

SCHOOL OF PHYSICS

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ON THE ONE-DIMENSIONAL BOSE GAS

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of the degree of Master of Science*

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# ABSTRACT

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The main work of this thesis involves the calculation, using the Bethe ansatz, of two of the signature quantities of the one-dimensional delta-function Bose gas. These are the density matrix and concomitantly its Fourier transform the occupation numbers, and the correlation function and concomitantly its Fourier transform the structure factor. The coefficient of the delta-function is called the coupling constant; these quantities are calculated in the finite-coupling regime, both expansions around zero coupling and infinite coupling are considered.

Further to this, the density matrix in the infinite coupling limit, and its first order correction, is recast into Toeplitz determinant form. From this the occupation numbers are calculated up to 36 particles for the ground state and up to 26 particles for the first and second excited states. This data is used to fit the coefficients of an ansatz for the occupation numbers.

The correlation function in the infinite coupling limit, and its first order correction, is recast into a form which is easy to calculate for any  $N$ , and is determined explicitly in the thermodynamic limit.



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## DECLARATION

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This is to certify that:

- (i) the thesis comprises only my original work towards the MSc except where indicated in the Statement of Contributions,
- (ii) due acknowledgement has been made in the text to all other material used,
- (iii) the thesis is less than 30,000 words in length, exclusive of table, maps, bibliographies, appendices and footnotes.

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*Melissa Irene Makin*



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## STATEMENT OF CONTRIBUTIONS

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This thesis topic and its theory, as presented in Chapters 3 and 4, were formulated and developed with my supervisors. In particular, I have been responsible for the numerical work and a number of analytic calculations, and collaborating in the interpretation of results.





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## PUBLICATIONS

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During the course of this project, the following article has been published, which is based on the work presented in this thesis. It is listed here for reference.

**Peter J. Forrester, Norman E. Frankel, Melissa I. Makin** *Analytic solutions of the one-dimensional finite-coupling delta-function Bose gas*, Physical Review A, **74** (2006) 043614.



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# CONTENTS

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<b>1</b>	<b>Introduction</b>	<b>1</b>
1.1	Bosons and fermions . . . . .	1
1.2	Experimental technique . . . . .	3
1.3	History . . . . .	4
1.4	This thesis . . . . .	5
<b>2</b>	<b>The Bethe ansatz</b>	<b>7</b>
2.1	Historical development . . . . .	7
2.1.1	$r = 0$ . . . . .	9
2.1.2	$r = 1$ . . . . .	9
2.1.3	$r = 2$ . . . . .	10
2.1.4	General $r$ . . . . .	13
2.2	The one-dimensional delta-function Bose gas . . . . .	14
<b>3</b>	<b>Density matrix and occupation numbers</b>	<b>21</b>
3.1	Specific examples . . . . .	22
3.1.1	$N = 2$ . . . . .	22
3.1.2	$N = 3$ . . . . .	25
3.1.3	$N = 4$ . . . . .	27
3.2	General $N$ small $cL$ expansion . . . . .	28
3.3	General $N$ large $cL$ expansion . . . . .	29
3.3.1	$\rho_N^{(0)}(x, 0)$ . . . . .	30
3.3.2	$\rho_N^{(1)}(x, 0)$ . . . . .	33
3.3.3	Occupation numbers . . . . .	35
3.3.4	Concluding remarks . . . . .	38

<b>4</b>	<b>Correlation functions and structure factors</b>	<b>41</b>
4.1	Specific examples . . . . .	42
4.1.1	$N = 2$ . . . . .	42
4.1.2	$N = 3$ . . . . .	44
4.1.3	$N = 4$ . . . . .	45
4.2	General $N$ small $cL$ expansion . . . . .	46
4.3	General $N$ large $cL$ expansion . . . . .	47
<b>5</b>	<b>Conclusions</b>	<b>57</b>
	<b>References</b>	<b>58</b>
<b>A</b>	<b>Bethe equation solutions</b>	<b>63</b>
<b>B</b>	<b>Multiple integrals and Toeplitz determinants</b>	<b>67</b>
<b>C</b>	<b>Fredholm determinants</b>	<b>69</b>
C.1	Notation . . . . .	69
C.2	Toeplitz determinant form . . . . .	70
<b>D</b>	<b>Numerical data</b>	<b>73</b>

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## LIST OF TABLES

---

2.1	The application of various spin operators on two basis vectors. These particles have only two spin states available, so that attempting to raise (lower) an up (down) spin will result in ‘destroying’ the state . . . . .	8
2.2	Some exact solutions to the Bethe equations (2.37) . . . . .	18
3.1	Parameters for the ansatz (3.47) . . . . .	37
D.1	Values of $c_0^{(0)}(N)$ and $c_0^{(1)}(N)$ for $N = 2, 3, 4, 5, 6, 7$ . Note that this Table extends Table II of [16] . . . . .	73
D.2	Values of $c_1^{(0)}(N)$ and $c_1^{(1)}(N)$ for $N = 2, 3, 4, 5, 6$ . . . . .	74
D.3	Values of $c_2^{(0)}(N)$ and $c_2^{(1)}(N)$ for $N = 2, 3, 4, 5, 6$ . . . . .	75
D.4	Values of $c_0^{(1,1)}(N)$ and $c_0^{(1,2)}(N)$ for $N = 2, 3, 4, 5, 6$ . . . . .	76
D.5	Values of $c_1^{(1,1)}(N)$ and $c_1^{(1,2)}(N)$ for $N = 2, 3, 4, 5, 6$ . . . . .	77
D.6	Values of $c_2^{(1,1)}(N)$ and $c_2^{(1,2)}(N)$ for $N = 2, 3, 4, 5, 6$ . . . . .	78
D.7	Numerical solutions for the ground state occupation numbers $c_0^{*(0)}(N)$ , $c_0^{*(1,1)}(N)$ , $c_0^{*(1,2)}(N)$ and $c_0^{*(1)}(N)$ , for $N = 2 - 36$ . . . . .	79
D.8	Numerical solutions for the first excited state occupation numbers $c_1^{*(0)}(N)$ , $c_1^{*(1,1)}(N)$ , $c_1^{*(1,2)}(N)$ and $c_1^{*(1)}(N)$ , for $N = 2 - 36$ . . . . .	80
D.9	Numerical solutions for the second excited state occupation numbers $c_2^{*(0)}(N)$ , $c_2^{*(1,1)}(N)$ , $c_2^{*(1,2)}(N)$ and $c_2^{*(1)}(N)$ , for $N = 2 - 36$ . . . . .	81

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# INTRODUCTION

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# 1

The advent of new experimental techniques to form one-dimensional gases of bosons in the laboratory motivates the theoretical work performed for this thesis.

The introduction contains four sections, Section 1.1 discusses the fundamental difference between bosons and fermions, Section 1.2 briefly describes the experimental setup, Section 1.3 considers the history of the theoretical development, and finally Section 1.4 outlines the work carried out for this thesis.

## 1.1 Bosons and fermions

The wave function  $\psi(x_1, x_2, \dots, x_n)$  of a system is a mathematical object which contains all of the information about that system. The wave function incorporates the wave-particle duality; the function has wave-like properties (e.g. by combining two of them, an interference pattern may be obtained) and it also has particle-like properties (e.g. it describes  $n$  particles at  $n$  positions in space  $x_1, x_2, \dots, x_n$ ). Two particles are identical if they have the same set of quantum numbers, but are not necessarily at the same position. Upon exchange of two identical particles, two cases arise which deserve special consideration. The first is the symmetric wave function

$$\psi(\dots, x_i, \dots, x_j, \dots) = \psi(\dots, x_j, \dots, x_i, \dots), \quad (1.1)$$

and the second is the antisymmetric wave function

$$\psi(\dots, x_i, \dots, x_j, \dots) = -\psi(\dots, x_j, \dots, x_i, \dots). \quad (1.2)$$



The Pauli exclusion principle states that two or more identical particles cannot exist at the same position. This principle was first introduced by Pauli in 1925 [38] for the specific case of electrons in an atom, and only later [39] was this generalised to any particle with half integer quantum spin<sup>1</sup>. Such particles are known as fermions. Examples of fermions are electrons, protons and neutrons. A wave function that describes a system of identical fermions is always antisymmetric [39]. It is possible to prove the Pauli exclusion principle using (1.2) for a system of identical particles. Consider a wave function describing a system of fermions. If two of these identical fermions exist at the same position,  $\psi(\dots, x, \dots, x, \dots)$ , then by applying (1.2) upon permutation of these two positions, one obtains  $\psi = -\psi$ , and hence  $\psi = 0$ . Physically this means that two identical fermions cannot occupy the same position in space.

Photons (with quantum spin 0) were proposed to be described by a symmetric wave function by Bose [6]. This was then generalised to all particles with integer quantum spin by Einstein [11], these particles became known as bosons. Bosons do not obey the Pauli exclusion principle; in fact in the ground state all bosons can exist in the same quantum state. When a number of bosons do this the system is said to be a Bose-Einstein condensate [12]. Other examples of bosons are W and Z gauge bosons, and certain composite particles such as mesons and certain nuclei.

In 1940, Pauli showed via special relativity that any half integer quantum spin particle is necessarily antisymmetric, while any whole integer quantum spin particle is necessarily symmetric [39]. Pauli did not show that these are the only two types of particles, however the symmetrisation postulate decrees that all particles are of two types: symmetric under exchange of two particles (bosons), or antisymmetric under exchange of two particles (fermions). This is surprising, yet firmly founded in empirical evidence, for example see [34]<sup>2</sup>.

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<sup>1</sup>The intrinsic angular momentum of a particle is called quantum spin. This is different to the classical angular momentum of a particle that is due to rotation. If we denote the (unitless) quantum spin by  $s$  (e.g.  $s = 0$  for a photon and  $s = 1/2$  for an electron), then the magnitude of the angular momentum of that particle is given by  $\hbar\sqrt{s(s+1)}$ .

<sup>2</sup>In  $\leq 2$  dimensions, this dichotomy can be generalised to a continuous range of particles, called anyons. An anyon has anyonic parameter  $\kappa$ , and obeys the wave function exchange symmetry given by  $\psi(\dots, x_i, \dots, x_j, \dots) = e^{i\kappa}\psi(\dots, x_j, \dots, x_i, \dots)$ . The existence of anyons has recently been inferred through studies of the fractional quantum Hall effect.

This thesis discusses the one-dimensional Bose gas, which in the limit of infinite coupling, is interesting in that it behaves like a one-dimensional Fermi gas; the coupling acts like an exclusion principle.

## 1.2 Experimental technique

Although the research done for this thesis is entirely theoretical in nature, it is worth briefly reviewing the experimental techniques and setup which correspond to the theoretical problem described in this thesis.

The two primary techniques needed to create a one-dimensional Bose gas in the laboratory are the ability to trap atoms, and the ability to cool atoms (laser cooling). The ability to trap particles was first demonstrated in 1970 [2]. The ability to laser cool particles was first predicted for the case of neutral atoms in 1974 [21], and this was first successfully put into practice in 1978 [48] (where a temperature of 40 K was achieved). The environment in which this temperature is achieved is typically smaller than a cubic millimetre. These techniques were combined to create the first Bose-Einstein condensate in 1995 [1].

A typical experimental setup, which our theoretical framework aims to approximate (first suggested by [36], and later actualised by [13, 26, 27, 37, 41, 47]) consists of trapping a Bose gas consisting of  $\sim 10^5$   $^{87}\text{Rb}$  atoms using an optical trap. Three lasers of wavelength  $\sim 810\text{--}826$  nm are aligned such that the Bose gas is confined tightly in the radial directions (the depth of the lattice potential is much deeper than the thermal fluctuations), and more loosely in the axial direction, forming a cigar-shaped trap.

One interesting aspect of this system is the quasi-momentum distribution. This cannot be measured directly. The technique for measuring this is achieved by suddenly switching off the confining potential and allowing the gas to expand freely, then waiting for some pre-specified time, (called the time-of-flight,  $\sim 7\text{--}25$  ms). After this time, the atoms will have spread according to their momentum so that the particles with higher momentum would have moved the furthest, and those with least momentum would have moved the least. An image of the gas cloud is taken, and optical depth (a measure of ‘cloudiness’) versus distance from the centre of the cloud is taken. This plot is proportional to an

(underestimated) density profile of the cloud. This distribution is interesting because it has the potential to be determined theoretically, see Chapter 3.

### 1.3 History

Girardeau first introduced the idea of the one-dimensional Bose and Fermi gases in 1960 [19], using a hard-core potential ( $\psi(x_1, \dots, x_N) = 0$  if  $|x_i - x_j| < a$ ,  $i \neq j$ ). This idea was extended just a few years later by Lieb and Liniger [33], who introduced the coupling constant  $c$ , using a delta-function potential (Girardeau's model corresponds to the limit  $c \rightarrow \infty, a \rightarrow 0$  of Lieb and Liniger's model). The Bethe ansatz was first introduced for the problem of the Heisenberg spin chain [5] (see Section 2.1), and is a powerful tool for finding energy eigenfunctions. Lieb and Liniger used Bethe's ansatz in [33] to find the energy eigenfunction for the one-dimensional delta-function Bose gas. They go on to examine the energy eigenvalues for various limits of the dimensionless expansion parameter  $\gamma = c/n$ , where  $n = N/L$  is the density of particles,  $N$  is the number of particles and  $L$  is the length of the system. Others have also determined the energy eigenvalues: in periodic boundary conditions for three particles [35] and up to 50 particles [40], and for hard wall boundary conditions for up to 37 particles [4].

The thermodynamic limit is the limit in which  $N \rightarrow \infty, L \rightarrow \infty$ , where the density  $n$  remains constant. This limit is important as boundary conditions should no longer impinge on the physics of the bulk. Yang and Yang [49] have examined the thermodynamic limit in the finite temperature regime of the one-dimensional delta-function Bose gas using integral equations.

A parallel line of study, beginning in the early seventies, is the Calogero-Sutherland model. The importance of both the Calogero-Sutherland model and the delta-function model is that they are exactly solvable models [3]. An exactly solvable model is attractive in that the framework is complex enough to describe a realistic physical situation, while also being simple enough to produce analytic results. The Calogero-Sutherland model is also a one-dimensional model, where the potential behaves like  $1/r^2$  in some limit, rather than the delta-function  $\delta(r)$ . Important contributions have been made by Calogero [7] and

Sutherland [42, 43, 44, 45].

Important contributions to the understanding of the one-dimensional delta-function Bose gas have been made for the case where  $cL = \infty$ , specifically by Lenard [30], Jimbo and Miwa [23], Korepin et al. [28], and three works by Forrester et al. [15, 16, 17]. This work is referred to in more detail in the remainder of this thesis.

## 1.4 This thesis

This thesis aims to build upon these works by bridging the gap between the free Bose gas ( $cL = 0$ ) and the impenetrable Bose gas ( $cL = \infty$ ) by making expansions around these two extrema. We go beyond the case of merely determining the energy eigenvalues, and instead intensively study the density matrix and its Fourier transform, the occupation numbers (Chapter 3), and the correlation function and its Fourier transform, the structure factor (Chapter 4).

Analytic results for all of these quantities are obtained completely for 2 particles (Subsections 3.1.1 and 4.1.1), partially for 3 particles (Subsections 3.1.2 and 4.1.2) and sparsely for 4 particles (Subsections 3.1.3 and 4.1.3). Extensions are then made for small  $cL$  expansions for arbitrary  $N$  (Sections 3.2 and 4.2). For large  $cL$ , expansions can be determined for arbitrary  $N$  of the correlation function (Section 4.3), and for the density matrix when recast into a form which is amenable to numerical calculation (Section 3.3). The occupation numbers for up to 36 particles are then calculated numerically (Subsection 3.3.3) and this information is fit by an ansatz. Mathematical techniques and tables of numerical data are placed in the appendices.

## 1. INTRODUCTION

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# THE BETHE ANSATZ

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# 2

The purpose of this chapter is to investigate how the Bethe ansatz was used when first introduced in 1931 [5], and to provide the background for why Lieb and Liniger [33] later choose to apply this method to the one-dimensional delta function Bose gas. The first section utilises the review of Karbach and Müller [25].

## 2.1 Historical development

The Bethe ansatz was first introduced as an ad-hoc calculational tool for diagonalising the Hamiltonian for the Heisenberg spin-wave chain - a one-dimensional representation of a ferromagnet. It has since become an incredibly useful tool utilised throughout much of statistical mechanics.

A ferromagnet is a material for which strong coupling exists between nearby spins, so that it is energetically favourable for any nearby spins to be pointing in the same direction. Common ferromagnetic materials include iron and nickel. It is out of such materials that permanent magnets are commonly made.

Let us now introduce the Hamiltonian that describes this physical problem in one dimension. The Heisenberg spin-wave chain is a one-dimensional chain of  $N$  spin  $1/2$  particles, called spinors. These spinors represent the electrons which provide the coupling in a real magnet. This coupling is specific to the particular material, and is denoted  $J$  (see London and Heitler [22] for a treatment of quantum mechanical forces between neutral atoms). Interaction between spinors in this model is restricted to nearest neighbours.

Periodic boundary conditions are chosen, so that for any function  $f$  (for example  $\mathbf{S}_n$ ,  $a(n)$ ,

$|n\rangle$ ) of any variable representing the position of a certain spinor  $n$ ,  $f(n \pm N) = f(n)$ . Also, any difference between two positions must be read as “mod  $N$ ”, for example  $n_2 - n_1 = 1$  should strictly read  $\text{mod}(n_2 - n_1, N) = 1$ .

Classically, the minimum energy state occurs when all spins point in the same direction. Each time a spinor opposes the direction of its neighbour, an increase in energy is introduced. The maximum energy state is obtained when half the spins are up and half are down; each spinor opposes the direction of its neighbour<sup>1</sup>. Quantum mechanically, the spin states aren't energy eigenstates, so it does not make sense to talk of their energy as such. The energy that is spoken of in this paragraph is the expectation value of the energy.

We introduce the notation  $|\uparrow\rangle$  ( $|\downarrow\rangle$ ) to represent a state which has spin parallel (antiparallel) to the  $z$  axis<sup>2</sup>. The operator  $S_n^i$  measures the component of spin of the  $n$ th spinor parallel to the  $i$ th axis. The raising and lowering operators are denoted  $S_n^\pm = S_n^x \pm iS_n^y$ , and the application of  $S_n^z, S_n^+$  and  $S_n^-$  on the states  $|\cdots \uparrow \cdots\rangle$  and  $|\cdots \downarrow \cdots\rangle$  is summarised in Table 2.1.

	$ \cdots \uparrow \cdots\rangle$	$ \cdots \downarrow \cdots\rangle$
$S_n^+$	0	$ \cdots \uparrow \cdots\rangle$
$S_n^-$	$ \cdots \downarrow \cdots\rangle$	0
$S_n^z$	$\frac{1}{2} \cdots \uparrow \cdots\rangle$	$-\frac{1}{2} \cdots \downarrow \cdots\rangle$

Table 2.1: The application of various spin operators on two basis vectors. These particles have only two spin states available, so that attempting to raise (lower) an up (down) spin will result in ‘destroying’ the state

The complete spin vector is given by  $\mathbf{S}_n = (S_n^x, S_n^y, S_n^z)$ . The Hamiltonian, in the absence of any external electric or magnetic fields, is given by a sum over the nearest-neighbour spin interactions

$$H = -J \sum_{n=1}^N \mathbf{S}_n \cdot \mathbf{S}_{n+1} = -J \sum_{n=1}^N \left[ \frac{1}{2} (S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+) + S_n^z S_{n+1}^z \right]. \quad (2.1)$$

This text describes only  $J > 0$ , where this Hamiltonian represents a ferromagnet. When

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<sup>1</sup>Of course if  $N$  is odd then within the maximum energy state there must exist two neighbouring spinors which point in the same direction.

<sup>2</sup>In Bethe's original paper [5] he used left and right spins rather than up and down.

$J < 0$  an anti-ferromagnet is described. The minimum (maximum) energy state of an anti-ferromagnet is equivalent to the maximum (minimum) energy state of a ferromagnet. An anti-ferromagnet will only exhibit magnetic behaviour (spontaneous spin-changing) if an electric field is applied.

The operator  $H$  can be represented as a matrix, where the elements of the matrix are given by the chosen basis. The most convenient basis to choose for initial analysis is the one where each spinor is either aligned or anti-aligned with the  $z$ -axis. However a basis for which the matrix representation of  $H$  is diagonal is much simpler to extract useful information from. The main purpose of the Bethe ansatz is to generate such a basis. One may do this by ordering according to the total spin  $S_T^z \equiv \sum_{n=1}^N S_n^z = N/2 - r$ , where  $r$  is the number of spins which point down. There are  $N!/(r!(N-r)!)$  states of the system given that there are  $r$  down spins. Let us now consider the diagonalisation for the specific cases  $r = 0, 1, 2$  and for general  $r$ .

### 2.1.1 $r = 0$

The state where all spinors are aligned with the  $z$ -axis may be denoted by  $|F\rangle = |\uparrow \cdots \uparrow\rangle$ . This is an eigenstate of  $H$  with eigenvalue  $E_0 = -JN/4$ .

### 2.1.2 $r = 1$

One can represent the states where only one spinor points down by  $|n\rangle = S_n^- |F\rangle$ . These states are not eigenstates of the Hamiltonian, but rather

$$H|n\rangle = -J \left[ \frac{1}{2}|n+1\rangle + \frac{1}{2}|n-1\rangle + \left( \frac{N}{4} - 1 \right) |n\rangle \right]. \quad (2.2)$$

This basis ( $|1\rangle, \dots, |N\rangle$ ) will obviously not produce a diagonal Hamiltonian. Let us search for an eigenstate of the Hamiltonian  $|\psi_k\rangle$ , given by a superposition of all states  $|1\rangle, \dots, |N\rangle$  with coefficients  $a(n)$ ,



$$|\psi_k\rangle = \sum_{n=1}^N a(n)|n\rangle. \quad (2.3)$$

By asserting that  $|\psi_k\rangle$  is an eigenstate of  $H$  with energy eigenvalue  $E$ , one can determine a recursion relation for  $a(n)$ . Applying (2.2) to the state (2.3) yields

$$2a(n)(E - E_0) = J[a(n) - a(n+1) - a(n-1)], \quad (2.4)$$

it is easily verified that this has solution  $a(n) = e^{ikn}$ , where  $k = 2\pi m/N$ ,  $m = 0, \dots, N-1$ . Energy eigenvalues are given by

$$E - E_0 = J(1 - \cos k). \quad (2.5)$$

With these values, the  $r = 1$  block is perfectly diagonalised.

At this point it is interesting to observe a point of difference between quantum mechanical and classical behaviour. Classical intuition tells us that each  $|n\rangle$  contains the same amount of energy. Taking an (albeit unusual) average (2.3) should yield the same amount of energy for  $|\psi_k\rangle$  regardless of the value of  $k$ . However, (2.5) clearly shows that this is not the case. This apparent problem is resolved by recognising that the states  $|n\rangle$  are not energy eigenstates, and so cannot be thought of as having a measurable energy. Part of the consequence of a state being an energy eigenstate is that the state will remain stationary as time progresses. A spin state with only one down spin is obviously not a stationary state, and so it must not be an energy eigenstate. The energy expectation value  $\langle n|H|n\rangle = E_0 + J$ , is however clearly independent of  $n$ , and in this case gives the intuitive, classical result.

### 2.1.3 $r = 2$

When two spins point down the appropriate spin states are designated by  $|n_1, n_2\rangle = S_{n_1}^- S_{n_2}^- |F\rangle$ . One must exhibit caution when two spins are down, as the case of the two spins being adjacent, and being separate, must be treated separately. These are also

not eigenstates. An application of  $H$  (2.1) to  $|n_1, n_2\rangle$  when the two spins are adjacent ( $n_2 - n_1 = 1$ ) gives

$$H|n_1, n_1 + 1\rangle = -J \left[ \frac{1}{2}|n_1, n_1 + 2\rangle + \frac{1}{2}|n_1 - 1, n_1 + 1\rangle + \left(\frac{N}{4} - 1\right)|n_1, n_1 + 1\rangle \right], \quad (2.6)$$

and when the two spins are separated ( $n_2 - n_1 > 1$ )

$$H|n_1, n_2\rangle = -J \left[ \frac{1}{2}|n_1 + 1, n_2\rangle + \frac{1}{2}|n_1, n_2 + 1\rangle + \frac{1}{2}|n_1 - 1, n_2\rangle + \frac{1}{2}|n_1, n_2 - 1\rangle + \left(\frac{N}{4} - 2\right)|n_1, n_2\rangle \right]. \quad (2.7)$$

If again one chooses a superposition of states

$$|\psi_{k_1, k_2}\rangle = \sum_{1 \leq n_1 < n_2 \leq N} a(n_1, n_2)|n_1, n_2\rangle, \quad (2.8)$$

and again enforces that  $|\psi_{k_1, k_2}\rangle$  is an eigenstate of  $H$  with energy eigenvalue  $E$ , one obtains two different recursion relations for  $a(n_1, n_2)$ , one when the two down-spins are adjacent ( $n_2 - n_1 = 1$ )

$$2(E - E_0)a(n_1, n_1 + 1) = J [2a(n_1, n_1 + 1) - a(n_1 - 1, n_1 + 1) - a(n_1, n_1 + 2)], \quad (2.9)$$

and one when the two down-spins are separated ( $n_2 - n_1 > 1$ )

$$2(E - E_0)a(n_1, n_2) = J [4a(n_1, n_2) - a(n_1 - 1, n_2) - a(n_1 + 1, n_2) - a(n_1, n_2 - 1) - a(n_1, n_2 + 1)]. \quad (2.10)$$

## 2. THE BETHE ANSATZ

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Now let us choose a trial solution, again composed of plane waves

$$a(n_1, n_2) = Ae^{i(k_1 n_1 + k_2 n_2)} + A'e^{i(k_2 n_1 + k_1 n_2)}, \quad (2.11)$$

this is called the Bethe ansatz. Either linearly independent component of (2.11) substituted into (2.10) determines the energy eigenvalue  $E$  as

$$E - E_0 = J \sum_{i=1}^2 (1 - \cos k_i). \quad (2.12)$$

We determine information about  $A$  and  $A'$  by noting that if one replaces  $n_2$  by  $n_1 + \Delta$  ( $1 < \Delta < N - 1$ )<sup>3</sup> in (2.10) and combine with (2.9) one may obtain an equation which no longer contains  $(E - E_0)$ . Substituting in (2.11) and solving for  $A$  and  $A'$  yields a solution free of  $\Delta$

$$\frac{A}{A'} = -\frac{e^{i(k_1 + k_2)} + 1 - 2e^{ik_1}}{e^{i(k_1 + k_2)} + 1 - 2e^{ik_2}} = e^{i\theta}, \quad (2.13)$$

where  $\theta$  is introduced as a phase factor between  $A$  and  $A'$  (dependent on  $k_1$  and  $k_2$ ), so that (2.11) becomes

$$a(n_1, n_2) = e^{i(k_1 n_1 + k_2 n_2 + \theta/2)} + e^{i(k_2 n_1 + k_1 n_2 - \theta/2)}. \quad (2.14)$$

It remains to determine an equation relating  $k_1$  and  $k_2$  with  $N$ . This is done by generating what are known as the Bethe equations. Using the boundary condition<sup>4</sup>  $a(n_1, n_2) = a(n_2, n_1 + N)$  on (2.14), which is solved by  $e^{i\theta} = e^{ik_1 N} = e^{-ik_2 N}$ , the Bethe equations are given by

$$-\frac{e^{i(k_1 + k_2)} + 1 - 2e^{ik_1}}{e^{i(k_1 + k_2)} + 1 - 2e^{ik_2}} = e^{ik_1 N} = e^{-ik_2 N}. \quad (2.15)$$

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<sup>3</sup>Note that in [5, 25],  $\Delta = 1$  is used, which although yielding the correct result, is not quite physical, so that this more cumbersome approach is taken here.

<sup>4</sup>This boundary condition is a combination of symmetry between spins,  $a(n_1, n_2) = a(n_2, n_1)$ , and periodic boundary conditions  $a(n_1, n_2) = a(n_1, n_2 + N)$ .

### 2.1.4 General $r$

Now, we extend this idea to general  $r$ , where the spin basis is given by  $|n_1, \dots, n_r\rangle = S_{n_1}^- \dots S_{n_r}^- |F\rangle$ . The first position in each adjacent pair is labelled  $n_{j_\alpha}$ , so that  $n_{j_\alpha+1} - n_{j_\alpha} = 1$ , and for all other down spin positions  $n_{j+1} - n_j > 1, j \neq j_\alpha$ . The number of adjacent pairs is denoted  $|\alpha|$  (this could be  $0, 1, \dots, r$ ). Note that this notation is valid for two or more adjacent down spins. The application of the Hamiltonian  $H$  (2.1) on  $|n_1, \dots, n_r\rangle$  is

$$\begin{aligned}
H|n_1, \dots, n_r\rangle = & -J \left\{ \sum_{\alpha} \left[ \frac{1}{2} |n_1, \dots, n_{j_\alpha} - 1, n_{j_\alpha+1}, \dots, n_r\rangle \right. \right. \\
& \left. \left. + \frac{1}{2} |n_1, \dots, n_{j_\alpha}, n_{j_\alpha+1} + 1, \dots, n_r\rangle \right] \right. \\
& \left. + \sum_{\substack{i \neq j_\alpha \\ i \neq j_{\alpha+1}}} \left[ \frac{1}{2} |n_1, \dots, n_i + 1, \dots, n_r\rangle + \frac{1}{2} |n_1, \dots, n_i - 1, \dots, n_r\rangle \right] \right. \\
& \left. + \left( \frac{N}{4} - r + |\alpha| \right) |n_1, \dots, n_r\rangle \right\}. \tag{2.16}
\end{aligned}$$

One may define a general superposition of spin states

$$|\psi_{k_1, \dots, k_r}\rangle = \sum_{1 \leq n_1 < \dots < n_r \leq N} a(n_1, \dots, n_r) |n_1, \dots, n_r\rangle. \tag{2.17}$$

By asserting that (2.17) is an eigenstate, one can develop recursion relations given by

$$\begin{aligned}
2(E - E_0)a(n_1, \dots, n_r) = & J \sum_{\substack{i \neq j_\alpha \\ i \neq j_{\alpha+1}}} [2a(n_1, \dots, n_r) - a(n_1, \dots, n_i + 1, \dots, n_r) \\
& - a(n_1, \dots, n_i - 1, \dots, n_r)] \\
& + J \sum_{\alpha} [2a(n_1, \dots, n_r) - a(n_1, \dots, n_{j_\alpha} - 1, n_{j_\alpha+1}, \dots, n_r) \\
& - a(n_1, \dots, n_{j_\alpha}, n_{j_\alpha+1} + 1, \dots, n_r)]. \tag{2.18}
\end{aligned}$$

The Bethe ansatz is now

$$a(n_1, \dots, n_r) = \sum_{p \in S_r} \exp \left( i \sum_{j=1}^r k_{p(j)} n_j + \frac{i}{2} \sum_{i < j} \theta_{p(i)p(j)} \right), \quad (2.19)$$

so that the energy of  $|\psi_{k_1, \dots, k_r}\rangle$  is determined to be

$$E - E_0 = J \sum_{j=1}^r (1 - \cos k_j). \quad (2.20)$$

An expression for  $\theta_{ij}$  is then determined as an implicitly defined equation of  $k_i$  and  $k_j$  as

$$e^{i\theta_{ij}} = - \frac{e^{i(k_i+k_j)} + 1 - 2e^{ik_i}}{e^{i(k_i+k_j)} + 1 - 2e^{ik_j}}. \quad (2.21)$$

Applying the boundary condition  $a(n_1, \dots, n_r) = a(n_2, \dots, n_r, n_1 + N)$  gives

$$e^{iNk_i} = e^{i \sum_{i < j}^N \theta_{ij}} = \prod_{1 \leq i < j \leq N} e^{i\theta_{ij}}, \quad (2.22)$$

so that the Bethe equations become

$$e^{iNk_i} = \prod_{1 \leq i < j \leq N} \left[ - \frac{e^{i(k_i+k_j)} + 1 - 2e^{ik_i}}{e^{i(k_i+k_j)} + 1 - 2e^{ik_j}} \right]. \quad (2.23)$$

So again, diagonalising the  $r$ th block of the Hamiltonian is reduced to solving for the set of numbers  $k_i$ ,  $i = 1, \dots, r$ . This implicitly defined equation is not analytically tractable in general, rather, for each value of  $N$ , numerical solutions must be found.

## 2.2 The one-dimensional delta-function Bose gas

The purpose of this section is to present the Bethe ansatz wave function and concomitantly the Bethe equations for the one-dimensional delta-function Bose gas in periodic boundary conditions, as derived in the seminal paper by Lieb and Liniger [33]. The wave function is extended to large  $cL$  (previously done by [23]) and small  $cL$  coupling.

The Schrödinger equation for this system with  $\hbar = 1, 2m = 1$  is

$$\left( -\sum_{i=1}^N \frac{\partial^2}{\partial x_i^2} + 2c \sum_{1 \leq i < j \leq N} \delta(x_i - x_j) \right) \psi_N(x_1, x_2, \dots, x_N) = E \psi_N(x_1, x_2, \dots, x_N), \quad (2.24)$$

where  $c$  controls the strength of the  $\delta$ -function. Throughout this thesis we consider only  $c \geq 0$ , the repulsive case.

Let us assume that  $\psi_N$  is continuous, and that its first and second derivatives with respect to any  $x_i$  are not continuous. For any pair of  $i, j$  values that satisfy the inequality  $1 \leq i < j \leq N$ ,

$$\lim_{\epsilon \rightarrow 0} \int_{-\epsilon}^{\epsilon} \left( -\frac{\partial^2}{\partial x_i^2} - \frac{\partial^2}{\partial x_j^2} + 2c \delta(x_i - x_j) \right) \psi_N d(x_i - x_j) = 0, \quad (2.25)$$

the terms in the integrand which are continuous have been discarded. This simplifies to

$$\left( \frac{\partial}{\partial x_j} - \frac{\partial}{\partial x_i} \right) \psi_N|_{x_j=x_i^+} - \left( \frac{\partial}{\partial x_j} - \frac{\partial}{\partial x_i} \right) \psi_N|_{x_j=x_i^-} + 2c \psi_N|_{x_j=x_i} = 0, \quad (2.26)$$

with the simpler differential equation

$$-\sum_{i=1}^N \frac{\partial^2}{\partial x_i^2} \psi_N(x_1, x_2, \dots, x_N) = E \psi_N(x_1, x_2, \dots, x_N). \quad (2.27)$$

There is a large amount of redundancy in the variable range of the wave function. By restricting the domain to

$$R_N : 0 \leq x_1 < \dots < x_N \leq L, \quad (2.28)$$

coupled with the symmetry of the wave function, equation (2.26) can be simplified markedly. This symmetry allows us to switch  $i$  and  $j$  in the first term of (2.26), to obtain

$$\left( \frac{\partial}{\partial x_{j+1}} - \frac{\partial}{\partial x_j} \right) \psi_N|_{x_{j+1}=x_j} = c \psi_N|_{x_{j+1}=x_j}. \quad (2.29)$$

The solution to (2.27) with boundary condition (2.29) and domain (2.28) under periodic boundary conditions is the Bethe ansatz

$$\psi_N(x_1, x_2, \dots, x_N) = \sum_{p \in S_N} a(p) \epsilon(p) e^{i \sum_{j=1}^N k_{p(j)} x_j}, \quad (2.30)$$

where  $S_N$  is the symmetric group on  $N$  symbols, and hence the wave function is a sum over  $N!$  quantities. The position and quasi-momenta of the  $j$ th particle is given by  $x_j$  and  $k_j$  respectively, the energy is given by  $E = \sum_{j=1}^N k_j^2$ , and the total momentum by  $\sum_{j=1}^N k_j$ . The function  $\epsilon(p)$  is the signature of the permutation  $p$ . Note the similarity to (2.19), where the  $a(p)\epsilon(p)$  term serves as the  $\exp(i/2 \sum \theta_{p(i)p(j)})$  term. The functional form of  $a(p)$  shall now be determined.

Consider the permutation  $p$  that takes  $\{k_1, k_2, \dots, k_N\}$  into  $\{\varrho, \varsigma, k_{p(3)}, \dots, k_{p(N)}\}$ , and the permutation  $q$  that takes  $\{k_1, k_2, \dots, k_N\}$  into  $\{\varsigma, \varrho, k_{p(3)}, \dots, k_{p(N)}\}$ .

Also consider the boundary condition (2.29) for  $j = 1$ . The two terms of the sum (2.30) corresponding to the permutations  $p$  and  $q$  are given by

$$a(p) e^{i(\varrho x_1 + \varsigma x_2 + \sum_{j=3}^N k_{p(j)} x_j)} - a(q) e^{i(\varsigma x_1 + \varrho x_2 + \sum_{j=3}^N k_{p(j)} x_j)}. \quad (2.31)$$

Substituting this into (2.29)<sup>5</sup> and discarding a factor of  $e^{i[(\varrho + \varsigma)x_1 + \sum_{j=3}^N k_{p(j)} x_j]}$  yields

$$i(\varsigma - \varrho)[a(p) + a(q)] = c[a(p) - a(q)], \quad (2.32)$$

and if  $a(q) = a(p)f(\varsigma, \varrho, c)$ , then

$$f = \frac{-(\varsigma - \varrho) - ic}{(\varsigma - \varrho) - ic} = e^{2i \arctan u}, \quad (2.33)$$

---

<sup>5</sup>All  $N!$  terms of (2.24) are linearly independent. Because of this, the remaining  $N! - 2$  terms need not be considered.

where  $u = (\varsigma - \varrho)/c$ . So,  $f$  is the ratio between  $a(p)$  and  $a(q)$ . To generalise to any permutation, one must use the boundary condition  $\psi_N(x_1, \dots, x_N) = \psi_N(x_2, \dots, x_N, x_1 + N)$ . Multiplying through by a factor of  $(\varsigma - \varrho) - ic^6$ , and including all the necessary permutations, gives

$$a(p) = \prod_{1 \leq i < j \leq N} \left[ 1 + \frac{i}{c} (k_{p(j)} - k_{p(i)}) \right]. \quad (2.34)$$

Note that  $a(p)$  may be given in a number of forms (any change absorbed into the normalisation), we choose (2.34) from Jimbo and Miwa [23]. Throughout this chapter we use the normalisation given by

$$\mathcal{N}^2 = \int_{R_{N-1}} dx_1 \dots dx_{N-1} |\psi_N(0, x_1, \dots, x_{N-1})|^2, \quad (2.35)$$

where  $R_{N-1}$  is the domain of integration specified by (2.28).

In this chapter we are concerned only with the ground state,  $\sum_{i=1}^N k_i = 0$ , so that

$$k_i = -k_{N+1-i} \quad \forall i = 1, \dots, N. \quad (2.36)$$

The  $k_i$  are ordered such that  $k_N > k_{N-1} > \dots > k_2 > k_1$ . The  $N$  (real) numbers  $k_i$  are determined as the solution of the Bethe equations. These can be given in many forms [23, 32, 33], we display that of [18]

$$k_j L = \sum_{\substack{l=1 \\ l \neq j}}^N 2 \arctan \left( \frac{c}{k_j - k_l} \right) \quad (2.37)$$

While these equations cannot be solved explicitly for  $k_j$  as a function of  $c$ , they can be solved for both small and large  $cL$  expansions, using the method of quadrature. We list explicit small  $cL$  expansions in Appendix A, and at this point we highlight that

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<sup>6</sup>A valid operation, as this change is absorbed into the normalisation.



$$k_j = \sqrt{\frac{2c}{L}} h_j^{(N)} \left( 1 - \frac{1}{24}(cL) + O(cL)^2 \right), \quad (2.38)$$

where  $h_j^{(N)}$  is the  $j$ th zero of the  $N$ th Hermite polynomial. The leading term in (2.38) is found in reference to this problem by Gaudin [18], for more detail refer to Szegő [46]. The coefficient  $-1/24$  in the next term of the expansion is new, and appears to be universal (see Appendix A).

Here we display the large  $cL$  expansion for  $k_j$  in its general  $N$  form as given in [23], for its particular utility in the following chapters

$$k_j = (2j - N - 1) \frac{\pi}{L} \left[ 1 - 2N \left( \frac{1}{cL} \right) + 4N^2 \left( \frac{1}{cL} \right)^2 + \left\{ -8N^3 + \frac{4}{3}N [2j^2 + (N+1)(N-2j)] \pi^2 \right\} \left( \frac{1}{cL} \right)^3 \right] + O \left( \frac{1}{cL} \right)^4. \quad (2.39)$$

We also list some exact solutions to the Bethe equations (2.37) in Table 2.2.

$N$	$cL$	$k_N L$
2	$\pi$	$\pi/2$
3	$\pi/2$	$\pi(\sqrt{17}-3)/4$
3	$\pi$	$\sqrt{2}\pi$
3	$3\pi/2$	$3\pi(\sqrt{17}+3)/4$

Table 2.2: Some exact solutions to the Bethe equations (2.37)

It is now possible to explicitly construct the wave function  $\psi_N(x_1, \dots, x_N)$  using (2.30) and (2.34). We close here by exhibiting the unnormalised wave function  $\psi_2(x_1, x_2)$  by way of example

$$\psi_2(x_1, x_2) = \left( 1 - \frac{2ik_2}{c} \right) e^{ik_2(x_2-x_1)} - \left( 1 + \frac{2ik_2}{c} \right) e^{-ik_2(x_2-x_1)}, \quad (2.40)$$

which has normalisation

$$\mathcal{N}^2 = 2L - \frac{\sin 2k_2 L}{k_2} - \frac{8 \sin^2 k_2 L}{c} + \frac{4k_2(2k_2 L + \sin 2k_2 L)}{c^2}. \quad (2.41)$$

## 2. THE BETHE ANSATZ

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# DENSITY MATRIX

## AND

# OCCUPATION NUMBERS

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# 3

This chapter outlines the definition of both the density matrix and its Fourier transform, the occupation numbers. Specific examples are given in Section 3.1 for 2, 3 and 4 particles. Polynomial structure is found for the  $n = 0$  occupation numbers for general  $N$ , small  $cL$  expansions in Section 3.2. Section 3.3 examines the general  $N$  large  $cL$  expansion, reformulating the original definition of the density matrix in such a way as to generate numerical results.

The normalised density matrix<sup>1</sup>  $\rho_N(x, 0)$  gives the density at position  $x$ , given that there is a particle at position 0. It is defined as

$$\rho_N(x, 0) = \frac{N}{L} \frac{1}{\mathcal{N}^2} \sum_{j=0}^{N-1} \int_{R_{N-1,j}(x)} dx_1 \dots dx_{N-1} \psi_N(0, x_1, x_2, \dots, x_{N-1}) \times \overline{\psi_N(x_1, \dots, x_j, x, x_{j+1}, \dots, x_{N-1})}, \quad (3.1)$$

where the overbar implies complex conjugation, the normalisation  $\mathcal{N}^2$  is specified by (2.35), and the domain of integration is specified by

$$R_{N,j}(x) : 0 \leq x_1 < \dots < x_j < x < x_{j+1} < \dots < x_N \leq L. \quad (3.2)$$

The density matrix is normalised such that  $\rho_N(0, 0) = \rho_0 = N/L$ . Hence to compute the density matrix for  $N$  particles, one must perform  $N$  lots of  $N-1$  dimensional integrals over

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<sup>1</sup>‘Density matrix’ is a shortened form of ‘one-body reduced density matrix’. This change in nomenclature explains why (3.1) is not a matrix [31].

$(N!)^2$  terms (e.g. 4 triple integrals over 576 terms for  $N = 4$ ). As this is a computationally expensive task, so only solutions up to  $N = 4$  are obtained using this method.

The occupation numbers  $c_n(N)$  are determined as a Fourier transform of the density matrix<sup>2</sup>

$$c_n(N) = \int_0^L \rho_N(x, 0) e^{2i\pi nx/L} dx = \int_0^L \rho_N(x, 0) \cos(2\pi nx/L) dx, \quad (3.3)$$

where  $n \in \mathbb{Z}$ . The occupation numbers have the physical interpretation of being the expectation value of the number of particles in mode  $n$ .

It is interesting here to consider the difference between the excited state of the whole system and the excited states of individual particles. This thesis studies only the ground state of the whole system, so that the total momentum is zero, or  $\sum_{j=1}^N k_j = 0$ . However within this individual particles can transition to excited states.

Note the normalisation property  $\sum_{n=-\infty}^{\infty} c_n(N) = N$ ; this result has been confirmed for all occupation number formulas that follow. It is sometimes useful to discuss occupation number per particle; the notation for this is  $c_n^*(N) = c_n(N)/N$ .

## 3.1 Specific examples

### 3.1.1 $N = 2$

Within Section 3.1, this subsection heralds the most complete set of results, with results for  $N = 3$  and  $N = 4$  becoming increasingly exiguous as the intricacies of the equations develop. For example, it is only possible to display the complete density matrix for  $N = 2$ , as for  $N = 3$  already the equation would take many pages to display. Utilising (2.37) one may obtain

$$c = 2k_2 \tan\left(\frac{k_2 L}{2}\right), \quad (3.4)$$

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<sup>2</sup>The density matrix  $\rho_N(x, 0)$  is an even function.

which is used to produce a concise form of the density matrix with (2.30), (2.34) and (3.1)

$$\rho_2(x, 0) = \frac{2}{L} \frac{k_2 x \cos(k_2(L-x)) + k_2(L-x) \cos(k_2 x) + \sin(k_2(L-x)) + \sin(k_2 x)}{k_2 L + \sin(k_2 L)}, \quad (3.5)$$

where  $0 \leq k_2 \leq \pi$ . This has corresponding occupation numbers from (3.3)

$$c_n(2) = 2 \frac{4(k_2 L)^3 (1 - \cos(k_2 L))}{(4n^2 \pi^2 - k_2^2 L^2)^2 (k_2 L + \sin(k_2 L))}. \quad (3.6)$$

The expansion of the density matrix for small  $cL$  is given using (A.1)

$$\rho_2(t, 0) = \frac{2}{L} \left[ 1 - \frac{t^2(\pi-t)^2}{24\pi^4} (cL)^2 + \frac{t^2(\pi-t)^2(t^2 - \pi t + 2\pi^2)}{360\pi^6} (cL)^3 \right. \\ \left. + \frac{t^2(\pi-t)^2(16\pi^4 - 24\pi^3 t + 27\pi^2 t^2 - 6\pi t^3 + 3t^4)}{40320\pi^8} (cL)^4 + O(cL)^5 \right]. \quad (3.7)$$

Note that we introduce here the unitless variable  $t = \pi x/L$ , henceforth we switch between  $t$  and  $x$  as appropriate. The corresponding occupation numbers for (3.7) are given by

$$c_n(2) = 2 \begin{cases} 1 - \frac{1}{720} (cL)^2 + \frac{1}{6048} (cL)^3 - \frac{11}{1209600} (cL)^4 + O(cL)^5 & \text{when } n = 0 \\ \frac{1}{16n^4\pi^4} (cL)^2 + \frac{3-n^2\pi^2}{96n^6\pi^6} (cL)^3 \\ \quad + \frac{4n^4\pi^4 - 30n^2\pi^2 + 45}{3840n^8\pi^8} (cL)^4 + O(cL)^5 & \text{when } n \neq 0. \end{cases} \quad (3.8)$$

Utilising (2.39), we obtain a large  $cL$  expansion for the density matrix

$$\rho_2(t, 0) = \frac{2}{L} \left\{ \frac{(\pi - 2t) \cos t + 2 \sin t}{\pi} + \frac{8(\pi - t)t \sin t}{\pi} \left( \frac{1}{cL} \right) + \frac{8 [(\pi^2 - 3\pi t + 2t^2)t \cos t - (\pi^2 + 6\pi t - 6t^2) \sin t]}{\pi} \left( \frac{1}{cL} \right)^2 + O \left( \frac{1}{cL} \right)^3 \right\}. \quad (3.9)$$

Note that in the limit  $cL \rightarrow \infty$ , we recover (20) of [16]. The corresponding occupation numbers for (3.9) are given by

$$c_n(2) = 2 \left[ \frac{8}{(4n^2 - 1)^2 \pi^2} - \frac{32(12n^2 + 1)}{(4n^2 - 1)^3 \pi^2} \left( \frac{1}{cL} \right) + \left\{ \frac{3072n^2 (4n^2 + 1)}{(4n^2 - 1)^4 \pi^2} - \frac{64(6n^2 - 1)}{(4n^2 - 1)^2} \right\} \left( \frac{1}{cL} \right)^2 + O \left( \frac{1}{cL} \right)^3 \right] \quad (3.10)$$

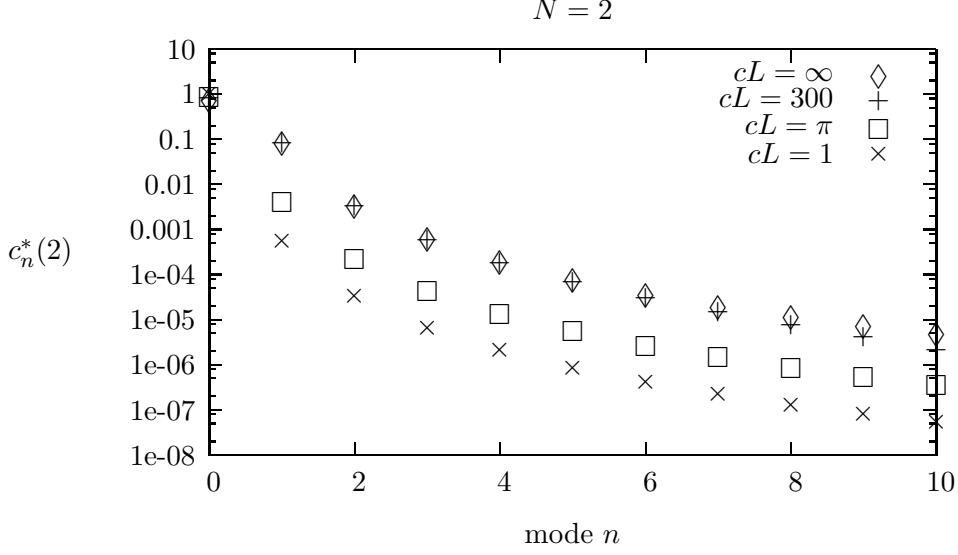
which in the limit  $cL \rightarrow \infty$  recovers (42) of [16]. We also display here the density matrix for the exact solution to (2.37) from Table 2.2, when  $cL = \pi, k_2 L = \pi/2$

$$\rho_2(t, 0) = \frac{2}{L} \frac{(-t + \pi + 2) \cos \frac{t}{2} + (t + 2) \sin \frac{t}{2}}{\pi + 2}, \quad (3.11)$$

and the corresponding occupation numbers are given by

$$c_n(2) = 2 \frac{16}{(16n^2 - 1)^2 \pi (\pi + 2)}. \quad (3.12)$$

Figure 3.1 provides a graphical representation of the results for the occupation numbers of  $N = 2$ . The case  $cL = 0$  is not displayed in this figure, it has  $c_0^*(2) = 1$ , with all higher modes having zero occupation. So when  $cL = 0$ , the system behaves purely like a free Bose gas in the ground state - all particles occupy  $n = 0$ . When  $cL = \infty$ , the system obeys the Pauli exclusion principle, as particles are forced to occupy individual states, so that a  $cL = \infty$  Bose gas acts like a Fermi gas. Note the smooth transition from  $cL = 0$  to  $cL = \infty$ .

Figure 3.1: Occupation numbers for  $N = 2$ 

### 3.1.2 $N = 3$

The small  $cL$  expansion of the density matrix is given here, using (3.1) and (A.2).

$$\begin{aligned} \rho_3(t, 0) = \frac{3}{L} & \left[ 1 - \frac{t^2(\pi - t)^2}{12\pi^4}(cL)^2 - \frac{t^2(\pi - t)^2(t^2 - \pi t - 3\pi^2)}{180\pi^6}(cL)^3 \right. \\ & \left. + \frac{t^2(\pi - t)^2(-101t^4 + 202\pi t^3 - 125\pi^2 t^2 + 24\pi^3 t + 54\pi^4)}{20160\pi^8}(cL)^4 + O(cL)^5 \right]. \end{aligned} \quad (3.13)$$

Note that the coefficient of the  $(cL)^p$  term is a polynomial in  $t$  of order  $2p$ , for  $p \geq 2$ . This structure is also repeated in (3.7).

The corresponding occupation numbers for (3.13) are given by

$$c_n(3) = 3 \begin{cases} 1 - \frac{1}{360}(cL)^2 + \frac{1}{1680}(cL)^3 - \frac{163}{1814400}(cL)^4 + O(cL)^5 & \text{when } n = 0 \\ \frac{1}{8n^4\pi^4}(cL)^2 - \frac{n^2\pi^2+3}{48n^6\pi^6}(cL)^3 \\ \quad + \frac{6n^4\pi^4+170n^2\pi^2-1515}{1920n^8\pi^8}(cL)^4 + O(cL)^5 & \text{when } n \neq 0. \end{cases} \quad (3.14)$$



We give here the large  $cL$  expansion of the density matrix, using (3.1) and (2.37)

$$\rho_3(t, 0) = \frac{3}{L} \left\{ \frac{2(\pi-2t)^2 + 12(\pi-2t) \sin 2t + 4(2t-\pi+2)(2t-\pi-2) \cos 2t + \cos 4t + 15}{6\pi^2} + \frac{4 \sin t [(\pi-2t)(1+8\pi t-8t^2) \cos t - (\pi-2t) \cos 3t + 8(\pi-t)t \sin t]}{\pi^2} \left( \frac{1}{cL} \right) + O\left( \frac{1}{cL} \right)^2 \right\}, \quad (3.15)$$

which in the limit  $cL \rightarrow \infty$  recovers (21) of [16].

The occupation numbers corresponding to (3.15) are given by

$$c_n(3) = 3 \begin{cases} \left( \frac{1}{9} + \frac{35}{6\pi^2} \right) + \left( \frac{8}{3} + \frac{35}{\pi^2} \right) \left( \frac{1}{cL} \right) + O\left( \frac{1}{cL} \right)^2 & \text{when } n = 0 \\ \frac{1}{9} - \left( \frac{4}{3} + \frac{35}{6\pi^2} \right) \left( \frac{1}{cL} \right) + O\left( \frac{1}{cL} \right)^2 & \text{when } |n| = 1 \\ \frac{35}{108\pi^2} - \frac{385}{36\pi^2} \left( \frac{1}{cL} \right) + O\left( \frac{1}{cL} \right)^2 & \text{when } |n| = 2 \\ \frac{2(3n^2+1)}{3n^2(n^2-1)^2\pi^2} - \frac{4(9n^6-28n^4-61n^2+8)}{n^2(n^2-1)^3(n^2-4)\pi^2} \left( \frac{1}{cL} \right) + O\left( \frac{1}{cL} \right)^2 & \text{when } |n| \geq 3, \end{cases} \quad (3.16)$$

which in the limit  $cL \rightarrow \infty$  recovers (45) of [16]. We also display here the density matrix for the exact solution to (2.37) from Table 2.2, when  $cL = \sqrt{2}\pi, k_3L = \pi$

$$\rho_3(t, 0) = \frac{3}{L} \frac{1}{48 + 3\phi\pi} \left\{ 8t^2 - 8\pi t + 2\phi(\pi - 2t) \cos t - 4 \cos 2t + 4 \left[ \pi \left( 2\sqrt{2}t + 5 \right) - 2\sqrt{2} \left( t^2 - 5 \right) \right] \sin t + \phi\pi + 52 \right\}, \quad (3.17)$$

where  $\phi = 10\sqrt{2} + 3\pi$ . The corresponding occupation numbers for (3.17) are given by

$$c_n(3) = 3 \begin{cases} \frac{5}{27} + \frac{4\sqrt{2}}{\pi} - \frac{4(299+71\sqrt{2}\pi)}{27(16+\phi\pi)} & \text{when } n = 0 \\ \frac{64\sqrt{2}+54\pi}{81\pi(16+\phi\pi)} & \text{when } |n| = 1 \\ \frac{4(-\pi+32n^4(2\sqrt{2}+\pi)-4n^2(12\sqrt{2}+\pi))}{3n^2\pi(4n^2-1)^3(16+\phi\pi)} & \text{when } |n| \geq 2. \end{cases} \quad (3.18)$$

The density matrices and occupation numbers for the other exact values listed in Table 2.2 for  $N = 3$ , although calculated, are too lengthy to display here.

Figure 3.2 displays a sample of results for the occupation numbers for  $N = 3$ . As in Subsection 3.1.1, the  $cL = 0$  case is not displayed, for it only has one non-zero point, at  $c_0^*(3) = 1$ . Refer to Subsection 3.1.1 for a further explanation of the features of this graph, which is similar to Figure 3.1.

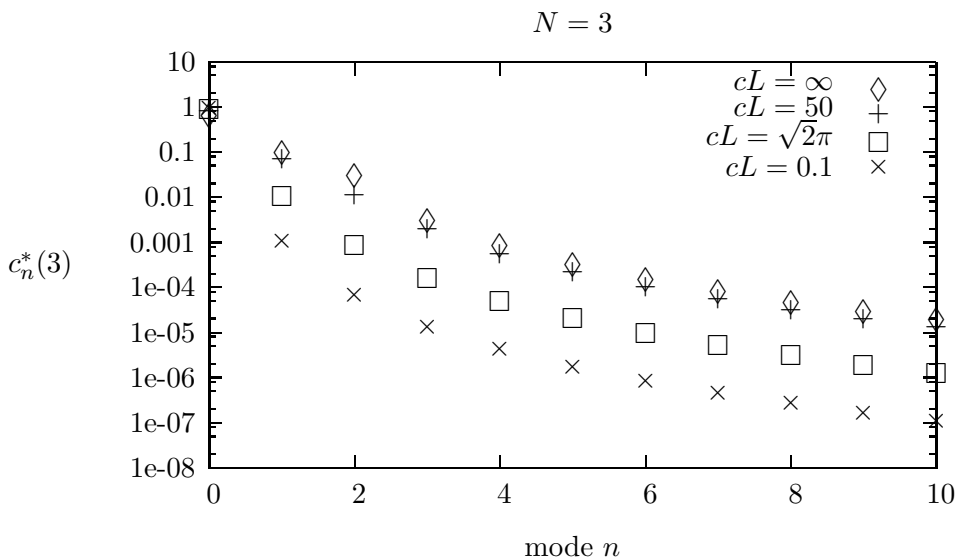


Figure 3.2: Occupation numbers for  $N = 3$

### 3.1.3 $N = 4$

The intricacy of the density matrix at this value of  $N$  is already so great that we go on to calculate the occupation numbers without explicitly exhibiting it, and as such we give only  $c_0(4)$ . We utilise (3.3) and (A.3) to produce the result

$$c_0(4) = 4 \left[ 1 - \frac{1}{240}(cL)^2 + \frac{13}{10080}(cL)^3 - \frac{383}{1209600}(cL)^4 + O(cL)^5 \right]. \quad (3.19)$$

## 3.2 General $N$ small $cL$ expansion

It is interesting to observe that, despite the presence of irrational numbers in the Bethe equations for small  $cL$  (Appendix A), when the final results for the occupation numbers appear they contain purely rational numbers. Upon close examination of (3.8), (3.14) and (3.19), the following polynomial structure for the small  $cL$  expansion of the  $n = 0$  occupation number for general  $N$  is obtained

$$\begin{aligned}
 c_0^*(N) = & 1 - \frac{N-1}{720}(cL)^2 + \frac{N-1}{720} \left( \frac{4(N-1)+1}{42} \right) (cL)^3 \\
 & - \frac{N-1}{720} \frac{1}{42} \left( \frac{45(N-1)^2 - 5(N-1) - 7}{120} \right) (cL)^4 + O(cL)^5. \quad (3.20)
 \end{aligned}$$

Equation (3.20) is written as given to emphasise the detailed structure of the coefficients in this expansion. Note that the coefficient of the  $(N-1)(cL)^p$  term is a polynomial of order  $p-2$  in  $N-1$  for  $p \geq 2$ . Therefore, to obtain, say, the coefficient of the  $(cL)^5$  term we would need  $c_0(N)$  for four specific values of  $N$  in their rational form. Though it was too computationally expensive to obtain any  $N-1$  polynomial for any higher order than  $(cL)^4$ , we conjecture that this pattern holds for all  $N \geq 2$ .

The observations that the coefficient of the  $(N-1)(cL)^p$  term appears to be a polynomial of degree  $p-2$  in  $N-1$  suggests that for any finite  $N$  there is always an interval  $cL \in [0, D_N)$  such that the series is convergent, but with  $D_N \rightarrow 0$  as  $N \rightarrow \infty$ . To quantify this last point, note that in the thermodynamic limit the dimensionless parameter is  $c/\rho_0 = \Gamma$  and the coefficient is proportional to  $N^{2p-1}$ , which suggests that the corresponding radius of convergence is proportional to  $1/N^2$ . In particular this means that no information can be gleaned as to the functional form of  $c_0^*(N)$  as a function of  $\Gamma$  about  $\Gamma=0$  except that it is not analytic.

### 3.3 General $N$ large $cL$ expansion

In Section 3.1, we gave large  $cL$  expansions for the density matrices and occupation numbers for  $N = 2$  and  $N = 3$ . Again, it was computationally prohibitive to go beyond  $N = 4$ . Furthermore, as can be seen from the coefficients in these expansions (and as can be witnessed in the Tables D.1-D.6 which we will refer to in what follows), that the numbers are highly irrational suggesting that there is little hope of finding an analogous pattern to that which we were fortunate enough to find in (3.20).

We therefore turn to a totally different mathematical strategy to obtain a large  $cL$  expansion for these quantities. In the impenetrable limit ( $cL = \infty$ , arbitrary  $L$ ), Lenard [30] developed the theory for the density matrix for arbitrary  $N$ , and went on to show that, for asymptotically large  $N$ ,  $c_0(N) \sim N^{1/2}$ .

In recent work [16] Lenard's theory was employed to obtain the results for the occupation numbers for a range of finite  $N$ , and from them determine the results for general  $N$ , which continue on to the asymptotically large  $N$  limit<sup>3</sup>.

To go beyond the impenetrable limit for these quantities, we turn to the very valuable work of Jimbo and Miwa [23]. Building upon the work of Lenard [30], they developed an expansion for the density matrix in the large  $cL$  limit for general  $N$  in principle. We say in principle because while their expansion is superb in the form given, it is as numerically prohibitive to use as was the method we employed in the previous section.

To resolve this difficulty we have recast their theory, using mathematical techniques developed in recent work [17] and presented in great detail by Forrester [14], into a new form that is readily amenable to numerical calculation. We will find in what follows that the specific results for  $N = 2$  and  $N = 3$ , in Section 3.1, are useful specific checks to the theory.

In Subsection 3.3.1 and 3.3.2, along with Appendix C, we present the full details of our derivation of the density matrix. Following that, in Subsection 3.3.3 we calculate the occupation numbers for a finite range of  $N$  values and from these results we determine the results for general  $N$  which again continue to asymptotically large  $N$ .

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<sup>3</sup>See [16] for a comprehensive list of references for the impenetrable limit.

The fact that  $|\psi_N|^2$  consists of  $(N!)^2$  terms means any method based on term-by-term integration must necessarily be restricted to small  $N$ . To overcome this, one must seek out structure in the form of  $\psi_N$ , and this structure must be used to reduce the computational expense required to compute  $\rho_N(x, 0)$ .

Let us introduce the notation

$$\rho_N(x, y) = \rho_N^{(0)}(x, y) + \left(\frac{1}{cL}\right) \rho_N^{(1)}(x, y) + O\left(\frac{1}{cL}\right)^2, \quad (3.21)$$

and now develop the mathematical path necessary to efficiently compute both  $\rho_N^{(0)}(x, 0)$  and  $\rho_N^{(1)}(x, 0)$ .

### 3.3.1 $\rho_N^{(0)}(x, 0)$

In the limit  $cL \rightarrow \infty$  there is structure in the wave function (2.30), for then the large  $cL$  expansion of  $k_j$  (2.39) gives  $k_j = (2j - N - 1)\pi/L$ , while (2.34) gives  $a(p) = 1$ , and so

$$\psi_N(x_1, \dots, x_N)|_{cL \rightarrow \infty} = \sum_{p \in S_N} \epsilon(p) \prod_{j=1}^N e^{i\pi(2j-N-1)x_{p(j)}/L}. \quad (3.22)$$

Strictly the magnitude of this wave function should be used [19, 31], hence this wave function can also be expressed

$$\left| \det(e^{i\pi(2j-N-1)x_p/L})_{j,p=1,\dots,N} \right| = \left| \det(e^{2i\pi j x_p/L})_{j,p=1,\dots,N} \right| \quad (3.23)$$

$$= \prod_{1 \leq p < j \leq N} \left| e^{2i\pi x_j/L} - e^{2i\pi x_p/L} \right| \quad (3.24)$$

where (3.23) is in the form of a Vandermonde determinant<sup>4</sup>, and (3.24) is related to (3.23) by the property of Vandermonde determinants expressed in [20]<sup>5</sup>.

The aim now is to express the density matrix in the limit  $cL \rightarrow \infty$  as a determinant (this method follows that of Lenard [30]).

Currently, our definition of the density matrix (where in the limit  $cL \rightarrow \infty$ ,  $\mathcal{N}^2 = NL^{N-1}$ ) appears in a slightly modified form from (3.1) as

$$\rho_N^{(0)}(x, y) = L^{-N} \int_0^L dx_1 \dots \int_0^L dx_{N-1} \psi_N(x_1, \dots, x_{N-1}, y)|_{cL \rightarrow \infty} \times \overline{\psi_N(x_1, \dots, x_{N-1}, x)}|_{cL \rightarrow \infty}, \quad (3.26)$$

where we no longer explicitly map out the sum which defines the ordering of the integration; it is now implicitly assumed that we must keep  $0 \leq x_1 < x_2 < \dots < x_N \leq L$ . It is useful to relate  $\psi_N$  to  $\psi_{N-1}$  using (3.24), to approach the form of a Fourier transform

$$\psi_N(x_1, \dots, x_N)|_{cL \rightarrow \infty} = \psi_{N-1}(x_1, \dots, x_{N-1})|_{cL \rightarrow \infty} \prod_{r=1}^{N-1} \left| e^{2\pi i x_r/L} - e^{2\pi i x_N/L} \right|. \quad (3.27)$$

It is also convenient to rescale variables, so that<sup>6</sup>

$$\rho_N^{(0)}(x, 0) = \frac{1}{L} R_N \left( \frac{2\pi x}{L} \right). \quad (3.28)$$

Also, let  $x = \alpha\pi/L$ ,  $y = -\alpha\pi/L$  and  $\theta_i = 2\pi x_i/L$ . Now  $R_N(\alpha)$ ,  $\alpha$  and  $\theta_i$  are all unitless,

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<sup>4</sup>A Vandermonde determinant is the determinant of a Vandermonde matrix, expressed in general as

$$\begin{pmatrix} x_1^0 & x_2^0 & \dots & x_n^0 \\ x_1^1 & x_2^1 & \dots & x_n^1 \\ x_1^2 & x_2^2 & \dots & x_n^2 \\ \vdots & \vdots & & \vdots \\ x_1^{n-1} & x_2^{n-1} & \dots & x_n^{n-1} \end{pmatrix} \quad (3.25)$$

<sup>5</sup>The determinant of any Vandermonde matrix as given above, is equivalent to  $\prod_{1 \leq i < j \leq n} (x_j - x_i)$ .

<sup>6</sup>Note that  $\rho_N(x, y) = \rho_N(x - y, 0)$ .

### 3. DENSITY MATRIX AND OCCUPATION NUMBERS

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and  $\alpha \geq 0$  throughout. So, using (3.24) and (3.27) the scaled density matrix becomes

$$R_N(\alpha) = L^{1-N} \int_0^{2\pi} \frac{L}{2\pi} d\theta_1 \dots \int_0^{2\pi} \frac{L}{2\pi} d\theta_{N-1} \prod_{1 \leq n < m}^{N-1} |e^{i\theta_n} - e^{i\theta_m}|^2 \times \prod_{r=1}^{N-1} \left| e^{i\theta_r} - e^{i\alpha/2} \right| \left| e^{i\theta_r} - e^{-i\alpha/2} \right|. \quad (3.29)$$

If we let

$$f(\theta, \alpha) = \left| e^{i\theta} - e^{i\alpha/2} \right| \left| e^{i\theta} - e^{-i\alpha/2} \right| = 2 \left| \cos \theta - \cos \frac{\alpha}{2} \right|, \quad (3.30)$$

then

$$R_N(\alpha) = (2\pi)^{1-N} \int_0^{2\pi} d\theta_1 \dots \int_0^{2\pi} d\theta_{N-1} \prod_{r=1}^{N-1} f(\theta, \alpha) \prod_{1 \leq n < m}^{N-1} \left| e^{i\theta_n} - e^{i\theta_m} \right|^2. \quad (3.31)$$

Now we can use the Toeplitz determinant technique of Appendix B to obtain

$$\rho_N(x) = \frac{(N-1)!}{L} \det_{1 \leq n, m \leq N-1} c_{n-m} \left( \frac{2\pi x}{L} \right), \quad (3.32)$$

where  $c_n(\alpha)$  is given by

$$\begin{aligned} c_n(\alpha) &= \frac{1}{2\pi} \int_0^{2\pi} e^{in\theta} f(\theta, \alpha) d\theta \\ &= 2\delta_{n,0} \cos(\alpha/2) - \delta_{n,1} - \delta_{n,-1} \\ &\quad + \frac{2}{\pi} \left[ g_{n+1}(\alpha) + g_{n-1}(\alpha) - 2 \cos(\alpha/2) g_n(\alpha) \right], \end{aligned} \quad (3.33)$$

where

$$g_n(\alpha) = \lim_{n' \rightarrow n} \frac{\sin(\frac{1}{2}n'|\alpha|)}{n'}. \quad (3.34)$$

The absolute value sign in (3.34) can be ignored, as  $\alpha \geq 0$ .

While the sum (3.22) consists of  $N!$  terms, the determinant (3.32) can be computed in  $O(N^3)$  arithmetic operations. This significantly reduces the numerical computation time in evaluating  $\rho_N^{(0)}(x, 0)$ .

### 3.3.2 $\rho_N^{(1)}(x, 0)$

It has been shown by Jimbo and Miwa [23] (see also Section 4.3 below) that determinant structures persist if  $\psi_N$  is expanded in large  $cL$ , and that this implies special structures for the expansion of the density matrix. In particular, it was shown in [23] that

$$\rho_N^{(1)}(x, 0) = -2\rho_0 x \frac{\partial}{\partial x} \rho_N^{(0)}(x, 0) + F_N(x), \quad (3.35)$$

where  $\rho_N^{(0)}(x, 0)$  is specified by (3.32) and (3.28) and

$$\begin{aligned} F_N(x) = \frac{1}{\Delta_0(-2)} & \left[ \frac{\partial}{\partial x} \Delta_1 \left( \begin{array}{c} x \\ 0 \end{array}; \lambda \right) \frac{\partial}{\partial \lambda} \Delta_0(\lambda) \right. \\ & + \frac{\partial}{\partial \lambda} \Delta_1 \left( \begin{array}{c} x \\ 0 \end{array}; \lambda \right) \frac{\partial}{\partial x} \Delta_0(\lambda) \\ & \left. - \Delta_1 \left( \begin{array}{c} x \\ 0 \end{array}; \lambda \right) \frac{\partial^2}{\partial x \partial \lambda} \Delta_0(\lambda) \right] \Bigg|_{\lambda=-2}. \end{aligned} \quad (3.36)$$

The functions  $\Delta_0$  and  $\Delta_1$  are Fredholm minors<sup>7</sup>, specifically,  $\Delta_0$  and  $\Delta_1$  are the zeroth Fredholm minor (or Fredholm determinant) and first Fredholm minor respectively.

It is desirable to compute  $\rho_N^{(1)}(x, 0)$  given in (3.35), however the form of  $\Delta_0$  and  $\Delta_1$  (C.1) required to calculate  $F_N(x)$  (3.36) prove particularly difficult for numerical calculation.

By noticing that  $\rho_N^{(0)}(x, 0)$  is related to  $\Delta_1$  by

<sup>7</sup>please refer to Section C.1 for a concise description of the notation.



$$\rho_N^{(0)}(x, 0) = -\frac{1}{2}\Delta_1\left(\begin{array}{c} x \\ 0 \end{array}; -2\right), \quad (3.37)$$

one can utilise properties of multi-dimensional integrals and Toeplitz determinants, based on Lenard's method [30] (given in Section 3.3.2), to cast both  $\Delta_0$  and  $\Delta_1$  into a form much more amenable to numerical calculation. This is done for general  $n$  in Appendix C. The resulting forms are given by, for  $\Delta_0$

$$\Delta_0(\lambda) = \det [A_0(j - k)]_{j,k=1,\dots,N}, \quad (3.38)$$

where

$$\begin{aligned} A_0(j) &= \frac{1}{L} \left( \int_0^L + \lambda \int_0^x \right) du \exp[2\pi i u j / L] \\ &= \begin{cases} 1 + \frac{\lambda x}{L} & \text{when } j = 0 \\ \frac{\lambda}{2i\pi j} (e^{2i\pi j x / L} - 1) & \text{when } j \neq 0, \end{cases} \end{aligned} \quad (3.39)$$

and for  $\Delta_1$

$$\Delta_1\left(\begin{array}{c} x \\ 0 \end{array}; \lambda\right) = \lambda e^{-i\pi(N-1)x/L} \det [A_1(j - k)]_{j,k=1,\dots,N-1}, \quad (3.40)$$

where

$$\begin{aligned}
A_1(j) &= \frac{1}{L} \left( \int_0^L + \lambda \int_0^x \right) du (e^{2\pi i u/L} - e^{2\pi i x/L}) (e^{-2\pi i u/L} - 1) e^{2\pi i u j/L} \\
&= \begin{cases} \frac{\lambda}{2\pi} \sin 2t - \frac{t\lambda}{\pi} - 1 & \text{when } j = -1 \\ 2e^{it} \left[ \left( \frac{t\lambda}{\pi} + 1 \right) \cos t - \frac{\lambda}{\pi} \sin t \right] & \text{when } j = 0 \\ e^{2it} \left[ \frac{\lambda}{2\pi} \sin 2t - \frac{t\lambda}{\pi} - 1 \right] & \text{when } j = 1 \\ \frac{2\lambda i e^{i(j+1)t}}{j(j^2-1)\pi} [j \cos jt \sin t - \cos t \sin jt] & \text{when } |j| \geq 2. \end{cases} \quad (3.41)
\end{aligned}$$

In [16] this determinant formula was used to compute the density matrix and the corresponding ground state occupation numbers up to  $N = 7$ .

The numerical complexity has been greatly reduced with these new forms, as  $\Delta_0$  and  $\Delta_1$  were previously composed of multi-dimensional integrals (C.1), and now are given by determinants containing no integrals (3.38) and (3.40).

With these determinant formulas  $F_N(x)$  is expressed in a computable form. This concludes the method necessary to construct the density matrix expanded in large  $cL$ . The following section applies this method to examine the occupation numbers.

### 3.3.3 Occupation numbers

The notation for the occupation number  $c_n(N)$  expanded in large  $cL$  is given as

$$c_n(N) = c_n^{(0)}(N) + \left( \frac{1}{cL} \right) c_n^{(1)}(N) + O\left( \frac{1}{cL} \right)^2. \quad (3.42)$$

Using (3.3) and (3.21),  $c_n^{(0)}(N)$  is related to  $\rho_N^{(0)}(x, 0)$  by

$$c_n^{(0)}(N) = \int_0^L \rho_N^{(0)}(x, 0) \cos\left( \frac{2\pi n x}{L} \right) dx. \quad (3.43)$$

The  $c_n^{(1)}(N)$  term can be expanded further as

$$\begin{aligned}
 c_n^{(1)}(N) &= \int_0^L \rho_N^{(1)}(x, 0) \cos\left(\frac{2\pi nx}{L}\right) dx \\
 &= \int_0^L \left(-2Nx \frac{\partial \rho_N^{(0)}(x, 0)}{\partial x} + F_N(x)\right) \cos\left(\frac{2\pi nx}{L}\right) dx \\
 &= c_n^{(1,1)}(N) + c_n^{(1,2)}(N),
 \end{aligned} \tag{3.44}$$

where  $F_N(x)$  may be computed using the expressions in Subsection 3.3.2 above. The  $c_n^{(1,1)}(N)$  term can be simplified using integration by parts to

$$c_n^{(1,1)}(N) = -2N^2 + 2Nc_n^{(0)}(N) - 4\pi nN \int_0^L \frac{x}{L} \sin(2\pi nx/L) \rho_n^{(0)}(x) dx. \tag{3.45}$$

The exact values of  $c_n^{(0)}(N)$  and  $c_n^{(1)}(N)$  for  $n = 0$  ( $N = 2, \dots, 7$ ) and  $n = 1, 2$  ( $N = 2, \dots, 6$ ) are listed in Tables D.1, D.2 and D.3. The exact values of  $c_n^{(1,1)}(N)$  and  $c_n^{(1,2)}(N)$  for  $n = 0, 1, 2$  with  $N = 2, \dots, 6$  are listed in Tables D.4, D.5 and D.6. All numerical values computed for  $c_n^{*(0)}(N)$ ,  $c_n^{*(1,1)}(N)$ ,  $c_n^{*(1,2)}(N)$  and  $c_n^{*(1)}(N)$  obtained for  $n = 0, 1, 2$  are presented in Tables D.7, D.8 and D.9. In these tables, the data is given to 6 significant figures for economy of presentation, while in point of fact, accuracy to 10 significant figures was needed for the analysis that now follows. This numerical accuracy was achieved for up to  $N = 36$  for the  $n = 0$  mode, and up to  $N = 26$  for the modes  $n = 1$  and  $n = 2$ . Note that  $c_n^{*(0)}(N)$  for  $n = 0, 1, 2$  reproduces the results of [16].

While 36 particles is an improvement on the 4 particles of Section 3.1, experiments are yet to use less than  $\sim 10^5$  particles (Section 1.2). Hence it is useful to predict the occupation numbers for large  $N$ . In [16], it was found that the occupation numbers in the large  $N$ ,  $cL = \infty$  limit are proportional to  $\sqrt{N}$  (49). They designed an ansatz containing a term proportional to  $\sqrt{N}$ , a term proportional to  $1/\sqrt{N}$ , and a constant term. The following ansatz extends their work by expanding the coefficients of two of these terms to  $O(1/cL)$

$$c_n(N) = A_{\infty,n} \left(1 + \frac{\alpha_n N}{cL}\right) N^{\frac{1}{2} + \frac{\beta_n N}{cL}} + C_{\infty,n} \left(1 + \frac{\gamma_n N}{cL}\right) \quad (3.46)$$

$$\begin{aligned} &= (A_{\infty,n} \sqrt{N} + C_{\infty,n}) \\ &\quad + N(A_{\infty,n} \alpha_n \sqrt{N} + A_{\infty,n} \beta_n \sqrt{N} \ln N + C_{\infty,n} \gamma_n) \left(\frac{1}{cL}\right) + O\left(\frac{1}{cL}\right)^2. \end{aligned} \quad (3.47)$$

It is now pertinent to determine bounds on  $\alpha_n$  and  $\beta_n$ , and a value for  $\gamma_n$ . Consider the set of three linear equations describing the  $1/cL$  term of (3.47) for three consecutive values of  $N$

$$\begin{pmatrix} \sqrt{N-1} & \sqrt{N-1} \ln(N-1) & 1 \\ \sqrt{N} & \sqrt{N} \ln(N) & 1 \\ \sqrt{N+1} & \sqrt{N+1} \ln(N+1) & 1 \end{pmatrix} \begin{pmatrix} A_{\infty,n} \alpha_n \\ A_{\infty,n} \beta_n \\ C_{\infty,n} \gamma_n \end{pmatrix} = \begin{pmatrix} c_n^{*(1)}(N-1) \\ c_n^{*(1)}(N) \\ c_n^{*(1)}(N+1) \end{pmatrix}, \quad (3.48)$$

and the set of two linear equations describing the  $1/cL$  term of (3.47) with  $C_{\infty,n} = 0$  for two consecutive values of  $N$

$$\begin{pmatrix} \sqrt{N} & \sqrt{N} \ln(N) \\ \sqrt{N+1} & \sqrt{N+1} \ln(N+1) \end{pmatrix} \begin{pmatrix} A_{\infty,n} \alpha_n \\ A_{\infty,n} \beta_n \end{pmatrix} = \begin{pmatrix} c_n^{*(1)}(N) \\ c_n^{*(1)}(N+1) \end{pmatrix}. \quad (3.49)$$

Values of  $A_{\infty,n}$  and  $C_{\infty,n}$  from [16] are displayed in Table 3.1. The solution for  $\alpha_n, \beta_n, \gamma_n$ , of (3.48) and the solution for  $\alpha_n, \beta_n$  for (3.49) for various values of  $N$  establish bounds on  $\alpha_n$  and  $\beta_n$ , and a value for  $\gamma_n$ . Numerical stability for these bounds is established by calculating them for  $N = 2$  up to  $N = 35$ . A fractional accuracy of  $\gtrsim 10^{-10}$  is necessary, and hence the parameters are calculated at  $N = 35$  for  $n = 0$ , and  $N = 25$  for  $n = 1$  and  $n = 2$ . These are presented in Table 3.1.

$n$	$A_{\infty,n}$	$C_{\infty,n}$	$\alpha_n$	$\beta_n$	$\gamma_n$
0	1.54273	-0.5725	$0.1561 < \alpha_0 < 0.1838$	$1.998 < \beta_0 < 2.003$	0.1599
1	0.5143	-0.5739	$-5.709 < \alpha_1 < -5.067$	$1.972 < \beta_1 < 2.094$	-1.109
2	0.3676	-0.5775	$-8.350 < \alpha_2 < -6.121$	$1.887 < \beta_2 < 2.313$	-2.736

Table 3.1: Parameters for the ansatz (3.47)

Note that  $\beta_n$  is very close to 2 for  $n = 0$ , and suggestive of the value 2 for  $n = 1$  and 2. We postulate that  $\beta_n = 2$  for all  $n$ . More is said about  $\beta_n$  in the following section.

### 3.3.4 Concluding remarks

The occupation numbers for the large  $cL$  limit given in (3.46) can be continued to the asymptotically large  $N$  limit giving

$$c_n(N) \sim N^{\frac{1}{2} + \frac{\beta_n N}{cL}}. \quad (3.50)$$

Very strong evidence for the exponent  $\beta_n$  having the integer value 2 was presented.

In constructing the ansatz for the occupation numbers, we chose to scale  $cL$  by  $N$  from the outset. This was done because the  $cL$  large limit is now compatible with the thermodynamic limit (unlike the small  $cL$  limit as discussed after (3.20)) and further to this we found that the numerical analysis, for any finite  $N$ , in constructing the ansatz, failed without this scaling.

The question then is, how does (3.50) compare with the thermodynamic limit. In a very nice work, at a time coincident with the seminal work of the Japanese group [23, 24], the density matrix first given by Lenard in the impenetrable limit [30], was extended to the  $1/c$  correction [9]. They used the quantum inverse-scattering method in concert with the very important work [24] on the impenetrable Bose gas in terms of Painlevé V theory, and obtained

$$\rho(\mathbf{x}) \sim \frac{1}{|\mathbf{x}|^{\frac{1}{2} + \frac{2k_F}{\pi c}}}. \quad (3.51)$$

The Fourier transform of (3.51) gives the momentum distribution, with the Fermi momentum,  $k_F = \pi\rho_0$ ,

$$c(\mathbf{k}) \sim \frac{1}{|\mathbf{k}|^{\frac{1}{2} + \frac{2k_F}{\pi c}}}. \quad (3.52)$$

Following the presentation given in [16], one can readily see that (3.50) is one-to-one with (3.52). An elementary way to see this immediately is to observe that  $|\mathbf{k}| \sim 1/L$  and thus in the thermodynamic limit  $|\mathbf{k}| \sim 1/N$ . Note the integer value of 2 for the coefficient of  $k_F/\pi c$  in the exponent (3.51) and (3.52).

In previous work on the impenetrable Bose gas [15, 16], the system was studied for various boundary conditions; periodic, Dirichlet, Neumann, as well as for the harmonically trapped system. In all cases, it was found that in the asymptotically large  $N$  limit that (3.50) held in the limit  $cL \rightarrow \infty$ . This firmly suggests that the exponent obtained in this large  $N$  limit is universal, being the same for all boundary conditions and (low lying)  $n$  modes. Therefore, one may anticipate the same is true now for (3.50).

The use of periodic boundary conditions, while facilitating the mathematics, is nonetheless a powerful pre-emptor of the analytical properties of the Bose gas.

### 3. DENSITY MATRIX AND OCCUPATION NUMBERS

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CORRELATION FUNCTIONS  
AND  
STRUCTURE FACTORS

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4

This chapter examines the correlation function and its Fourier transform the structure factor. Specific examples are given in Section 4.1 for 2, 3 and 4 particles. Polynomial structure for the general  $N$ , small  $cL$  expansion is given in Section 4.2. Finally the correlation function in the general  $N$ , large  $cL$  expansion is derived in general in Section 4.3, and examined in the thermodynamic limit.

The definition of the two-point correlation function  $g_N(x, 0)$  is

$$g_N(x, 0) = \frac{1}{\mathcal{N}^2} \sum_{j=0}^{N-2} \int_{R_{N-2,j}(x)} dx_1 \dots dx_{N-2} |\psi_N(0, x_1, \dots, x_j, x, x_{j+1}, \dots, x_{N-2})|^2, \quad (4.1)$$

where the normalisation  $\mathcal{N}^2$  is specified by (2.35) and the domain of integration by (3.2). Equation (4.1) has the property

$$\int_0^L g_N(x, 0) dx = N - 1, \quad (4.2)$$

in keeping with the interpretation of  $g_N(x, 0)$  as the density of particles at position  $x$ , given there is a particle at the origin. The structure factor is defined by

$$\mathcal{S}_n(N) = \frac{1}{N} \frac{1}{\mathcal{N}^2} \int_{R_{N-1,j}} dx_1 \dots dx_{N-2} \left| \sum_{j=0}^{N-1} e^{2i\pi x_j n/L} \right|^2 |\psi_N(0, x_1, \dots, x_{N-1})|^2, \quad (4.3)$$



where  $x_0 = 0$ , which can be written in terms of  $g_N(x, 0)$  to read

$$\mathcal{S}_n(N) = 1 + \int_0^L g_N(x, 0) \cos(2\pi nx/L) dx. \quad (4.4)$$

In view of (4.2) this gives  $\mathcal{S}_0(N) = N$ .

## 4.1 Specific examples

### 4.1.1 $N = 2$

This subsection yields the most complete set of results within Section 4, with the set of results for  $N = 3$  and  $N = 4$  becoming increasingly limited. For  $N = 4$ , we display only the small  $cL$  expansion of the correlation function and structure factor.

It is possible to produce a simple, exact form of the correlation function for  $N = 2$  by utilising (3.4) and (4.1) to obtain

$$g_2(x, 0) = \frac{2k_2 \cos^2[\frac{1}{2}k_2(L - 2x)]}{k_2L + \sin(k_2L)}, \quad (4.5)$$

which has corresponding structure factor

$$\mathcal{S}_n(2) = \begin{cases} 2 & \text{when } n = 0 \\ 1 + \frac{k_2^2 L^2 \sin(k_2L)}{(k_2^2 L^2 - n^2 \pi^2)(k_2L + \sin(k_2L))} & \text{when } n \neq 0. \end{cases} \quad (4.6)$$

The correlation function, expanded about small  $cL$  using (A.1), is given by

$$g_2(x, 0) = \frac{1}{L} \left[ 1 + \left( -\frac{x^2}{L^2} + \frac{x}{L} - \frac{1}{6} \right) (cL) + \left( \frac{x^4}{3L^4} - \frac{2x^3}{3L^3} + \frac{x^2}{2L^2} - \frac{x}{6L} + \frac{1}{60} \right) (cL)^2 \right. \\ \left. + \left( -\frac{2x^6}{45L^6} + \frac{2x^5}{15L^5} - \frac{7x^4}{36L^4} + \frac{x^3}{6L^3} - \frac{7x^2}{90L^2} + \frac{x}{60L} - \frac{1}{945} \right) (cL)^3 + O(cL)^4 \right], \quad (4.7)$$

and hence the structure factor is given by

$$\mathcal{S}_n(2) = \begin{cases} 2 & \text{when } n = 0 \\ 1 - \frac{1}{2n^2\pi^2}(cL) + \frac{n^2\pi^2-6}{12n^4\pi^4}(cL)^2 \\ -\frac{n^4\pi^4-15n^2\pi^2+60}{120n^6\pi^6}(cL)^3 + O(cL)^4 & \text{when } n \neq 0. \end{cases} \quad (4.8)$$

The large  $cL$  expansion of the correlation function is given using (2.39)

$$g_2(t, 0) = \frac{1}{L} \left\{ 2 \sin^2 t + 8 \sin t [(\pi - 2t) \cos t - \sin t] \left( \frac{1}{cL} \right) + O \left( \frac{1}{cL} \right)^2 \right\}, \quad (4.9)$$

taking the Fourier transform then yields the structure factor

$$\mathcal{S}_n(2) = \begin{cases} 2 & \text{when } n = 0 \\ \frac{1}{2} + 3 \left( \frac{1}{cL} \right) + O \left( \frac{1}{cL} \right)^2 & \text{when } |n| = 1 \\ 1 - \frac{4}{(n^2-1)} \left( \frac{1}{cL} \right) + O \left( \frac{1}{cL} \right)^2 & \text{when } |n| \geq 2. \end{cases} \quad (4.10)$$

The correlation function for the special values  $cL = \pi$ ,  $k_2L = \pi/2$ , (see Table 2.2) is

$$g_2(t, 0) = \frac{\pi (\sin t + 1)}{L(\pi + 2)}, \quad (4.11)$$

and hence the structure factor is

$$\mathcal{S}_n(2) = \begin{cases} 2 & \text{when } n = 0 \\ 1 - \frac{2}{(4n^2-1)(\pi+2)} & \text{when } n \neq 0. \end{cases} \quad (4.12)$$

**4.1.2**  $N = 3$ 

Given the length of the full correlation function for  $N = 3$ , it is not practical to display the full result here, however we shall display the small and large  $cL$  expansions for both the correlation function and the structure factor.

The small  $cL$  expansion of the correlation function is given, using (A.2)

$$g_3(x, 0) = \frac{2}{L} \left[ 1 + \left( -\frac{x^2}{L^2} + \frac{x}{L} - \frac{1}{6} \right) (cL) + \left( \frac{x^4}{12L^4} - \frac{x^3}{6L^3} + \frac{x^2}{4L^2} - \frac{x}{6L} + \frac{1}{40} \right) (cL)^2 + \left( \frac{x^6}{5L^6} - \frac{3x^5}{5L^5} + \frac{5x^4}{8L^4} - \frac{x^3}{4L^3} + \frac{x}{40L} - \frac{1}{280} \right) (cL)^3 + O(cL)^4 \right], \quad (4.13)$$

and hence the structure factor by

$$\mathcal{S}_n(3) = \begin{cases} 3 & \text{when } n = 0 \\ 1 - \frac{1}{n^2\pi^2}(cL) + \frac{2n^2\pi^2-3}{12n^4\pi^4}(cL)^2 \\ -\frac{n^4\pi^4+15n^2\pi^2-180}{40n^6\pi^6}(cL)^3 + O(cL)^4 & \text{when } n \neq 0. \end{cases} \quad (4.14)$$

The large  $cL$  expansion for the correlation function is given using (2.39)

$$g_3(t, 0) = \frac{2}{L} \left\{ \frac{4(2 + \cos 2t) \sin^2 t}{3} - \frac{8 \sin t [-2(\pi - 2t)(2 \cos t + \cos 3t) + 3 \sin t + 4 \sin 3t]}{3} \left( \frac{1}{cL} \right) + O\left( \frac{1}{cL} \right)^2 \right\}, \quad (4.15)$$

which yields the structure factor

$$\mathcal{S}_n(3) = \begin{cases} 3 & \text{when } n = 0 \\ \frac{1}{3} + \frac{32}{9} \left(\frac{1}{cL}\right) + O\left(\frac{1}{cL}\right)^2 & \text{when } |n| = 1 \\ \frac{2}{3} + \frac{38}{9} \left(\frac{1}{cL}\right) + O\left(\frac{1}{cL}\right)^2 & \text{when } |n| = 2 \\ 1 - \frac{16(n^2-2)}{(n^2-4)(n^2-1)} \left(\frac{1}{cL}\right) + O\left(\frac{1}{cL}\right)^2 & \text{when } |n| \geq 3. \end{cases} \quad (4.16)$$

We now display the correlation function for the special values  $k_3L = \pi$ ,  $cL = \sqrt{2}\pi$ , (from Table 2.2)

$$g_3(t, 0) = -\frac{2\pi}{L(16 + 16\sqrt{2}\pi + 9\pi^2)} \left[ 2(4\sqrt{2} - \pi) \cos t - \pi \cos 2t \right. \\ \left. - 4(2 + \sqrt{2}\pi) \sin t + 2(6 + \sqrt{2}\pi) \sin 2t - 9\pi - 8\sqrt{2} \right], \quad (4.17)$$

and the corresponding structure factor

$$\mathcal{S}_n(3) = \begin{cases} 3 & \text{when } n = 0 \\ 1 - \frac{32+16\sqrt{2}\pi-3\pi^2}{48+48\sqrt{2}\pi+27\pi^2} & \text{when } |n| = 1 \\ 1 - \frac{16(2+\sqrt{2}\pi)}{(4n^2-1)(16+16\sqrt{2}\pi+9\pi^2)} & \text{when } |n| \geq 2. \end{cases} \quad (4.18)$$

#### 4.1.3 $N = 4$

Due to increasing complexities, here we display only the correlation function for the small  $cL$  expansion of  $N = 4$

$$g_4(x, 0) = \frac{3}{L} \left[ 1 + \left( -\frac{x^2}{L^2} + \frac{x}{L} - \frac{1}{6} \right) (cL) + \left( -\frac{x^4}{6L^4} + \frac{x^3}{3L^3} - \frac{x}{6L} + \frac{1}{30} \right) (cL)^2 \right. \\ \left. + \left( \frac{7x^6}{18L^6} - \frac{7x^5}{6L^5} + \frac{47x^4}{36L^4} - \frac{2x^3}{3L^3} + \frac{19x^2}{180L^2} + \frac{x}{30L} - \frac{1}{135} \right) (cL)^3 + O(cL)^4 \right], \quad (4.19)$$

and its corresponding structure factor

$$\mathcal{S}_n(4) = \begin{cases} 4 & \text{when } n = 0 \\ 1 - \frac{3}{2n^2\pi^2}(cL) + \frac{n^2\pi^2+3}{4n^4\pi^4}(cL)^2 \\ -\frac{2n^4\pi^4+60n^2\pi^2-525}{40n^6\pi^6}(cL)^3 + O(cL)^4 & \text{when } n \neq 0. \end{cases} \quad (4.20)$$

## 4.2 General $N$ small $cL$ expansion

Through close examination of the small  $cL$  expansions of the correlation function for  $N = 2$  (4.7),  $N = 3$  (4.13) and  $N = 4$  (4.19), we find the following polynomial structure

$$\begin{aligned} g_N(x, 0) = & \frac{N-1}{L} \left\{ 1 - f(x)(cL) \right. \\ & + \left[ \left( -\frac{N}{4} + \frac{5}{6} \right) f(x)^2 + \left( \frac{N}{12} - \frac{1}{9} \right) f(x) + \left( \frac{N}{720} - \frac{1}{216} \right) \right] (cL)^2 \\ & + \left[ \left( -\frac{N^2}{36} + \frac{23N}{60} - \frac{7}{10} \right) f(x)^3 + \left( \frac{N^2}{36} - \frac{7N}{40} + \frac{1}{5} \right) f(x)^2 \right. \\ & \left. \left. + \left( -\frac{N^2}{144} + \frac{13N}{720} - \frac{1}{120} \right) f(x) + \left( -\frac{N^2}{6804} + \frac{79N}{90720} - \frac{1}{1080} \right) \right] (cL)^3 + O(cL)^4 \right\} \end{aligned} \quad (4.21)$$

where  $f(x) = x^2/L^2 - x/L + 1/6$ . We conjecture that this structure continues for all  $N$ . This has corresponding structure factor

$$\mathcal{S}_n(N) = \begin{cases} N & \text{when } n = 0 \\ 1 - \frac{(N-1)}{2n^2\pi^2}(cL) + \frac{(N-1)(2n^2\pi^2+9N-30)}{24n^4\pi^4}(cL)^2 \\ -\frac{(N-1)(Nn^4\pi^4+75Nn^2\pi^2-180n^2\pi^2+75N^2-1035N+1890)}{240n^6\pi^6}(cL)^3 \\ +O(cL)^4 & \text{when } n \neq 0 \end{cases} \quad (4.22)$$

We have not proceeded further than  $N = 4$  for the large  $cL$  expansion as similar difficulties are encountered as in the case of the density matrix in Chapter 3. There is now, once again, a powerful way to proceed to develop such an expansion for general  $N$ , and we

present the derivation in the following section. The special case of  $N = 2$  (4.9) and  $N = 3$  (4.15) provide useful checks.

### 4.3 General $N$ large $cL$ expansion

In Section 3.3 results from Jimbo and Miwa [23] were used to express the  $O(1/cL)$  correction to the density matrix in the form of Toeplitz determinants, which could then be numerically analysed. The method of [23] can also be applied to the calculation of the  $O(1/cL)$  correction to the two-point correlation function (4.1), yielding in fact a closed form analytic expression. To derive this, we follow the working in [23], and begin by noting that the  $O(1/cL)$  expansion of (2.30) is

$$\psi_N(x_1, x_2, \dots, x_N) = \left[ 1 + \frac{1}{cL} \hat{G} + O\left(\frac{1}{cL}\right)^2 \right] \det[e^{ik_j x_l}], \quad (4.23)$$

where the det term is understood throughout this section to be expanded about  $j$  and  $l$  over all particles, and where  $\hat{G}$  is an operator given by

$$\hat{G} = L \sum_{l=1}^N (-N + 2l - 1) \frac{\partial}{\partial x_l} - 2N \sum_{l=1}^N x_l \frac{\partial}{\partial x_l}. \quad (4.24)$$

Putting  $N \rightarrow N + 2$  (for convenience), the sums given in  $\hat{G}$  now run from 0 to  $N + 1$ . We label the particles as

$$0 < y < x_1 < \dots < x_j < x < x_{j+1} < \dots < x_N < L. \quad (4.25)$$

In the definition of  $g_{N+2}(x, 0)$ ,  $x$  will be the variable as in (4.25) and we will take  $y \rightarrow 0$ . With these labels and  $N \rightarrow N + 2$  the operator in (4.23) reads

$$\begin{aligned} \hat{G} = & -L(N+1)\frac{\partial}{\partial y} + L\sum_{l=1}^j(-N+2l-1)\frac{\partial}{\partial x_l} + L(-N+2j+1)\frac{\partial}{\partial x} \\ & + L\sum_{l=j+1}^N(-N+2l+1)\frac{\partial}{\partial x_l} - 2(N+2)\left(\sum_{l=1}^N x_l\frac{\partial}{\partial x_l} + x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y}\right). \end{aligned} \quad (4.26)$$

The determinant in (4.23) has the translation invariance property

$$\det\begin{pmatrix} e^{ik_j y} \\ e^{ik_j x_k} \end{pmatrix} = \det\begin{pmatrix} 1 \\ e^{ik_j(x_k - y)} \end{pmatrix}, \quad (4.27)$$

since  $\sum k_j = 0$ . This means that we can write

$$\frac{\partial}{\partial y} = -\frac{\partial}{\partial x} - \sum_{l=1}^N \frac{\partial}{\partial x_l}, \quad (4.28)$$

and as  $y \rightarrow 0$ , the operator (4.26) becomes

$$\hat{G} = L\sum_{l=1}^j 2l\frac{\partial}{\partial x_l} + 2L(1+j)\frac{\partial}{\partial x} + \sum_{l=j+1}^N 2L(1+l)\frac{\partial}{\partial x_l} - 2(N+2)\left(\sum_{l=1}^N x_l\frac{\partial}{\partial x_l} + x\frac{\partial}{\partial x}\right). \quad (4.29)$$

In keeping with (4.1), by definition

$$g_{N+2}(x, 0) = \frac{1}{\mathcal{N}^2} \lim_{y \rightarrow 0} \sum_{j=0}^N \int_{R_{N,j}(y,x)} dx_1 \dots dx_N |\psi_{N+2}(y, x_1, \dots, x_j, x, x_{j+1}, \dots, x_N)|^2, \quad (4.30)$$

where  $\mathcal{N}^2$  is the normalisation, defined by (2.35), and  $R_{N,j}(y, x)$  is the region of integration specified by

$$R_{N,j}(y, x) : 0 \leq y \leq x_1 \leq \dots \leq x_j \leq x \leq x_{j+1} \leq \dots \leq x_N \leq L. \quad (4.31)$$

Again relabel the particles as  $(\tilde{x}_1, \tilde{x}_2, \dots, \tilde{x}_{N+2}) = (0, x_1, \dots, x_j, x, x_{j+1}, \dots, x_N)$ , and introduce

$$\hat{A} = \sum_{l=1}^N x_l \frac{\partial}{\partial x_l} + x \frac{\partial}{\partial x}, \quad (4.32)$$

$$\hat{B}_j = L \sum_{l=1}^j 2l \frac{\partial}{\partial x_l} + 2L(1+j) \frac{\partial}{\partial x} + L \sum_{l=j+1}^N 2(1+l) \frac{\partial}{\partial x_l}, \quad (4.33)$$

so (4.29) then can be expressed

$$\hat{G} = \hat{B}_j - 2(N+2)\hat{A}, \quad (4.34)$$

so that the limit in (4.30) becomes

$$\begin{aligned} \lim_{y \rightarrow 0} |\psi_{N+2}(y, \tilde{x}_2, \tilde{x}_3, \dots, \tilde{x}_{N+2})|^2 &= \left| \left( 1 + \left( \frac{1}{cL} \right) \hat{G} + O\left( \frac{1}{cL} \right)^2 \right) |\det[e^{ik_j \tilde{x}_l}]|^2 \right|^2 \\ &= |\det[e^{ik_j \tilde{x}_l}]|^2 - \frac{2(N+2)}{cL} \hat{A} \left( |\det[e^{ik_j \tilde{x}_l}]|^2 \right) \\ &\quad + \frac{1}{cL} \hat{B}_j \left( |\det[e^{ik_j \tilde{x}_l}]|^2 \right) + O\left( \frac{1}{cL} \right)^2. \end{aligned} \quad (4.35)$$

The normalisation (2.35) was first expanded in large  $cL$  by [23]. We display here the first two orders

$$\mathcal{N}^2 = (\mathcal{N}^{(\infty)})^2 \left[ 1 + \left( \frac{1}{cL} \right) 2(N+2)(N+1) + O\left( \frac{1}{cL} \right)^2 \right], \quad (4.36)$$

where  $(\mathcal{N}^{(\infty)})^2 = (N+2)!L^{N+1}$  is the normalisation (2.35) in the limit  $cL \rightarrow \infty$ . Substi-



tuting (4.35) and (4.36) into (4.30) shows that to  $O(1/cL)$

$$\begin{aligned}
 g_{N+2}(x, 0) &= g_{N+2}^{(\infty)}(x, 0) - \left(\frac{1}{cL}\right) 2(N+2)(N+1)g_{N+2}^{(\infty)}(x, 0) \\
 &\quad - \left(\frac{1}{cL}\right) 2(N+2) \frac{1}{(\mathcal{N}^{(\infty)})^2} \sum_{j=0}^N \int_{R_{N,j}(x)} dx_1 \dots dx_N \hat{A} \left( |\det[e^{ik_j \tilde{x}_l}]|^2 \right) \\
 &\quad + \left(\frac{1}{cL}\right) \frac{1}{(\mathcal{N}^{(\infty)})^2} \sum_{j=0}^N \int_{R_{N,j}(x)} dx_1 \dots dx_N \hat{B}_j \left( |\det[e^{ik_j \tilde{x}_l}]|^2 \right).
 \end{aligned} \tag{4.37}$$

Observe that

$$g_{N+2}^{(\infty)}(x, 0) = \frac{1}{N!} \frac{1}{(\mathcal{N}^{(\infty)})^2} \int_0^L dx_1 \dots dx_N |\det[e^{ik_j \tilde{x}_l}]|^2 = \frac{N+2}{L} (1 - \tilde{K}_{N+2,L}(x, 0)^2), \tag{4.38}$$

where  $\tilde{K}$  is related to the  $K$  given in (C.3) by

$$\tilde{K}_{N,L}(x, y) = \frac{L}{N} K_{N,L}(x, 0) = \frac{\sin(N\pi(x-y)/L)}{N \sin(\pi(x-y)/L)}. \tag{4.39}$$

Note that (4.38) and (4.39) also appear in the circular unitary ensemble (CUE), given by Dyson [10].

To proceed further consider  $|\det[e^{ik_j \tilde{x}_l}]|^2$  as a function of  $x_l$ , ( $l = 1, \dots, N$ ). This function vanishes at the three points  $x_l = 0, x_j, L$  ( $j \neq l$ ).

It follows that

$$\int_{R_{N,j}(x)} dx_l x_l \frac{\partial}{\partial x_l} |\det[e^{ik_j \tilde{x}_l}]|^2 = - \int_{R_{N,j}(x)} dx_l |\det[e^{ik_j \tilde{x}_l}]|^2, \tag{4.40}$$

while

$$\int_{R_{N,j}(x)} dx_l \frac{\partial}{\partial x_l} |\det[e^{ik_j \tilde{x}_l}]|^2 = 0. \quad (4.41)$$

Hence

$$\begin{aligned} g_{N+2}(x, 0) &= g_{N+2}^{(\infty)}(x, 0) - \left(\frac{1}{cL}\right) 2(N+2)(N+1)g_{N+2}^{(\infty)}(x, 0) \\ &\quad - \left(\frac{1}{cL}\right) 2(N+2) \left(x \frac{\partial}{\partial x} - N\right) g_{N+2}^{(\infty)}(x, 0) \\ &\quad + \frac{1}{cL} \frac{L}{(\mathcal{N}^{(\infty)})^2} \sum_{j=0}^N 2(j+1) \frac{\partial}{\partial x} \int_{R_{N,j}(x)} dx_1 \dots dx_N |\det[e^{ik_j \tilde{x}_l}]|^2 \end{aligned} \quad (4.42)$$

$$= g_{N+2}^{(\infty)}(x, 0) - \left(\frac{1}{cL}\right) 2(N+2) \left(x \frac{\partial}{\partial x} + 1\right) g_{N+2}^{(\infty)}(x, 0) \quad (4.43a)$$

$$+ \frac{2}{cL} \frac{L}{(\mathcal{N}^{(\infty)})^2} \frac{\partial}{\partial x} \sum_{j=0}^N \frac{(j+1)}{j!(N-j)!} \int_{\tilde{R}_{N,j}(x)} dx_1 \dots dx_N |\det[e^{ik_j \tilde{x}_l}]|^2, \quad (4.43b)$$

where the new domain  $\tilde{R}_{N,j}(x)$  has broken the strict ordering of (3.2) on either side of  $x$ , i.e.

$$\tilde{R}_{N,j}(x) = 0 \leq x_1, \dots, x_j \leq x \leq x_{j+1}, \dots, x_N \leq L. \quad (4.44)$$

It remains to simplify (4.43b). Introducing  $\xi$  yields

$$\begin{aligned} &\frac{1}{N!} \frac{\partial}{\partial x} \frac{\partial}{\partial \xi} \sum_{j=0}^N \xi^{j+1} \binom{N}{j} \int_{\tilde{R}_{N,j}(x)} dx_1 \dots dx_N |\det[e^{ik_j \tilde{x}_l}]|^2 \Big|_{\xi=1} \\ &= \frac{1}{N!} \frac{\partial}{\partial x} \frac{\partial}{\partial \xi} \xi \prod_{l=1}^N \left( \int_x^L + \xi \int_0^x \right) dx_l |\det[e^{ik_j \tilde{x}_l}]|^2 \Big|_{\xi=1}. \end{aligned} \quad (4.45)$$

Using the product rule, one can obtain

$$= \frac{1}{N!} \frac{\partial}{\partial x} \int_0^L dx_1 \dots dx_N |\det[e^{ik_j \tilde{x}_l}]|^2 \quad (4.46a)$$

$$+ \frac{1}{N!} \frac{\partial}{\partial x} \frac{\partial}{\partial \xi} \prod_{l=1}^N \left( \int_x^L + \xi \int_0^x \right) dx_l |\det[e^{ik_j \tilde{x}_l}]|^2 \Big|_{\xi=1}. \quad (4.46b)$$

Hence (4.46a) is equal to

$$(\mathcal{N}^{(\infty)})^2 \frac{\partial}{\partial x} g_{N+2}^{(\infty)}(x, 0). \quad (4.47)$$

Regarding (4.46b), note that

$$\frac{\partial}{\partial \xi} \prod_{l=1}^N \left( \int_x^L + \xi \int_0^x \right) dx_l |\det[e^{ik_j \tilde{x}_l}]|^2 \Big|_{\xi=1} \quad (4.48)$$

$$= \frac{\partial}{\partial \xi} \left( \prod_{l=1}^N \int_0^L dx_l |\det[e^{ik_j \tilde{x}_l}]|^2 + \sum_{l=1}^N \int_0^x dx_l (\xi - 1) \prod_{\substack{j=1 \\ j \neq l}}^N \int_0^L dx_j |\det[e^{ik_j \tilde{x}_l}]|^2 + O((\xi - 1)^2) \right) \Big|_{\xi=1} \quad (4.49)$$

$$= \sum_{l=1}^N \int_0^x dx_l \prod_{\substack{j=1 \\ j \neq l}}^N \int_0^L dx_j |\det[e^{ik_j \tilde{x}_l}]|^2 \quad (4.50)$$

$$= N \int_0^x dx_1 \int_0^L dx_2 \dots \int_0^L dx_N |\det[e^{ik_j \tilde{x}_l}]|^2. \quad (4.51)$$

Therefore, (4.46b) is equal to

$$\frac{1}{(N-1)!} \frac{\partial}{\partial x} \int_0^x dx_1 \int_0^L dx_2 \dots \int_0^L dx_N |\det[e^{ik_j \tilde{x}_l}]|^2. \quad (4.52)$$

For the free Fermi system the 3-point correlation function is specified by

$$g_{3,(N+2)}^{(\infty)}(x, 0, x_1) = \frac{1}{(N-1)!} \frac{1}{(\mathcal{N}^{(\infty)})^2} \int_0^L dx_2 \dots \int_0^L dx_N |\det[e^{ik_j \tilde{x}_l}]|^2 \quad (4.53)$$

$$= \left(\frac{N+2}{L}\right)^2 \det \begin{pmatrix} 1 & \tilde{K}_{N+2,L}(x, 0) & \tilde{K}_{N+2,L}(x_1, 0) \\ \tilde{K}_{N+2,L}(x, 0) & 1 & \tilde{K}_{N+2,L}(x, x_1) \\ \tilde{K}_{N+2,L}(x_1, 0) & \tilde{K}_{N+2,L}(x, x_1) & 1 \end{pmatrix} \quad (4.54)$$

$$= \left(\frac{N+2}{L}\right)^2 [1 - \tilde{K}_{N+2,L}(x, 0)^2 - \tilde{K}_{N+2,L}(x_1, 0)^2 - \tilde{K}_{N+2,L}(x, x_1)^2 + 2\tilde{K}_{N+2,L}(x, 0)\tilde{K}_{N+2,L}(x_1, 0)\tilde{K}_{N+2,L}(x, x_1)], \quad (4.55)$$

where  $\tilde{K}_{NL}(x, y)$  is specified by (4.39). Note that this definition is only valid for  $N \geq 1$ ; a 3-point correlation function for a system of 2 particles does not make physical sense, as  $g_{3,2}^{(\infty)}(x, 0, x_1) = 0$ . Using (4.53), (4.52) reduces to

$$(\mathcal{N}^{(\infty)})^2 \frac{\partial}{\partial x} \int_0^x dx_1 g_{3,(N+2)}^{(\infty)}(x, 0, x_1). \quad (4.56)$$

Finally, adding up all contributions gives the sought closed form expression for  $g_N(x, 0)$  (here we revert to  $N+2 \rightarrow N$ )

$$g_N(x, 0) = g_N^{(\infty)}(x, 0) + \left(\frac{1}{cL}\right) \left[ 2 \left( L \frac{\partial}{\partial x} - x \frac{\partial}{\partial x} - 1 \right) g_N^{(\infty)}(x, 0) + 2L \frac{\partial}{\partial x} \int_0^x dx_1 g_{3,N}^{(\infty)}(x, 0, x_1) \right] + O\left(\frac{1}{cL}\right)^2 \quad (4.57)$$

correct to  $O(1/cL)$ , valid for all  $N \geq 2$ . This gives equivalent results for the cases  $N = 2$  and  $N = 3$ , given by (4.9) and (4.15). Using (4.38) and (4.55), (4.57) can be written in the simpler form

$$\begin{aligned}
 g_N(x, 0) = & \frac{N}{L} (1 - \tilde{K}_{N,L}(x, 0)^2) \\
 & + 4N \left( \frac{1}{cL} \right) \left\{ -\tilde{K}_{N,L}(x, 0) \left[ \left( \frac{N}{L} + \frac{\partial}{\partial x} \right) \tilde{K}_{N,L}(x, 0) \right] \right. \\
 & \left. + \frac{N}{L} \frac{\partial}{\partial x} \left[ \tilde{K}_{N,L}(x, 0) \int_0^x \tilde{K}_{N,L}(x_1, 0) \tilde{K}_{N,L}(x, x_1) dx_1 \right] \right\} + O \left( \frac{1}{cL} \right)^2
 \end{aligned} \tag{4.58}$$

which is valid for all  $N \geq 3$ . We have confirmed that this result recovers (4.15). Now (4.58), and concomitantly its structure factor, can be readily computed for any  $N \geq 3$ . The structure factor in the limit  $cL \rightarrow \infty$ , is given by

$$\mathcal{S}_n(N) = \begin{cases} N & \text{when } n = 0 \\ |n|/N & \text{when } 0 < |n| < N \\ 1 & \text{when } |n| \geq N. \end{cases} \tag{4.59}$$

In the thermodynamic limit,  $\tilde{K}$  becomes

$$\tilde{K}_\infty(x, y) = \frac{\sin(\rho_0\pi(x-y))}{\rho_0\pi(x-y)}, \tag{4.60}$$

where  $\rho_0 = N/L$ , and now the correlation function follows from (4.58) and is (using the appropriate scaled variable  $\rho_0/c$ )

$$\begin{aligned}
 g_\infty(x, 0) = & \rho_0 \left( 1 - \frac{\sin^2 \bar{x}}{\bar{x}^2} \right) - 4\rho_0 \left\{ \frac{\sin \bar{x}}{\bar{x}^3} [\pi \bar{x} \cos \bar{x} + (\bar{x} - \pi) \sin \bar{x}] \right. \\
 & \left. + \frac{\partial}{\partial x} \left[ \tilde{K}_\infty(x, 0) \int_0^x \tilde{K}_\infty(x_1, 0) \tilde{K}_\infty(x, x_1) dx_1 \right] \right\} \left( \frac{\rho_0}{c} \right) + O \left( \frac{\rho_0}{c} \right)^2,
 \end{aligned} \tag{4.61}$$

where  $\bar{x} = \rho_0\pi x$ . This equation is in agreement with that first given by Korepin [29]. Recently in [8], using the random phase approximation (RPA), which they indicated is

valid to the  $\rho_0/c$  correction, the structure factor was calculated in the thermodynamic limit from which (4.61) is recovered.

Here we explicitly evaluate the integral in (4.61) using (4.60)

$$\int_0^x \tilde{K}_\infty(x_1, 0) \tilde{K}_\infty(x, x_1) dx_1 = \frac{\sin(\bar{x})\text{Si}(2\bar{x}) + \cos(\bar{x})[\text{Ci}(2\bar{x}) - \log(2\bar{x}) - \gamma]}{\rho_0\pi\bar{x}}, \quad (4.62)$$

where  $\gamma$  is Euler's constant, and Si and Ci are the sine integral and cosine integral functions, respectively.

#### 4. CORRELATION FUNCTIONS AND STRUCTURE FACTORS

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## CONCLUSIONS

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# 5

In this thesis, we find the density matrix, occupation numbers, correlation function and structure factor completely for 2 particles, partially for 3 particles, and sparingly for 4 particles. These are calculated exactly and as analytic expansions around  $cL = 0$  and  $cL = \infty$ .

The density matrix expanded in large  $cL$  is originally calculated using a multiple integral expression. This expression is reformulated using a Toeplitz determinant technique, enabling subsequent calculation of the occupation numbers (which are the Fourier transform of the density matrix) for up to 36 particles for the ground state, and 26 particles for the first and second excited states. This data is used to determine the coefficients of an ansatz which generalises the  $1/cL$  expansion of the occupation numbers, and to show that one important coefficient has  $\beta_n = 2 \forall n$ , we conjecture that this is true for all  $N$ .

The correlation function is manipulated into a form that is readily calculated for any  $N$ , and the thermodynamic limit is also shown.



## 5. CONCLUSIONS

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# BETHE EQUATION SOLUTIONS

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# A

Equation (2.38) gives the quasi-momenta expanded to order  $(cL)$ . We present here the quasi-momenta up to  $(cL)^4$ , for up to 8 particles. These are solutions to equation (2.37), obtained using the method of quadrature.

$N = 2$

$$k_2 = \sqrt{\frac{c}{L}} \left[ 1 - \frac{1}{24}(cL) + \frac{11}{5760}(cL)^2 - \frac{17}{322560}(cL)^3 - \frac{281}{154828800}(cL)^4 + O(cL)^5 \right] \quad (\text{A.1})$$

$N = 3$

$$k_3 = \sqrt{\frac{3c}{L}} \left[ 1 - \frac{1}{24}(cL) + \frac{19}{5760}(cL)^2 - \frac{299}{967680}(cL)^3 + \frac{11077}{464486400}(cL)^4 + O(cL)^5 \right] \quad (\text{A.2})$$

$N = 4$

$$k_4 = \sqrt{\left(3 + \sqrt{6}\right) \frac{c}{L}} \left[ 1 - \frac{1}{24}(cL) + \frac{31 - 2\sqrt{6}}{5760}(cL)^2 + \frac{-879 + 86\sqrt{6}}{967680}(cL)^3 + \frac{63381 - 5500\sqrt{6}}{464486400}(cL)^4 + O(cL)^5 \right] \quad (\text{A.3a})$$

$$k_3 = \sqrt{\left(3 - \sqrt{6}\right) \frac{c}{L}} \left[ 1 - \frac{1}{24}(cL) + \frac{31 + 2\sqrt{6}}{5760}(cL)^2 + \frac{-879 - 86\sqrt{6}}{967680}(cL)^3 + \frac{63381 + 5500\sqrt{6}}{464486400}(cL)^4 + O(cL)^5 \right] \quad (\text{A.3b})$$

$N = 5$

$$k_5 = \sqrt{(5 + \sqrt{10}) \frac{c}{L}} \left[ 1 - \frac{1}{24}(cL) + \frac{39 - 2\sqrt{10}}{5760}(cL)^2 + \frac{-1511 + 118\sqrt{10}}{967680}(cL)^3 + \frac{165589 - 13196\sqrt{10}}{464486400}(cL)^4 + O(cL)^5 \right] \quad (\text{A.4a})$$

$$k_4 = \sqrt{(5 - \sqrt{10}) \frac{c}{L}} \left[ 1 - \frac{1}{24}(cL) + \frac{39 + 2\sqrt{10}}{5760}(cL)^2 + \frac{-1511 - 118\sqrt{10}}{967680}(cL)^3 + \frac{165589 + 13196\sqrt{10}}{464486400}(cL)^4 + O(cL)^5 \right] \quad (\text{A.4b})$$

$N = 6$

$$k_6 = 3.3242 \sqrt{\frac{c}{L}} [1 - 0.041667(cL) + 0.0067532(cL)^2 - 0.0017543(cL)^3] \quad (\text{A.5a})$$

$$k_5 = 1.8892 \sqrt{\frac{c}{L}} [1 - 0.041667(cL) + 0.0093511(cL)^2 - 0.0028885(cL)^3] \quad (\text{A.5b})$$

$$k_4 = 0.61671 \sqrt{\frac{c}{L}} [1 - 0.041667(cL) + 0.010458(cL)^2 - 0.0035594(cL)^3] \quad (\text{A.5c})$$

$N = 7$

$$k_7 = 3.7504 \sqrt{\frac{c}{L}} [1 - 0.041667(cL) + 0.0077897(cL)^2 - 0.0024201(cL)^3] \quad (\text{A.6a})$$

$$k_6 = 2.3668 \sqrt{\frac{c}{L}} [1 - 0.041667(cL) + 0.010729(cL)^2 - 0.0039343(cL)^3] \quad (\text{A.6b})$$

$$k_5 = 1.1544 \sqrt{\frac{c}{L}} [1 - 0.041667(cL) + 0.012211(cL)^2 - 0.0049975(cL)^3] \quad (\text{A.6c})$$

$N = 8$

$$k_8 = 4.1445 \sqrt{\frac{c}{L}} [1 - 0.041667(cL) + 0.0087926(cL)^2 - 0.0031697(cL)^3] \quad (\text{A.7a})$$

$$k_7 = 2.8025 \sqrt{\frac{c}{L}} [1 - 0.041667(cL) + 0.012030(cL)^2 - 0.0050758(cL)^3] \quad (\text{A.7b})$$

$$k_6 = 1.6365 \sqrt{\frac{c}{L}} [1 - 0.041667(cL) + 0.013827(cL)^2 - 0.0065475(cL)^3] \quad (\text{A.7c})$$

$$k_5 = 0.53908 \sqrt{\frac{c}{L}} [1 - 0.041667(cL) + 0.014656(cL)^2 - 0.0073260(cL)^3] \quad (\text{A.7d})$$

The leading term of  $k_j$  is precisely related to the  $j$ th zero of the  $N$ th Hermite polynomial, as mentioned in Section 2.2. If we begin with (2.37), and let  $k_j = a_j \sqrt{2c/L}$ , then by expanding to order  $cL$  on both sides, one obtains

$$a_j = \sum_{l=1}^N \frac{1}{a_j - a_l}. \quad (\text{A.8})$$

The solution to this equation is the  $j$ th zero of the  $N$ th Hermite polynomial [46], so that  $a_j = h_j^{(N)}$ .

Note that the second order term is  $-1/24$  up to  $N = 8$ . Assuming that

$$k_j = \sqrt{\frac{2c}{L}} h_j^{(N)} (1 - cL/24) \quad (\text{A.9})$$

for all  $N$ , and expanding (2.37) to order  $(cL)^2$ , one obtains

$$-h_j^{(N)} = \sum_{\substack{l=1 \\ l \neq j}}^N \frac{(h_j^{(N)} - h_l^{(N)})^2 - 4}{(h_j^{(N)} - h_l^{(N)})^3}. \quad (\text{A.10})$$

We conjecture that (A.10) is true for all  $N$ . This has been checked numerically up to  $N = 100$ .



## A. BETHE EQUATION SOLUTIONS

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MULTIPLE INTEGRALS  
AND  
TOEPLITZ DETERMINANTS

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# B

A Toeplitz determinant is the determinant of any Toeplitz matrix, where the element in the  $j$ th row and the  $i$ th column is given by  $c_{j-i}$ , i.e.

$$\begin{pmatrix} c_0 & c_1 & c_2 & \dots & c_N \\ c_{-1} & c_0 & c_1 & \dots & c_{N-1} \\ c_{-2} & c_{-1} & c_0 & \dots & c_{N-2} \\ \vdots & \vdots & \vdots & & \vdots \\ c_{-N} & c_{-N+1} & c_{-N+2} & \dots & c_0 \end{pmatrix}. \quad (\text{B.1})$$

This appendix demonstrates how to manipulate the general multiple integral

$$\int_0^{2\pi} d\psi_1 \dots \int_0^{2\pi} d\psi_N \prod_{j=1}^N f(\psi_j) \prod_{1 \leq m < n \leq N} |e^{2i\psi_m} - e^{2i\psi_n}|^2, \quad (\text{B.2})$$

where  $f(\psi_j)$  is some well-behaved function, into a Toeplitz determinant form - which is simpler to calculate numerically. This technique is useful for determining a simple way to calculate  $\rho_N^{(0)}(x, y)$  (Subsection 3.3.1), and a simple way to express  $\Delta_n$  (Section C.2).

We begin by noting that the final term of (B.2) can be rewritten using

$$\prod_{1 \leq m < n \leq N} (e^{2i\psi_m} - e^{2i\psi_n}) = \sum_{p \in S_N} \epsilon(p) \prod_{j=1}^N e^{2ij\psi_{p(j)}}, \quad (\text{B.3})$$

where  $S_N$  is the symmetric group on  $N$  symbols, and  $\epsilon(p)$  is the signature of the permutation  $p$ . Hence

$$\prod_{1 \leq m < n \leq N} |e^{2i\psi_m} - e^{2i\psi_n}|^2 = \sum_{p \in S_N} \sum_{q \in S_N} \epsilon(p)\epsilon(q) \prod_{j=1}^N e^{2ij\psi_{p(j)}} e^{-2ij\psi_{q(j)}}. \quad (\text{B.4})$$

Now define the function

$$t(r) = \int_0^{2\pi} e^{ir\psi} f(\psi) d\psi. \quad (\text{B.5})$$

Therefore (B.2) becomes

$$\begin{aligned} & \sum_{p \in S_N} \sum_{q \in S_N} \epsilon(p)\epsilon(q) \prod_{j=1}^N \int_0^{2\pi} d\psi e^{2i(p(j)-q(j))\psi} f(\psi) \\ &= \sum_{p \in S_N} \sum_{q \in S_N} \epsilon(p)\epsilon(q) \prod_{j=1}^N t(p(j) - q(j)), \end{aligned} \quad (\text{B.6})$$

where we have dropped the subscript of  $\psi$ . One sum just introduces a factor of  $N!$ , so that (B.2) is equivalent to

$$N! \det_{1 \leq n, m \leq N} t(n - m), \quad (\text{B.7})$$

which is in the form of a Toeplitz determinant.

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# FREDHOLM DETERMINANTS

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# C

## C.1 Notation

The  $n$ th Fredholm minor is given by [23]

$$\Delta_n \begin{pmatrix} x_1 & \dots & x_n \\ x'_1 & \dots & x'_n \end{pmatrix} ; \lambda = \sum_{l=0}^{N-n} \frac{\lambda^{n+l}}{l!} \int_0^x dz_1 \dots \int_0^x dz_l \times \quad (C.1)$$

$$K_{NL} \begin{pmatrix} x_1 & \dots & x_n & z_1 & \dots & z_l \\ x'_1 & \dots & x'_n & z_1 & \dots & z_l \end{pmatrix},$$

where the function  $K_{NL}$  is given by

$$K_{NL} \begin{pmatrix} x_1 & \dots & x_l \\ x'_1 & \dots & x'_l \end{pmatrix} = \det[K_{NL}(x_i, x'_j)]_{1 \leq i, j \leq l} \quad (C.2)$$

and  $K_{NL}(x, y)$  by

$$K_{NL}(x, y) = \frac{1}{L} \sum_{j=1}^N e^{-i\pi(2j-N-1)(x-y)/L} \quad (C.3)$$

$$= \frac{\sin[N\pi(x-y)/L]}{L \sin[\pi(x-y)/L]}.$$

Note that the termination of the integrals in (C.1) ensures that all Fredholm minors depend on  $x$ .

## C.2 Toeplitz determinant form

The aim of this section is to manipulate the general Fredholm minor (C.1) into a form involving Toeplitz determinants. The latter of these forms is significantly simpler to calculate numerically. Let us begin by noting the property of the determinant  $K_{NL}$  from [23]

$$K_{NL} \begin{pmatrix} x_1 & \cdots & x_n \\ x'_1 & \cdots & x'_n \end{pmatrix} = \frac{1}{L^N (N-n)!} \int_0^L \cdots \int_0^L dy_{n+1} \cdots dy_N \times \frac{f_{NL}(x_1, \dots, x_n, y_{n+1}, \dots, y_N)}{f_{NL}(x'_1, \dots, x'_n, y_{n+1}, \dots, y_N)}, \quad (\text{C.4})$$

where

$$\begin{aligned} f_{NL}(x_1, \dots, x_n) &= \det[e^{i\pi(-N+2j-1)x_l/L}]_{j,l=1,\dots,n} \\ &= e^{-i(N-1)\pi \sum_{i=1}^n x_i/L} \prod_{1 \leq j < k \leq n} (e^{2i\pi x_k/L} - e^{2i\pi x_j/L}). \end{aligned} \quad (\text{C.5})$$

Using this, (C.1) becomes

$$\begin{aligned} \Delta_n \begin{pmatrix} x_1 & \cdots & x_n \\ x'_1 & \cdots & x'_n \end{pmatrix} ; \lambda &= \frac{1}{L^N} \sum_{l=0}^{N-n} \frac{\lambda^{n+l}}{l!(N-n-l)!} \int_0^x dz_1 \cdots \int_0^x dz_l \times \\ &\int_0^L dy_{n+l+1} \cdots \int_0^L dy_N \frac{f_{NL}(x_1, \dots, x_n, z_1, \dots, z_l, y_{n+l+1}, \dots, y_N)}{f_{NL}(x'_1, \dots, x'_n, z_1, \dots, z_l, y_{n+l+1}, \dots, y_N)}. \end{aligned} \quad (\text{C.6})$$

Now by replacing all the  $z_i \rightarrow y_{i+n}$ , and using the bilinear theorem, one may obtain,

$$\Delta_n \begin{pmatrix} x_1 & \dots & x_n \\ x'_1 & \dots & x'_n \end{pmatrix} ; \lambda = \frac{\lambda^n}{L^{N+1}(N-n)!} \left( \int_0^L + \lambda \int_0^x \right) dy_n \dots \left( \int_0^L + \lambda \int_0^x \right) dy_N \times \overline{f_{NL}(x_1, \dots, x_n, y_n, \dots, y_N)} f_{NL}(x'_1, \dots, x'_n, y_n, \dots, y_N). \quad (\text{C.7})$$

The integrand of (C.7) is obtained using (C.5)

$$\begin{aligned} \overline{f_{NL}(x_1, \dots, x_n, y_n, \dots, y_N)} f_{NL}(x'_1, \dots, x'_n, y_n, \dots, y_N) = \\ \overline{f_{NL}(x_1, \dots, x_n)} f_{NL}(x'_1, \dots, x'_n) \times \\ \prod_{j=n}^N \prod_{k=1}^n (e^{2i\pi y_j/L} - e^{2i\pi x'_k/L}) (e^{-2i\pi y_j/L} - e^{-2i\pi x_k/L}) \times \\ \prod_{n \leq j < k \leq N} |e^{2i\pi y_k/L} - e^{2i\pi y_j/L}|^2, \end{aligned} \quad (\text{C.8})$$

letting

$$g(u) = (1 + \lambda \chi_{[0,x]}^{(u)}) \prod_{k=1}^n (e^{2i\pi u/L} - e^{2i\pi x'_k/L}) (e^{-2i\pi u/L} - e^{-2i\pi x_k/L}), \quad (\text{C.9})$$

where  $\chi_{[0,x]}^{(u)} = 1$  for  $u \in [0, x]$  and 0 otherwise, (C.7) becomes

$$\begin{aligned} \Delta_n \begin{pmatrix} x_1 & \dots & x_n \\ x'_1 & \dots & x'_n \end{pmatrix} ; \lambda = \frac{\lambda^n}{L^{N+1}(N-n)!} \times \\ \overline{f_{NL}(x_1, \dots, x_n)} f_{NL}(x'_1, \dots, x'_n) \times \\ \int_0^L \dots \int_0^L dy_n \dots dy_N \prod_{l=n}^N g(y_l) \prod_{n \leq j < k \leq N} |e^{2i\pi y_k/L} - e^{2i\pi y_j/L}|^2 \end{aligned} \quad (\text{C.10})$$

which, by the Toeplitz determinant technique of Appendix B, is

$$\Delta_n \begin{pmatrix} x_1 & \dots & x_n \\ x'_1 & \dots & x'_n \end{pmatrix} ; \lambda = \left( \frac{\lambda}{L} \right)^n \overline{f_{NL}(x_1, \dots, x_n)} \times \quad (C.11)$$

$$f_{NL}(x'_1, \dots, x'_n) \det[A_n(j-k)]_{j,k=1, \dots, N-n},$$

where

$$\begin{aligned} A_n(j) &= \frac{1}{L} \int_0^L du g(u) e^{2i\pi u j/L} \\ &= \frac{1}{L} \left( \int_0^L + \lambda \int_0^x \right) du \prod_{k=1}^n (e^{2i\pi u/L} - e^{2i\pi x'_k/L}) \times \quad (C.12) \\ &\quad (e^{-2i\pi u/L} - e^{-2i\pi x_k/L}) e^{2i\pi u j/L}. \end{aligned}$$

The specific cases  $\Delta_0(\lambda)$  and  $\Delta_1 \begin{pmatrix} x \\ 0 \end{pmatrix} ; \lambda$  are of particular use in Subsection 3.3.2.

# NUMERICAL DATA

# D

$N$	$c_0^{(0)}(N)$		$c_0^{(1)}(N)$	
2	$\frac{16}{\pi^2}$	1.62114...	$\frac{64}{\pi^2}$	6.48456...
3	$\frac{1}{3} + \frac{35}{2\pi^2}$	2.10645...	$8 + \frac{105}{\pi^2}$	18.6387...
4	$-\frac{2097152}{19845\pi^4} + \frac{320}{9\pi^2}$	2.51766...	$-\frac{16777216}{19845\pi^4} + \frac{138752}{315\pi^2}$	35.9512...
5	$\frac{1}{5} + \frac{7436429}{129600\pi^4} + \frac{4459}{216\pi^2}$	2.88069...	$\frac{16}{3} + \frac{7436429}{12960\pi^4} + \frac{249613}{540\pi^2}$	58.0593...
6	$\frac{193507848058308060419981312}{12748157814913474078125\pi^6} - \frac{38494793629696}{21739843125\pi^4} + \frac{4144}{75\pi^2}$	3.20923...	$\frac{774031392233232241679925248}{4249385938304491359375\pi^6} - \frac{55397943205615894528}{2589628373206875\pi^4} + \frac{85085248}{75075\pi^2}$	84.6855...
7	$\frac{1}{7} + \frac{85760621135804297813}{40663643328000000\pi^6} - \frac{46891706849}{317520000\pi^4} + \frac{79679}{3000\pi^2}$	3.51155...	$\frac{24}{5} + \frac{85760621135804297813}{2904545952000000\pi^6} + \frac{1528761661843}{2716560000\pi^4} + \frac{641803}{875\pi^2}$	115.607...

Table D.1: Values of  $c_0^{(0)}(N)$  and  $c_0^{(1)}(N)$  for  $N = 2, 3, 4, 5, 6, 7$ . Note that this Table extends Table II of [16]



Table D.2: Values of  $c_1^{(0)}(N)$  and  $c_1^{(1)}(N)$  for  $N = 2, 3, 4, 5, 6$ 

$N$	$c_1^{(0)}(N)$		$c_1^{(1)}(N)$	
2	$\frac{16}{9\pi^2}$	0.180127...	$-\frac{832}{27\pi^2}$	-3.12219...
3	$\frac{1}{3}$	0.333333...	$-4 - \frac{35}{2\pi^2}$	-5.77312...
4	$\frac{-6318718976}{22325625\pi^4} + \frac{832}{25\pi^2}$	0.466435...	$\frac{-52781507411968}{7032571875\pi^4} + \frac{1382912}{2025\pi^2}$	-7.85498...
5	$\frac{1}{5} - \frac{18059899}{129600\pi^4} + \frac{3871}{216\pi^2}$	0.585231...	$\frac{28}{9} - \frac{574729727}{151200\pi^4} + \frac{47201}{180\pi^2}$	-9.34192...
6	$\frac{4458566781285863348987439874048}{315703029023206220155134375\pi^6} - \frac{14163619272982528}{7456766191875\pi^4} + \frac{7984}{147\pi^2}$	0.693364...	$\frac{317603131762611117568514042882856845312}{850617087107250872660154262734375\pi^6} - \frac{90755550267618998878208}{1722102868182571875\pi^4} + \frac{8618142656}{6131125\pi^2}$	-10.2255...

Table D.3: Values of  $c_2^{(0)}(N)$  and  $c_2^{(1)}(N)$  for  $N = 2, 3, 4, 5, 6$ 

$N$	$c_2^{(0)}(N)$		$c_2^{(1)}(N)$	
2	$\frac{16}{225\pi^2}$	0.00720506...	$\frac{-3136}{3375\pi^2}$	-0.0941461...
3	$\frac{35}{36\pi^2}$	0.0985067...	$\frac{-385}{12\pi^2}$	-3.25072...
4	$\frac{-7408644521984}{132368630625\pi^4} + \frac{27584}{3675\pi^2}$	0.185917...	$\frac{3710310553890062336}{458657305115625\pi^4} - \frac{6735912448}{7640325\pi^2}$	-6.28072...
5	$\frac{1}{5} - \frac{1062347}{127008\pi^4} + \frac{325}{216\pi^2}$	0.266582...	$-\frac{52}{9} + \frac{30358690219}{17781120\pi^4} - \frac{221909}{1080\pi^2}$	-9.06869...
6	$\frac{16076943096817340218487564310413312}{821143578489359378623504509375\pi^6} - \frac{47388412779564105728}{19395048865066875\pi^4} + \frac{990928}{19845\pi^2}$	0.34121...	$\frac{4194702189111033289475552785337770452189184}{2212455043565959519789061237372109375\pi^6} - \frac{2887827552035815814833635328}{13437568680428608340625\pi^4} + \frac{18544396881344}{8442559125\pi^2}$	-11.5824...

Table D.4: Values of  $c_0^{(1,1)}(N)$  and  $c_0^{(1,2)}(N)$  for  $N = 2, 3, 4, 5, 6$

$N$	$c_0^{(1,1)}(N)$		$c_0^{(1,2)}(N)$	
2	$-8 + \frac{64}{\pi^2}$	-1.51544...	8	8
3	$-16 + \frac{105}{\pi^2}$	-5.36128...	24	24
4	$-32 - \frac{16777216}{19845\pi^4} + \frac{2560}{9\pi^2}$	-11.8587...	$32 + \frac{16384}{105\pi^2}$	47.8100...
5	$-48 + \frac{7436429}{12960\pi^4} + \frac{22295}{108\pi^2}$	-21.1931...	$\frac{160}{3} + \frac{23023}{90\pi^2}$	79.2524...
6	$-72 + \frac{77403139223322241679925248}{4249385938304491359375\pi^6} - \frac{153979174518784}{7246614375\pi^4} + \frac{16576}{25\pi^2}$	-33.4892...	$72 - \frac{74481467421360128}{517925674641375\pi^4} + \frac{7061504}{15015\pi^2}$	118.175...

Table D.5: Values of  $c_1^{(1,1)}(N)$  and  $c_1^{(1,2)}(N)$  for  $N = 2, 3, 4, 5, 6$ 

$N$	$c_1^{(1,1)}(N)$		$c_1^{(1,2)}(N)$	
2	$\frac{8}{3} - \frac{832}{27\pi^2}$	-0.455527...	$-\frac{8}{3}$	-2.66667...
3	$-1 - \frac{35}{2\pi^2}$	-2.77312...	-3	-3....
4	$-\frac{352}{15} - \frac{52781507411968}{7032571875\pi^4} + \frac{65129984}{70875\pi^2}$	-7.40762...	$\frac{352}{15} - \frac{16728064}{70875\pi^2}$	-0.447369...
5	$-\frac{109}{3} - \frac{574729727}{151200\pi^4} + \frac{64757}{108\pi^2}$	-14.6032...	$\frac{355}{9} - \frac{91091}{270\pi^2}$	5.26130...
6	$-\frac{2232}{35} + \frac{317603131762611117568514042882856845312}{850617087107250872660154262734375\pi^6}$ $-\frac{40373418531338728767488}{803648005151866875\pi^4} + \frac{30246667072}{18393375\pi^2}$	-24.5196...	$\frac{2232}{35} - \frac{2698870354841096421376}{1095883643388909375\pi^4}$ $-\frac{399294464}{1672125\pi^2}$	14.2941...

$N$	$c_2^{(1,1)}(N)$		$c_2^{(1,2)}(N)$	
2	$\frac{8}{15} - \frac{3136}{3375\pi^2}$	0.439187...	$-\frac{8}{15}$	-0.533333...
3	$4 - \frac{385}{12\pi^2}$	0.749279...	-4	-4
4	$\frac{2272}{105} + \frac{3710310553890062336}{458657305115625\pi^4} - \frac{39711774208}{38201625\pi^2}$	-0.641704...	$-\frac{2272}{105} + \frac{6032211968}{38201625\pi^2}$	-5.63902...
5	$\frac{31}{3} + \frac{30358690219}{17781120\pi^4} - \frac{238405}{756\pi^2}$	-4.09068...	$-\frac{145}{9} + \frac{830687}{7560\pi^2}$	-4.97802...
6	$-\frac{3592}{105} + \frac{4194702189111033289475552785337770452189184}{2212455043565959519789061237372109375\pi^6} - \frac{98659506842974376305885184}{418057692280001148375\pi^4} + \frac{13193444962112}{2814186375\pi^2}$	-9.82321...	$\frac{3592}{105} + \frac{1983596175418523964988719104}{94062980763000258384375\pi^4} - \frac{21035938004992}{8442559125\pi^2}$	-1.75923...

Table D.6: Values of  $c_2^{(1,1)}(N)$  and  $c_2^{(1,2)}(N)$  for  $N = 2, 3, 4, 5, 6$

$N$	$c_0^{*(0)}(N)$	$c_0^{*(1,1)}(N)$	$c_0^{*(1,2)}(N)$	$c_0^{(1)}(N)$
2	0.810569...	-0.757722...	4	3.24228...
3	0.702151...	-1.78709...	8	6.21291...
4	0.629414...	-2.96469...	11.9525...	8.98781...
5	0.576137...	-4.23863...	15.8505...	11.6119...
6	0.534872...	-5.58153...	19.6958...	14.1143...
7	0.50165...	-6.9769...	23.4922...	16.5153...
8	0.474130...	-8.41392...	27.2440...	18.8301...
9	0.450832...	-9.88502...	30.9548...	21.0698...
10	0.430766...	-11.3847...	34.6282...	23.2435...
11	0.413239...	-12.9087...	38.2671...	25.3583...
12	0.397753...	-14.4539...	41.8741...	27.4202...
13	0.383935...	-16.0177...	45.4517...	29.4340...
14	0.371504...	-17.5979...	49.0018...	31.4039...
15	0.360239...	-19.1928...	52.5264...	33.3335...
16	0.349968...	-20.8010...	56.0269...	35.2259...
17	0.34055...	-22.4213...	59.5049...	37.0836...
18	0.331874...	-24.0525...	62.9616...	38.9091...
19	0.323844...	-25.6939...	66.3983...	40.7044...
20	0.316385...	-27.3446...	69.8160...	42.4715...
21	0.309431...	-29.0039...	73.2157...	44.2118...
22	0.302927...	-30.6712...	76.5983...	45.9271...
23	0.296826...	-32.3460...	79.9645...	47.6185...
24	0.291088...	-34.0278...	83.3151...	49.2874...
25	0.285677...	-35.7161...	86.6509...	50.9348...
26	0.280564...	-37.4106...	89.9724...	52.5618...
27	0.275723...	-39.1110...	93.2802...	54.1692...
28	0.271128...	-40.8168...	96.5749...	55.7581...
29	0.266761...	-42.5279...	99.8570...	57.3292...
30	0.262603...	-44.2438...	103.127...	58.8832...
31	0.258637...	-45.9645...	106.385...	60.4207...
32	0.254849...	-47.6896...	109.632...	61.9426...
33	0.251227...	-49.4190...	112.868...	63.4493...
34	0.247757...	-51.1525...	116.094...	64.9414...
35	0.244430...	-52.8899...	119.309...	66.4194...
36	0.241237...	-54.6310...	122.515...	67.8839...

Table D.7: Numerical solutions for the ground state occupation numbers  $c_0^{*(0)}(N)$ ,  $c_0^{*(1,1)}(N)$ ,  $c_0^{*(1,2)}(N)$  and  $c_0^{*(1)}(N)$ , for  $N = 2 - 36$

D. NUMERICAL DATA

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$N$	$c_1^{*(0)}(N)$	$c_1^{*(1,1)}(N)$	$c_1^{*(1,2)}(N)$	$c_1^{(1)}(N)$
2	0.0900633...	-0.227763...	-1.33333...	-1.56110...
3	0.111111...	-0.924374...	-1	-1.92437...
4	0.116609...	-1.85190...	-0.111842...	-1.96375...
5	0.117046...	-2.92064...	1.05226...	-1.86838...
6	0.115561...	-4.08661...	2.38235...	-1.70426...
7	0.113315...	-5.32460...	3.82394...	-1.50066...
8	0.110796...	-6.61868...	5.34600...	-1.27269...
9	0.108225...	-7.95803...	6.92912...	-1.02891...
10	0.105704...	-9.33488...	8.56031...	-0.774574...
11	0.103278...	-10.7435...	10.2304...	-0.513070...
12	0.100969...	-12.1794...	11.9327...	-0.246672...
13	0.0987797...	-13.6392...	13.6622...	0.0230389...
14	0.0967099...	-15.1200...	15.4150...	0.294935...
15	0.0947542...	-16.6196...	17.1878...	0.568195...
16	0.0929060...	-18.1360...	18.9782...	0.842211...
17	0.0911579...	-19.6677...	20.7842...	1.11653...
18	0.0895030...	-21.2133...	22.6041...	1.39080...
19	0.0879343...	-22.7715...	24.4363...	1.66475...
20	0.0864452...	-24.3415...	26.2797...	1.93819...
21	0.0850299...	-25.9223...	28.1333...	2.21096...
22	0.0836828...	-27.5132...	29.9961...	2.48292...
23	0.0823990...	-29.1133...	31.8673...	2.75400...
24	0.0811738...	-30.7222...	33.7464...	3.02411...
25	0.0800030...	-32.3393...	35.6325...	3.29320...
26	0.0788828...	-33.9641...	37.5254...	3.56123...
27	0.0778098...	-35.5961...	39.4243...	3.82817...
28	0.0767809...	-37.2350...	41.3290...	4.09399...
29	0.0757931...	-38.8803...	43.2390...	4.35868...
30	0.0748437...	-40.5318...	45.1762...	4.64439...
31	0.0739304...	-42.1891...	47.0737...	4.88464...
32	0.0730510...	-43.8519...	48.9978...	5.14590...
33	0.0722034...	-45.5201...	50.9260...	5.40589...
34	0.0713858...	-47.1931...	52.8581...	5.66498...
35	0.0705964...	-48.8710...	54.7939...	5.92294...
36	0.0698336...	-50.5537...	56.7332...	6.17953...

Table D.8: Numerical solutions for the first excited state occupation numbers  $c_1^{*(0)}(N)$ ,  $c_1^{*(1,1)}(N)$ ,  $c_1^{*(1,2)}(N)$  and  $c_1^{(1)}(N)$ , for  $N = 2 - 36$

$N$	$c_2^{*(0)}(N)$	$c_2^{*(1,1)}(N)$	$c_2^{*(1,2)}(N)$	$c_2^{(1)}(N)$
2	0.00360253...	0.219594...	-0.266667...	-0.0470731...
3	0.0328356...	0.249760...	-1.33333...	-1.08357...
4	0.0464792...	-0.160426...	-1.40975...	-1.57018...
5	0.0533164...	-0.818135...	-0.995603...	-1.81374...
6	0.0568683...	-1.63720...	-0.293205...	-1.93041...
7	0.0586798...	-2.57138...	0.598918...	-1.97246...
8	0.0595055...	-3.59273...	1.62585...	-1.96689...
9	0.0597461...	-4.68294...	2.75391...	-1.92903...
10	0.0596284...	-5.82927...	3.96095...	-1.86831...
11	0.0592871...	-7.02245...	5.23161...	-1.79084...
12	0.0588057...	-8.25550...	6.55476...	-1.70074...
13	0.0582372...	-9.52303...	7.92208...	-1.60095...
14	0.0576162...	-10.8207...	9.32717...	-1.49356...
15	0.0569656...	-12.1451...	10.7650...	-1.38014...
16	0.0563009...	-13.4934...	12.2315...	-1.26189...
17	0.0556325...	-14.8632...	13.7235...	-1.13973...
18	0.0549676...	-16.2524...	15.2380...	-1.01437...
19	0.0543109...	-17.6594...	16.7730...	-0.886401...
20	0.0536657...	-19.0827...	18.3264...	-0.756273...
21	0.0530340...	-20.5210...	19.8966...	-0.624366...
22	0.0524171...	-21.9732...	21.4822...	-0.490990...
23	0.0518158...	-23.4383...	23.0819...	-0.356402...
24	0.0512305...	-24.9153...	24.6945...	-0.220815...
25	0.0506612...	-26.4037...	26.3193...	-0.0844091...
26	0.0501078...	-27.9026...	27.9552...	0.0526638...
27	0.0495701...	-29.4114...	29.6016...	0.190274...
28	0.0490476...	-30.9295...	31.2578...	0.328313...
29	0.0485400...	-32.4564...	32.9231...	0.466684...
30	0.0480469...	-33.9918...	34.5971...	0.605307...
31	0.0475677...	-35.5348...	36.2791...	0.744267...
32	0.0471020...	-37.0856...	37.9688...	0.883173...
33	0.0466492...	-38.6436...	39.6657...	1.02209...
34	0.0462090...	-40.2085...	41.3695...	1.16098...
35	0.0457808...	-41.7797...	43.0798...	1.30008...
36	0.0453641...	-43.3572...	44.7963...	1.43904...

Table D.9: Numerical solutions for the second excited state occupation numbers  $c_2^{*(0)}(N)$ ,  $c_2^{*(1,1)}(N)$ ,  $c_2^{*(1,2)}(N)$  and  $c_2^{*(1)}(N)$ , for  $N = 2 - 36$





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