation and operators according to

$$b_p = \left(\frac{2\pi}{L|p|}\right)^{\frac{1}{2}} \sum_r \theta(rp)\rho_r(p), \qquad b_p^\dagger = \left(\frac{2\pi}{L|p|}\right)^{\frac{1}{2}} \sum_r \theta(rp)\rho_r^\dagger(p), \qquad p \neq 0. \tag{C.18}$$

All fermionic operators can be expressed in the boson basis, which is proved to be complete (Giamarchi, 2003). Consider first the Hamiltonian. Using the fermionic anticommutation relations (C.7a) (assuming, for instance, that $p > 0$),

$$\begin{aligned}[b_p, H_0] &= \left(\frac{2\pi}{L|p|}\right)^{\frac{1}{2}} \sum_k v_F k \left[\rho_R(p),\, c^\dagger_{R,k} c_{R,k}\right] \\ &= \left(\frac{2\pi}{L|p|}\right)^{\frac{1}{2}} \sum_{k,k'} v_F k \left[c^\dagger_{R,k'} c_{R,k'+p},\, c^\dagger_{R,k} c_{R,k}\right] \\ &= v_F p \left(\frac{2\pi}{L|p|}\right)^{\frac{1}{2}} \sum_k c^\dagger_{R,k} c_{R,k+p} = v_F p\, b_p. \end{aligned} \tag{C.19}$$

Since the basis generated by the b_p operators is complete, this results defines completely the Hamiltonian in the boson basis. From the bosonic commutation relations it follows that the operator which satisfies Eq. (C.19) is

$$H_0 \simeq \sum_{p\neq 0} v_F |p| b_p^\dagger b_p \tag{C.20}$$

where $\simeq$ means up to factors commuting with b_p. This shows that the energy of the free fermions, that is normally quadratic in fermion operators, can also be expressed by (C.20), which is quartic in fermion operators and quadratic in boson operators. This remarkable property is the main interest of bosonization, because any interaction term, which is quartic

in fermion operators, will also be quadratic in boson operators. Thus solving the interacting problem is not more complicated than obtaining the free Hamiltonian.

The field operators can be determined by the same method. Since

$$\left[\rho_r^\dagger(p), \psi_r(x)\right] = \frac{1}{\sqrt{L}} \sum_{k,k'} \mathrm{e}^{ikx} \left[c_{r,k'}^\dagger c_{r,k'-p}, c_{r,k}\right] = -\mathrm{e}^{ipx}\psi_r(x), \tag{C.21}$$

by using the fact that if $c = [A, B]$ commutes with A and B, $[A, \mathrm{e}^{\lambda B}] = \lambda c\, \mathrm{e}^{\lambda B}$, we get

$$\psi_r(x) = \eta_r \mathrm{e}^{\sum_p (\frac{2\pi}{rpL}) \mathrm{e}^{ipx} \rho_r(p)}. \tag{C.22}$$

Here η_r are fermionic operators such that they commute with the boson operators and $\eta_r^\dagger$ adds one fermion of species r. They are known as Klein factors. In Eq. (C.22), the operator η_r suppresses a charge uniformly, while the factors in the exponential (which conserve the number of fermions of each species) ensure that the charge will be moved, that is, added at some points in space and removed at some others, to ensure that the charge is only destroyed at point x.

Rather than working directly in terms of the boson operators, it is convenient to introduce the real fields

$$\phi(x),\, \theta(x) = \mp(N_R \pm N_L)\frac{\pi x}{L} \mp \frac{i\pi}{L} \sum_{p\neq 0} \frac{1}{p} \mathrm{e}^{-\alpha|p|/2 - ipx} \left(\rho_R^\dagger(p) \pm \rho_L^\dagger(p)\right). \tag{C.23}$$

Using these fields (or the boson operators) the exact expressions of the fermionic field operator and the Hamiltonian are

$$\psi_r(x) = \frac{\eta_r}{\sqrt{2\pi\alpha}} \mathrm{e}^{-ir\pi x/L} \mathrm{e}^{i[\theta(x) - r\phi(x)]}, \tag{C.24}$$

$$H_0 = \sum_{p\neq 0} v_F |p| b_p^\dagger b_p + \frac{\pi v_F}{L}(N_R^2 + N_L^2). \tag{C.25}$$

Here $\alpha \sim 1/\Lambda$ is the regularizing cutoff that prevents the momentum from becoming too large. Strictly speaking, one should take the limit $\alpha \to 0$. Using Eq. (C.18), the fields $\phi(x)$, $\theta(x)$ can be rewritten in terms of the boson operators as

$$\begin{aligned}
\phi(x) &= -(N_R + N_L)\frac{\pi x}{L} - \frac{i\pi}{L} \sum_{p\neq 0} \left(\frac{L|p|}{2\pi}\right)^{\frac{1}{2}} \frac{1}{p} \mathrm{e}^{-\alpha|p|/2 - ipx} (b_p^\dagger + b_{-p}), \\
\theta(x) &= (N_R - N_L)\frac{\pi x}{L} + \frac{i\pi}{L} \sum_{p\neq 0} \left(\frac{L|p|}{2\pi}\right)^{\frac{1}{2}} \frac{1}{|p|} \mathrm{e}^{-\alpha|p|/2 - ipx} (b_p^\dagger - b_{-p}).
\end{aligned} \tag{C.26}$$

Hereafter we shall take the limit $L \to \infty$. In this limit we easily get from Eq. (C.26)

$$[\phi(x), \theta(x')] = \frac{i\pi}{2}\mathrm{sgn}(x' - x), \qquad [\phi(x), \partial_x\theta(x')] = i\pi\delta(x' - x). \tag{C.27}$$

This shows that the conjugate momentum $\Pi(x)$ to the field $\phi(x)$ is $\Pi(x) = \partial_x\theta(x)/\pi$. From Eq. (C.23) we get

$$\partial_x\phi(x) = -\pi\left[\rho_R(x) + \rho_L(x)\right], \qquad \partial_x\theta(x) = \pi\left[\rho_R(x) - \rho_L(x)\right]. \tag{C.28}$$

These can be inverted to write the densities as

$$\rho_R(x) = -\frac{1}{2\pi}\partial_x[\phi(x) - \theta(x)], \qquad \rho_L(x) = -\frac{1}{2\pi}\partial_x[\phi(x) + \theta(x)]. \tag{C.29}$$

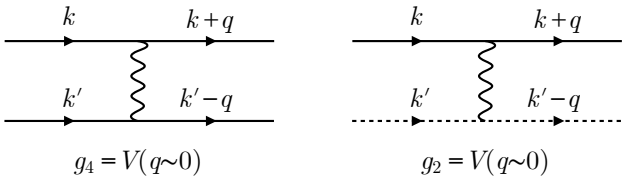


Figure C.2: Diagrams representing g_4 and g_2 processes. A full line represents a right-moving fermion, a dashed line represents a left-moving fermion.

Using Eq. (C.18), the Hamiltonian can be rewritten as $H_0 = 2\pi v_F \int dx\,(\rho_R^2(x) + \rho_L^2(x))$. Using Eq. (C.29) this becomes

$$H_0 = \frac{v_F}{2\pi} \int dx \left[(\partial_x \theta(x))^2 + (\partial_x \phi(x))^2\right]. \tag{C.30}$$

Since we have now a mapping between fermions and bosons, we can look at the effect of interactions. The interaction is of the form $H_{\rm int} = \int dx\, V(x-x')\rho(x)\rho(x')$. Let us consider for instance a contact interaction, that is $V(x-x') = g\delta(x-x')$. For spinless fermions we only have two types of low-energy processes (Fig. C.2):

(i) The 'g_4 process', in which we scatter right-movers (left-movers) producing right-movers (left-movers),

$$H_{\rm int}^{(g_4)} \quad = \quad \frac{g_4}{2} \int dx \;:\rho_R(x)::\rho_R(x): \quad \text{or} \quad \frac{g_4}{2} \int dx \;:\rho_L(x)::\rho_L(x):. \tag{C.31}$$

(ii) The 'g_2 process', in which we scatter a right- and a left-mover producing a right- and a left-mover,

$$H_{\rm int}^{(g_2)} = g_2 \int dx \;:\rho_R(x)::\rho_L(x):. \tag{C.32}$$

The sum of these processes gives

$$H_{\rm int} = H_{\rm int}^{(g_4)} + H_{\rm int}^{(g_2)} = \frac{1}{(2\pi)^2} \int dx \Big[(g_4 - g_2)(\partial_x\theta(x))^2 + (g_4+g_2)(\partial_x\phi(x))^2\Big] \tag{C.33}$$

and the Luttinger liquid Hamiltonian

$$H_{\rm LL} = H_0 + H_{\rm int} = \frac{u}{2\pi} \int dx \left[K(\partial_x\theta(x))^2 + \frac{1}{K}(\partial_x\phi(x))^2\right], \tag{C.34}$$

where u (the renormalized velocity) and K (the dimensionless Luttinger parameter) are given by

$$u = v_F \sqrt{\left(1 + \frac{g_4}{2\pi v_F}\right)^2 - \left(\frac{g_2}{2\pi v_F}\right)^2}, \qquad K = \sqrt{\frac{1 + \frac{g_4}{2\pi v_F} - \frac{g_2}{2\pi v_F}}{1 + \frac{g_4}{2\pi v_F} + \frac{g_2}{2\pi v_F}}} \leq 1. \tag{C.35}$$

Thus we see that the Hamiltonian remains quadratic even in the presence of interactions. The physics of such an interacting system is thus described by free bosonic excitations. As mentioned before, this is one of the main interests of the bosonization method. The net effect of the interactions amounts to a modification of the velocity and of the relative weights of the $(\partial_x\theta)^2$ and $(\partial_x\phi)^2$ terms in the Hamiltonian. Notice that a g_4 process affects only the velocity.

The parameter u/K is related to the compressibility κ_S of the system, which is

$$\kappa_S = -\frac{1}{L}\frac{\partial L}{\partial P} = \frac{1}{\varrho^2}\frac{\partial \varrho}{\partial \mu}, \tag{C.36}$$

where $\varrho = mn$ is the mass density. A uniform chemical potential adds to the Hamiltonian the term

$$-\mu \int dx\, \rho(x), \tag{C.37}$$

where $\rho(x) = \psi^\dagger(x)\psi(x) = \rho_R(x) + \rho_L(x) + \mathrm{e}^{-2ip_F x}\psi_R^\dagger(x)\psi_L(x) + \text{h.c.}$. The rapidly oscillating factors $\mathrm{e}^{\pm 2ip_F x}$ vanish upon integration, thus in Eq. (C.37) we can safely take

$$\rho(x) = \rho_R(x) + \rho_L(x) = -\frac{1}{\pi}\partial_x\phi(x). \tag{C.38}$$

The mass density is then simply

$$\varrho = \frac{m}{L}\int dx\, \langle\rho(x)\rangle = -\frac{m}{\pi}\langle\partial_x\phi(x_0)\rangle, \tag{C.39}$$

since the average is independent of the point x_0. In the bosonic representation, Eq. (C.37) becomes

$$\frac{\mu}{\pi}\int dx\, \partial_x\phi(x). \tag{C.40}$$

One can absorb this term in the Hamiltonian (C.34) by shifting the field ϕ as

$$\phi_{\text{shift}}(x) = \phi(x) + \mu\frac{K}{u}x, \tag{C.41}$$

and therefore the compressibility is

$$\kappa_S = \frac{1}{\varrho^2}\frac{\partial\varrho}{\partial\mu} = \frac{m}{\varrho^2}\frac{K}{u\pi}. \tag{C.42}$$

C.2 Bosonization with band curvature

We now go beyond the Luttinger liquid, and consider the additional term in the Hamiltonian coming from band curvature, i.e. from the quadratic component of the spectrum (C.1),

$$\begin{aligned} H_{\text{bc}} &= \sum_p \frac{p^2}{2m}\left(:c_{R,p}^\dagger c_{R,p}: + :c_{L,p}^\dagger c_{L,p}:\right) \\ &= -\frac{1}{2m}\int dx\left[:\psi_R^\dagger(x)\partial_x^2\psi_R(x): + :\psi_L^\dagger(x)\partial_x^2\psi_L(x):\right]. \end{aligned} \tag{C.43}$$

We derive the bosonized version of a general band curvature term following Pereira et al. (2007). Consider the operator

$$\begin{aligned} \mathcal{P}_r(x,\epsilon) \equiv \psi_r^\dagger\left(x+\frac{\epsilon}{2}\right)\psi_r\left(x-\frac{\epsilon}{2}\right) &= \sum_{j=0}^\infty \frac{1}{j!}\left(\frac{\epsilon}{2}\right)^j \partial_x^j\psi_r^\dagger(x)\sum_{k=0}^\infty\frac{1}{k!}\left(-\frac{\epsilon}{2}\right)^k\partial_x^k\psi_r(x) \\ &= \sum_{n=0}^\infty\left(-\frac{\epsilon}{2}\right)^n\psi_r^\dagger(x)\partial_x^n\psi_r(x)\sum_{m=0}^n\frac{1}{m!(n-m)!} + \cdots \\ &= \sum_{n=0}^\infty\frac{(-1)^n}{n!}\epsilon^n\psi_r^\dagger(x)\partial_x^n\psi_r(x) + \cdots \end{aligned} \tag{C.44}$$

where $\cdots$ is a total derivative. According to Eq. (C.24), $\psi_r(x) \sim (2\pi\epsilon)^{-1/2}\mathrm{e}^{i(\theta(x)-r\phi(x))}$, therefore the operator $\mathcal{P}_r(x,\epsilon)$ is also equal to

$$\mathcal{P}_r(x,\epsilon) = \frac{1}{2\pi\epsilon}\mathrm{e}^{-i[\theta(x+\epsilon/2)-r\phi(x+\epsilon/2)]}\mathrm{e}^{i[\theta(x-\epsilon/2)-r\phi(x-\epsilon/2)]}. \tag{C.45}$$

We can write the product of two exponentials in Eq. (C.45) as a single exponential by using the Baker-Campbell-Hausdorff formula, $\mathrm{e}^{A}\mathrm{e}^{B} = \mathrm{e}^{A+B+[A,B]/2}$. According to Eq. (C.27), $[-i\theta(x+\frac{\epsilon}{2})+ir\phi(x+\frac{\epsilon}{2}),\, i\theta(x-\frac{\epsilon}{2})-ir\phi(x-\frac{\epsilon}{2})] = ri\pi$, hence in our case $e^{[A,B]/2} = \mathrm{e}^{ri\pi/2} = ri$. Introducing the field

$$\varphi_r(x) \equiv -\theta(x) + r\phi(x), \tag{C.46}$$

we can then rewrite Eq. (C.45) as

$$\begin{aligned}
\mathcal{P}_r(x,\epsilon) &= -\frac{r}{2\pi i\epsilon}\mathrm{e}^{i[\varphi_r(x+\epsilon/2)-\varphi_r(x-\epsilon/2)]} \\
&= -\frac{r}{2\pi i\epsilon}\sum_{\ell=0}^{\infty}\frac{i^\ell}{\ell!}\left[2\sum_{j=1,3,\ldots}\left(\frac{\epsilon}{2}\right)^j\frac{\partial_x^j\varphi_r(x)}{j!}\right]^\ell \\
&= -\frac{r}{2\pi i\epsilon}\sum_{\ell=0}^{\infty}\frac{(2i)^\ell}{\ell!}{\sum_{\{m_j\}}}'\frac{\ell!}{\prod_j' m_j!}\left(\frac{\epsilon}{2}\right)^{\sum_j' jm_j}\prod_{j=1,3,\ldots}\left(\frac{\partial_x^j\varphi_r(x)}{j!}\right)^{m_j}
\end{aligned} \tag{C.47}$$

with $j = 1, 3, \ldots$ and $\sum_{j=1,3,\ldots} m_j = \ell$, having used in the last line the multinomial theorem. From (C.44) and the coefficient of the ϵ^n term in Eq. (C.47), we have

$$\psi_r^\dagger(x)\partial_x^n\psi_r(x) = \frac{r(-1)^{n+1}n!}{2^{n+1}2\pi i}{\sum_{\{m_j\}}}'\frac{(2i)^{\sum_j' m_j}}{\prod_j' m_j!}\prod_{j=1,3,\ldots}\left(\frac{\partial_x^j\varphi_r(x)}{j!}\right)^{m_j}, \tag{C.48}$$

where the m_j's obey the constraint $\sum_{j=1,3,\ldots} jm_j = n+1$. In particular, for $n = 2$ the sum contains only two terms, namely $m_1 = 3$, $m_3 = 0$ and $m_1 = 0$, $m_3 = 1$, which give

$$\psi_r^\dagger(x)\partial_x^2\psi_r(x) = \frac{r}{6\pi}(\partial_x\varphi_r(x))^3 - \frac{r}{24\pi}\partial_x^3\varphi_r(x). \tag{C.49}$$

The last term is a total derivative and can be omitted from the Hamiltonian. With Eqs. (C.46) and (C.49), the bosonized version of the Hamiltonian (C.43) is then

$$H_{\mathrm{bc}} = -\frac{1}{6\pi m}\int dx\,\Big[3(\partial_x\theta(x))^2\partial_x\phi(x) + (\partial_x\phi(x))^3\Big]. \tag{C.50}$$

Thus we see that as soon as the band curvature terms are taken into account, an exact diagonalization of the Hamiltonian $H_{\mathrm{LL}} + H_{\mathrm{bc}}$ in terms of the fields θ and ϕ is no longer possible, as the interacting fermion system is mapped to an interacting boson system. The terms in H_{bc} correspond in fact to three-boson interaction vertices.

A very effective way to treat this problem is to move to a basis of fermionic quasiparticles (Rozhkov, 2005; Imambekov et al., 2012). To illustrate the origin of the fermionic quasiparticle representation of the Luttinger model, let us first consider just H_{LL}. Performing the Bogoliubov transformation

$$\tilde\theta(x) = \sqrt{K}\,\theta(x), \qquad \tilde\phi(x) = \frac{1}{\sqrt{K}}\phi(x), \tag{C.51}$$

we can reabsorb the Luttinger parameter K, so that H_{LL} in the new variables $\tilde\theta$ and $\tilde\phi$ is indistinguishable from the bosonized version of the Hamiltonian of free fermions with linear spectrum and Fermi velocity u. The densities of such right- and left-moving quasiparticles are

$$\tilde\rho_{R,L}(x) = -\frac{1}{2\pi}\partial_x(\tilde\phi \mp \tilde\theta) = (1-\delta_+)\rho_{R,L} + \delta_-\rho_{L,R}, \tag{C.52}$$

where the phase shifts δ_+, δ_- are given by

$$\delta_+ = 1 - \frac{1}{2\sqrt{K}} - \frac{\sqrt{K}}{2}, \qquad \delta_- = \frac{1}{2\sqrt{K}} - \frac{\sqrt{K}}{2}. \tag{C.53}$$

We define the right- and left-moving fermionic quasiparticles by applying the bosonization identity (C.24) on the rescaled bosonic fields, obtaining

$$\tilde{\psi}_r(x) \sim \exp\left\{i\left[\tilde{\theta}(x) - r\tilde{\phi}(x)\right]\right\} = \exp\{i\Phi_r(x)\}\psi_r(x), \tag{C.54}$$

where

$$\Phi_{R,L}(x) = \pm 2\pi \int_{-\infty}^{x} dy\ \left[\delta_{\pm}\tilde{\rho}_R(y) + \delta_{\mp}\tilde{\rho}_L(y)\right]. \tag{C.55}$$

In terms of quasiparticles, $H_{\rm LL}$ is then

$$H_{\rm LL} = -iu \int dx \left[:\tilde{\psi}_R^\dagger(x)\partial_x\tilde{\psi}_R(x): - :\tilde{\psi}_L^\dagger(x)\partial_x\tilde{\psi}_L(x): \right]. \tag{C.56}$$

The quadratic spectrum of the physical fermions, whose bosonized version gives $H_{\rm bc}$, leads to additional terms in the fermion quasiparticle Hamiltonian (Rozhkov, 2005, 2006). Most importantly, there is a band curvature term

$$\tilde{H}_{\rm bc} = -\frac{1}{2m^*} \int dx \left[:\tilde{\psi}_R^\dagger(x)\partial_x^2\tilde{\psi}_R(x): + :\tilde{\psi}_L^\dagger(x)\partial_x^2\tilde{\psi}_L(x): \right]. \tag{C.57}$$

The effective mass m^* is related to the Luttinger parameters by the phenomenological expression

$$\frac{1}{m^*} = \frac{u}{K}\frac{\partial}{\partial\mu}\left(u\sqrt{K}\right), \tag{C.58}$$

where μ is the chemical potential (Pereira et al., 2007; Imambekov et al., 2012)[2]. From Eq. (C.42) for the compressibility we then have

$$\frac{\partial n}{\partial\mu} = \frac{K}{u\pi}, \tag{C.59}$$

which allows us to rewrite the effective mass in the form

$$\frac{1}{m^*} = \frac{1}{\pi}\frac{\partial}{\partial n}\left(u\sqrt{K}\right). \tag{C.60}$$

In addition, the quasiparticles are interacting through

$$\tilde{H}_{\rm int} = i\tilde{g} \int dx \left[:\rho_R(x)::\tilde{\psi}_L^\dagger(x)\overleftrightarrow{\partial_x}\tilde{\psi}_L(x): - :\rho_L(x)::\tilde{\psi}_R^\dagger(x)\overleftrightarrow{\partial_x}\tilde{\psi}_R(x): \right], \tag{C.61}$$

where $f\overleftrightarrow{\partial_x}g = f\partial_x g - (\partial_x f)g$. However, since it involves particles on opposite branches, at low energy this additional term is rather harmless. In the scattering between two quasiparticles with momenta $p + p_F$ and $-p_F$, $\tilde{H}_{\rm int}$ in momentum space is proportional to p, therefore for $|p| \ll p_F$ this interaction term produces only a small additional phase shift of order $|p|/p_F \ll 1$. We conclude that even in presence of band curvature of the physical fermions, near the Fermi points the quasi particles are essentially free, with the spectrum

$$\tilde{\epsilon}(p) = u(p - p_F) + \frac{(p - p_F)^2}{2m^*}. \tag{C.62}$$

[2]The fact that Eq. (C.58) coincides with the exact expression of the effective mass of the Lieb-Liniger model, derived from the Bethe Ansatz in Appendix A, is highly non-trivial; see the discussion in the main text, Section 4.3.2.

Appendix D

Ratios of matrix elements

Given the Bethe state $|\{\lambda\}_N\rangle$, let us now consider a different Bethe state $|\{\lambda'\}_N\rangle$, obtained from the former by changing some quantum numbers. We are interested in the ratio

$$\frac{\rho'(0)}{\rho(0)} = \frac{\langle\{\mu\}_N|\hat{\rho}(0)|\{\lambda'\}_N\rangle}{\langle\{\mu\}_N|\hat{\rho}(0)|\{\lambda\}_N\rangle}, \tag{D.1}$$

where it is understood that the Bethe states are normalized. According to Eq. (5.29), in the large c limit this is given by

$$\frac{\rho'(0)}{\rho(0)} = \left(\frac{\mathcal{P}'}{\mathcal{P}}\right)^N \frac{\prod_{j>k}|\lambda'_{jk}|}{\prod_{j,k}(\mu_j-\lambda'_k)} \frac{\prod_{j,k}(\mu_j-\lambda_k)}{\prod_{j>k}|\lambda_{jk}|}. \tag{D.2}$$

The change in rapidities to order $1/L$ can be written as

$$\lambda'_j = \lambda_j + \frac{d_j}{L}, \tag{D.3}$$

where the displacements d_j are determined by taking the difference of the Bethe equations for $(\{I'\}_N, \{\lambda'\}_N)$ and $(\{I\}_N, \{\lambda\}_N)$. In particular, according to Eq. (5.23),

$$d_j = 2\pi(I'_j - I_j) - \frac{2N}{c}\left[\frac{2\pi}{L}(I'_j - I_j) - \frac{P_{\rm ex}}{N}\right] + O(L^{-2}, c^{-2}), \tag{D.4}$$

where $P_{\rm ex} = P_{\{\lambda'\}} - P_{\{\lambda\}}$. Substituting Eq. (D.3) into Eq. (D.2) and expanding up to the order $1/L$, we obtain[1]

$$\frac{\rho'(0)}{\rho(0)} \simeq \left(1+\frac{P_{\rm ex}}{\mathcal{P}}\right)^N \left|1+\frac{1}{L}\sum_{j>k}\frac{d_{jk}}{\lambda_{jk}}\right| \left(\frac{c}{2\mathcal{P}}\sum_{j\notin\{h\}} d_j\right)^{-1}. \tag{D.5}$$

Now let $\{a\}$ be the set of indices j corresponding to the quantum numbers such that $I'_j - I_j \neq 0$, i.e. the quantum numbers by which the states $\{\lambda\}$ and $\{\lambda'\}$ differ (assuming that

[1] We use the fact that $\mathcal{P}'/\mathcal{P} = (1 + P_{\rm ex}/\mathcal{P})$,

$$\frac{\rho'(0)}{\rho(0)} \simeq \left(1+\frac{P_{\rm ex}}{\mathcal{P}}\right)^N \left|1+\frac{1}{L}\sum_{j>k}\frac{d_{jk}}{\lambda_{jk}}\right| \left(1-\frac{1}{L}\sum_{j,k}\frac{d_k}{\mu_j-\lambda_k}\right)^{-1},$$

and that in the large c limit, according to Eq. (5.31),

$$\sum_{j,k}\frac{d_k}{\mu_j-\lambda_k} = \sum_{j\notin\{h\}}\frac{d_j}{\mu_j-\lambda_j} + \sum_{j\in\{h\}}\frac{d_j}{\mu_j-\lambda_j} + \sum_{j\neq k}\frac{d_k}{\mu_j-\lambda_k} = -\frac{cL}{2\mathcal{P}}\sum_{j\notin\{h\}} d_j + O(1).$$

we keep unchanged the indices of the quantum numbers that remain occupied). Exploiting Eq. (D.4) we then obtain[2]

$$\frac{\rho'(0)}{\rho(0)} \simeq \left(1+\frac{P_{\rm ex}}{\mathcal{P}}\right)^N \frac{\mathcal{P}}{\pi c}\left[\sum_{\substack{j\notin\{h\}\\ j\in\{a\}}}(I'_j-I_j)+(N-n)\frac{P_{\rm ex}}{\pi c}\right]^{-1}\left|1+\frac{2\pi}{L}\sum_{\substack{j\neq k\\ j\in\{a\}}}\frac{I'_j-I_j}{\lambda_{jk}}\right|. \quad \text{(D.6)}$$

As an illustration, let us consider the simplest case where the set $\{I'\}$ differs from $\{I\}$ by only one element. Then $I'_j - I_j = \Delta_a \delta_{ja}$ and $P_{\rm ex} = 2\pi\Delta_a/L$. We have to distinguish two cases: (i) $a \in \{h\}$, i.e. the quantum number by which $\{\lambda\}$ and $\{\lambda'\}$ differ belongs to the set of quantum numbers by which $\{\lambda\}$ and $\{\mu\}$ differ; (ii) $a \notin \{h\}$. Eq. (D.6) gives

$$\text{(i)} \qquad \left.\frac{\rho'(0)}{\rho(0)}\right|_{I'_j-I_j=\Delta_a\delta_{ja}} \simeq \left(1+\frac{2\pi\Delta_a}{L\mathcal{P}}\right)^N \frac{L\mathcal{P}}{(N-n)2\pi\Delta_a}\left|1+\frac{2\pi\Delta_a}{L}\sum_{k\neq a}\frac{1}{\lambda_{ak}}\right| \quad \text{(D.7a)}$$

$$\text{(ii)} \qquad \left.\frac{\rho'(0)}{\rho(0)}\right|_{I'_j-I_j=\Delta_a\delta_{ja}} \simeq \left(1+\frac{2\pi\Delta_a}{L\mathcal{P}}\right)^N \frac{\mathcal{P}}{\pi c\Delta_a}\left|1+\frac{2\pi\Delta_a}{L}\sum_{k\neq a}\frac{1}{\lambda_{ak}}\right| \quad \text{(D.7b)}$$

At arbitrary interaction strength, things are more complicated. The ratio (D.1) is

$$\begin{aligned}\frac{\rho'(0)}{\rho(0)} = \frac{\|\{\lambda\}_N\|}{\|\{\lambda'\}_N\|}\frac{\mathcal{P}'}{\mathcal{P}}\prod_j\left(\frac{V_j'^+-V_j'^-}{V_j^+-V_j^-}\right)\\ \times\prod_{j,k}\left[\frac{(\lambda'_{jk}+ic)(\mu_j-\lambda_k)}{(\mu_j-\lambda'_k)(\lambda_{jk}+ic)}\right]\left(\frac{V_p^+-V_p^-}{V_p'^+-V_p'^-}\right)\frac{\det_N(\delta_{jk}+U'_{jk}(\lambda'_p))}{\det_N(\delta_{jk}+U_{jk}(\lambda_p))}.\end{aligned} \quad \text{(D.8)}$$

Expanding rapidity differences up to order $1/L$ as before, we have

$$K'_{jk} = K_{jk}+\frac{1}{L}\delta K_{jk}, \qquad V_j'^{\pm} = V_j^{\pm}-\frac{1}{L}\delta V_j^{\pm}, \qquad \frac{\mu_m-\lambda'_j}{\lambda'_{mj}} = \frac{\mu_m-\lambda_j}{\lambda_{mj}}+\frac{1}{L}\delta B_{mj}, \quad \text{(D.9)}$$

where

$$\delta K_{jk} = -4c\,\frac{\lambda_{jk}d_{jk}}{(\lambda_{jk}^2+c^2)^2}, \quad \text{(D.10)}$$

$$\delta V_j^{\pm} = \sum_m \frac{1}{\lambda_{mj}\pm ic}\left(\frac{\mu_m-\lambda_j\pm ic}{\lambda_{mj}\pm ic}\,d_{mj}+d_j\right)\prod_{l\neq m}\frac{\mu_l-\lambda_j\pm ic}{\lambda_{lj}\pm ic}, \quad \text{(D.11)}$$

$$\delta B_{mj} = -\frac{1}{\lambda_{mj}}\left(\frac{\mu_m-\lambda_j}{\lambda_{mj}}d_{mj}+d_j\right). \quad \text{(D.12)}$$

This gives us

$$U'_{jk}(\lambda'_p) = U_{jk}(\lambda_p)+\frac{1}{L}\delta U_{jk}(\lambda_p), \quad \text{(D.13)}$$

[2] We have

$$\sum_{j\notin\{h\}} d_j = (N-n)\frac{2P_{\rm ex}}{c}+\sum_{\substack{j\notin\{h\}\\ j\in\{a\}}}2\pi(I'_j-I_j)\left(1-\frac{2N}{cL}\right)+O(L^{-2},c^{-2})$$

and therefore

$$\left(\frac{c}{2\mathcal{P}}\sum_{j\notin\{h\}}d_j\right)^{-1} \simeq \frac{\mathcal{P}}{\pi c}\left[\sum_{\substack{j\notin\{h\}\\ j\in\{a\}}}(I'_j-I_j)+(N-n)\frac{P_{\rm ex}}{\pi c}\right]^{-1}.$$

Moreover,

$$\sum_{j>k}\frac{d_j-d_k}{\lambda_{jk}} = 2\pi\left(1-\frac{2N}{cL}\right)\sum_{\substack{j\neq k\\ j\in\{a\}}}\frac{I'_j-I_j}{\lambda_{jk}}.$$

where

$$\delta U_{jk}(\lambda_p) = \frac{i(\mu_j - \lambda_j)}{V_j^+ - V_j^-}\Bigg[\prod_{m\neq j}\left(\frac{\mu_m - \lambda_j}{\lambda_{mj}}\right)(\delta K_{jk} - \delta K_{pk}) + \left(\sum_{m\neq j}\delta B_{mj}\prod_{l\neq m}\frac{\mu_l - \lambda_j}{\lambda_{lj}}\right)(K_{jk} - K_{pk})\Bigg] + \frac{i}{V_j^+ - V_j^-}\left[\frac{\mu_j - \lambda_j}{V_j^+ - V_j^-}(\delta V_j^+ - \delta V_j^-) - d_j\right]\prod_{m\neq j}\left(\frac{\mu_m - \lambda_j}{\lambda_{mj}}\right)(K_{jk} - K_{pk}). \tag{D.14}$$

The most challenging term to compute is the ratio of determinants

$$\frac{\det(\mathbb{1} + U')}{\det(\mathbb{1} + U)} = \det\left(\mathbb{1} + L^{-1}\delta U(\mathbb{1} + U)^{-1}\right). \tag{D.15}$$

In general, the determinant of the sum of two $N \times N$ matrices A and B can be written as

$$\det(A + B) = \sum_{P_L, P_C}\det(A + B)_{P_L P_C} \tag{D.16}$$

(Korepin et al., 1993). Here P_L is a partition of the rows of $A + B$ into two subsets, rows of type A and rows of type B, and P_C is a similar partition of the columns of $A + B$ into columns of type A and columns of type B. The partitions P_L and P_C are independent, except for the condition that the number n_A of rows of type A is equal to the number of columns of type A. The same is true for B, and we denote the number of rows and columns of type B by n_B ($n_A + n_B = N$). Given P_L and P_C, the matrix $(A + B)_{P_L P_C}$ is obtained from $A + B$ as follows. For each matrix element $(A + B)_{jk}$, if row j and column k are both of type A (B) we replace $(A + B)_{jk}$ by A_{jk} (B_{jk}), whereas if row j is of type A and column k is of type B, or vice versa, we replace $(A + B)_{jk}$ by 0.

Now let us consider $\det(A+B)_{P_L P_C}$. We can rearrange the positions of the rows in such a way to move all the A rows to the top and all the B rows to the bottom. The parity of this permutation will be denoted by $[P_L]$. In a similar way we can change the order of the columns, moving all the A columns at the left and all B columns to the right. The parity of this permutation will be denoted by $[P_C]$. After these permutations of rows and columns, $\det(A + B)_{P_L P_C}$ will acquire a factor $(-1)^{[P_L]+[P_C]}$, and the matrix $(A + B)_{P_L P_C}$ will be block diagonal,

$$\begin{pmatrix} A_{P_L P_C} & 0 \\ 0 & B_{P_L P_C} \end{pmatrix}. \tag{D.17}$$

The matrix $A_{P_L P_C}$ has dimension $n_A \times n_A$ and can be obtained from A by removing all B rows and B columns according to the partitions P_L and P_C. Similarly, the matrix $B_{P_L P_C}$ has dimension $n_B \times n_B$ and can be obtained from B by removing all A rows and A columns. The determinant of the matrix (D.17) is equal to the product of $\det A_{P_L P_C}$ and $\det B_{P_L P_C}$, thus we can rewrite Eq. (D.16) in the form

$$\det(A + B) = \sum_{P_L, P_C}(-1)^{[P_L]+[P_C]}\det A_{P_L P_C}\det B_{P_L P_C}. \tag{D.18}$$

We now apply this formula to rewrite the right-hand side of Eq. (D.15). In this case $A = \mathbb{1}$ and $B = L^{-1}M$, where $M = \delta U(\mathbb{1} + U)^{-1}$. We notice that $\det \mathbb{1}_{P_L P_C}$ is either zero (if some columns or rows are zero) or one (if $\mathbb{1}_{P_L P_C}$ is still an identity matrix), thus we have

$$\det(\mathbb{1} + L^{-1}M) = \sum_{P_L, P_C}{}' (-1)^{[P_L]+[P_C]}\frac{1}{L^{n_M}}\det M_{P_L P_C}, \tag{D.19}$$

where the prime indicates that the sum is restricted to partitions such that $\det \mathbb{1}_{P_L P_C} = 1$. At leading order we keep just the terms up to order $1/L$, which corresponds to $n_M = 1$ and $n_{\mathbb{1}} = N - 1$. For these values of n_M and $n_{\mathbb{1}}$, $\det \mathbb{1}_{P_L P_C}$ is zero unless the index of the only M row is equal to the index of the only M column. In this case $[P_L] = [P_C]$, which implies that $(-1)^{[P_L]+[P_C]} = 1$, and $M_{P_L P_C}$ is obtained from M by removing all elements except one along the diagonal. We conclude that

$$\det(\mathbb{1} + L^{-1}M) = 1 + \frac{1}{L}\sum_i M_{ii} + O(1/L^2). \tag{D.20}$$

We have

$$M_{ii} = \sum_j \delta U_{ij}(\mathbb{1} + U)^{-1}_{ji} = \frac{1}{\det(\mathbb{1} + U)}\sum_j (-1)^{i+j}\delta U_{ij} \det(\mathbb{1} + U)^{i,j}, \tag{D.21}$$

where $\det(\mathbb{1} + U)^{i,j}$ is the (i, j) minor of $\mathbb{1} + U$, and therefore

$$\frac{\det(\mathbb{1} + U')}{\det(\mathbb{1} + U)} = 1 + \frac{1}{L\,\det(\mathbb{1} + U)}\sum_{i,j} (-1)^{i+j}\delta U_{ij} \det(\mathbb{1} + U)^{i,j}. \tag{D.22}$$

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