A primer on the study of one dimensional systems, Bethe ansatz and integrability

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Abstract

El objetivo de este trabajo es introducir y familiarizar al lector con las técnicas y fundamentos del estudio de sistemas cuánticos unidimensionales de muchos cuerpos. El análisis de este tipo de sistemas comenzó poco después de la formulación ondulatoria de la mecánica cuántica de Schrödinger (1926), y uno de los pioneros en este área fue Hans Bethe (1931). En su estudio del magnetismo cuántico introdujo su famoso ansatz, el cual constituyó la primera solución completa a un problema de muchos cuerpos en interacción. Su contribución pasaría desapercibida hasta que, en 1963, Lieb y Liniger utilizaran las ideas desarrolladas por Bethe para resolver el problema de N bosones en una dimensión interactuando a través de un potencial tipo delta de Dirac. Esto abrió un nuevo campo de estudio tanto en la física de sistemas cuánticos fuertemente interactuantes como en el estudio de gases cuánticos. La reciente realización experimental de sistemas de este tipo ha provocado el aumento de los esfuerzos técnicos para la obtención de sistemas más variados, así como intensos avances teóricos para proporcionar una descripción más detallada de su dinámica. La importancia de trabajar con sistemas unidimensionales no está solo en la mayor probabilidad de admitir una solución analítica, sino en los nuevos fenómenos que es posible observar en una dimensión, por ejemplo, el proceso de fermionización.

La primera parte del trabajo está dedicada a introducir al lector a la teoría de colisiones, describiendo los elementos básicos necesarios, y haciendo un especial enfásis en el análisis de problemas unidimensionales.

En la siguiente parte del trabajo introduciremos el concepto de integrabilidad. Surge en el estudio de sistemas hamiltonianos clásicos y ha sido un área en el que los avances se han dado, en su mayoría, desde una perspectiva matemática. El método de Bethe y sus generalizaciones nos proveen con técnicas para determinar si un sistema cuántico es integrable o no. El estudio de la integrabilidad en sistemas cuánticos se ha convertido en un área de intensa investigación por las profundas implicaciones que tiene en la física estadística cuántica. Se estudia, cualitativamente, la relación entre el ansatz de Bethe, la integrabilidad del sistema y el proceso de termalización, analizando los mecanismos que permiten, o no, que se den estos procesos.

El segundo paso, una vez introducido el ansatz de Bethe y sus propiedades será usarlo para resolver el modelo de Lieb-Liniger original, tanto para un sistema de N bosones como para el estado fundamental del límite termodinámico. Se utilizarán métodos numéricos para resolver las ecuaciones obtenidas en ambos casos y se discuten los resultados obtenidos. Aquí se obtiene por primera vez un indicio de la relación entre el espectro de sistemas integrables y la distribución de autovalores de matrices aleatorias.

El siguiente objetivo del trabajo será realizar un análisis similar al anterior pero para un sistema en el que tres bosones interactúan a través de un potencial Gaussiano y no a través de una delta de Dirac. Estudios teóricos han obtenido que el sistema sigue siendo integrable para ciertos valores de los parámetros del sistema. En este trabajo obtenemos resultados numéricos que respaldan esto, así como indicios de la ruptura de la integrabilidad para valores medio-altos de la densidad. Estas conclusiones se obtienen a partir del estudio

del espectro de este modelo modificado.

In this work we will be introducing important concepts, techniques and procedures related to the study of one dimensional quantum many body systems. The study of this kind of systems started shortly after Schrödinger's seminal paper (1926) with the work of Hans Bethe (1931). He introduced a novel technique, the Bethe ansatz, that would stay unrecognized until the paradigmatic work of Lieb and Liniger (1963). They were able to solve, without any approximation, a many body quantum system analytically, both for a finite system of bosons as well as in the thermodynamic limit. This opened a new research field that has helped to understand the physics of strongly correlated quantum systems as well as the dynamics of dilute gases. Moreover, the recent experimental realization of systems of this kind has fueled not just intense experimental efforts to reproduce more diverse one dimensional systems but also theoretical ones. The importance of dealing with one dimensional systems is that they exhibit exotic phenomena that are not present in 2D and 3D systems, as we shall see, in the process of fermionization. Moreover, one dimensional systems are more prone to admit an analytical solution, making it easier to understand the dynamics of the system.

Another topic that we will be covering is integrability. Coming from the theory of classical Hamiltonian systems it has been an elusive topic for physicists, and some advances have been done with more mathematically-oriented purposes. Bethe's method and its generalizations (Nested, Thermodynamic, Algebraic, Coordinate Bethe Ansatz) allow us to determine whether a system is integrable or not, because solvability by the ansatz is a clear signature of the system being integrable. The study of integrability in quantum systems has become a topic of great interest because of the deep implications it has in quantum statistical mechanics. The relation between integrability and thermalization is yet under study and the mechanisms that enable one or the other are to be discovered, although some hypothesis, as the Eigenstate thermalization hypothesis, have been proposed.

The main motivation of this work is to serve as an introduction to this vast topic. We begin with a brief review of scattering theory, introducing some useful results and how these can be used to solve one dimensional problems. The next step is an overview of the problem of thermalization: when should one expect a system to thermalize? Which mechanisms are responsible? The link between integrability, thermalization and quantum collisions is established here, qualitatively.

Our following task is to study Bethe's method, initially giving a general description and why it being a solution implies that the system is integrable. Then, we solve the problem of a system of N bosons in a ring with delta interaction [1], both for finite N and in the thermodynamic limit. We study the spectrum of this model and find some relations between the distribution of Bethe's rapidities and the spectrum of random matrices, which serve us to introduce the concept of level repulsion and distribution of level spacing. After some calculations we proceed to study a slightly modified model for a system of three bosons, where we substitute the delta potential by a Gaussian. We repeat the same analysis as for the Lieb-Liniger model and analyze the similarities and differences between them. Theoretical research on this topic has found that the system is integrable for certain regimes. We study the statistics of the energy spectrum for different values of the parameters of the system, comparing the results with the integrable or non integrable expected results.

1. Scattering theory

En este capítulo introduciremos algunas herramientas básicas de la teoría de colisiones cuánticas que necesitaremos para entender correctamente los conceptos que se introduciran más adelante. En concreto, describiremos la condición asintótica para los estados de scattering, el teorema de ortogonalidad y el de completitud asintótica. Justificamos así la definición de la matriz S y presentamos algunas de las propiedades más importantes de esta.

1.0.1 What is scattering?

Many of the groundbreaking quantum experiments of all times rely on what we may call quantum collisions. Quantum scattering experiments allow to probe the properties of quantum/microscopic matter at different length scales, depending on the energy.

Non-relativistic quantum scattering theory provides a formalism in which the outgoing state of a system, after the interaction (for a limited time) with a potential, can be completely characterized in terms of the properties of the incoming state.

1.1 Basics of scattering theory

In this section we describe, at a basic level, some of the general results of scattering theory. They are all intuitive, but the formal proofs are quite involved and out of the scope of our discussion, so we will limit ourselves to stating them and sketching some procedures. Most of the topics covered in this section can be found in [2].

As in the classical case, when the interaction potential is not known, information about it can be extracted by a statistical analysis of the resulting states. A complete theory of quantum scattering has not yet been stated, and some advanced results depend on the particular conditions imposed on the potential. However, most of the important results can be derived for a potential satisfying the following conditions:

- The potential can only depend on r, that is a *spherically-symmetric potential*.
- $V(r) = O(r^{-3-\epsilon})$ as $r \to \infty, \quad \epsilon > 0$.
- $V(r) = O(r^{-3/2+\epsilon})$ as $r \to 0, \quad \epsilon > 0$.
- V(r) is continuous for all r $(r > 0)$ but it can have a finite number of finite discontinuities.

This set of three conditions allows us to state, without further comment, a list of relevant results. But it is quite important to take into account that more complex or singular potentials can also be used (as we shall do).

1.1.1 The asymptotic condition

Let $|\psi\rangle$ represent the actual solution to the scattering problem, that is, $|\psi(t)\rangle$ is the solution of the time-dependent Schrödinger equation. In the limit $t \to \pm\infty$, that is, when far from the interaction region, this state approaches:

$$\lim_{t\to\pm\infty} U(t)\,|\psi(t)\rangle = U_0(t)\,|\psi_{out/in}\rangle\,,$$

where U and U_0 are, respectively, the evolution and free evolution operators, while $|\psi_{out/in}\rangle$ may represent the out or in asymptote. This may be taken as the definition of asymptotes, it is the state that is approached by the actual solution long after/before interacting.

The asymptotic conditions guarantee that for every possible wavepacket there is an actual solution of the scattering problem that satisfies that condition. This allows us to write:

$$|\psi\rangle = \Omega_{\mp}\,|\psi_{out/in}\rangle = \left(\lim_{t\to\pm\infty} U^{\dagger}(t)U_0(t)\right)|\psi_{out/in}\rangle\,. \tag{1.1}$$

The operators $\Omega_{\pm}$ are called the Møller operators, and relate the in- and outgoing asymptotes with the actual state at $t = 0$. This operators are isometric but not unitary. This is because although they preserve the norm, they map every vector in $\mathcal{H}$ to a unique scattering state, but as we shall see shortly, the scattering states are just a subset of the entire Hilbert space.

1.1.2 Orthogonality theorem

Given some potential V that satisfies the former conditions. If we call $\mathcal{B}$ the set of all bound states and $\mathcal{D}_{\pm}$ the sets with, respectively, in and out asymptotes. Then the theorem asserts that:

$$\mathcal{B} \perp \mathcal{D}_{+} \quad \text{and} \quad \mathcal{B} \perp \mathcal{D}_{-}.$$

1.1.3 Asymptotic completeness

Last but not least, we present the asymptotic completeness theorem. This is by far the most difficult result to prove. The interested reader may found the procedure in [3]. This theorem states that:

$$\mathcal{D}_{+} = \mathcal{D}_{-} = \mathcal{D} \perp \mathcal{B}.$$

That is, the set of states with *in-asymptote* is the same as the set of states with *out-asymptote*, and due to the orthogonality theorem, they are all orthogonal to the bound states of the system. In short we would say that our Hilbert space is separable in scattering and bound states. A scattering theory is said to be asymptotically complete if it satisfies this condition.

1.1.4 The S-Matrix

All these results allow us to define the central object of the scattering theory, the scattering operator or the S-matrix:

$$S = \Omega_{-}^{\dagger}\,\Omega_{+}. \tag{1.2}$$

And why is this definition useful? Looking at the foregoing results we can directly write:

$$|\psi_{out}\rangle = \Omega_-^\dagger |\psi\rangle = \Omega_-^\dagger \Omega_+ |\psi_{in}\rangle ,$$

that is to say:

$$|\psi_{out}\rangle = S |\psi_{in}\rangle . \tag{1.3}$$

Now it is clear why this object is important in our description of the scattering process. It allows us to relate the incoming and outgoing asymptotic states, that is, what we send towards the potential and what we measure afterwards. These are essentially free wave packets. The operator S contains all the possible information about the potential and its coupling with the system undergoing the collision. So if we are able to completely characterize the S-matrix, we would obtain all the information that can be extracted from the experiment.

For example, if we wish to calculate the probability of obtaining the asymptotic state $|\theta_{out}\rangle$ given that the incoming asymptotic state is $|\phi_{in}\rangle$ we would proceed as follows. We evolve this asymptotic state into the actual state at $t = 0$, that is, when interacting with the potential:

$$|\phi\rangle = \Omega_+ |\phi_{in}\rangle .$$

Now we calculate the overlap with the actual state that would give rise to the desired asymptotic state when leaving the region of action of the potential. That is, the probability of obtaining the *out-asymptote* $|\theta_{out}\rangle$ given the *in-asymptote* $|\phi_{in}\rangle$ is:

$$P(\phi_{in} \to \theta_{out}) = \langle\theta|\phi\rangle = \langle\theta_{out}|\Omega_-^\dagger\Omega_+|\phi_{in}\rangle\,| = \langle\theta_{out}|S|\phi_{in}\rangle\,|^2. \tag{1.4}$$

In this way the operator S gives us all the information of interest about the problem.

1.1.5 The operator S is unitary

This is a very important property as we shall see in the coming sections. In our current position, the proof of this statement is easy because we have the strong asymptotic completeness theorem. Let us see why the S operator is unitary.

The Møller operators map the states from $\mathcal{H}$ into the scattering states $\mathcal{D}$. Moreover, as they are isometric, they preserve the inner product. Therefore we have the following chain:

$$S : \mathcal{H} \xrightarrow{\Omega_+} \mathcal{D} \xrightarrow{\Omega_-^\dagger} \mathcal{H} .$$

Hence we have an operator that maps $\mathcal{H}$ into $\mathcal{H}$ and preserves the norm, so we conclude that S is unitary. The core of this proof is contained in the asymptotic completeness theorem, that has been taken as a result directly, so this can be regarded as a corollary of the main theorem.

1.1.6 The phase-shift

We will neglect the spin degrees of freedom for simplicity. In a situation with a central potential, as we considered in the conditions at the beginning of section 1.1, we can work in the basis of common eigenstates of $\{H_0, \mathbf{L}^2, L_z\}$, where H_0 is the free Hamiltonian, $\mathbf{L}^2$ is the

modulus squared of the orbital angular momentum and L_z its z-component. Since S is solely determined by the potential it must commute too with these three observables. So we must have:

$$\langle E', l', m'|S|E, l, m\rangle = \delta(E - E')\delta_{ll'}\delta_{mm'}s_l(E). \tag{1.5}$$

The independence of the quantum number m stems from the spherical symmetry of the configuration. Now, since S is a unitary operator, all its eigenvalues must have unit modulus, so we are allowed to write them as:

$$s_l(E) = e^{2i\delta_l(E)}. \tag{1.6}$$

We rewrite the outgoing state in terms of the incoming one:

$$|\psi_{out}\rangle = S\,|\phi_{in}\rangle\,.$$

Projecting onto the basis previously defined we have:

$$\langle E, l, m|\psi_s\rangle = \langle E, l, m|S|\phi_{in}\rangle = \sum_{E',l',m'} \langle E, l, m|S|E', l', m'\rangle\, c_{E',l',m'},$$

where the summation over the energies must be understood as an integral, since we are dealing with the continuous part of the spectrum. Using equations (1.5,1.6) we write:

$$\langle E, l, m|\psi_{out}\rangle = e^{2i\delta_l(E)}c_{E,l,m} = e^{2i\delta_l(E)}\,\langle E, l, m|\phi_{in}\rangle\,. \tag{1.7}$$

That is, each one of the spherical components of the scattered wave just suffers a phase shift with respect to the corresponding component of the incoming state. This is a very important result that will sustain what is to come. Let us see one last important property of this phase shift. We can write it as a function of k as well as a function of E, since they are related by the dispersion relation, so we write:

$$s_l(E) = e^{2i\delta_l(k)} \tag{1.8}$$

Each spherical component picks up a phase shift $\delta_l(k)$ (which must be real in a scattering process) when traversing the potential with momentum k. Then we can also argue that, if once on the other side we reverse time, then we are changing $k \to -k$. As we should recover the original wavepacket, without phase-shift, we must conclude that:

$$\delta_l(-k) = -\delta_l(k)$$

That is, the phase-shift is antisymmetric in k as a result of the time reversal invariance of the system. It is also important to note that, due to the periodicity of the exponential, we phase shift here is defined mod π. We will choose the branch that gives us: $\delta(0) = 0$.

2. One dimensional problems

En este capítulo particularizaremos los conceptos desarrollados en el anterior para el estudio de sistemas unidimensionales. Usando los métodos desarrollados se resuelve el problema del potencial delta, obteniendo el desfasaje correspondiente. A continuación, se trasladan estos resultados a la interacción de dos partículas a través de este potencial y, finalmente, se introduce el problema de colisiones de un número arbitrario de partículas en una dimensión. Aquí se menciona por primera vez el término difractivo de la función de onda y se discuten sus implicaciones.

When coming down to just one dimension we no longer have a well defined orbital angular momentum, but we do have a well defined parity. For a symmetric potential, that is $V(x) = V(-x)$, the S matrix must also commute with the parity operator Π, using the same argument as in the general proof for the spherical symmetry. So again, we conclude that the effect of the potential in each one of the parity-component of the wavefunction is a phase-shift.

Here, instead of using the previous description in terms of wavepackets we will focus on a plane-wave description, because in any case we can reconstruct the scattered wavepacket from the scattered plane-wave. In this terms we can understand the incoming *asymptotic* states as the familiar plane-waves: $e^{\pm ikz}$, the positive sign when it comes from the left and negative one when it comes from the right.

When under the effect of the potential its form will change, but we can relate the *asymptotic* outgoing state with the incoming one through the S-matrix, as we stated in (1.3).

Now, if $\Psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}$ is the wavefunction, where ψ_+ is to be used in the region $x \ll 0$ and ψ_- in $x \gg 0$, we write the scattering process as:

$$\Psi = \begin{pmatrix} e^{ikz} \\ e^{-ikz} \end{pmatrix} + S \begin{pmatrix} e^{-ikz} \\ e^{ikz} \end{pmatrix}. \tag{2.1}$$

In the second term the order is reversed because for $x \gg 0$, the incoming state is the one that comes from $x \ll 0$. Because we are allowing scattering from both directions (it will be useful in future discussions) we have two terms in each region, unlike in (1.3). Since we are working with time-independent states, we would multiply by e^{-iwt} if we want to switch to a time-dependent description. To change the direction of motion of the wavepacket we would change $k \to -k$, this amounts to taking the complex conjugate of the spatial component of the whole state.

The neat result about phase-shifts that we derived applies for the parity eigenvectors. We could consider, for example, the following decomposition:

$$\phi_e = e^{-ik|x|},$$

$$\phi_o = \text{sign}(x) e^{-ik|x|}.$$

Let us see how we can recover well known results from this more general considerations. In the coordinate representation we have some wavefunction $\psi(x)$, that we split into its even and odd components: ψ_e and ψ_o. Now, the asymptotic state can be written as:

$$\Psi = \begin{pmatrix} \psi_e \\ \psi_o \end{pmatrix} = \begin{pmatrix} \phi_e \\ \phi_o \end{pmatrix} + S \begin{pmatrix} \phi_e^* \\ \phi_o^* \end{pmatrix},$$

where the complex conjugation has the same origin as before.

Since the potential is symmetric, the S matrix is diagonal in this representation, and we already conclude that in this basis its effect is purely a phase-shift:

$$\Psi = \begin{pmatrix} e^{-ik|x|} - e^{ik|x|+2i\delta_+} \\ \text{sign}(x)\left(e^{-ik|x|} - e^{ik|x|+2i\delta_-}\right) \end{pmatrix} = \begin{pmatrix} \sin(k|x| + \delta_+) \\ \text{sign}(x)\sin(k|x| + \delta_-) \end{pmatrix}. \tag{2.2}$$

Where we have redefined the phase shift as: $-e^{2i\delta_-(k)}$, introducing a negative sign with respect to (1.8). With this powerful result, let us see how to solve some problems.

2.1 The delta potential

Throughout this whole discussion we have been referring to asymptotic states, but we have not explicitly defined when we will consider that we are in the asymptotic region. We will typically work with finite-ranged potentials, so if $V(x) = 0$ for every $|x| > R$, with R fixed, then $|x| > R$ defines our asymptotic region.

For the case of the delta potential, every x except the origin constitutes the asymptotic region. In order to determine the phase shift we will simply have to use the boundary condition imposed by the delta potential. The stationary Schrödinger equation reads:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + g\delta(x)\psi(x) = E\psi(x). \tag{2.3}$$

Integrating on the interval $[-\epsilon, \epsilon]$ we obtain:

$$-\frac{\hbar^2}{2m}\left(\frac{d\psi}{dx}(\epsilon^+) - \frac{d\psi}{dx}(\epsilon^-)\right) + g\psi(0) = E\int_{-\epsilon}^{\epsilon}\psi(x)dx,$$

taking the limit as $\epsilon \to 0^+$ we derive:

$$\frac{d\psi}{dx}(0+) - \frac{d\psi}{dx}(0-) = \frac{2mg}{\hbar^2}\psi(0) \equiv 2c\psi(0), \quad c = \frac{mg}{\hbar^2} = -\frac{2}{a}, \tag{2.4}$$

where a is the scattering length (therefore c^{-1} gives a length scale). Now it is time to use our asymptotic states. Let us begin by the antisymmetric wavefunction, intuitively one anticipates that this component needs to be unaffected by the potential, because it vanishes at the origin. But let us see how to treat it for the sake of completeness:

- Antisymmetric component

  The wavefunction is $\psi(x) = \phi_o = \text{sign}(x)\sin(k|x| + \delta_-)$, and the boundary condition reads:

  $$k\cos(\delta_-) - k\cos(\delta_-) = 0 = 2c\sin(\delta_-).$$

This way we see that the only solution, if we take $\delta_- \in [0, \pi)$, is $\delta_- = 0$. Hence the potential has no effect, as it does not depend on k.

- Symmetric component

  This time the wavefunction is: $\phi_e(x) = \sin(k|x| + \delta_-)$ and the boundary condition imposes that:

  $$k\cos(\delta_+) + k\cos(\delta_+) = 2c\sin(\delta_+).$$

  Finally, our scattering phase-shift can be obtained as:

  $$\delta_+(k) = \arctan\left(\frac{k}{c}\right).$$

  Here we see how in the limit $c \to \infty$ we recover the result for the antisymmetric wavefunction. We will see some implications of this result in the coming section.

This is a quite useful result that we will use repeated times throughout this work. How can we recover other familiar expressions like the transmission and reflection coefficients? Let us suppose that our particle is coming from $x < 0$ (incoming) and no particle comes from $x > 0$ (outgoing), as usual. The trick is to note that we can write the *incoming* and *outgoing* as:

$$\psi_{incoming/outgoing} = \frac{1}{2}\left(\psi_{even} - \psi_{odd}\right) = \frac{1}{2}\left((1 - \text{sign}(x))e^{-ik|x|} - \frac{e^{2i\delta_+(k)} + \text{sign}(x)e^{2i\delta_-}}{2}e^{ik|x|}\right).$$

Explicitly we have:

$$\begin{pmatrix}\psi_{incoming}\\ \psi_{outgoing}\end{pmatrix} = \begin{pmatrix}e^{ikx} + \frac{1}{2}\left(e^{2i\delta_-(k)} - e^{2i\delta_+}\right)e^{-ikx}\\ -\frac{1}{2}\left(e^{2i\delta_+(k)} + e^{2i\delta_-}\right)e^{ikx}\end{pmatrix},$$

here we clearly identify:

$$t = -\frac{e^{2i\delta_+(k)} + e^{2i\delta_-}}{2},$$
$$r = \frac{e^{2i\delta_-(k)} - e^{2i\delta_+}}{2},$$

and we recover immediately the result:

$$|t|^2 + |r|^2 = 1.$$

This is because the unitarity of S expresses, concisely, and in a general way the property of conservation of probability in scattering processes.

2.2 Two-body problems

We can link these results about the interaction of a particle with a potential with those of the scattering of two particles. Let us use the delta potential as an example, what we may

call *contact interaction*. The Hamiltonian this time reads:

$$H = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2}\right) + g\delta(x_1 - x_2),$$

where both particles have the same mass and their positions are, respectively, x_1, x_2. The natural choice is to change to the center of mass and relative coordinates:

$$x = x_1 - x_2, \qquad X = \frac{x_1 + x_2}{2},$$

for the momenta we have:

$$k_{12} = \frac{k_1 - k_2}{2}, \qquad K = k_1 + k_2.$$

Then we rewrite the Hamiltonian as:

$$H = -\frac{\hbar^2}{2(2m)}\frac{\partial^2}{\partial X^2} - \frac{\hbar^2}{2(m/2)}\frac{\partial^2}{\partial x^2} + g\delta(x) = H_{CM} + H_{rel}.$$

The solution to the center of mass problem is the usual plane wave, so we will focus on the relative problem. We will consider the case of identical particles, so the exchange symmetry is a concern for us. Again, the asymptotic region is everywhere with the exception of $x = 0$, so we can use our expression (2.2).

Let us first consider the **sector** $x > 0$, that is: $x_1 < x_2$. We write the asymptotic wavefunction as:

$$\psi(x) = e^{ikx} - e^{-ikx+2i\delta(k)}.$$

As we are dealing with identical particles, the sector determined by $x < 0$ is obtained by interchanging the particles. So to determine the wavefunction in this new **sector** we use the exchange-symmetry associated with the kind of particles we are considering. For the case of bosons we would use the symmetric wavefunction, and the antisymmetric one for the case of fermions. From the results of the former section we already know that the fermions are unaffected by a *contact interaction*, a conclusion that could also have been achieved by arguments regarding the exclusion principle. A more interesting result is that, as we have argued before, in the limit $c \to \infty$, a system of bosons with contact interaction approaches asymptotically that of free fermions, because all phase shifts vanish.

For the development of future concepts, let us write explicitly the wavefunction for bosons in the sector $x_1 < x_2$ in terms of the coordinates of the particles:

$$\psi(x_1, x_2) = e^{i(k_1+k_2)(x_1+x_2)/2}\left(e^{i(k_1-k_2)(x_1-x_2)/2} - e^{-i(k_1-k_2)(x_1-x_2)/2+2i\delta(k_1-k_2)}\right),$$

performing this product we obtain:

$$\psi(x_1, x_2) = e^{i(k_1x_1+k_2x_2)} - e^{2i\delta(k_{12})}e^{i(k_1x_2+k_2x_1)}. \tag{2.5}$$

We see that the momenta in the second term are permuted, but did we not say that the effect of the potential was just to introduce a phase shift? Well, here we are dealing just with the wavefunction in just one **sector**: $x_1 < x_2$ and more importantly, we are dealing

with identical particles. This last concept has to make us decouple the k_i momenta from the i-th particle. The system has two momenta k_1, k_2, and we are ordering the real line so that $x_1 < x_2$, one particle is at x_1 and the other at x_2. For the sake of visualization, let us consider that $k_1 > 0$ and $k_2 < 0$, so that we can picture the particle at x_1 going with momentum k_1 towards positive values of the coordinate, and the particle at x_2 going with momentum k_2 to the negative ones. After interacting the particle that leaves towards the negative coordinates has to be the one at x_1, because $x_1 < x_2$, and it must do it with momentum k_2. This way we can reasonably understand this separation in sectors and the permutation of momenta.

In the case of two-body collisions this effect of permuting momenta is readily derived from the conservation of momentum and energy, two conditions that fix the two possible values of the momentum. But we have derived it on more general grounds using the S-matrix formalism.

2.3 The general scattering problem in 1D.

Until now we have focused on the problem of a system of two identical particles with a two-body potential. But what happens when we add more and more particles and retain a two body potential? Should we expect the same type of solutions? Certainly not and this is because, apart from two body interactions, the higher the number of particles the larger the probability of the simultaneous interaction of three or more particles is to occur. Let us find an estimate of the probability of these events to occur, as measured by the mean free path. Let $n = N/L$ be the density of particles and λ the characteristic interaction distance.

- Two-body collisions: this is the usual magnitude that is considered. For a uniform density we can take the average interparticle distance as: $l_2 \sim \frac{1}{n}$.

- Three body collisions: now we want to estimate the distance a particle has to travel in order to meet a pair of particles. So we will approximate this value by the product of the average interparticle distance and the probability of two particles being within a distance λ, being this of the order of potential's range. The first term is the aforementioned l_2 mean free path. The second term is obtained by reasoning the following: $n\lambda$ gives us the number of particles within the interacting region, so $\frac{1}{n\lambda}$ must be the probability of having a pair of particles in interaction. We finally write:

$$l_3 \sim \frac{1}{\lambda n^2}.$$

We can follow this reasoning to give an expression for the four-body collision mean free path, but it is of no interest for the moment. We already see the $1/\lambda$ dependence so we see how much less likely to occur the three body collisions are in comparison with the two-body collisions. Of course, this is a semi-classical consideration, but it can give us a intuitive idea of the situation when the De-Broglie wavelength is small compared with l_2.

2.3.1 Scattering with diffraction

Let us briefly analyze the case of $N = 3$ particles taking into these possible three body interactions. Our Hamiltonian can be written as:

$$H = \frac{-\hbar^2}{2m} \sum_{i=1}^{3} \frac{\partial}{\partial x_i} + v\left(x_1, x_2, x_3\right),$$

where $v(x_1, x_2, x_3)$ is a potential that must depend on the relative distances between particles, but not necessarily of just a particular relative distance. When far apart from each other we can think of defining an asymptotic wavefunction, as we did before. Let us take our momenta to be: $k_1 > k_2 > k_3$ and our sector $Q: \ x_1 < x_2 < x_3$. This way we make sure that we have an interaction, classically speaking. The total energy and total momentum are found to be:

$$K = k_1 + k_2 + k_3, \tag{2.6}$$

$$E = \frac{\hbar^2}{2m}\left(k_1^2 + k_2^2 + k_3^2\right). \tag{2.7}$$

In general, for this setup, these are the only restrictions upon the possible values of the momenta. So now let us try to write our asymptotic wavefunction. This has to be a superposition of all the possible ways the particles may scatter from one another. So first we consider the case in which the particles undergo two body scattering. We know that its effect is just a permutation of the momenta with a phase shift. Furthermore we need to include also the possibility of the three particles meeting at the same time, the outgoing momenta from this interaction is the triad of real numbers (k_1', k_2', k_3') that satisfies the conditions (2.6, 2.7). Each of these possible triads will be pondered by the corresponding scattering amplitude of the event. Putting this reasoning on mathematical grounds we write the asymptotic wavefunction as:

$$\psi(x_1, x_2, x_3) = \sum_{\{P\}} \Psi(P) e^{i(k_{P_1}x_1 + k_{P_2}x_2 + k_{P_3}x_3)} + \int\int_{E,K \text{ fixed}} S(k_1', k_2', k_3') e^{i(k_1'x_1 + k_2'x_2 + k_3'x_3)}. \tag{2.8}$$

Here $\{P\}$ represent the set of all possible permutation of $(1, 2, 3)$ and P_i the i-th element of the P permutation. $S(k_1, k_2, k_3)$ is the S-matrix element of the collision of three particles with momenta (k_1, k_2, k_3). We have introduced a new notation for the two body scattering. Following the one presented in [4], these new coefficients are related to our previous results through relations of the form:

$$\frac{\Psi(213)}{\Psi(123)} = -e^{2i\delta(k_{12})}.$$

Of course, we can concatenate collisions by adding their respective phase shifts, we must only take into account that the scattering can only happen between neighbouring particles:

$$\frac{\Psi(312)}{\Psi(123)} = e^{2i\delta(k_{23}) + 2i\delta(k_{13})}.$$

The last term on the expression (2.8) is called the diffractive term and will be responsible for the termalization for the system, as we will discuss on the coming chapters.

3. Thermalization and the Bethe Ansatz

Comenzaremos dando una descripción del fenómeno de la termalización desde un punto de vista clásico. Se discuten las hipótesis sobre las que se sustenta la física estadística y su relación con el proceso de termalización. Se introduce entonces el problema de la termalización en sistemas cuánticos y se establece la relación entre este fenómeno y el concepto de integrabilidad y se discute, cualitativamente, qué permite a un sistema termalizar o no. A continuación se presenta la técnica del ansatz de Bethe, explicando y derivando algunas de sus propiedades básicas. Por último, derivamos las ecuaciones de Bethe (BAE) para un sistema de N partículas con condiciones periódicas de contorno.

Once we have introduced all the tools needed for the study of quantum collisions it is time to analyze the effect of quantum collisions on the evolution of systems. We will begin with a general description of the phenomenon of thermalization, followed by a discussion of its effects in classical macroscopic systems and finally a presentation of the problem in quantum systems.

Whenever we have a macroscopic system in equilibrium we will be able to find a set of parameters $(x_1, ...x_N)$ that allow us to characterize its state. A number of these parameters may be volume, pressure, temperature, energy, chemical potential... This statement, when analyzed carefully carries a very deep concept that will be central to this work.

Let us suppose we have an ensemble of boxes each containing an ideal gas. The boxes are equal in volume and they are all put at the same temperature. In each one of them we are allowed to arrange the particles as we prefer, without any limitations. In classical "particle"-physics this difference in the initial conditions advocate us, certainly, to totally different dynamics. A clear example of the sensitivity on initial conditions is the N-body problem. When doing a statistical analysis a remarkable feature of (almost) all systems is the eventual erasure of all trace of the initial conditions. Said ensemble of boxes will eventually reach the same stationary state, so its density, distribution of velocities, energies and so on will all be identical *on average*. Regardless of the different initial conditions and uniquely determined by this intrinsic factors (energy, volume, temperature) that we took to be equal. This process of reaching a stationary state is called thermalization.

In classical systems the evolution to this equilibrium state is well understood through statistical mechanics, the basic foundations of this field are rather experimental and no definitive theoretical explanation has been given. One of the paths followed to explain it is tipicality [5]: since we are certainly sure, from observation, that macroscopic systems thermalize, then we want to explain why. A very reasonable assumption is the "equal probability a priori". Given some set of macroscopic constraints, such as energy, volume..., the system has equal probability to be found in any of the microstates compatible with said set of constraints. This condition is normally assumed without further comment but it is at the heart of the thermalization process, because the acceptance of the "a priori equal probability" erases all the information of the initial conditions, being just one possible configuration among the

enormous number of compatible microstates in a macroscopic system. This statement allows us to easily define the microcanonical ensemble. Together with the ergodic hypothesis these two conditions are at the very heart of statistical physics, and allow one to derive a great number of results.

But so far, we have not explained how a system thermalizes. We have just explained why a system might thermalize and its consequences. The process of thermalization is of an irreversible character (although most of the microscopic processes are reversible). The a priori equal probability condition already anticipated this when talking about the erasure of initial conditions. The process of thermalization is always achieved through the interaction of the constituents of the system, so there must exist a coupling between them. For example, strictly speaking an ideal gas cannot thermalize and we must assume that collisions between particles are taking place. So it is the coupling between the different parts of a system that allow the microscopic properties to be distributed so that the thermal state is reached.

In the quantum regime the field of statistical physics is also perfectly established and many results can be obtained by using this formalism. Loosely speaking, the previous paragraph, although it uses classical concepts, is approximately what we have in quantum statistical mechanics. The principle of equiprobability is also used and a microcanonical ensemble, from which one can construct much of the theory, can be defined.

The problem that concerns us is that quantum statistical mechanics starts by assuming that the system is in thermal equilibrium, as in the classical case, but: how does a quantum system reach this thermal state? Classically the answer is known, and Boltzmann equation gives account of it, but what are the differences in the quantum regime? In order to thermalize a system must redistribute its microscopic properties according to some macroscopic constraints, so it is therefore natural to think that if all the microscopic properties are conserved we should not expect the system to thermalize.

Let us explain this a bit better, we can use as an example the previous one dimensional system of fermions with contact interaction. As we proved, this type of coupling between fermions has no effect on the dynamics of the system, since by symmetry properties they are not allowed to be in "contact". We conclude that the momentum of each one of the particles is a constant of motion, i.e, $[p_i, H] = 0$. This implies that the system will not be able to accommodate the distribution of the microscopic momenta to be in accordance with the predicted ensemble distribution, so the system cannot thermalize. Following this line of thought one defines what are called integrable systems. In classical mechanics the definition is well established. If a system of N degrees of freedom has N constant of motion in involution, then it is said to be integrable. We can make a canonical transformation to action-angle variables and predict a periodic motion in phase space. In quantum mechanics the definition is more subtle because, for example, any function of the Hamiltonian would be a constant of motion, so a more precise definition must be given. We will leave this definition for what is to come, and retain the idea that in order to thermalize we must not have many constants of motion and that a system has indeed thermalized if the average value of quantities are determined by ensemble averages. We will try to understand the thermalization from a practical point of view, indicating which phenomena would allow or not the final objective of the process.

As we discussed in the classical case, leaving aside systems of spin chains and some other special configurations, the main mean of redistribution of microscopic properties are

collisions. More generally, we speak about scattering. We already know some basics about scattering so we can jump directly to the link between scattering and thermalization.

As we saw previously, scattering requires the existence of a potential between particles. What kind of potential will we consider? Mainly we will work with short-ranged potentials. The definition is deliberately vague but we will exclude Coulomb-like potentials but will allow contact interaction, finite-ranged potentials... Additionally we will make use only of local and pair potentials.

As we did before, let us consider a system of N interacting particles, each one of them initially with energies e_i, and momenta k_i. Since we are dealing with short-ranged or contact potentials we can assume that there must be two-body collisions. That is, we study the interaction between two particles independently from the rest of the system. In the collision the total energy and momenta are conserved, so if we name the interacting particles 1 and 2 then:

$$K = k_1 + k_2,$$

$$E = e_1 + e_2,$$

hence the resulting momenta has to be still the set $\{k_1, k_2\}$. This result was already derived in the former chapter. So we see that two-body collisions do not change the values of the momenta of the system. We conclude therefore that, in one dimension, two-body collisions cannot thermalize a system of particles. Two degrees of freedom with two constants of motion leads to no redistribution.

Logically the next step is to consider three body collisions. Again, we can treat this encounter of three particles independently from the rest of the system, so we can write:

$$K = k_1 + k_2 + k_3,$$

$$E = e_1 + e_2 + e_3.$$

This time these two conditions do not allow us to fix all the possible momenta in the system. This is a result that was already presented to us when we wrote the wave function for the scattering of three particles eq. (2.8). There we saw that a new, somewhat mysterious, diffractive term appeared. This is precisely how the redistribution of momenta takes place, and as we explained before, this must be at the heart of the process of thermalization. Intuitively we can understand it with the following example. Suppose that $k_3 \ggg k_1, k_2$, so that $K \approx k_3$. After the collision k_1 and k_2 may acquire (almost) any possible value, so they are allowed to redistribute themselves according to the expected equilibrium distribution.

3.1 This is an open problem.

Here we must stress the fact that thermalization at the quantum level is not yet fully understood, and several objections to the description we have given here can be risen. For example, our explanation highly relies on the concept that the particles can be somewhat localised so that we can say that at some times they are not within the interaction range and some times they are. In a wave theory, such as quantum mechanics, this kind of description only makes sense in some restricted regimes, for example, in the semiclassical limit or in the low density regime. But the reality is that most systems thermalize, so although our description may not

be completely precise, the system must somewhat make use of the concepts explained before to redistribute its microscopic properties and reach an stationary state. The main objective of this work is not to attempt to give this complete description, but rather to unravel the connection between thermalization and the specific form of the interparticle potential. We will study a well known integrable problem, in which thermalization cannot occur and study the response of the system to perturbations on the specific form of the interparticle potential.

3.2 The Bethe Ansatz

This will be our main tool to discriminate whether a system reaches a thermal state or not. It basically assumes that in a system of particles, the asymptotic state is reached through consecutive two-body collisions (interactions in the general case of spins). As we have seen, two body interaction does not allow redistribution of microproperties, so if the Bethe ansatz turns out to be a solution to our problem, we can assure that the system will not thermalize.

This type of solution was first proposed by Hans Bethe in 1931 [6] when studying the quantum origin of magnetism. It was one of the first exact solution to a many-body problem in quantum physics and revealed profound aspects of the underlying physical processes. The Heisenberg chain model in one dimension consists on an array of spins with nearest-neighbour interactions.

For our purposes we will not describe in detail this model but one based on quantum collisions. Let us consider a ring of size L in which we place N particles, bosons for concreteness. If the particles are at $x_1, x_2, ..., x_N$, respectively, with $x_1 < x_2 ... < x_N$. The Bethe ansatz says that in the sector Q: $x_1 \ll x_2 \ll ... \ll x_N$, the wavefunction may be written as:

$$\psi(x_1, x_2 ..., x_N) = \sum_{\{P\}} (-1)^{\text{sign(P)}} A(P)\, e^{\sum_j^N ik_{P_j} x_j}, \tag{3.1}$$

where $\{P\}$ denotes the set of all possible permutations of the first N integers, P_j denotes the j-th element of said permutations and the $A(P)$ are complex numbers. The coefficients relates as follows: if P and P' are permutations differing only in the exchange of the $j-th$ and $j+1-th$ elements, then:

$$\frac{A(P')}{A(P)} = e^{2i\delta\left(k_{P_j} - k_{P_{j+1}}\right)}, \tag{3.2}$$

here δ_k denotes a phase-shift. In all the other sectors the wavefunction can be obtained by using the statistics of the particles. This form, although intimidating at first, have been encountered before in this work. If we take $N = 2$ we would write:

$$\psi(x_1, x_2) = e^{ik_1 x_1 + ik_2 x_2} - e^{ik_2 x_1 + ik_1 x_2 + \delta_{k_{12}}},$$

where we have factored out one of the phase shifts in order to get full resemblance with the wavefunction presented in eq. (2.5).

What situation is this wavefunction describing? First we waited long enough for the system to reach a stationary state and then label the particles according with the prescription given by our fundamental sector. This wavefunction tell us that this stationary situation has

been reached through a sequence of two body collisions, because no diffractive term appears here. That is, the scattering of one particle off all the other particles can be described sequentially by two body scattering processes, about which we already know that their effect is just picking up a phase shift. In the general case of N particles we must then consider all possible reorganisation (not redistribution) of the *initial* momenta k_i, that is why the permutations are introduced. From the discussions presented before we can understand here that if the Bethe ansatz turns out to be a solution to the system considered, then we can say the system is indeed integrable. Being, for example, N (non-trivial) conserved quantities the momenta (more precisely, rapidities or pseudo-momenta) that appear in the Bethe ansatz.

Keeping in mind the vast possibilities that the Bethe Ansatz has in more advanced topics like QFT we can reformulate the Bethe Ansatz by saying that the scattering matrix S of the entire system factors out into a sequence of two body scattering matrices.

3.2.1 When can the Bethe Ansatz be useful? Fundamental equation

When not dealing with the thermodynamic limit the precise value of N and L are important and will limit the usefulness of the Bethe Ansatz. To be precise what we have presented here is called the asymptotic Bethe Ansatz [4]. When the particles are within the range of the interparticle potential the wavefunction can only be obtained by solving the stationary Schrödinger equation of the full system. We restrict our work to short-ranged potentials so we are able to define some region: $x_1 \ll x_2 ... \ll x_N$, where we can regard the particles to be free. One must here clarify that we are not neglecting the potential between particles, the ansatz takes that into account, the only requirement is that after interacting with each other the particles almost propagates freely until they meet another particle. That is, we have to let the wavefunction reach its asymptotic form within the limits of the box they are contained in. Another important point is that we are usually interested in taking the thermodynamic limit of our system after being able to determine whether the Bethe ansatz is a solution or not for a finite number of particles. This way, we are allowed to choose whatever boundary conditions we prefer, so as usual, periodic boundary conditions (PBC, analogue to a ring) will be our choice.

Our focus will be on the study of a one dimensional system of N indistinguishable particles, confined in a box of length L with periodic boundary conditions. Given this setup we are in a position to derive one of our fundamental equations. Our particles will be ordered so that: $x_1 < x_2 ... < x_N$. If one of the particles, the j-th for example, is moved around the ring, undergoing scattering from all other particles, and again brought to the exact same position then the wavefunction must be left unchanged, since we have periodic boundary conditions. We must therefore consider the phase-shift caused by the displacement of length L and the accumulated effect of all the scattering phase-shifts. Here we must remember that we initially defined our wavefunction for the fundamental sector Q, so the match that we are considering is:

$$\psi(x_1, ..., x_j, ..., x_N) = (\pm 1)^{N-1} \psi(x_1, ..., x_j + L, ..., x_N), \tag{3.3}$$

for bosons and fermions respectively. This is because the LHS is written for the sector $Q : x_1 < ... < x_j < ... < x_N$ and the RHS for $Q' : x_1 < ... < x_{j-1} < x_{j+1} < ... < x_N < x_j + L$,

and we have stated that in order to change sectors we must use the statistics of the particles. We can write the right hand side as:

$$\psi(x_1, ..., x_j + L, ..., x_N) = \sum_{P'} (-1)^{\mathrm{P'}} B(P') e^{-ik_j L} e^{i \sum_j k_{P'_j} x_j},$$

where we use a different a notation for the coefficients since we are now in a different sector. The next step is to identify the factors that precede the exponentials with the same argument. This is key in the derivation. Since in the current situation the particle at x_j has travelled through all the ring, it must have permuted with both every particle at its left and at its right. So even though the ordering may seem the same it have suffered $N-1$ permutations. Therefore we may write:

$$\frac{(-1)^{\mathrm{sign(P')}}}{(-1)^{\mathrm{sign(P)}}} = (-1)^{N-1}. \tag{3.4}$$

Now we have to consider where the phase shifts may appear. Appealing to the former reasoning, after each scattering collision it picks up an exponential factor, so after reaching again the same position we must have:

$$B(P') = B(P) = \prod_{l \neq j}^{N} e^{2i\delta(k_j - k_l)} A(P).$$

Therefore our equation for the periodic boundary conditions turns out to be:

$$1 = (\pm 1)^{N-1} e^{ik_j L} \prod_{l \neq j}^{N} \left(e^{2i\delta(k_j - k_l)} \right),$$

where the minus sign corresponds to bosons and the positive one to fermions. This is because in the second case the $(-1)^{N-1}$ coming from (3.4) combines with the one appearing due to the fermionic statistics in eq. (3.3) giving rise to the identity.

If we take logarithms, for bosons we arrive at:

$$0 = -2i\pi I_j + ik_j L + (N-1)i\pi + \sum_{l \neq j} 2i\delta(k_j - k_l).$$

While for fermions the middle term does not appear:

$$0 = -2i\pi I_j + ik_j L + \sum_{l \neq j} 2i\delta(k_j - k_l).$$

The numbers I_j are a set of integers that arises due to the 2π periodicity of the complex exponential. Let us see that in the expression for bosons we can easily do the following manipulation:

$$ik_j L = 2i\pi \left(I_j - \frac{N-1}{2} \right) - \sum_{l \neq j} 2i\delta(k_j - k_l),$$

we see that if N is odd the number in brackets is an integer while otherwise it is a half-odd-

integer $(1/2, 3/2...)$. So we can write our equation for the two types of particles as:

$$k_j L = 2\pi n_j - 2\sum_{l \neq j} \delta(k_j - k_l) \tag{3.5}$$

Where the n_j are integers except for an even number of bosons, that are half-odd-integers. This is our fundamental equation, let us understand why. The phase shifts may be determined analytically or numerically by means of the boundary conditions imposed by the potentials. So we can obtain them in terms of the momenta k_i. Introducing them in the above equation we have a set of N coupled and (possibly) non-linear equations for the k_i that we can solve numerically. Here we should mention that being able to obtain a solution for this equation does not always imply that the system is integrable. This is only true if the solution to the time independent Schrödinger equation is the Bethe ansatz. This equation is used in approximation methods for many body problems. We must also take into account that we must introduce before-hand the set of n_j values that will take the role of the quantum numbers characterizing a particular state. A lot can be said in general about the different distributions that these quantum numbers may have, but before doing so, let us consider a concrete system, derive the expression for the phase shift, and then discuss about the different properties of the system that we can readily derived.

4. The Lieb-Liniger Model

En este capítulo se describe y resuelve el modelo de Lieb y Liniger para un gas de bosones interactuando a través de un potencial delta en una dimensión. Tras esto se deriva analíticamente la expresión que nos da la distribución de momentos en el límite termodinámico, se resuelve numéricamente y se discuten los resultados. Se realiza un análisis del espectro en ambos regímenes, y se encuentran las primeras trazas de la relación entre integrabilidad y la teoría de matrices aleatorias.

4.1 Solving the Bethe Ansatz Equations (BAE)

It describes a system of N bosons with contact interaction and periodic boundary conditions. Explicitly we would write, in first quantized form, the Hamiltonian of this model as:

$$H = -\sum_{j}^{N} \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x_j^2} + \sum_{i<j}^{N} g\delta(x_i - x_j). \tag{4.1}$$

We left a consideration of the possible experimental realization of this system for the ending part of the text. This model was first solved by Lieb and Liniger [1] and soon after by McGuire [7] using a different method.

We will consider them to be trapped in a ring of circumference L. It is a generalization of the system of two particles studied in the first part of this work. In that simpler model we derived, without having introduced the Bethe Ansatz, an explicit expression for the phase shift due to the scattering process. Our work now will be to analyze if, in the general case, the scattering problem can still be factorized into a series of two-body processes. That is, to study whether the Bethe wavefunction can provide us with a solution of the problem. Before using the ansatz we must take care of the boundary conditions. When studying the scattering of two particles one often writes the problem in the relative coordinate, then the typical boundary condition for the delta potential is precisely written in this relative coordinate:

$$\frac{\partial\psi}{\partial\Delta x_j}(\epsilon) - \frac{\partial\psi}{\partial\Delta x_j}(-\epsilon) = \frac{2mg}{\hbar^2}\psi(\Delta x_j = 0) \equiv 2c\psi(\Delta x_j = 0)\ , \quad j = 1, 2, ..., N-1,$$

where we have written: $\Delta x_j = x_{j+1} - x_j$, $\epsilon \to 0^+$ and $c = \frac{mg}{\hbar^2}$. The second term is defined on another sector, because $x_{j+1} < x_j$. The wavefunction is obtained through symmetry considerations. Since we are working with bosons, the derivative is an antisymmetric function. Therefore the two terms are equal and we are left with:

$$\frac{\partial\psi}{\partial\Delta x_j}(\epsilon) = c\psi(\Delta x_j = 0).$$

Since we want to work with the x_i, we introduce the change of variables to obtain:

$$\left(\frac{\partial\psi}{\partial x_{j+1}} - \frac{\partial\psi}{\partial x_j}\right)_{x_{j+1}=x_j} = c\psi(x_{j+1} = x_j) \quad , \quad j = 1, 2..., N-1. \tag{4.2}$$

Given the wavefunction:

$$\psi(x_1, ...x_N) = \sum_P (-1)^{\text{sign(P)}} A(P) e^{i\sum_n k_{P_n} x_n},$$

plugging it into the above equation we obtain:

$$\sum_P (-1)^{\text{sign(P)}} \left(ik_{P_{j+1}} - ik_{P_j} - c\right) A(P) \exp\left(ik_{P_1}x_1 + ... + i(k_{P_j} + k_{P_{j+1}})x_j + ...ik_{P_N}x_N\right) = 0.$$

All the complex exponential will be different except for the pair of permutations P and P', where P' exchange the $j-th$ and $j+1-th$ elements of P. Therefore, we can equate to 0 the corresponding coefficients:

$$\left(ik_{P_{j+1}} - ik_{P_j} - c\right) A(P) - \left(ik_{P_j} - ik_{P_{j+1}} - c\right) A(P') = 0.$$

From this it follows that:

$$A(P') = -\frac{ik_{P_j} - ik_{P_{j+1}} + c}{ik_{P_j} - ik_{P_{j+1}} - c} A(P) = \frac{1 + i\frac{k_{P_j} - k_{P_{j+1}}}{c}}{1 - i\frac{k_{P_j} - k_{P_{j+1}}}{c}} A(P).$$

We see that the change between coefficients is indeed a phase shift. Since we defined previously for the Bethe Ansatz: $A(P')/A(P) = \exp(2i\delta)$, we can then equate:

$$\exp(2i\delta(k_{P_j} - k_{P_{j+1}})) = \frac{1 + i\frac{k_{P_j} - k_{P_{j+1}}}{c}}{1 - i\frac{k_{P_j} - k_{P_{j+1}}}{c}},$$

isolating the phase shift, we obtain:

$$\delta(k_j - k_{j+1}) = -\frac{i}{2}\log\left(\frac{1 + i\frac{k_j - k_{j+1}}{c}}{1 - i\frac{k_j - k_{j+1}}{c}}\right),$$

where we have chosen $P = 123...N$ for concreteness and changed the notation accordingly. Using the representation of the arctangent: $\arctan(x) = \frac{i}{2}\log([1 - ix]/[1 + ix])$. We can finally write:

$$\delta(k_j - k_{j+1}) = \arctan\left(\frac{k_j - k_{j+1}}{c}\right). \tag{4.3}$$

The first thing that sparks our minds is that this result fully resembles the one we obtained for the scattering of a single particle off a delta potential. This was to be expected, since that problem can be understood as a reduction of the scattering of one particle off another particle through a delta potential expressed in the relative coordinate. This is precisely what we have here. For completeness, the total energy of the system and the total momentum are given by the following expressions:

$$E = \frac{\hbar^2}{2m} \sum_i^N k_i^2, \tag{4.4}$$

$$K = \sum_i^N k_i. \tag{4.5}$$

This can be easily seen by noting that within a sector we have just a combination of plane waves.

As said at the beginning of this section, after deriving the phase shift, we must analyze the conclusions we can draw from our fundamental equation. Introducing this result we have:

$$k_j L = 2\pi n_j - 2\sum_{l\neq j} \arctan\left(\frac{k_j - k_l}{c}\right). \tag{4.6}$$

We can readily verify that, as we stated in the first chapter, the phase shift is antisymmetric in the relative momenta. The first property that we are going to discuss is that all the Bethe momenta must be different to have a nontrivial solution. This proof is easy if we note that the Bethe wavefunction in a particular sector is also antisymmetric in the momenta. Obviously, if two momenta are equal the phase shift is zero. For $N = 2$ we have:

$$\frac{A(21)}{A(12)} = e^{2i\delta} = 1 \rightarrow \psi(x_1, x_2) = e^{ik_1x_1+ik_1x_2} - e^{ik_1x_1+ik_1x_2} = 0.$$

For $N = 3$, taking $k_1 = k_2$ we have:

$$\begin{aligned}\psi = e^{ik_1x_1+ik_1x_2+ik_3x_3} &- e^{ik_1x_1+ik_1x_2+ik_3x_3+\delta_{12}} \\ &+ e^{ik_1x_1+ik_3x_2+ik_1x_3+\delta_{12}+\delta_{13}} - e^{ik_3x_1+ik_1x_2+ik_1x_3+\delta_{12}+\delta_{13}+\delta_{23}} \\ &+ e^{ik_3x_1+ik_1x_2+ik_1x_3+\delta_{12}+\delta_{13}+\delta_{23}+\delta_{21}} - e^{ik_1x_1+ik3x_2+ik_1x_3+\delta_{12}+\delta_{13}+\delta_{23}+\delta_{21}+\delta_{31}},\end{aligned} \tag{4.7}$$

where we have written: $\delta(k_i - k_j) = \delta_{ij}$. Now, we make the simplifying assumption $\delta_{12} = 0$, $\delta_{23} = \delta_{13}$, so:

$$\begin{aligned}\psi = e^{ik_1x_1+ik_1x_2+ik_3x_3} &- e^{ik_1x_1+ik_1x_2+ik_3x_3} \\ &+ e^{ik_1x_1+ik_3x_2+ik_1x_3+\delta_{13}} - e^{ik_3x_1+ik_1x_2+ik_1x_3+\delta_{13}+\delta_{13}} \\ &+ e^{ik_3x_1+ik_1x_2+ik_1x_3+\delta_{13}+\delta_{13}} - e^{ik_1x_1+ik_3x_2+ik_1x_3+\delta_{13}+\delta_{13}+\delta_{31}} = 0.\end{aligned} \tag{4.8}$$

We see that using the antisymmetry property of the phase shift in the last exponential, all terms in the above expression cancel by pairs. This result generalizes to arbitrary N. For every possible element of the set of permutations P, there exists another permutation in which the two elements with equal momentum are interchanged. Therefore this two permutations have different parity so there is a minus sign between their coefficients. Moreover, since the two momenta are equal, the phase shift that would appear due to the permutation is zero, so this way all terms cancel by pairs. This allows us to conclude too that the quantum numbers n_j must all be different given that the momenta must be different, this can be seen if we take the difference between the fundamental equation for two momenta.

It can also be shown [8] that there exists a unique set of k_i for each set of quantum numbers n_j. We will be interested too in the distribution of quantum numbers that gives us the ground state of the system. Qualitatively we can argue the following. Since the n_j arises exclusively due to the periodicity of the exponential they must be independent of the strength of the coupling. In the limit $c \to \infty$ we see that the solution for the momenta is:

$$k_j = \frac{2\pi}{L} n_j, \tag{4.9}$$

so a symmetric distribution of this quantum numbers around zero gives us a state with zero total momentum and also the state with lowest energy, as can be seen by writing:

$$h = \left(\frac{L}{2\pi}\right)^2 \frac{2m}{\hbar^2} E = \sum_i n_i^2 = n_0^2 + n_1^2 + ... + n_N^2.$$

The lower the numbers in the sum, being all of them different, the lower the sum. To extrapolate this result to an arbitrary c we notice the following. As we change the value of c the value of the k_i will vary as a new term appear in expression (4.6). Nonetheless the above configuration of n_j is still valid and since, in the absence of internal degrees of freedom, the ground state is never degenerate the initial ground state cannot cross another energy level, so it remains as the ground state of the system. It is remarkable to note too that this is precisely the momentum distribution of a system of free fermions on a ring. In the limit of $c \to \infty$, called the Tonks-Girardeau gas [9] (experimentally obtained in [10]), the system of bosons suffer what is a called a statistical transmutation and the behaviour resemble that of free fermions. However it should be stressed that the wavefunction is different in both cases, since one of them is symmetric and the other antisymmetric, nonetheless we can write in all sectors: $\psi_{\text{bosons}} = |\psi_{\text{fermions}}|$ for the ground state.

The first remarkable property of the spectrum of this system, that we are going to study deeper in the posterior numerical analysis, is that most levels are doubly degenerate. This is because for every string of quantum numbers $\{n_j\}$ we have the string $\{-n_j\}$ which has the exact same energy. The states with a symmetric distribution of the quantum numbers are non-degenerate because these two sets would be equal. A departure from integrability should imply a breaking of this degeneracy.

4.1.1 The thermodynamic limit of the ground state

We can easily obtain the macroscopic limit of this system using our fundamental equation (4.6). In the limit $N, L \to \infty$ with $n = N/L$ fixed, the momenta will be distributed almost continuously along the real axis so it would useful and legitimate to define a density function of this momenta. Using the fact that $\Delta k_j \approx \Delta k \to 0$, we can write:

$$\sum_{\{k\}} = L \sum_{\{k\}} \Delta k \frac{1}{L\Delta k} = L \int dk \rho(k). \tag{4.10}$$

That is, the integral of $\rho = \lim_{\Delta k \to 0} \frac{1}{L\Delta k}$ over all possible momenta and over the length of the container equals the number of particles considered. So we start by doing this change to

the sums and by getting rid of the subindices:

$$kL = 2\pi n_k - 2L\int_{-Q}^{Q} dk'\rho(k')\delta(k-k'), \qquad (\delta \text{ is the phase shift}).$$

The limits of the integral are chosen using the evenness of the ground state distribution. The value of Q is yet to be determined. Now the trick is to note that, since we are looking for the momentum distribution of the ground state, the quantum numbers $\{n_j\}$ are related to the total number of particles in such a way that:

$$n_k = \sum_{0<k_j<k} 1,$$

This is natural because in the ground state the i-th momentum will occupy the i-th integer starting from $k_0 = 0$. Taking the thermodynamic limit we would write:

$$n_k = L\int_0^k dk'\rho(k').$$

Then our fundamental equation reads:

$$kL = 2\pi L\int_0^k dk'\rho(k') - 2L\int_{-Q}^{Q} dk'\rho(k')\delta(k-k').$$

We can differentiate this expression with respect to k (not k') to obtain:

$$1 = 2\pi\rho(k) - 2\int_{-Q}^{Q} dk'\rho(k')\frac{c}{c^2+(k-k')^2}. \tag{4.11}$$

This is an integral equation for the density of the ground state and Q that must be solved under the restriction imposed by the fixed density of particles:

$$n = \int_{-Q}^{Q}\rho(k)dk. \tag{4.12}$$

Now it is useful to define the following:

$$k = Qx, \quad c = Q\lambda, \quad f(x) = \rho(Qx), \tag{4.13}$$

so that we can rewrite our set of equations as:

$$\frac{1}{2\pi} = f(x) - \frac{\lambda}{\pi}\int_{-1}^{1} dy\frac{f(y)}{\lambda^2+(x-y)^2}, \tag{4.14}$$

$$n = \frac{c}{\lambda}\int_{-1}^{1} f(x)dx \to \lambda = \gamma\int_{-1}^{1} f(x)dx, \tag{4.15}$$

where we have defined the Lieb parameter: $\gamma = c/n$. The important thing to note here is that through this change, if we solve for a fixed λ, the two equations decouple making this solution much easier. We will fix λ instead of a more experimentally tuneable parameter like n just

for mathematical purposes. Once we obtain $f(x)$ for a certain λ using the first equation, we solve for γ using the second equation. Having initially fixed c, which only depends on the nature of the interaction, we can obtain immediately n. So repeating this process for a number of λ we can obtain a relation of the form $\gamma = \gamma(\lambda)$, which can be inverted to obtain $\lambda = \lambda(n)$, the desired result.

The numerical scheme that will be used to solve this integral equation is the Nyström method, which has proven to be very useful. We will first approximate the integral by a finite sum. Given that the integrand is a smooth function of the dummy variable, the Gauss-Legendre quadrature should give us good results. We can write then, using an order-N Gaussian quadrature rule:

$$f(x) = \frac{1}{2\pi} + \frac{\lambda}{\pi} \sum_{j=1}^{N} w_j \frac{f(y_j)}{\lambda^2 + (x - y_j)^2}, \tag{4.16}$$

where the w_j and x_j are the quadrature weights and the roots of the Legendre polynomials, respectively. The next step consists of evaluating both sides precisely at the Gaussian integration points $\{x_i\}$, that is:

$$f(x_i) = \frac{1}{2\pi} + \frac{\lambda}{\pi} \sum_{j=1}^{N} w_j \frac{f(y_j)}{\lambda^2 + (x_i - y_j)^2}. \tag{4.17}$$

In this way we have reduced the integral equation to a set of N coupled linear equations for the set $\{f(x_i)\}$. The simplicity of the method allows us to choose a high value of N without rising too much the computational costs, but the Nyström method provides us with a more elegant method to determine $f(x)$ at other points without using polynomial interpolation formulas. The answer is, once we have solved eq. (4.17), we go back to eq. (4.16) and use it as the interpolation formula.

After having determined the adimensional density at the interpolation points we can obtain the Lieb parameter as:

$$\gamma = \frac{\lambda}{\sum_j w_j f(x_j)}.$$

Moreover, relevant quantities, as the total energy can be computed as:

$$E = L \int_{-Q}^{Q} dk \rho(k) \frac{k^2}{2}. \tag{4.18}$$

Introducing the change of variables above presented we rewrite this integral as:

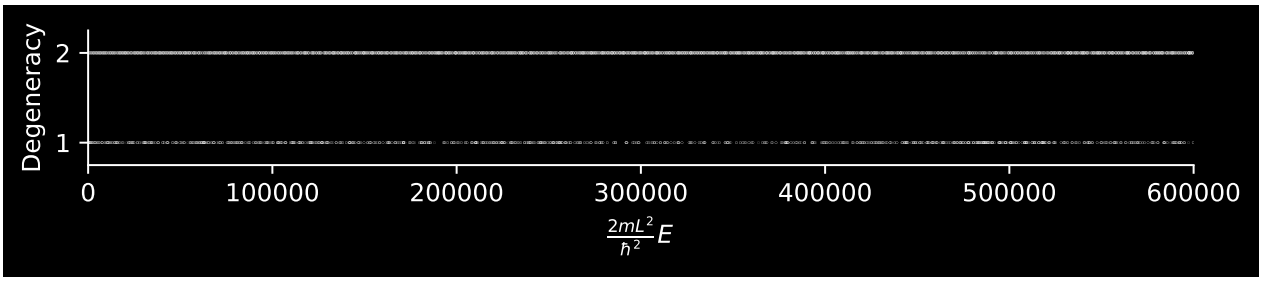
$$E = LQ^3 \int_{-1}^{1} dx f(x) \frac{x^2}{2} = \frac{Ln^3\gamma^3}{\lambda^3} \int_{-1}^{1} dx f(x) \frac{x^2}{2},$$

which allow us to define the useful energy per unit particle:

$$e = \frac{E}{N} = n^2 \frac{\gamma^3}{\lambda^3} \int_{-1}^{1} dx f(x) \frac{x^2}{2}.$$

A beautiful article where also the excitation spectrum is presented is [11].

Figure 4.1: Lieb Liniger model spectrum. On the X-axis we have the adimensional energies, while on the Y-axis we have the degeneracy of each level. Parameter $\gamma = 1/3$.



4.2 Unveiling the spectrum of the model

In this section we will present the asymptotic expression in the limit of both strong and weak coupling, as well as the transition from a finite system to the thermodynamic limit. This way we will be able to appreciate some important features of the spectrum that are deeply rooted in the integrable nature of the system.

4.2.1 Finite system of bosons.

We will be interested in the study of a system of three bosons, but first we will study more generally the spectrum. We rewrite here the LL equations, eq (4.6), that allow us to determine the rapidities of the Bethe ansatz:

$$k_j L = 2\pi n_j - 2\sum_{l\neq j} \arctan\left(\frac{k_j - k_l}{c}\right).$$

We will solve them for a fixed value of the total momentum, in particular, for $K = \sum_i k_i = 0$. We will now show why we can get all the features of the spectrum even with this restriction. The first thing to note is that, since the Bethe ansatz has proven to be a solution and it is just a combination of plane waves, each one of the rapidities is a conserved quantity. Therefore the total momentum K must be also a conserved quantity. The Hamiltonian therefore is block diagonal with respect to each value of the total momentum. We will first note that a given value of the K is determined solely by the sum of the quantum numbers $\{n_j\}$:

$$2\pi \sum_j n_j = L\sum_j k_j + 2\sum_{j,l} \arctan\left(\frac{k_j - k_l}{c}\right) = L\sum_j k_j. \tag{4.19}$$

Where we have summed over j and included the term $l = j$ because it is just 0. Since the arctangent is odd in its argument the double sum cancel by pairs. Therefore speaking of a state with zero total momentum is just saying that $\sum_j n_j = 0$. Therefore, if we want to compare states with different total momentum we just have to shift their quantum numbers: $n'_j = n_j + \alpha$. This way we have:

$$K' = \frac{2\pi}{L}\sum_j n'_j = \frac{2\pi}{L}\sum_j n_j + \beta = K + \beta,$$

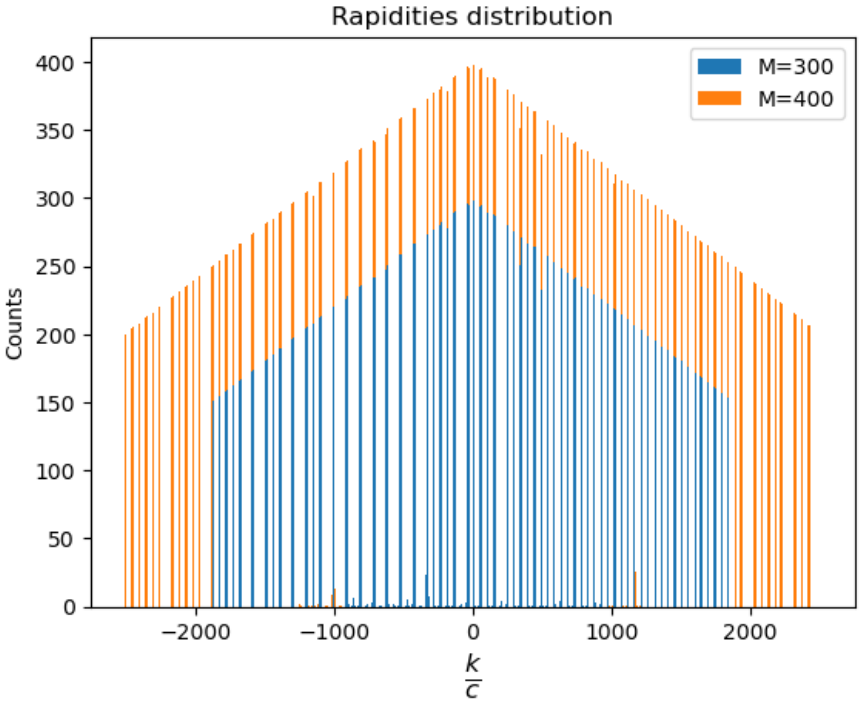


Figure 4.2: Distribution of the Bethe momenta for a system of three particles. The parameters of the system are $N = 3$ and $Lc = 1$.

but more importantly, for K' the Bethe equations take the following form:

$$k'_j L = 2\pi n'_j - 2\sum_l \arctan\left(\frac{k'_j - k'_l}{c}\right).$$

If we just change $n'_j \to n_j$ we immediately see that this equation is satisfied by $k'_j = k_j + \frac{2\pi\alpha}{L}$:

$$2\pi(n_j + \alpha) = L(k_j + \frac{2\pi\alpha}{L}) + 2\sum_l \arctan\left(\frac{k_j - k_l}{c}\right).$$

It is crucial that the phase shift depends just on the difference of momenta. So, if we shift the total momentum by β we have to do the same by shifting each rapidity by $\theta = \frac{2\pi\alpha}{L}$. Therefore, the energy for each set of quantum numbers is, respectively:

$$E = \frac{\hbar^2}{2m}\sum_j k_j^2,$$

$$E' = \frac{\hbar^2}{2m}\sum_j k_j'^2 = \frac{\hbar^2}{2m}\sum_j (k_j + \theta)^2 = E + aK + b.$$

Therefore changing the total momentum just amounts to a constant shift in the energy levels. We can make our statistical analysis for a definite value of the total momentum without restricting the possible results.

In fig. 4.1 we computed the rapidities for every combination of three integers up to $M = 300$ whose sum equals 0. As can be seen, one of the most notable properties of this spectrum (emphasized by the way of plotting) is the great clustering of doubly degenerate

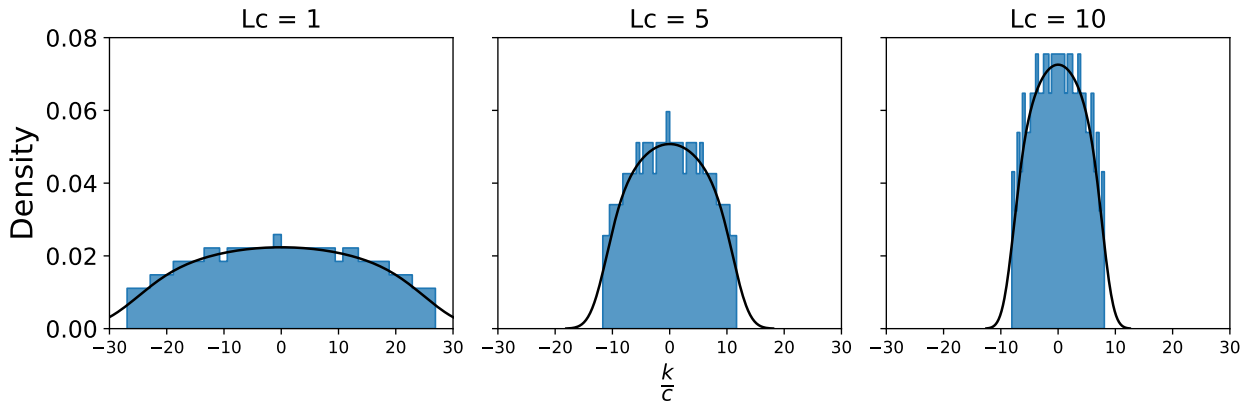


Figure 4.3: Momentum distribution for N= 201 particles and parameters given in each plot.

levels, specially when compared with single ones. It is worth mentioning that we have cut out the higher part of the spectrum in order to avoid the cut-off effect produced by the use of finite M. It is also interesting to analyze the distribution of the momenta that gives rise to said energies, this is presented in fig. 4.2. This has been computed for N=3 and the M cut-off indicated in the figure. We see in the "spiked-shape" that this symmetric distribution shows a clear cluttering around certain values of the momentum. The slope of the histogram has certainly its origin in the cut-off selected. For the shake of comparison the distribution for two different values of M are presented. We see that the two shapes seem to have just suffered a scaling transformation. It is remarkable to note that although the values of the quantum number are higher for $M = 400$, it still introduces a lot of new low lying momentum values.

In prevision of what we will find when analyzing numerically the properties of the ground state in the thermodynamic limit, we will present here also the distribution of momenta but for a higher number of particles and varying the defining parameter of the system γ, fig. 4.3. It is interesting to analyze the underlying reason for the shrinking of the distribution when the density gets smaller. This can be understood easily just by noting that the ground state in a system of non-interacting bosons would have them all with zero momentum. By taking the $\gamma \gg 1$ limit with such a short-ranged coupling we are doing nothing but reducing the effect of the interparticle potential, which can be understood as taking $c \to \infty$, the particle cannot tunnel through each other, or $L \to \infty$, they probability of a collision goes to zero.

We already explained what we should expect in the limit $\gamma \to \infty$. What about the exact opposite limit? The result is quite surprising and will open us the door to the underlying connection of integrability and random matrices. The momentum distribution approaches asymptotically (only exact in the thermodynamic limit at vanishing strength) the Wigner's semicircular distribution given by:

$$P(x; R) = \frac{2}{\pi R^2}\sqrt{R^2 - x^2}. \tag{4.20}$$

The comparison can be more clearly seen in the figure fig. 4.4, where for the radius R we have chosen a somewhat larger value than the largest k. KDE stands for Kernel Density Estimation and is just a fit using a Gaussian kernel in order to approximate the underlying smooth probability distribution that gives rise to the observed binning.

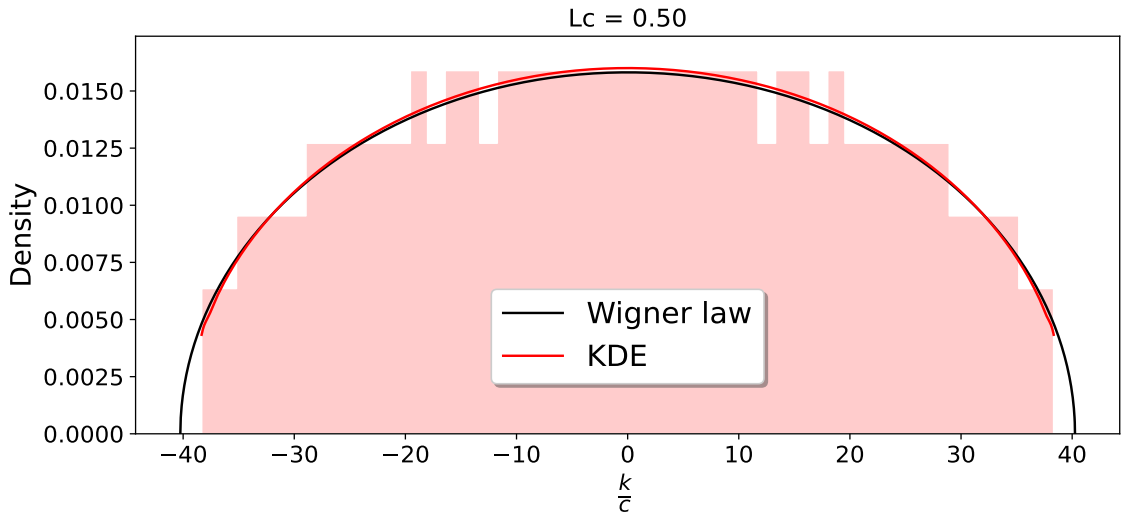


Figure 4.4: Comparison between the Wigner semicircle law and the momentum distribution.

This relation was absolutely not expected and derivations can be found in [11]. This distribution is also the one followed by the eigenvalues of random symmetric matrices as their dimension approaches infinity. This way we can start the following links: an integrable model has uncorrelated levels that in certain regimes can be related to properties of random matrices.

Following this first hint about the relation of the spectra of the Lieb-Liniger model and the one of symmetric random matrices one may study also the nearest neighbour spacing of eigenvalues (NNS), which we present in fig. 4.5. For a certain class of random matrices one finds that the level spacing follows either the Gaussian Orthogonal Ensemble (GOE), Gaussian Unitary Ensemble (GUE) or the Gaussian Symplectic Ensemble (GSE). Research on this topic [12] has found that non-integrable systems often follow one these distributions.

The study of the NNS gives us a clear view of the correlation between energy levels. For example, in an integrable model, as the levels are identified by the set of conserved quantities they are completely uncorrelated, while for a non integrable model, there appear couplings between energy levels, leading to repulsion among them. Therefore, in the first case is reasonable to expect clustering of levels, but not in the second case. This is represented in the strong slope near the zero spacing limit. How may we derive the expression for this distribution? Let us present an heuristic derivation given initially by Wigner that can be found in [12]. Given an energy level at E and the distance to the following level S. The probability that there is a level in $(E+S, E+S+dS)$ can be written as:

$$P(S)dS = P(1 \in dS | 0 \notin S) P(0 \in S),$$

where $P(n \in A | m \in B)$ is the conditional probability that there are n levels within the A interval given that there m within B. $P(n \in A)$ is the probability of n levels being in A. We see that we have just applied Bayes' theorem. The second term is the probability of the level spacing being greater than S, therefore it is just $\int_S^\infty P(x)dx$. For the first term we make the following educated guess:

$$P(1 \in dS | 0 \notin S) = r_{10}(S)dS.$$

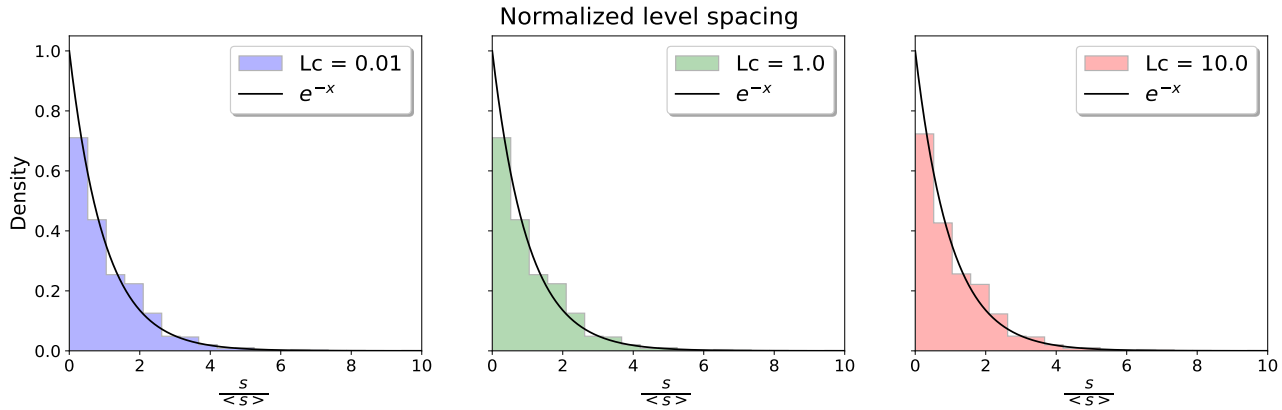


Figure 4.5: Normalized level spacing for various strength of the Lieb Liniger model. We have taken just unique levels, that is, degeneracy has been removed up to numerical precision.

That is, the probability is a function of S and proportional to the interval dS, seems reasonable. Therefore we have:

$$P(S) = r_{10}(S) \int_S^\infty P(x)dx.$$

Differentiating this expression and using the starting definition to get rid of the integral we arrive at:

$$P'(S) = -r_{10}(S)P(S) + P(S)\frac{r'_{10}(S)}{r_{10}}.$$

Which can be integrated between 0 and S to give:

$$P(S) = Cr_{10}(S) \exp\left(-\int_0^S r_{10}(x)dx\right), \tag{4.21}$$

with C a numerical constant.

In this expression we can already observe some typical properties of almost all spectra. The spacing between levels has an exponential decay, as it is rare to find two subsequent levels far apart from each other. The role of the r_{10} is just a measure of the level repulsion. For suitable forms of this function we will be just shifting the maximum value of the probability distribution from 0 ($r_{10} = \text{constant}$) to a higher value. For example:

$$r_{10} = \text{constant} \to P(S) = \exp(-S) \qquad \text{Poisson decay.} \tag{4.22}$$

Which has its maximum at $S = 0$. This would be the case if we had the levels randomly distributed and therefore uncorrelated, as it is the case for integrable systems, since each levels is characterized by a set of N quantities. If we have linear repulsion of levels the distribution is:

$$r_{10} = aS \to P(S) = bS \exp\left(-\alpha S^2\right) \qquad \text{Wigner decay,} \tag{4.23}$$

which has its maximum value at $S = 1/\sqrt{2b}$. This way we can understand easier where the name level repulsion comes from. Nonetheless, it should be stressed that this is just an heuristic explanation and may not fit well all Hamiltonians. In fig. 4.5 we see how the Poisson decay clearly fits the empirical distribution for the normalized level spacing [1].

[1] When we deal with normalized spacing we have just, after removing the degeneracy, divided the spacing

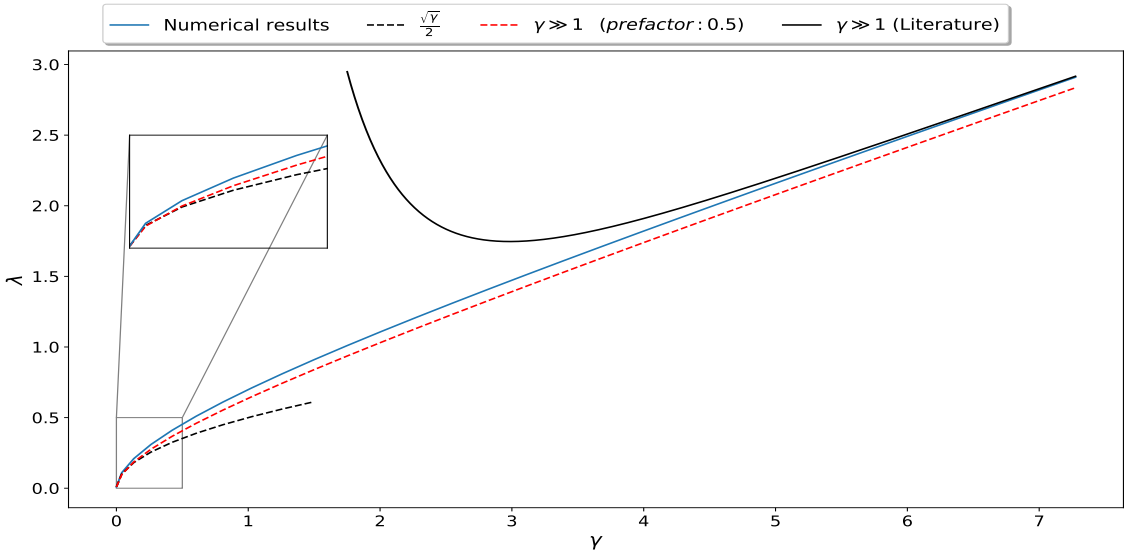


Figure 4.6: Numerical results and analytical approximations for the functional relation $\lambda = \lambda(\gamma)$.

4.2.2 Results in the thermodynamic limit

In this section we will numerically solve the equations presented in Sec. 1.1 and compare with analytical approximations for, both the limit of strong and weak coupling strength. The solution method is the one presented in the corresponding section, namely, the Nyström method. Obtaining precise expressions in the weak coupling limit is a specially difficult task because of the divergence of the integral kernel in eq. (4.14). Nonetheless, accurate asymptotic expressions have been obtained and can be found, for example, in [13]. There, it can be found how one has to deal with the renormalization of divergent series to obtain the ultimate results.

The expressions that we will be using to compare are now presented. In the strong coupling limit the momenta density distribution is approximated by:

$$f(x) \overset{\lambda\to\infty}{\approx} \frac{1}{2\pi} + \frac{1}{\pi^2\lambda} + \frac{2}{\pi^3\lambda^2} + \frac{12-\pi^2}{3\pi^4\lambda^3} + \frac{8-2\pi^2}{\pi^5\lambda^4} - x^2\left(\frac{1}{\pi^2\lambda^3} + \frac{2}{\pi^3\lambda^4}\right). \tag{4.24}$$

For the weak coupling limit it is found:

$$f(x) \overset{\lambda\to 0}{\approx} \frac{\sqrt{1-x^2}}{2\pi\lambda} + \frac{1}{4\pi^2\sqrt{1-x^2}}\left[x\log\left(\frac{1-x}{1+x}\right) + \log\left(\frac{16\pi}{\lambda}\right) + 1\right]. \tag{4.25}$$

We will be interested too in the relation $\lambda = \lambda(\gamma)$. For the strong coupling regime we can find in the literature [11] the following expression:

$$\lambda = \frac{\gamma}{\pi} + \frac{2}{\pi} - \frac{4\pi}{3\gamma^2} + \frac{16\pi}{(3\gamma^3)}.$$

Which we represent in fig. 4.6. For the weak coupling limit no expression could be found,

by its mean value.

nonetheless we tried to obtain it by using equation (4.15), inserting the weak coupling expression for $f(x)$ and solving for the desired relation. Only if we retain just the first order an analytical expression can be found, and it is: $\lambda = \sqrt{\gamma}/2$. It can be seen in the figure that the fit is only good for extremely low values of γ. However, when trying to apply the same procedure to obtain the relation for the strong coupling regime the following expression was found:

$$\lambda = 0.5 \left(\frac{\gamma}{\pi} + \sqrt{\frac{\gamma^2}{\pi^2} + \frac{8\gamma}{\pi^2}} \right).$$

We see that we obtain a better fit for **low** values of γ in comparison, although we are using the strong coupling approximation.

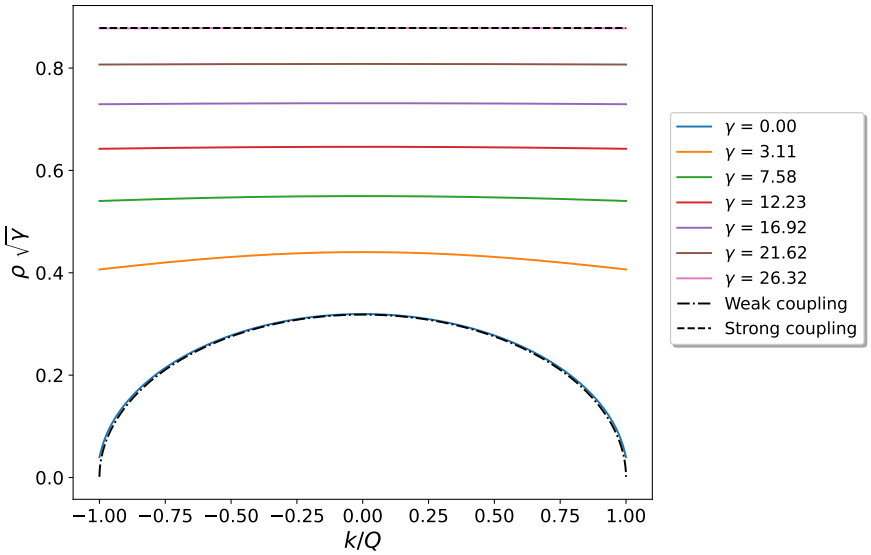


Figure 4.7: Ground state density distribution for the momenta of the system. The broken lines represent the approximation for both the weak and strong coupling limit.

In fig. 4.7 can be clearly seen the transition between both limiting regimes. The semicircular distribution, characterizing its integrable nature, and the flat profile as the fermionization process dictate. The scale is chosen as to be able the appreciate more clearly the transition between both regimes.

5. Tuning the potential: Departure from integrability?

En esta última sección se utiliza el código desarrollado por uno de los tutores para determinar las energías de un sistema de 3 bosones con interacción Gaussiana. Este modelo, en el límite de Gaussiana muy estrecha o muy bajas densidades, se aproxima asintóticamente al de Lieb-Liniger. Se estudia el espectro de este sistema en distintos regímenes y se compara con las predicciones teóricas presentadas en [14] así como con los resultados obtenidos para el modelo de Lieb-Liniger.

Disclaimer: The code for the numerical computation of the energies for an arbitrary potential has been entirely developed by Dr. Manuel Valiente Cifuentes.

The code is able to obtain the energies of a system of three particles (both distinguishable and indistinguishable) given the matrix elements of the potential in the momentum space. It decomposes the wavefunction using a truncated basis of plane waves and solves the resulting matrix equation directly in this space in order to obtain the energy eigenvalues. Since we are not interested in the reconstruction of the wavefunction there is no need to apply any Fourier transform, and using the symmetry properties of a system of bosons lighten the calculations noticeably.

An advantage of working with a delta potential is that it can be computed as the limit of an exponential, making much easier the computation of the matrix element in momentum space, as we present shortly. First, we will approximate the delta function by:

$$\delta(x) \approx \frac{1}{\epsilon\sqrt{\pi}} e^{-\frac{x^2}{\epsilon^2}} \quad , \ \epsilon \to 0^+. \tag{5.1}$$

For the computation of the matrix element we need the closure relation in the space representation: $|x\rangle \langle x| = \int_{-\infty}^{\infty} dx$. Now we proceed as usual:

$$\langle k'|\delta(X)|k\rangle = \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' \, \langle k'|x'\rangle \, \langle x'|\frac{1}{\sqrt{\pi}\epsilon} e^{-\frac{X^2}{\epsilon^2}}|x\rangle \, \langle x|k\rangle \, .$$

Writing explicitly the inner products in the expression:

$$\langle k'|\delta(X)|k\rangle = \frac{1}{\sqrt{\pi}\epsilon} \int_{-\infty}^{\infty} dx \int_{-\infty}^{\infty} dx' e^{-ik'x'+ikx} \delta(x-x') e^{-\frac{x^2}{\epsilon^2}}.$$

From which it is inmediate to derive:

$$\langle k'|\delta(X)|k\rangle = \frac{1}{\sqrt{\pi}\epsilon} \int_{-\infty}^{\infty} dx e^{i(k-k')x - \frac{x^2}{\epsilon^2}} = \exp\left(-\frac{\epsilon^2(k-k')^2}{4}\right).$$

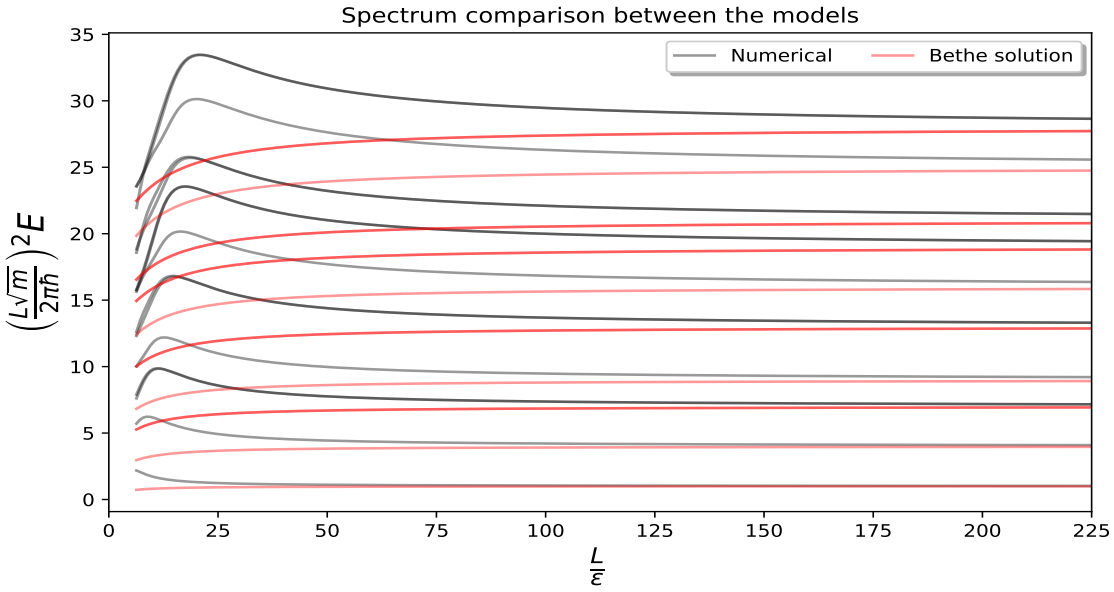


Figure 5.1: For the MLL model the parameters have been chosen so that : $\frac{\epsilon^2}{4} \cdot c^2 = 22.5$. The solution for the LL model are plotted in red.

So for the numerical purposes we will be considering a matrix element of the form:

$$\langle k'|V(X)|k\rangle = c \exp\left(-\frac{\epsilon^2(k-k')^2}{4}\right). \tag{5.2}$$

So we are able to tune both the strength of the potential and its width, we will refer to the system defined by this potential as MLL (Modified Lieb-Liniger). In fig. 5.2 we can see a comparison between the ground state energy of the Lieb Liniger model and the MLL, with parameters given in the figure in accordance to the expression presented in eq. (5.2).

Precisely in fig. 5.2 we see see the transition between the high and low density regimes. We can get a proper sense of how fast the low density regime makes both energies converge, as the narrow exponential potential is no appreciably different from a point-like interaction when the distances are large, while the higher the density the more noticeable the difference between the two models.

We are also interested in the excitation spectrum of this model. We can get a full view of the spectra of both models in fig. 5.1. There are a couple of features that are worth mentioning. First, we see that as in fig. 5.2 the ground state for the LL model gives the minimum energy at every length of the ring, this appear to hold for every value of the coupling strength. If we want to pair the corresponding LL-energy to each MLL-solution we have to examine the large L limit. By distinguishing degeneracy by the opacity of the line we see that indeed the single and doubly degenerate levels of the LL model are approached from above by the corresponding single and doubly degenerate energies of the MLL model. We have to be careful when speaking of the degeneracy of these numerical solutions because it is only exact in the $L \to \infty$ limit. And even more interesting situation can be found when we get closer to the high density region.

First, we notice that at the very beginning of the plot every MLL energy crosses LL levels, but this only occurs between non paired (levels that do not converge in the low density limit) set of levels. Nonetheless a much steeper descent can be observed in the MLL levels as L gets

smaller so it remains to study whether they indeed intersect the corresponding LL level in this limit. We are not in a position to study this at the moment because one of the conditions that must be imposed in the tuned potential is that it must fully contained within the ring's length. With the set of chosen parameters the minimum length that we can reasonably use is around $L/\epsilon \approx 4$. If we change the parameters to make the potential narrower, the possible crossing will move to even lower values of L, so we would end up in the same situation.

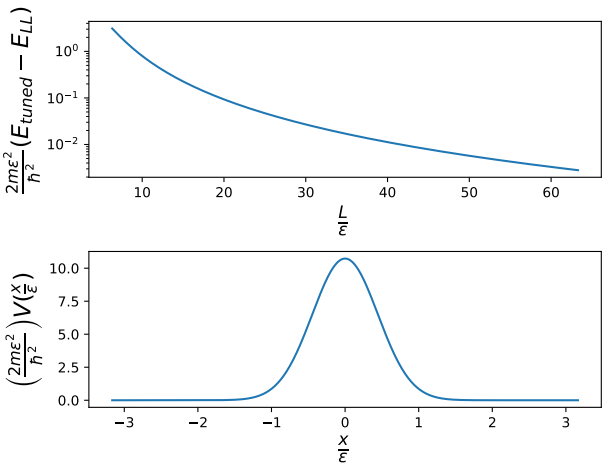


Figure 5.2: On the upper panel the difference between the ground state energy of the MLL model and the Lieb-Liniger one are represented. On the lower one we have plotted the potential over the smallest ring's length, for comparison. Parameters: $\frac{\epsilon^2}{4} \cdot c^2 = 22.5$.

Before presenting the structure of the repulsion of a set of levels, it is worth mentioning the peak that every MLL present between $L/\epsilon \approx 10$ and $L/\epsilon \approx 20$, being this value larger when analyzing higher excited states. How could we qualitatively understand this maxima on the quantity L^2E? When the box gets narrower our description of the system in terms of a scattering theory starts to lose sense. Classically speaking the particles no longer interact for a limited time and then move freely, in this case they start to probe the details of the potential, as they are not allowed to get away from it. The continuous presence of the interparticle potential is what causes this extreme on the quantity L^2E (one should remember that E is always decreasing with L, with no extremes). Moreover, we should note that this bump takes place at larger values of L for higher excited states. This is also reasonable since fast moving wavepackets are more frequently under the range of action of the other potentials, making this phenomenon appear sooner.

Much more interesting is that, in this bigger picture, we can appreciate certainly the level repulsion for high values of the density. This phenomenon appears not just between "degenerate" MLL levels but also between those corresponding to different LL levels. In fig. 5.3 we compute with finer detail the region of interest. The general theory that explains the structure of the repulsion is condensed in the Von-Neumann-Wigner theorem. Qualitatively we can interpret the following: the MLL model can be understood as a perturbation of the LL model, specially in the limit of the width of the Gaussian approaching zero. We can write the following relation:

$$H = H_{LL} + W_{MLL} = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} + \begin{pmatrix} 0 & W \\ W^* & 0 \end{pmatrix}.$$

Where we restrict ourselves to the subspace spanned by the eigenvectors associated with the eigenvalues under study. The perturbation couples both levels through the non-diagonal matrix elements (diagonal elements has been ignored on purpose). This is reflected in the spectrum of the resulting matrix which now has as eigenvalues:

$$E_+ = \frac{E_1 + E_2}{2} + 0.5\sqrt{(E_1 - E_2)^2 + 4|W|^2},$$

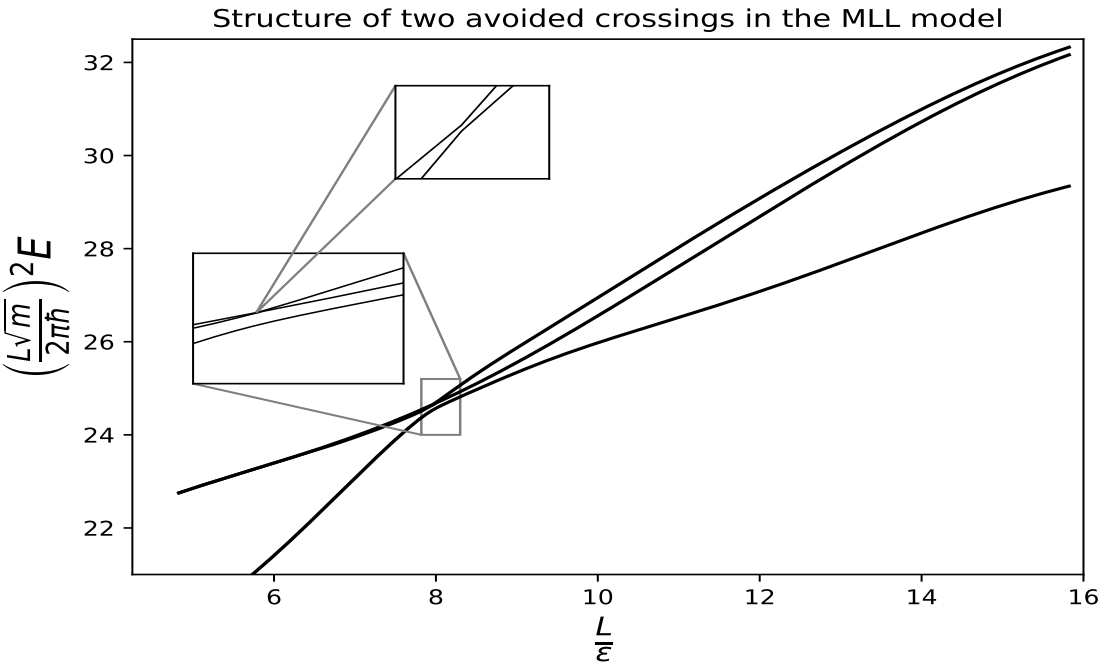


Figure 5.3: We plot a smaller region of fig. 5.1 where level repulsion appears. We see that it is present at two different scales of energies and lengths.

$$E_- = \frac{E_1 + E_2}{2} - 0.5\sqrt{(E_1 - E_2)^2 + 4|W|^2}.$$

These results explain both the separation of initially degenerate eigenvalues, $E_1 = E_2$, as well as the repulsion between non degenerate eigenvalues, $E_1 \neq E_2$. As the coupling weakens, in this case due to the variation of density, we recover the initial eigenvalues, situation that we have in the low density limit.

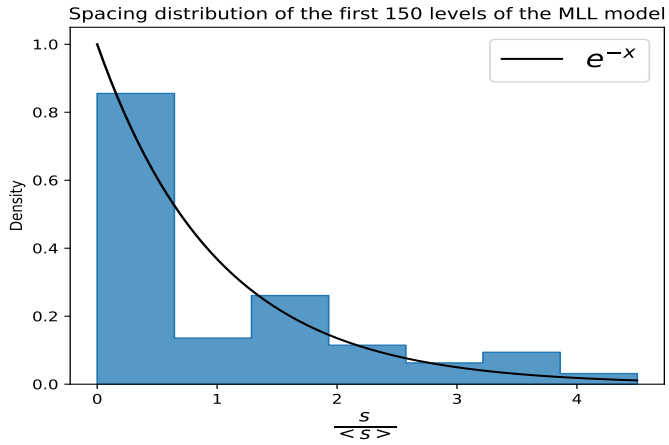


Figure 5.4: Normalized spacing statistics of the MLL model for the first 150 levels. The parameters are: $\frac{\epsilon^2}{4} \cdot c^2 = 22.5$ and $Lc = 600.0$. The Poisson distribution has been plotted for comparison.

It should be mentioned here that, given the width of the potential used and length of the ring, as we mentioned before, the particles have no room to propagate freely but they are always under the influence of the interparticle potential. This is the reason why the coupling between levels is stronger in the high density regime. As it is also seen in fig. 5.1, no repulsion is observed when both models converge.

The last topic that we would like to review of the MLL model is the statistics of the level spacing distribution. Does the perturbation in the potential have an appreciable effect on this distribution? Does it remain Poissonian? Does the spacing follow one of the GOE, GSE or GUE distributions?

Research on this topic [14] has proven that for small values of ϵ the MLL remains integrable

(given that interparticle distances are much larger than the Gaussian). In that paper they solve the MLL (including also internal DOFs) using the asymptotic Bethe ansatz, and explain in the conclusions that the decay has to be fast enough as to be able to use this form for the wavefunction. Until now we have indeed observed this change of regime in the phenomenon of level repulsion. Being only present, precisely, when the potential does not decay fast enough as to have: $|x_i - x_j| \gg \epsilon$.

The study of the level spacing may help us gain some insights about the model. For the MLL model with parameters $\frac{\epsilon^2}{4} \cdot c^2 = 22.5$ and $Lc = 600.0$, it is found the distribution shown in fig. 5.4. The fit may not be as good as the one we had for the LL model but it is reasonable to say that the spacing does indeed has a Poisson (or Poisson-like) decay, with yet a great clustering of levels.

The parameters are chosen such that, as we have explained before, the use of results from scattering theory is reasonable. Moreover, we have chosen to study just low lying energy levels. This is because at higher energies the effect of the potential becomes negligible and therefore we should not expect this energy levels to reflect notably the nature of the system.

For comparison we present too the level spacing distribution for a much lower γ, $Lc = 105.0$, fig. 5.5. This was in the range of values where we were able to appreciate the level repulsion shown in fig. 5.3, so the result we obtain is very reasonable, an apparent departure from the Poisson distribution.

It should be also mentioned that none of the other distributions mentioned (GOE, GSE, GME) fit any better this one. Specially if one takes into account that the maximum should be somewhat apart from zero. We propose two reasons to explain this situation. The first one has been already mentioned and it is that we are working with such small boxes that predictions coming from scattering theory may not be as accurate as one may think at first. The second one is that we are working with a system of just a few particles. Although in the integrable limit the empirical distribution and the theoretical one have a good agreement, it should be no surprise that predictions coming from the theory of random matrices, made in the limit of infinite dimension, cannot be perfectly accommodated in this three particle system.

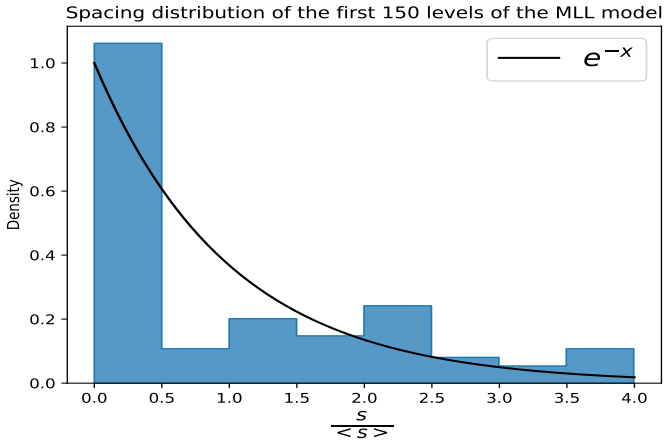


Figure 5.5: Normalized spacing statistics of the MLL model for the first 150 levels. The parameters are $\frac{\epsilon^2}{4} \cdot c^2 = 22.5$ and $Lc = 105.0$. The Poisson distribution has been plotted for comparison.

6. Conclusions

La intención de este trabajo ha sido dar una introducción al tema de sistemas cuánticos en una dimensión, integrabilidad y termalización. Tras la introducción a la teoría de scattering y la descripción del Ansatz de Bethe se ha sido capaz de resolver analíticamente el modelo de Lieb y Liniger, obteniendo en primer lugar los desfasajes para este sistema y después usando las ecuaciones de Bethe para obtener, numéricamente, los pseudomomentos de Bethe. El análisis estadístico del espectro de este modelo reveló resultados conocidos para sistemas integrables, como la distribución del espaciado entre niveles así como la presencia de estados degenerados.

El uso del código para la resolución numérica del modelo con interacción gaussiana arrojó resultados interesantes que, nuevamente, se corresponden con las predicciones teóricas. Pudimos estudiar el comportamiento de este sistema a lo largo de todo el rango de densidades, dándonos acceso a distintas respuestas del sistema.

El estudio de sistemas cuánticos de muchos cuerpos es un campo muy complicado y de mucho interés científico desde comienzos del milenio. Las herramientas y técnicas que se usan son muy sofisticadas, el objetivo de este trabajo es hacer una descripción y dar algunos ejemplos de uso de estos métodos para personas que quieran iniciarse en el tema.

The goal of this work is to give a basic introduction to the relation between the origin of quantum thermodynamics, scattering theory and integrability. The study of one dimensional systems, specially strongly correlated ones, is a very active field of research which has gain a lot of popularity in recent years thanks to the advances in experimental techniques. Most of the bibliography found on this topic is dedicated to graduate students or researchers so in this work we have tried to bridge the knowledge of the undergraduate curriculum to current investigations in physics.

After introducing the main tool, the Bethe ansatz, we solved analytically the LL model and verified numerically some properties about its spectrum that are strongly related to its integrable nature. Once we have seen that indeed it fulfills all the characteristic indicators of an integrable model (wavefunction given by the Bethe ansatz, structure of the level spacing...), we tweak the potential a bit and did a brief numerical analysis on the resulting system. We recovered results that are supported by theoretical studies [14] in the low density regime and were also capable of obtaining signs of the departure from the integrable limit in the structure of the level spacing of the system, better illustrated in the phenomenon of level repulsion.

Although the Lieb-Liniger model is a very particular one and the method of solution may not be immediately used in the solution of harder problems, it does indeed provide the path that one must follow. More refined techniques, such as the nested Bethe ansatz, the algebraic Bethe ansatz... ultimately take the ideas from the general scheme presented here. Moreover,

an explanation of the implications of the integrability of a system has been given. Also the link between conserved quantities and thermalization in the quantum regime was established. We hope that the insights gained in this work can help the reader understand more easily advanced methods such as the Yang-Baxter equation which uses the two-body separability of the S-matrix to prove integrability, a topic that we have discussed here; and the method of Lax's Pairs, a matrix equation that once solved allows one to find N constants of motion for an N D.O.F. system, another result that implies integrability, as we have also discused.

A. Experimental realization: ultracold atoms.

En este apartado se hace una descripción y se proporciona bibliografía para entender como se trasladan los modelos teóricos analizados en el trabajo a la práctica experimental usando sistemas de átomos ultrafríos.

In this appendix we present briefly some advances in the field of ultracold atoms and one dimensional systems as well as bibliography to do a more extensive research on this, specially we highly recommend the review [15].

When one aims to study many-body quantum physics experimentally one find that often numerical techniques are so computationally expensive that they are no longer a resource for the study of certain systems [16]. The community has found in the use of ultracold atoms a remarkable alternative for the simulation of quantum systems. The importance of this approach is mainly the ability to tune the parameters of the system such as the kind of interaction (contact, spin-dependent, velocity dependent...) [17] and strength (using Feschbach resonances [18]), use of different atomic species and, even more impressively, the capability to change the effective dimension of the system. This last point is mainly achieved by means of optical lattices, generated by the interference of laser fields, although magnetic trapping is also commonly used. The versatility that using ultracold atoms provides has allowed researchers to simulate a great number of systems ranging from Bose-Einstein condensates, Fermi degenerate gases to Tonks-Girardeau gases and many more.

Specially important for our work is the last contribution. Prior to these experiments Bose-Einstein condensates in one dimension [19] had been already obtained experimentally, which can be understood as the regime for which $\gamma \ll 1$ in the LL model. Another research group [20] was able to maintain an array of one dimensional Bose gases were $\gamma \approx 1$, in between both limiting regimes. To complete the description of this model the group lead by I. Bloch [10] designed an experiment that allowed them to obtain a Bose gas where $\gamma \gg 1$, that is, in the limit of a Tonks-Girardeau gas. In this last setup they were able to obtain experimental evidence of the fermionization of a 1D Bose gas, a result that we have seen, for a simplified model, in this work.

We have seen therefore how the topics we have introduced in this work have provided important theoretical support to actual experiments in current physics problems.

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