Finite one dimensional impenetrable Bose systems: Occupation numbers

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Bosons in the form of ultra cold alkali atoms can be confined to a one dimensional (1d) domain by the use of harmonic traps. This motivates the study of the ground state occupations $\lambda_i$ of effective single particle states $\phi_i$ in the theoretical 1d impenetrable Bose gas. Both the system on a circle and the harmonically trapped system are considered. The $\lambda_i$ and $\phi_i$ are the eigenvalues and eigenfunctions respectively of the one body density matrix. We present a detailed numerical and analytic study of this problem. Our main results are the explicit scaled forms of the density matrices, from which it is deduced that for fixed $i$ the occupations $\lambda_i$ are asymptotically proportional to $\sqrt{N}$ in both the circular and harmonically trapped cases.

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I. INTRODUCTION

The Bose Gas, whose genesis we gratefully owe to Bose and Einstein, is an icon of statistical physics. The Bose-Einstein condensate (BEC) has found its very special place in nature as the fundamental mechanism underlying the properties of a very special system, superfluid helium. In the past decade, a new chapter has been opened with the experimental realization of ultracold atomic Bose gases [1, 2, 3].

As such, new and intriguing possibilities for the Bose gas have arisen. As these systems require harmonic traps, it is possible to fashion them to constrain the bosons in low dimensional configurations. In particular, Olshanii [4] has pointed out that a one dimensional (1d) configuration can be obtained and maintained by making an elongated trap where one of the harmonic trap frequencies, $\omega_z$, is much much less than the other frequency $\omega_\perp$. The experimental realization of a 1d ultra cold atomic Bose gas has now made this a physical reality [5, 6, 7].

This exciting prospect has now brought back into prominence the noted quantum mechanical $N$-body problem, the impenetrable 1d Bose gas. This system was introduced by Girardeau [8] and Lieb and Liniger [9]. It was solved by Lenard in his two classic works [10, 11] and in the ensuing major works of Sutherland [12, 13, 14], Vadiya and Tracy [15, 16, 17] and Jimbo et al [18].

In [9], a 1d system of $N$ bosons in box of length $L$ interacting via a repulsive delta-function potential of strength, $g$, was studied. It was shown that in the limit $\epsilon_F/\hbar g \rightarrow 0$ the impenetrable Bose gas was obtained, where $\epsilon_F$ is the Fermi energy and $n = N/L$ is the number density. This limit corresponds to the condition $n a_1 \rightarrow 0$ where $g = \hbar^2/ma_1$ and $a_1$ is the 1d $s$-wave scattering length [10]. To constrain the bosons to a 1d configuration the condition $\epsilon_F/\hbar \omega_\perp \rightarrow 0$ must be obtained. This limit corresponds to the condition $n l_0 \rightarrow 0$ where $l_0 = \sqrt{\hbar/m \omega_\perp}$, the characteristic range of the harmonic trap. These and concomitant matters are discussed in [4, 19, 20]. Appendix A gives the ground state energy and $\epsilon_F$ values for the finite $N$ and large $N$ limit systems.

The signature of the 1d impenetrable Bose system is the set of particle occupation numbers, which correspond in the untrapped system to the momentum distribution of the bosons but which is quite different for the harmonically trapped system.

Section II presents our comprehensive study of the occupation numbers for the finite $N$ and large $N$ limit untrapped impenetrable boson systems. Section III with Appendix B presents our comprehensive study of the occupation numbers for the finite $N$ and large $N$ limit harmonically trapped boson systems. Section IV presents concluding remarks.

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II. IMPENETRABLE BOSONS ON A CIRCLE

A. Properties of the density matrix

1. The wave function

We are interested in the ground state of a one dimensional many body Bose system which satisfies the free-particle Schrödinger equation, and also a condition of impenetrability which prevents two bosons occupying the same point in space. This system of impenetrable bosons is confined to lie in a box of length \( L \), and satisfy periodic boundary conditions, i.e.

\[
\psi_N^C(x_1,\ldots, x_k + L, \ldots, x_N) = \psi_N(x_1,\ldots, x_k, \ldots, x_N),
\]

\[
k = 1, 2, \ldots, N
\]

which may be interpreted as confining the particles to move on a circle of circumference length \( L \).

The impenetrability condition states that the wave function for our \( N \) body system must vanish whenever two coordinates coincide,

\[
\psi_N^C(x_1, x_2, \ldots, x_N) = 0 \quad \text{for} \quad x_j = x_k \quad (j \neq k).
\]

For spin-less point particles however this condition is equivalent to the Pauli exclusion principle. Hence for any fixed ordering of the particles, e.g.

\[
x_1 < x_2 < \ldots < x_N,
\]

there is no distinction between impenetrable bosons and free fermions\[8\]. Therefore for the ordering \( \{j\} \), the ground state of the system of impenetrable bosons can be constructed from a Slater determinant of distinct single particle plane wave states, which has zero total momentum and minimum total energy,

\[
\psi_N^C(x_1, x_2, \ldots, x_N) = \begin{cases} 
(L^N N!)^{-1/2} \frac{\det [e^{2\pi i x_j/L}]}{j=1}^{j=N} & \text{N odd} \\
(L^N N!)^{-1/2} \frac{\det [e^{2\pi i (k+1/2)x_j/L}]}{k=-\frac{N-1}{2}}^{k=\frac{N-1}{2}} & \text{N even} 
\end{cases}
\]

\[
= (L^N N!)^{-1/2} \prod_{1 \leq j < k \leq N} 2i \sin[\pi (x_k - x_j)/L].
\]

Ignoring irrelevant constant phase factors, we note that in the region of configuration space which we are considering, defined by condition \( \{3\} \), the function \( \{3\} \) is non-negative. This property of non-negativity distinguishes the ground state in Bose systems. Imposing the condition that the wave function for a system of bosons be symmetric under particle interchange, \( x_j \leftrightarrow x_k \quad (j \neq k) \), we then deduce from \( \{3\} \) that for general ordering of the particles, the properly normalized \( N \) body wave function for our system is

\[
\psi_N^C(x_1, x_2, \ldots, x_N) = (N! L^N)^{-1/2} \prod_{1 \leq j < k \leq N} 2|\sin[\pi (x_k - x_j)/L]| 
\]

\[
= (N! L^N)^{-1/2} \prod_{1 \leq j < k \leq N} |e^{2\pi i x_k/L} - e^{2\pi i x_j/L}|.
\]

This result was first obtained by Girardeau \[8\].

2. Toeplitz determinant form for the density matrix

The one body density matrix for a system of \( N \geq 2 \) particles is obtained by integrating out \((N - 1)\) degrees of freedom from the product \( \psi_N(x_1, x_2, \ldots, x_{N-1}, x)\psi_N(x_1, x_2, \ldots, x_{N-1}, x') \). Since the periodic boundary conditions imply translational invariance the one body density matrix will be a function of one variable only. Specifically, for the wave function \( \{3\} \) we have

\[
\rho_N^C(x - y) = N \int_0^L dx_1 \ldots \int_0^L dx_{N-1} \psi_N(x_1, x_2, \ldots, x_{N-1}, x)\psi_N(x_1, x_2, \ldots, x_{N-1}, y)
\]

\[
N \int_0^L dx \rho_N^C(x - y).
\]
where \( t = \pi(x - y)/L \), and to obtain (11) we have made a change of variables and utilized the periodicity of the integrand. The normalization of (9) is chosen so that

\[
\rho_N(t) := L \rho^C_N(x).
\]

By utilizing the following general result it is straightforward to express \( \rho_N(t) \) as the determinant of a Toeplitz matrix [21], a result first noted by Lenard [10],

\[
\frac{1}{N!} \int_0^{2\pi} d\theta_1 \cdots \int_0^{2\pi} d\theta_N \prod_{l=1}^{N} f(\theta_l) \prod_{1 \leq j < m \leq N} |e^{i\theta_j} - e^{i\theta_k}|^2 = \det \left[ \int_0^{2\pi} d\theta f(\theta) e^{i\theta(j-k)} \right]_{j,k=1,2,...,N}.
\]

The result (11) can be obtained by identifying the double product as the squared modulus of the Vandermonde determinant, which implies that the left hand side of (11) is

\[
\frac{1}{N!} \int_0^{2\pi} d\theta_1 \cdots \int_0^{2\pi} d\theta_N \prod_{l=1}^{N} f(\theta_l) \sum_{P \in S_N} \sum_{Q \in S_N} \varepsilon(P) \varepsilon(Q) \prod_{l=1}^{N} e^{i\theta_l[P(l)-Q(l)]}
\]

\[
= \frac{1}{N!} \sum_{P \in S_N} \sum_{Q \in S_N} \varepsilon(P) \varepsilon(Q) \prod_{l=1}^{N} \int_0^{2\pi} d\theta f(\theta) e^{i\theta[P(l)-Q(l)]}
\]

\[
= \det \left[ \int_0^{2\pi} d\theta f(\theta) e^{i\theta(j-k)} \right]_{j,k=1,...,N}
\]

where \( S_N \) is the group of all permutations on \( N \) objects, and \( \varepsilon(P) \) is the signature of the permutation \( P \). In obtaining (11) from (13) we have used the general result that

\[
\frac{1}{N!} \sum_{P \in S_N} \sum_{Q \in S_N} \varepsilon(P) \varepsilon(Q) \prod_{l=1}^{N} a_{P(l),Q(l)} = \det [a_{j,k}]_{j,k=1,...,N}.
\]

Applying (11) to (3) and explicitly computing the one dimensional integrals we arrive at (11)

\[
\rho_N(t) = \det [\gamma_{j-k}(t)]_{j,k=1,...,N-1}
\]

with \( \gamma_n(t) \) given by

\[
\gamma_n(t) = \frac{1}{\pi} \int_0^{2\pi} |\cos(u) - \cos(t)| e^{iun} \, du
\]

\[
\gamma_n(t) = 2\delta_{n,0}\cos(t) - \delta_{n,1} - \delta_{n,-1} - \frac{4\cos(t) \sin(n|t|)}{\pi n}
\]

\[
+ \frac{2}{\pi} \left( \frac{\sin([n+1]|t|)}{(n+1)} + \frac{\sin([n-1]|t|)}{(n-1)} \right).
\]

The succinct expressions (16) and (18) are well suited for our numerical investigations of the momentum distribution, to be discussed in Section II.B.3.

Expanding out the determinant (16) we find explicitly

\[
\varrho_2(t) = \frac{2}{\pi} [(\pi - 2t) \cos(t) + 2 \sin(t)],
\]

\[
\varrho_3(t) = \frac{1}{2\pi^2} \left[ (15 + 2(\pi - 2t)^2 + 4(2 + \pi - 2t)(\pi - 2(1+t)) \cos(2t) + \cos(4t)) \right]
\]
Specifically, as a consequence of the detailed discussion in [22] it can be seen that the function $VI$ formulation of the sixth Painlevé equation, $P_I$, of this equation. Hence we obtain as a corollary an explicit differential equation characterization for our $\rho_N(t)$, such an average is expressible in terms of a specific $\tau$-function occurring in the Hamiltonian formulation of the sixth Painlevé equation, $P_{VI}$, and thus can be characterized by the Jimbo-Miwa-Okamoto $\sigma$-form of this equation. Hence we obtain as a corollary an explicit differential equation characterization for our $\rho_N(t)$. Specifically, as a consequence of the detailed discussion in [22] it can be seen that the function

$$\phi_N(t) = \frac{e^{2it} - 1}{2it} \frac{d}{dt} \log \rho_N(t),$$

satisfies the second order nonlinear differential equation

$$\left(1 - e^{-2it}\right)^2 \left(-2i \phi_N'(t) + \phi_N''(t)\right)^2 = 16 \left(1 + \phi_N(t) + \frac{i}{2} \left(1 - e^{-2it}\right) \phi_N(t)\right) \times \left(2i e^{-2it} \left(\phi_N(t) + \frac{i}{2} \phi_N'(t)\right) \phi_N'(t) + (N - 1)(N + 1) \left(\phi_N(t) + \frac{i}{2} \left(1 - e^{-2it}\right) \phi_N(t)\right)\right).$$

The expression (22) can be inverted for $\rho_N(t)$ to yield

$$\rho_N(t) = N e^{2i \int_0^t ds \frac{2i}{e^{2is} - 1} \phi_N(s)}.$$

If we substitute $u = e^{2it}$ into (23), and define

$$\sigma_N(u) = \phi_N(t) = u(u - 1) \frac{d}{du} \log \rho_N(t)|_{e^{2it}=u},$$

then the resulting equation is precisely of the Jimbo-Miwa-Okamoto $\sigma$-form for $P_{VI}$.

It is interesting to note [23] that if in (22) we replace $\phi_N(t)$ with the one body density matrix for the free Fermi system, $\rho_N^F(t)$, then this function is also a solution of the differential equation (23), albeit with a different boundary condition. The boundary condition required to complete the characterization of $\rho_N(t)$ or $\rho_N^F(t)$ in terms of (22) and (24) is provided by knowing the first few terms of their small $t$ expansion. For $\rho_N^F(t)$ this is trivial since we simply have

$$\rho_N^F(t) = \frac{\sin(Nt)}{\sin(t)} = N \left(1 - \frac{(N^2 - 1)}{6} t^2 + \frac{(3N^4 - 10N^2 + 7)}{360} t^4 + O(t^6)\right).$$

To obtain the small $t$ expansion for $\rho_N(t)$ we utilize the result, originally due to Lenard [11, 22], that $\rho_N^F(x)$ can be written in terms of an expansion over integrals of the $n$-body density matrix of the free Fermi system, which we denote here by $\rho_N^F(x_1, x_2, x_3, ..., x_n) = L^{-(n+1)} \rho_N^F(t_1, t_2, t_3, ..., t_n)$, with the obvious extension of our notation $t_j = \pi x_j/L$. Recall that $\rho_N^F(t_1, t_2, t_3, ..., t_{n+1})$ has the following determinantal expression in terms of $\phi_N(t)$

$$\rho_N^F(t_1, t_2, t_3, ..., t_{n+1}) = \det \left(\phi_N^F(t_j - t_k)\right)_{j=2,3, ..., n+1} = \det \left(\phi_N^F(t_j - t_k)\right)_{j=2,3, ..., n+1}. $$

For larger $N$, expanding out the determinant for $\rho_N(t)$ quickly becomes unwieldy. We use the expressions [19]-[21] in Section [2B] to find the corresponding exact expressions for the momentum distribution.

3. A differential equation for $\rho_N(t)$

We present in this section a characterization of $\rho_N(t)$ via a second order, second degree differential equation. This is a consequence of the identification [22] of $\rho_{N+1}(t)$ with a certain well studied average over the eigenvalue probability density function of the circular unitary ensemble of $N \times N$ random matrices. It has recently been demonstrated [24] that for a given $N$ such an average is expressible in terms of a specific $\tau$-function occurring in the Hamiltonian formulation of the sixth Painlevé equation, $P_{VI}$, and thus can be characterized by the Jimbo-Miwa-Okamoto $\sigma$-form of this equation. Hence we obtain as a corollary an explicit differential equation characterization for our $\rho_N(t)$. Specifically, as a consequence of the detailed discussion in [22] it can be seen that the function

$$\rho_N(t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\sigma \rho_N(t) \left(1 - e^{-2it}\right)^2 \frac{\phi_N'(t) + \phi_N''(t)}{2i} \phi_N(t) + (N - 1)(N + 1) \left(\phi_N(t) + \frac{i}{2} \left(1 - e^{-2it}\right) \phi_N(t)\right),$$

satisfies the second order nonlinear differential equation

$$\left(1 - e^{-2it}\right)^2 \left(-2i \phi_N'(t) + \phi_N''(t)\right)^2 = 16 \left(1 + \phi_N(t) + \frac{i}{2} \left(1 - e^{-2it}\right) \phi_N(t)\right) \times \left(2i e^{-2it} \left(\phi_N(t) + \frac{i}{2} \phi_N'(t)\right) \phi_N'(t) + (N - 1)(N + 1) \left(\phi_N(t) + \frac{i}{2} \left(1 - e^{-2it}\right) \phi_N(t)\right)\right).$$

The expression (23) can be inverted for $\rho_N(t)$ to yield

$$\rho_N(t) = N e^{2i \int_0^t ds \frac{2i}{e^{2is} - 1} \phi_N(s)}.$$

If we substitute $u = e^{2it}$ into (23), and define

$$\sigma_N(u) = \phi_N(t) = u(u - 1) \frac{d}{du} \log \rho_N(t)|_{e^{2it}=u},$$

then the resulting equation is precisely of the Jimbo-Miwa-Okamoto $\sigma$-form for $P_{VI}$.

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$$\rho_N^F(t) = \frac{\sin(Nt)}{\sin(t)} = N \left(1 - \frac{(N^2 - 1)}{6} t^2 + \frac{(3N^4 - 10N^2 + 7)}{360} t^4 + O(t^6)\right).$$

To obtain the small $t$ expansion for $\rho_N(t)$ we utilize the result, originally due to Lenard [11, 22], that $\rho_N^F(x)$ can be written in terms of an expansion over integrals of the $n$-body density matrix of the free Fermi system, which we denote here by $\rho_N^F(x_1, x_2, x_3, ..., x_n) = L^{-(n+1)} \rho_N^F(t_1, t_2, t_3, ..., t_n)$, with the obvious extension of our notation $t_j = \pi x_j/L$. Recall that $\rho_N^F(t_1, t_2, t_3, ..., t_{n+1})$ has the following determinantal expression in terms of $\phi_N(t)$

$$\rho_N^F(t_1, t_2, t_3, ..., t_{n+1}) = \det \left(\phi_N^F(t_j - t_k)\right)_{j=2,3, ..., n+1} = \det \left(\phi_N^F(t_j - t_k)\right)_{j=2,3, ..., n+1}. $$

For larger $N$, expanding out the determinant for $\rho_N(t)$ quickly becomes unwieldy. We use the expressions [19]-[21] in Section [2B] to find the corresponding exact expressions for the momentum distribution.
In the above, \( j \) and \( k \) refer to the row and column elements respectively, so that for example \( \rho_N^F(t)_{j=2,3,...,n+1} \) is an \( n \) dimensional row vector and \( \rho_N^F(t_j-t_k)_{j,k=2,3,...,n+1} \) is an \( n \times n \) matrix.

The one-body density matrix for the impenetrable Bose system then has the form

\[
\rho_N(t) = \sum_{n=0}^{\infty} \frac{(-2)^n}{n!} \int_0^t dt_2 \ldots \int_0^t dt_{n+1} \rho_N^F(t, t_2, t_3, \ldots, t_{n+1}).
\] (28)

We remark that the right hand side of (28) is exactly proportional to the first Fredholm minor for the kernel \( V \). Using (26)-(28), it is straightforward to deduce that \( \rho_N(t) \) has the small \( t \) behavior

\[
\frac{\rho_N(t)}{\rho_N(0)} = 1 - \left( \frac{N^2 - 1}{6} \right) t^2 + \frac{N (N^2 - 1)}{9\pi} t^3 + \ldots
\] (29)

which then serves as the boundary condition characterizing \( \rho_N(t) \) in terms of (22) and (23).

4. Asymptotic expansions of \( \rho_N(t) \), and the thermodynamic limit

One important application of the differential equation (23), is that it provides a far more expedient way of deriving the corrections to the small \( t \) expansion (24) than the does the expression (28). By substituting a small \( t \) power series ansatz for \( \phi_N(t) \) into the differential equation (23), we obtain equations which define all but one of the coefficients. In particular the resulting equation for the coefficient of \( t^4 \) vanishes identically, and to fix this parameter we require the boundary condition (23), obtained from (28). However the differential equation then provides an extremely efficient way of obtaining a large number of higher order terms in the small \( t \) expansion. We found it straightforward to obtain the first twenty terms of \( \rho_N(t) \) in this manner, although it would require far too much space to exhibit all these here. Using the relationship (23) we obtain the corresponding small \( t \) expansion of \( \rho_N(t) \), and include here terms up to and including \( t^9 \),

\[
\frac{\rho_N(t)}{\rho_N(0)} = 1 - \left( \frac{N^2 - 1}{6} \right) t^2 + \frac{N (N^2 - 1)}{9\pi} t^3 + \frac{3N^4 - 10N^2 + 7}{360} t^4
\]

\[
- \frac{N (11N^4 - 40N^2 + 29)}{1350\pi} t^5 - \frac{(3N^6 - 21N^4 + 49N^2 - 31)}{15120} t^6
\]

\[
+ \frac{N (N^2 - 1) (183N^4 - 1210N^2 + 2227)}{793800\pi} t^7
\]

\[
+ \left( \frac{N^2 - 1}{} \left( \frac{5N^6 - 55N^4 + 239N^2 - 381}{1814400} \right) + \frac{N^2 (N^2 - 4) (N^2 - 1)^2}{24300\pi^2} \right) t^8
\]

\[
- \frac{N (N^2 - 1) (253N^6 - 3017N^4 + 13867N^2 - 22863)}{71442000\pi} t^9 + O(t^{10}).
\] (30)

Comparing this expansion with the expansion for \( \rho_N^F(t) \) given in (22), we see that while the terms with an odd power of \( t \) in (30) arise purely from the Bose nature of the system and are not present in the expansion of \( \rho_N^F(t) \), the even terms in (30) up to and including \( t^6 \), are precisely just the corresponding free Fermi terms from (22). The coefficient of \( t^6 \) however is seen to be a composed of two pieces, the first is simply the corresponding free Fermi term which is rational, where as the second is irrational and dependent on the Bose nature of the system. Precisely the same behavior is observed in the well known small \( x \) expansion in the thermodynamic limit.

Our differential equation (23) and small \( t \) expansion (30) for the finite system can be seen to reduce to the corresponding results in the thermodynamic limit as follows. We define

\[
\sigma_V(s) = \lim_{N \to \infty} \phi_N(s/N) = \lim_{N \to \infty} \sigma_N(\rho^{2is/N})
\] (31)

and denote the density matrix for the system in the thermodynamic limit by \( \rho(x) \). Taking \( N \to \infty \) in (23) and (24), and retaining only leading order terms, we respectively recover both the expression for \( \rho(x) \) in terms of \( \sigma_V(s) \), and the correct \( \sigma \)-form of the fifth Painlevé equation characterizing \( \sigma_V(s) \), as discussed in the celebrated work of Jimbo et al[8]. Further, recalling that the thermodynamic limit corresponds to \( N \to \infty \) with the Fermi momentum \( k_F = \pi N/L \) held finite, we can replace \( Nt \) with \( k_F x \) in (30) and then noting that only the highest powers of \( N \) in each coefficient of (30) will survive in this limit, we recover the corresponding small \( x \) asymptotic expansion for \( \rho(x) \) due to Vaidya and Tracy[17].
In their tour de force \cite{17}, Vaidya and Tracy were also able to systematically construct the large $x$ asymptotic expansion for $\rho(x)$, the leading term of which is

$$\frac{\rho(x)}{\rho(0)} \sim \rho_\infty |k_F x|^{-1/2}. \quad (32)$$

The corresponding result for the finite system is a good deal more subtle, as we deal with competing behavior of large $x$ and large $N$. Starting with the Toeplitz form \cite{16}, a delicate analysis due to Lenard\cite{24}, rigorously justified by Widom\cite{25}, gives the surprisingly simple result

$$\rho_N(t) := L \rho_N^C(x) \sim N \rho_\infty \left| N \sin \left( \frac{k_F x}{N} \right) \right|^{-1/2} = \rho_\infty \sqrt{N} |\sin(t)|^{-1/2} \quad (33)$$

with

$$\rho_\infty = \frac{G^4(3/2)}{\sqrt{2}} = \frac{\pi e^{1/2} 2^{-1/3} A^{-6}}{2} \approx 0.92418 \quad (34)$$

where $G(z)$ is the Barnes G function\cite{26}, $A \approx 1.2824271$ is Glaisher’s constant and we have noted the identity \cite{26, 27}\cite{26, 27}

$$G(3/2) = \frac{\pi^{1/4} e^{1/8} 2^{1/4}}{A^{-3/2}} \approx 1.06922. \quad (35)$$

It is now known that \cite{16} is a special case of a class of Toeplitz determinants with singular generating functions for which the asymptotics can be computed (see for e.g. \cite{28}). We note too that in the thermodynamic limit the expression \cite{33} reduces to \cite{32}. It is still an open question however, as to how to obtain the correction terms to \cite{33} and thus generalize the expansion of $\rho(x)$ of Vaidya and Tracy to the finite system. These correction terms are important for investigating the large $N$ behavior of the momentum distribution.

**B. Momentum distribution**

1. Preliminaries

Due to our choice of periodic boundary conditions the Fourier coefficients of $\rho_N^C(x)$,

$$c_n(N) = \int_0^L dx \rho_N^C(x) \exp \left( \frac{-2n \pi x i}{L} \right) = \frac{1}{\pi} \int_0^\pi dt \varrho_N(t) \cos(2nt), \quad (36)$$

have the physical interpretation of being the expectation of the number of particles in the single particle state of momentum $2\pi n \hbar / L$. In terms of these momentum state occupations, we have the Fourier expansion for $\varrho_N(t)$ given by

$$\varrho_N(t) = \sum_{n=-\infty}^{\infty} c_n(N) \cos(2nt). \quad (37)$$

Recalling our normalization convention, $\varrho_N(0) = N$, a direct consequence of \cite{37} is that

$$N = \sum_{n=-\infty}^{\infty} c_n(N), \quad (38)$$

$$\varrho_N(\pi/2) = \sum_{n=-\infty}^{\infty} (-1)^n c_n(N). \quad (39)$$

The expression \cite{38} simply states that the sum over the occupations of all momentum modes for our system is equal to the total number of particles $N$. It is of interest to compare the asymptotic occupation of the even modes versus that of the odd modes, for large $N$. By subtracting \cite{39} from \cite{38}, and observing that \cite{33} implies $\varrho_N(\pi/2) \sim \sqrt{N}$, we obtain

$$\sum_{n=-\infty}^{\infty} c_{2n+1}(N) = \frac{N}{2} - \frac{\varrho(\pi/2)}{2} \sim \frac{N}{2}. \quad (40)$$
Hence for large $N$ the total occupation of the odd modes is half the total number of particles, and so in this limit the particles are evenly distributed among both the odd and even modes.

It is straightforward to obtain an exact expression for $c_n(2)$ for all $n$ by performing the integration (30) with $\rho_2(t)$ given by (19), to obtain

$$c_n(2) = \frac{16}{(4n^2 - 1)^2\pi^2}. \quad (41)$$

We pause here to mention a mathematically interesting observation regarding the structure of the Fourier series for $\rho_2(t)$ at the special values $t = 0$, and $t = \pi/2$. By definition we know $\rho_N(0) = N$, and as discussed in [22] the exact value of $\rho_N(\pi/2)$ can be expressed in closed form for all $N$. For $N = 2$ the particular expressions (11) and (37) yield

$$\rho_2(0) = \frac{16}{\pi^2}E_1(2) = 2 \quad \text{and} \quad \rho_2(\pi/2) = \frac{16}{\pi^2}E_2(1) = \frac{16}{\pi^2}\arctan(1) = \frac{4}{\pi} \quad (42)$$

where $E_1(s)$ and $E_2(s)$ are the celebrated series studied by Euler [29, 30]

$$E_1(s) = \sum_{k=0}^{\infty} \frac{1}{(2k + 1)^s} = (1 - 2^{-s})\zeta(s) \quad s > 1, \quad E_2(s) = \sum_{k=0}^{\infty} \frac{(-1)^k}{(2k + 1)^s}, \quad (43)$$

which have the property that the sum of $E_1(s)$ for even $s \geq 2$, and the sum of $E_2(s)$ for odd $s \geq 1$ are both rational multiples of $\pi^s$.

It is possible to obtain exact closed form expressions of $c_n(N)$ for other small values of $N$, however the complexity of the corresponding $\rho_N(t)$ obviously prohibits us from taking this procedure too far, and indeed already by $N = 4$ the expression for $c_n(4)$ is quite a complicated object. Explicitly,

$$c_n(3) = \begin{cases} \frac{35}{2\pi^2}n_0, & |n| \leq 1 \\ \frac{1}{4\pi^2}n_1, & |n| \geq 1 \end{cases} \quad (44)$$

$$c_n(4) = \frac{64}{(16n^4 - 40n^2 + 9)^2\pi^2} \left( 80n^4 - 8n^2 + 45 \right) \left( \frac{18874368 (16n^2 (88n^2 (21n^2 - 137) + 15613) - 179455) - 55125}{(16n^4 - 296n^2 + 1225)^2 (16n^4 - 40n^2 + 9)^4 \pi^4} \right). \quad (45)$$

2. Large $N$ asymptotics of $c_n(N)$

Utilizing the large $N$ asymptotic form for $\rho_N(t)$ given by (33), we can obtain the asymptotic behavior of $c_n(N)$ for $N \gg n$,

$$c_n(N) \sim \frac{\rho_\infty}{\pi} \sqrt{N} \int_0^\pi dt \cos(2nt) \sin^{-1/2}(t). \quad (46)$$

This integral is expressible in terms of the beta function [31], $B(x, y)$, and so

$$c_n(N) \sim \frac{\rho_\infty}{\pi} \frac{2\sqrt{2}\pi \cos(n\pi)}{B(n + 3/4, -n + 3/4)} \sqrt{N} \quad (47)$$

$$c_n(N) \sim \frac{\rho_\infty}{\sqrt{\pi}} \frac{\Gamma(n + 1/4)}{\Gamma(n + 3/4)} \sqrt{N}. \quad (48)$$

Thus the leading order large $N$ behavior of $c_0(N)$ is

$$c_0(N) \sim \frac{\sqrt{2\pi} \rho_\infty}{\Gamma(2\pi (3/4))} \sqrt{N} \approx 1.54269\sqrt{N} \quad N \to \infty. \quad (49)$$

A consequence of our lack of correction terms to the asymptotic result (33) for $\rho_N(t)$, is that only the leading order large $N$ behavior of $c_n(N)$ is available to us via this argument. In Section II.B.3 we use numerical results to conjecture the form of the correction terms to (48).
Manipulating (48) we find that the ratio of gamma functions \([46]\) reduces to a simple rational product and thus we obtain the following very tidy expression for the large \(N\) behavior of \(c_n(N)\) in terms of that of \(c_0(N)\) as follows

\[
\frac{c_n(N)}{c_0(N)} \sim \prod_{l=1}^{n} \frac{(4l - 3)}{(4l - 1)}.
\]  

(50)

If \(n\) also is asymptotically large, so that \(N \gg n \gg 1\), we can simplify things further still by applying Stirling’s formula to (48) which yields

\[
\frac{c_n(N)}{c_0(N)} \sim \frac{\rho_\infty \sqrt{N}}{\sqrt{\pi} \sqrt{n}} \left[ 1 - \frac{1}{64n^2} + O(n^{-3}) \right].
\]

(51)

\[
\implies \frac{c_n(N)}{c_0(N)} \sim \frac{\Gamma^2(3/4)}{\sqrt{2\pi} \sqrt{n}} \frac{1}{\sqrt{n}} \left[ 1 - \frac{1}{64n^2} + O(n^{-3}) \right].
\]

(52)

It is important to observe that there are no corrections linear in \(n^{-1}\) in the expressions (51) and (52), which is a consequence of the fact that the first correction terms in the Stirling expansions of \(\Gamma(n + 1/4)\) and \(\Gamma(n + 3/4)\) are identical. The practical consequence of this is that (52) provides an extremely good approximation of (50) even for small \(n\), in particular even for \(n = 1\). To demonstrate this remarkable agreement we list in Table I the values of \(c_n(N)/c_0(N)\) evaluated via both (50) and (52), for \(n = 1, 2, 3, 5\).

Finally, we compare our results for the finite system when \(N \gg n > 0\) with the continuum momentum distribution constructed using the large \(x\) expansion [32] for \(\rho(x)\) of Vaidya and Tracy [17]. Denoting the momentum distribution in the thermodynamic limit by \(c(k)\), we find the following small \(|k|\) behaviour

\[
c(k) = \int_{-\infty}^{\infty} e^{-ikx} \rho(x) dx \sim \rho_\infty \int_{-\infty}^{\infty} e^{-ikx}|k_Fx|^{-1/2} dx = \sqrt{\frac{2}{\pi}} \rho_\infty \left| k/k_F \right|^{-1/2}.
\]

(53)

Substituting \(k = 2\pi n/L\), consistent with our periodic boundary conditions, into (53) results in the leading term of (51). This is consistent since even with \(n \gg 1\), if \(N \gg n\) this implies that \(k \ll k_F\).

3. Numerical calculation of \(c_0(N)\), \(c_1(N)\) and \(c_2(N)\)

In order to gain further insight into the occupations of the low lying momentum modes, we have performed the Fourier integral (54) over the Toeplitz determinant (14) numerically, for various values of \(N\), for the cases \(c_0(N)\), \(c_1(N)\), and \(c_2(N)\). The results are shown in Figs. 1, 2 and 3 where the dots represent the result of performing the numerical integration and the line represents a fit of this data to the ansatz

\[
c_n(N) \approx a_1 \sqrt{N} + a_2 + a_3 N^{-1/2} + a_4 N^{-1} + ...
\]

(54)

We also list in Table I the exact values of \(c_0(N)\) for \(N = 2, 3, 4, 5, 6, 7\).

As discussed in Section 1B.2, analytic arguments lead to \(\sqrt{N}\) leading order behavior for the large \(N\) asymptotics of \(c_n(N)\). The coefficients of \(\sqrt{N}\) for \(c_0(N)\), \(c_1(N)\), and \(c_2(N)\) given in our numerical fits below match very well with those derived by such arguments.

\[
c_0(N) \approx 1.54273 \sqrt{N} - 0.5725 + \frac{0.003677}{\sqrt{N}}
\]

(55)

\[
c_1(N) \approx 0.514345 \sqrt{N} - 0.5739 + \frac{0.01128}{\sqrt{N}}
\]

(56)

\[
c_2(N) \approx 0.367622 \sqrt{N} - 0.5775 + \frac{0.02948}{\sqrt{N}}
\]

(57)
FIG. 1: The zeroth mode of the momentum distribution $c_0(N)$ vs $N$.

FIG. 2: The first mode of the momentum distribution $c_1(N)$ vs $N$.

The fits (55)-(57) were constructed using only the data for $N > 30$ so as to obtain asymptotic information for large $N$, however as can be seen from the plots they match up very well with all the data. Indeed, the $\chi^2$ value for each fit is of the order $10^{-10}$. We note that the coefficient of the $N^{-1/2}$ term in each of (55)-(57) is considerably smaller than the coefficient of the leading term or the constant. Also we remark that the constant term is very similar in all three fits, and that a very similar constant again appears in the fits of the occupation numbers for the system of harmonically trapped impenetrable bosons to be discussed in Section II B 3. This suggests that the first correction term to the occupation of the low lying states as a function of $N$ may well be a universal constant common to both of these systems.

4. Large $n$ asymptotics of $c_n(N)$

The occupation numbers, $c_n(N)$, depend on the two parameters $n$ and $N$. In Section II B 2 we found the asymptotic behaviour of $c_n(N)$ for $N \gg n$. In this section, by contrast, we seek an expression for the large $n$ behaviour of $c_n(N)$, with $n \gg N$. Observing the large $n$ behaviour of the exact results for $c_n(2)$, $c_n(3)$ and $c_n(4)$, given respectively by
FIG. 3: The second mode of the momentum distribution $c_2(N)$ vs $N$.

| $N$ | Exact $c_0(N)$ | Numerical $c_0(N)$ |
|-----|----------------|--------------------|
| 2   | $\frac{1}{2}$   | 1.62114...         |
| 3   | $\frac{1}{2} + \frac{1}{\pi^2}$ | 2.10645...         |
| 4   | $\frac{1}{2} + \frac{1}{\pi^2} + \frac{1}{\pi^4}$ | 2.35196...         |
| 5   | $\frac{1}{2} + \frac{1}{\pi^2} + \frac{1}{2 \pi^4}$ | 2.88069...         |
| 6   | $\frac{1}{2} + \frac{1}{\pi^2} + \frac{1}{2 \pi^4} + \frac{1}{3 \pi^6}$ | 3.20923...         |
| 7   | $\frac{1}{2} + \frac{1}{\pi^2} + \frac{1}{2 \pi^4} + \frac{1}{3 \pi^6} + \frac{1}{4 \pi^8}$ | 3.51155...         |

TABLE II: Values of $c_0(N)$ for $N = 2, 3, 4, 5, 6, 7$

To obtain the coefficients $a_1, a_2, ...$ we construct a small $t$ expansion of $\varrho_N(t)$ by applying the Mellin transform technique to its Fourier series representation (37) with Fourier coefficients given by (58), and then compare this result with (30).

Beginning with (37) we insert the Mellin integral representation of $\cos(2\pi nt)$ which yields

$$\varrho_N(t) = c_0(N) + \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds \ 2^{-s} \Gamma(s) \cos(\pi s/2) g(s) t^{-s}, \quad 0 < c < 1$$

where we have defined

$$g(s) = \sum_{n=1}^{\infty} \frac{c_n(N)}{n^s} = \sum_{j=1}^{\infty} a_j \zeta(s + 2j + 2)$$

and in the last step we have swapped orders of summation and identified the series representation of the Riemann zeta function, $\zeta(s)$, which is finite everywhere on our contour of integration in (59).

Closing the contour of (59) to the left results in a small $t$ expansion. The poles of the integrand in the left half plane are all simple, and lie at $s = 0, -2, -3, -4, -5, ...$. We note that the term arising from the residue at $s = 0$ combines with $c_0(N)$ to produce $\varrho_N(0)$. Since $\Gamma(s) \cos(\pi s/2)$ is analytic when $s$ is odd, the poles at $s = -(2k + 1), k \geq 1$, arise purely from the $a_k$ term in the zeta function expansion of $g(s)$. Hence the corresponding $t^{2k+1}$ term in the small $t$ expansion of $\varrho_N(t)$ will contain $a_k$, so that we can obtain the values of all the $a_k$ simply by considering the odd terms. We note that as discussed in Section 1A, it is precisely the odd terms in the small $t$ expansion of $\varrho_N(t)$ which arise purely from the Bose nature of the system and do not appear in the corresponding free Fermi expansion. The poles at even values of $s$ arise from $\Gamma(s)$, since $g(s)$ is analytic then, and so the residues at these values will contain the
entire $g(s)$ series, \(60\)). Calculating the required residues then, we obtain the following expansion

$$\frac{g_N(t)}{g_N(0)} \sim 1 - \frac{4g(-2)}{N} t^2 + \frac{4\pi}{3N}a_1 t^3 + \frac{4g(-4)}{3N} t^4 - \frac{4\pi}{15N}a_2 t^5 - \frac{8g(-6)}{45N} t^6$$

$$+ \frac{8\pi}{315(N+1)}a_3 t^7 + \frac{4g(-8)}{315N} t^8 - \frac{4\pi}{2835N}a_4 t^9. \quad (61)$$

Comparing \((61)\) with \((34)\) we deduce

$$c_n(N) \sim \frac{N^2 (N^2 - 1)}{12\pi^2} \frac{1}{n^6} + \frac{N^2 (N^2 - 1) (-29 + 11N^2)}{360\pi^2} \frac{1}{n^8}$$

$$+ \frac{N^2 (N^2 - 1) (2227 - 1210N^2 + 183N^4)}{20160\pi^2} \frac{1}{n^{10}} + \frac{N^2 (N^2 - 1) (-22863 + 13867N^2 - 3017N^4 + 253N^6)}{100800\pi^2} \frac{1}{n^{12}}. \quad (62)$$

Going out to higher orders is a straightforward matter, but the resulting expressions obtained for \(a_k\) become increasingly cumbersome.

Feeding the explicit values of \(a_k\) from \((62)\) into \(g(s)\) and comparing the even terms in \((61)\) with the corresponding even terms in \((34)\) we obtain a consistency check on the validity of our ansatz.

We note that for the values \(N = 2, 3, 4\), the large \(n\) expansion \((62)\) recovers the large \(n\) expansions one obtains from the exact exact results \((41)\), \((44)\) and \((45)\). Further, we can also recover from \((62)\) the large \(c\) behaviour of the continuum momentum distribution, \(c(k)\), just as we recovered the small \(c\) behaviour of \(c(k)\) from \((51)\) in Section II B 2. If we apply the following asymptotic result\[32\]

$$\rho(x) \sim \rho(0) \sum_{s=0}^{\infty} b_s (k_F x)^s, \quad x \to 0 \quad (63)$$

$$\implies \int_0^\infty \rho(x) \cos(kx) \, dx \sim \frac{1}{\pi} \sum_{s=0}^{\infty} (-1)^{s+1} (2s + 1) b_{2s+1} \left(\frac{k_F}{k}\right)^{2(s+1)}, \quad k \to \infty \quad (64)$$

to the small \(x\) asymptotic expansion for \(\rho(x)\) of Vaidya and Tracy\[17\]

$$\frac{\rho(x)}{\rho(0)} = 1 - \frac{(k_F x)^2}{6} + \frac{|k_F x|^3}{9\pi} + \frac{(k_F x)^4}{120} - \frac{11 |k_F x|^5}{1350\pi} - \frac{(k_F x)^6}{5040} + \frac{122 |k_F x|^7}{105\pi^7}$$

$$+ \left( \frac{1}{24300\pi^2} + \frac{1}{9!} \right) (k_F x)^8 - \frac{253}{98000\pi^2} |k_F x|^9 + O((k_F x)^{10}) \quad (65)$$

we deduce that

$$c(k) \sim \frac{4}{3\pi^2} \left(\frac{k_F}{k}\right)^4 + \frac{88}{45\pi^2} \left(\frac{k_F}{k}\right)^6 + \frac{244}{105\pi^2} \left(\frac{k_F}{k}\right)^8 + \frac{4048}{1575\pi^2} \left(\frac{k_F}{k}\right)^{10}. \quad (66)$$

Substituting \(k = 2\pi n/L\), which implies \(N/n = 2k_F/k\), into \((62)\) and taking \(N \to \infty\) retaining only leading order terms then recovers \((60)\).

We can thus summarise the asymptotic behaviour of the occupation of the \(n\)th single particle momentum state for a system of impenetrable bosons on a circle as follows: for large \(N\) and fixed \(n\), \(c_n(N)\) diverges as \(\sqrt{N}\), whilst it tends to zero like \(n^{-4}\) when \(n \gg N\). As will become evident in Section III, this summary also describes the behaviour of a system of harmonically trapped impenetrable bosons on a line.
III. IMPENETRABLE BOSONS TRAPPED IN A HARMONIC WELL

A. The analytic structure of the density matrix

1. The wave function

The wave function for a system of $N$ impenetrable bosons on a line confined by a harmonic potential is defined by the Hamiltonian (in reduced units)

$$-\sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} + \sum_{j=1}^{N} x_j^2$$  \hspace{1cm} (67)

and the impenetrability condition discussed in Section (II A 1). The well known single particle eigenstates of (67) have the form

$$e^{-x^2/2} \frac{H_j(x)}{\sqrt{\pi^2 j!}} \quad j = 0, 1, 2, ...$$  \hspace{1cm} (68)

where $H_j(x)$ is the $j$th Hermite polynomial. The ground state wave function for the harmonically trapped non-interacting Fermi system is obtained by forming the Slater determinant of the functions (68) with $j = 0, 1, ..., N-1$. Arguing then as in Section (II A 1) we obtain the ground state wave function for the impenetrable bosons by simply taking the modulus of this Slater determinant.

The Vandermonde determinant formula states that

$$\det[p_j - 1(x_k)]_{j,k=1,...,N} = \prod_{1 \leq j,k \leq N} (x_k - x_j)$$  \hspace{1cm} (69)

for any set $\{p_j(x)\}$ with $p_j(x)$ a monic polynomial of degree $j$, i.e. a polynomial of degree $j$ for which the coefficient of $x^j$ is 1. In particular, (69) is true for $\{p_j\} = \{2^{-j}H_j(x)\}$ and $\{p_j(x)\} = \{x^j\}$. Applying (69) to the Slater determinant over (68) we see that the ground state wave function for $N$ harmonically trapped impenetrable bosons can be expressed as

$$\psi_0^H(x_1, x_2, ..., x_N) = \frac{1}{C_N^H} \prod_{k=1}^{N} e^{-x_k^2/2} \prod_{1 \leq j < k \leq N} |x_j - x_k|,$$  \hspace{1cm} (70)

where

$$(C_N^H)^2 = N! \prod_{m=0}^{N-1} 2^{-m}\sqrt{\pi m}.$$  \hspace{1cm} (71)

2. The one body density matrix

The one body density matrix is defined as in (8) with the domain of integration now $\mathbb{R}$,

$$\rho_N^H(x, y) = N \int_{-\infty}^{\infty} dx_1 ... \int_{-\infty}^{\infty} dx_{N-1} \psi_N^H(x_1, ... x_{N-1}, x) \psi_N^H(x_1, ... x_{N-1}, y).$$  \hspace{1cm} (72)

and is now genuinely a function of two variables. We are again able to find a closed form expression for $\rho_N^H(x, y)$ in terms of a determinant, analogous to the result on the circle, this time the determinant being of Hankel type rather than Toeplitz type. To make this identification it is advantageous to note the following general result, in analogy to (11)

$$\frac{1}{N!} \prod_{l=1}^{N} \int_{-\infty}^{\infty} dx_l g(x_l) \left( \det[f_j - 1(x_k)]_{j,k=1,...,N} \right)^2 = \det \left[ \int_{-\infty}^{\infty} dt g(t) f_{j-1}(t) f_{k-1}(t) \right]_{j,k=1,...,N},$$  \hspace{1cm} (73)
which can be obtained by simply expanding the determinants and recalling (72) so that left hand side becomes

\[
\frac{1}{N!} \sum_{P \in S_N} \sum_{Q \in S_N} \varepsilon(P) \varepsilon(Q) \prod_{l=1}^{N} \int_{-\infty}^{\infty} dx_l \ g(x_l) f_{Q(l)} f_{P(l-1)}(x_l) \tag{74}
\]

\[
= \det \left[ \int_{-\infty}^{\infty} dt \ g(t) f_{j-1}(t) f_{k-1}(t) \right]_{j,k=1,\ldots,N} . \tag{75}
\]

To obtain a closed form for \( \rho_N^H(x,y) \) we proceed as follows. Consider \( \psi_N^H(x_1,\ldots,x_{N-1},x) \) from (74) and factor out the pieces that depend upon \( x \), then apply (73) to obtain

\[
\rho_N^H(x,y) = \frac{N}{C_N} \ e^{-x^2/2-y^2/2} \prod_{l=1}^{N-1} \int_{-\infty}^{\infty} dx_l \ e^{-x_l^2} |x-x_l||y-y_l| (\det \left[ x_k^{-1} \right]_{j,k=1,\ldots,N-1})^2 \tag{76}
\]

and hence \( \rho_N^H(x,y) = \frac{2^{N-1}}{\sqrt{\pi} \Gamma(N)} \ e^{-x^2/2-y^2/2} \det \left[ \frac{2^{(j+k)/2}}{2^{(j+k)/2}} \text{det} \left[ b_{j,k}(x,y) \right] \right]_{j,k=1,\ldots,N-1} \tag{77}
\]

where in the last step use has been made of (73). The elements of the determinant have the following explicit form \( \text{det} \left[ b_{j,k}(x,y) \right] \)

\[
b_{j,k}(x,y) = \int_{-\infty}^{\infty} dt \ e^{-t^2} |x-t||y-t| t^{j+k-2} \quad 1 \leq j, k \leq N-1 \tag{78}
\]

\[
b_{j,k}(x,y) = \int_{-\infty}^{\infty} dt \ e^{-t^2} (x-t)(y-t) t^{j+k-2} - 2 \text{sgn}(y-x) \int_{x}^{y} dt \ e^{-t^2} (x-t)(y-t) t^{j+k-2} \tag{79}
\]

\[
b_{j,k}(x,y) = f_{j,k}(x,y) - 2 \text{sgn}(y-x) xy \mu_{j+k-2}(x,y) - (x+y) \mu_{j+k-1}(x,y) + \mu_{j+k}(x,y) \tag{80}
\]

where for clarity we have introduced

\[
f_{j,k}(x,y) := \int_{-\infty}^{\infty} dt \ e^{-t^2} (x-t)(y-t) t^{j+k-2} \tag{81}
\]

\[
= \begin{cases} 
\Gamma \left( \frac{j+k-1}{2} \right) xy + \Gamma \left( \frac{j-k+1}{2} \right) & j+k \text{ even} \\
-\Gamma \left( \frac{j+k}{2} \right) (x+y) & j+k \text{ odd} 
\end{cases} \tag{82}
\]

\[
\mu_m(x,y) := \int_{x}^{y} dt \ e^{-t^2} t^m \tag{83}
\]

\[
= \frac{(\text{sgn}(y))^{m+1}}{2} \gamma \left( \frac{m+1}{2}, y^2 \right) - \frac{(\text{sgn}(x))^{m+1}}{2} \gamma \left( \frac{m+1}{2}, x^2 \right) \\
= \frac{y^{m+1}e^{-y^2}}{(m+1)} \text{F}_1 \left( 1, \frac{m+3}{2}, y^2 \right) - \frac{x^{m+1}e^{-x^2}}{(m+1)} \text{F}_1 \left( 1, \frac{m+3}{2}, x^2 \right) \tag{84}
\]

and where \( \gamma \) and \( \text{F}_1 \) respectively denote the incomplete gamma function and confluent hypergeometric function.

There are some properties of \( \rho_N^H(x,y) \) worthy of note. Firstly, as is clear from the form of (74), \( |\psi_N^H(x_1,x_2,\ldots,x_N)|^2 \) is precisely the probability density function for the distribution of eigenvalues of the Gaussian Unitary Ensemble (GUE) of random matrix theory, and hence \( \rho_N^H(x,y) \) can be interpreted as a certain average over the GUE [22]. Secondly it is obvious that since the ground states of the noninteracting Fermi and impenetrable Bose systems differ only in the presence of the absolute value in the wave function of the latter, we see by comparing (74) with (73) that the density matrix for a harmonically trapped noninteracting Fermi system is given by (74) with \( b_{j,k}(x,y) \) replaced by \( f_{j,k}(x,y) \). From this observation it is immediately clear that the densities for the Fermi and Bose cases are identical.
since on setting $x = y$ in (84) we see that $b_{j,k}(x,x) = f_{j,k}(x, x)$. The global large $N$ limit of the density in this case results in the Wigner semi circle law\[33, 34\]

$$\rho^H_N(x, x) = \frac{\sqrt{2N}}{\pi} \sqrt{1 - \frac{x^2}{2N}}, \quad |x| \leq \sqrt{2N},$$

(85)

while for $|x| > \sqrt{2N}$ we have $\rho^H_N(x, x) = 0$ to leading order. An oscillatory correction to this leading global asymptotic form has been given in [35]. Finally we note from the second equality in (84) that since the $1F_1$ function is entire, $\rho^H_N(x, y)$ is analytic everywhere in the finite $(x, y)$ plane except along the diagonal $y = x$, where it has discontinuities in its first derivatives. Such observations are important in choosing a numerical quadrature method.

3. Occupation numbers

Quite generally, for a many body quantum system the eigenvalue equation

$$\int \rho_N(x, y)\phi_j(y)dy = \lambda_j\phi_j(x), \quad j = 0, 1, 2, ...$$

(86)

defines the natural orbitals, $\phi_j(x)$, which have the physical interpretation of being effective single particle states, and the eigenvalues $\lambda_j$ which are interpreted as the occupation numbers for these natural orbitals. When the system lies on a circle the periodicity implies that the natural orbitals are simply plane waves, and so the eigenvalues are given by the Fourier coefficients of $\rho_N(x - y)$ and hence the momentum distribution and the set of natural orbital occupations coincide. In the general case, in which $\rho_N(x, y)$ is not translationally invariant, this is no longer true. Recent work\[30, 31\] has focused attention on the computation and analysis of the momentum distribution for harmonically trapped impenetrable bosons. A more demanding task is the investigation of the $N$ dependence of the occupation of the lowest natural orbital, $\lambda_0$, the fundamental quantity of interest in discussing BEC-like coherence. We undertake a numerical analysis of $\lambda_0$ in Section III B, and then in Section III D we go on to discuss how a new analytic result, obtained in Section III C, yields its large $N$ scaling.

B. Numerical investigation of the eigenvalues of $\rho^H_N(x, y)$

The integral equation (84) was solved numerically for $2 \leq N \leq 30$ to obtain the corresponding values of $\lambda_0(N)$ and $\lambda_1(N)$. In the present section we carefully analyse this numerical data in order to determine the $N$ dependence of $\lambda_0(N)$ and $\lambda_1(N)$. Before getting under way however, a few comments are in order.

1. Perfunctory remarks

Since our ultimate goal is to infer from the sequence of computed $\lambda_0(N)$ and $\lambda_1(N)$ values how these quantities grow with increasing $N$, it is not only the accuracy and number of the computed $\lambda$ values that are obtained that is important, but equally important is how we infer the large $N$ behaviour from these computed values. Naive approaches such as fitting the data to a log/log plot in order to obtain the exponent in $\lambda_0 \sim N^\alpha$\[35\] prove to be of no use. A striking demonstration of this fact occurs if we attempt to apply this procedure to our numerical $c_0(N)$ data for the system on a circle. In this case we know a priori by analytic arguments that the exponent is precisely 1/2. However, fitting the $c_0(N)$ data with $2 \leq N \leq 70$ via a log/log plot predicts an exponent of $\alpha = 0.64$, and even using $2 \leq N \leq 10$ only forces the exponent to drop to $\alpha = 0.60$. A similar analysis for the harmonically trapped system produces analogous results. Clearly such an approach will only be useful for very large $N$, and more suitable methods of analysis are required.

The method we shall use to analyse the $N$ dependence of the computed $\lambda_0$ and $\lambda_1$ values is motivated by series analysis techniques. We assume an ansatz for $\lambda_0(N)$ of the form

$$\lambda_0(N) = aN^p + b + \frac{c}{N^x},$$

(87)

and similarly for $\lambda_1(N)$. We then fit our numerical data to this ansatz, varying the parameters $p$ and $x$ and seeking to minimise the $\chi^2$ value for the fit. We have already noted that the fits of the numerical data for the system on the circle to this form of ansatz are in very good agreement with the known analytic results. We shall see in Section III D that again our numerical fits to this ansatz agree remarkably with analytic results that we obtain via independent means.
2. Numerical Results

To numerically solve
\[ \int_{-\infty}^{\infty} \rho_N^H(x, y) \phi_j(y) dy = \lambda_j \phi_j(x), \quad j = 0, 1, 2, \ldots \]

we used the so-called quadrature method \[39\] which replaces the integral equation with an approximate matrix equation. Specifically, we factored out \( e^{-y^2/2} \) in \[7\] and applied a Gaussian-Hermite quadrature (with abscissae \( \xi_i \), weights \( w_i \) and \( 1 \leq i \leq Z \)) to \( e^{y^2/2} \rho_N^H(x, y) \phi(y) \). Setting \( x = \xi_i \) in \[88\] for each \( i \), we thus obtain \( Z \) linear equations, which then defines a matrix approximation to our integral operator. This matrix, \( S \), can be so chosen that

\[
S_{l,m} = e^{-x_l^2/4-z_m^2/4} \sqrt{w_l w_m} \frac{2^{N-1}}{\sqrt{\pi} \Gamma(N)} \det \left[ \frac{2^{(j+k)/2}}{2 \sqrt{\pi} \Gamma((j+k)/2)} b_{j,k}(\xi_l, \xi_m) \right]_{j,k=1,\ldots,N-1}
\]

\[l, m = 1, 2, \ldots, Z,\]

where a suitable transformation has been used to force \( S \) to be symmetric, since such a transformation makes the numerical computations more efficient. We computed the required \( b_{j,k}(\xi_l, \xi_m) \) using the representation in terms of incomplete gamma functions \[80\] with \[84\].

Due to the complexity of \( S \), each of its elements being given in terms of an \((N-1)\) dimensional determinant, we find that as \( Z \) and \( N \) are increased round-off error becomes an important obstacle. For \( N = 30 \) convergence was down to two significant figures and by \( N = 35 \) we found that 64 bit precision became insufficient and to obtain higher values of \( N \) a multiprecision routine would be necessary. As \( N \) approached \( N = 30 \) the fits of the data to \[57\] became rather sensitive to the precision of the \( \lambda_j \) used. Due to this we chose to fit only the data \( 2 \leq N \leq 27 \) to the ansatz \[57\] since for this set we could be sure that the precision was at least three significant figures (actually considerably more for the lower \( N \) values). With the computed \( \lambda_j \) analysed according to \[57\] however, it turns out that a good deal of large \( N \) asymptotic information is already present even at these relatively low values of \( N \). This will become evident in Section \ref{sec:asymp}.

Systematically varying the parameters \( p \) and \( x \) in \[57\], we observed a dramatic dip of three to four orders of magnitude in the \( \chi^2 \) of the fit when \( p \) hit the critical value of \( p = 0.5 \). For \( p = 0.45 \) and \( p = 0.55 \) the best \( \chi^2 \) values as \( x \) was varied were of the order \( 10^{-3} \), and these \( \chi^2 \) values became larger as \( p \) was moved away from \( p = 0.5 \) on either side. At \( p = 0.5 \) however, the best \( \chi^2 \) value was of the order \( 10^{-7} \), which occurred for \( x \) in the neighbourhood of \( 2/3 \). This very steep dip in \( \chi^2 \) exactly at \( p = 0.5 \) indicates that the exponent of the leading order behaviour of \( \lambda_0 \) with \( N \) is in fact \( 1/2 \), just as is the case on the circle. A similar analysis performed for \( \lambda_1 \) yielded the same sharp drop in \( \chi^2 \) at \( p = 0.5 \), again dropping from around \( 10^{-3} \) on either side of \( p = 0.5 \) to around \( 10^{-7} \) at \( p = 0.5 \). The coefficients of the correction terms for \( \lambda_1 \) turn out to be identical, to two decimal places, to those for \( \lambda_0 \), however it now appears that the best value of \( x \) is in the neighbourhood of \( x = 4/3 \). Specifically, fitting the computed \( \lambda_0 \) and \( \lambda_1 \) values with \( 2 \leq N \leq 27 \) we obtained

\[
\lambda_0(N) = 1.43 \sqrt{N} - 0.56 + \frac{0.12}{N^{2/3}}, \quad (90)
\]

\[
\lambda_1(N) = 0.61 \sqrt{N} - 0.56 + \frac{0.12}{N^{4/3}}, \quad (91)
\]

with \( \chi^2 \approx 10^{-7} \). Again we remark that the similarity of the constant in these fits with that for the case of the uniform system, \[53\] and \[54\], is quite suggestive.

In FIGS. \[45\] we plot the computed numerical values for \( \lambda_0(N) \) and \( \lambda_1(N) \) for \( 2 \leq N \leq 30 \) together with the fits \[90, 91\].

Recently Papenbrock \[35\] discussed the computation of the density matrix using a form similar to \[77\]. Information regarding the leading \( N \) behaviour of \( \lambda_0 \) was inferred indirectly from a numerical investigation of the momentum distribution, by way of an interesting scaling argument, rather than by analysing the \( \lambda_0(N) \) directly as we have done. This argument predicts that \( \lambda_0 \propto \sqrt{N} \) for large \( N \), in agreement with our analytical study to be presented below.

In the next Section we construct the large \( N \) asymptotic form for \( \rho_N^H(x, y) \). This result allows the \( \sqrt{N} \) scaling of \( \lambda_j \) to be put on a firm analytic footing as a straightforward corollary.
C. Global asymptotics from a log-gas picture

We would like to derive the analogue of the asymptotic formula (33) for the impenetrable Bose gas in a harmonic trap. Now the latter is given as a determinant by (77). To our knowledge unlike the situation for the Toeplitz determinant (16), there is no known general theorem giving the asymptotic form of determinants of the type (77), or equivalently multidimensional integrals of the form (72). (If each factor $|x-x'_l||y-x'_l|$ in (72) is replaced by $e^{-g(x'_l)}$ for $g$ analytic, such general asymptotics are known [40]). However, as we will now demonstrate, a Coulomb gas argument which can be used to give a heuristic derivation of (33) does carry over to the case of the density matrix for the impenetrable Bose gas in a harmonic trap, thus allowing the global asymptotics of the latter to be predicted.

Let us first revise the derivation of the asymptotic form (33), slightly modified relative to the presentation in [41] so it is best adapted to application in the harmonic trap case. The starting point is the multidimensional integral formula (4) for $\varrho_N(t)$. Put

$$Z_n^C ((\phi_1,q_1),(\phi_2,q_2)) := |e^{i\phi_1} - e^{i\phi_2}|^{2q_1,q_2}$$
\begin{align*}
\times \int_0^{2\pi} d\theta_1 \ldots \int_0^{2\pi} d\theta_n \prod_{i=1}^n |e^{i\phi_i} - e^{i\theta_i}|^2 |q_i|^2 e^{-e^{i\theta_i}|2q_2|} \\
\times \prod_{1 \leq j < k \leq n} |e^{i\theta_k} - e^{i\theta_j}|^2 
\end{align*}

This is the classical configuration integral for \( n \) mobile unit charges, and two fixed impurity charges (at angles \( \phi_1, \phi_2 \) and of charge \( q_1, q_2 \)) on the unit circle interacting via the logarithmic potential \(-q_a q_b \log |e^{i\theta_a} - e^{i\theta_b}|\) at inverse temperature \( \beta = 2 \). In terms of this notation, and that of (33), we can write

\[ g_N(t) = \frac{2\pi N}{|1 - e^{2it}|^{1/2}} \frac{Z_N^{C_{-1}((0, 1/2), (2t, 1/2))}}{Z_N^{C_{N-1}}} \]

where

\[ Z_N^C := Z_N^C((\cdot, 0), (\cdot, 0)) = (2\pi)^N N! \]

Now for \( N \) large and \( t \) fixed the impurity charges are effectively separated by a macroscopic amount (in units of the mean interparticle separation) so we expect the factorization

\[ \frac{Z_N^{C_{-1}((0, 1/2), (2t, 1/2))}}{Z_N^C} \sim \frac{Z_N^{C_{N-1}((0, 1/2))}}{Z_N^{C_{N-1/2}}} \frac{Z_N^{C_{N-1/2}}}{Z_N^{C_{N-1}}} = \left( \frac{Z_N^{C_{N-1/2}}}{Z_N^{C_{N-1}}} \right)^2 \]

Now the reason for \( N - 1/2 \) in the classical configuration integral of the denominators is to exactly balance the total charge in the numerator but this is immediate from the original expression (33). Of course to evaluate \( Z_{N-1/2}^C \) we must analytically continue off the integers and so this is immediate from the exact evaluation in (94). Furthermore, we know from (34) that

\[ Z_{N-1}^C((0, 1/2)) = (2\pi)^{N-1} \left( \frac{G(N + 1)G(3/2)}{G(N + 1/2)} \right)^2 \sim (2\pi)^{N-1/2} N^{-1/4} e^{-N N^N (G(3/2))^2} \]

while it follows from (34) and Stirling’s formula that

\[ Z_{N-1}^C = (2\pi)^{N-1/2} \Gamma(N + 1/2) \sim (2\pi)^N N^{-1} e^{-N} \]

and so

\[ \frac{Z_{N-1}^C((0, 1/2))}{Z_N} \sim \frac{(G(3/2))^2}{\sqrt{2\pi N^{1/4}}} \]

Substituting (38) and (96) in (33) then substituting the result in (33) reclaims (33).

This log-gas argument readily generalises to provide the global asymptotics for

\[ g^H(X, Y) := (2N)^{1/2} \rho_N(\sqrt{2NX}, \sqrt{2NY}) \]

with \(-1 < X, Y < 1\) fixed and \( N \to \infty \). Let us write

\[ Z_{n,m}^H((X_1, q_1), (X_2, q_2)) := |X_1 - X_2|^{2q_1 q_2} e^{-mq_1 X_1^2/2} e^{-mq_2 X_2^2/2} \times \int_{-2}^{2} dx_1 \ldots \int_{-2}^{2} dx_n \prod_{i=1}^n e^{-m x_i^2/2} |X_1 - x_i|^{2q_1} |X_2 - x_i|^{2q_2} \times \prod_{1 \leq j < k \leq n} |x_k - x_j|^2 \]

where \( m = n + q_1 + q_2 \). This is the classical configuration integral for \( n \) mobile unit charges and two fixed impurity charges (of charge \( q_1, q_2 \) at \( X_1, X_2 \) respectively) interacting on the interval \([-2, 2]\) via the logarithmic potential.
\(-q_aq_b \log |x_a - x_b|\) at inverse temperature \(\beta = 2\). The charges are also subject to the one body potential \((mq_a/4)x_a^2\).

(We work in the scaled interval \([-2,2]\) as this is the convention used in [12], the results of which we will be using subsequently.) Now it is well known from the random matrix interpretation of \(|\psi_N^H|^2\) (recall [12]) that the support for the density is the interval \([-\sqrt{2N}, \sqrt{2N}]\). Doing this then changing variables shows

\[
\varrho(X, Y) = \frac{2N}{|2X - 2Y|^{1/2}} \frac{Z_{N-1,N}^H((2X,1/2),(2Y,1/2))}{Z_{N,N}^H} \tag{101}
\]

where

\[
Z_{n,m}^H = Z_{n,m}^H((\cdot, 0), (\cdot, 0)).
\]

Now analogous to [12], for \(N\) large and \(-2 < X, Y < 2\) fixed we expect the factorisation

\[
\frac{Z_{N-1,N}^H((2X,1/2),(2Y,1/2))}{Z_{N,N}^H} \sim \frac{Z_{N-1,N-1/2}^H((2X,1/2))}{Z_{N-1/2,N-1/2}^H} \frac{Z_{N-1,N-1/2}^H((2Y,1/2))}{Z_{N-1/2,N-1/2}^H} \tag{102}
\]

But in the notation of Brezin and Hikami (Eq. (46) of [12])

\[
\frac{Z_{N-1,N-1/2}^H((2X,1/2))}{Z_{N-1/2,N-1/2}^H} = \frac{(N - 1/2)!}{N!} M_1(2X) \tag{103}
\]

and it is shown in [12] (see also [13]) that

\[
M_1(2X) \sim (2\pi)^{-1/2}(2N(1 - X^2)^{1/2})^{1/4}(G(3/2))^2 \tag{104}
\]

where we have used the fact [11]

\[
\prod_{l=0}^{K-1} \frac{l!}{(K+l)!} = \frac{(G(K + 1))^2}{G(2K + 1)}
\]

Substituting (104) in (103) and noting that \((N - 1/2)!/N! \sim N^{-1/2}\), we then obtain from (102) and (101) the sought asymptotic formula

\[
\varrho^H(X, Y) \sim N^{1/2} \frac{(G(3/2))^4 (1 - X^2)^{1/8}(1 - Y^2)^{1/8}}{\pi |X - Y|^{1/2}} \tag{105}
\]

### D. Occupation numbers and natural orbitals as \(N \to \infty\)

Using (105) we can determine the large \(N\) behaviour of the occupation numbers and natural orbitals. Taking the large \(N\) limit of the integral equation (88), utilising (105) and (99) we obtain

\[
\frac{(G(3/2))^4}{\pi} \int_{-1}^{1} dX \frac{(1 - X^2)^{1/8}(1 - Y^2)^{1/8}}{|X - Y|^{1/2}} \varphi_j(X) = \frac{\lambda_j}{\sqrt{N}} \varphi_j(Y), \tag{106}
\]

where we have defined the scaled limiting large \(N\) natural orbitals

\[
(2N)^{1/4} \varphi_j(x) \to \varphi_j(X). \tag{107}
\]

This scaling for \(\varphi_j(x)\) arises since for large \(N\) the density matrix \(\rho_N^H(x,y)\) has support \([-\sqrt{2N}, \sqrt{2N}]\), and so the integral equation (88) tells us that \(\varphi_j(x)\) must also, hence normalising \(\varphi_j(x)\) on this interval implies (107).

From (106), the large \(N\) scaling of \(\lambda_j\) is immediate. Since both the left hand side of (106) and \(\varphi_j(Y)\) are independent of \(N\), we must have that for large \(N\)

\[
\lambda_j \propto \sqrt{N}. \tag{108}
\]

We note that this argument has regarded \(j\) as a fixed parameter. For \(j \gg N\) we expect the behaviour of \(\lambda_j\) to be similar to that of \(c_j(N)\) given by (82), since very excited states should not feel the presence of the trap.
FIG. 6: Comparison of the limiting large $N$ natural orbital $\varphi_0(X)$, denoted by the dashed line, with the the scaled natural orbital $\sqrt{2N}\varphi_0(x)$ for $N = 25$.

Hence from a knowledge of the asymptotic behaviour of $\rho^H_{xy}(x,y)$ we have demonstrated not only that $\lambda_0 \sim \sqrt{N}$, but that the other low lying modes must also display this $N$ dependence. We can go one step further however and numerically solve (106) to obtain the proportionality constants missing from (108).

Factoring out the exact constants, (106) becomes

$$\int_{-1}^{1} dX \; \varphi_j(X)(1 - X^2)^{1/8} = \bar{\lambda}_j \varphi_j(Y) (1 - Y^2)^{1/8},$$

where

$$\lambda_j = \frac{[G(3/2)]^4}{\pi} \bar{\lambda}_j \sqrt{N}.$$  

We solved (109) using a similar method to that discussed in Section III B 2 to obtain

$$\bar{\lambda}_0 = 3.438... \quad \bar{\lambda}_1 = 1.47... \quad \bar{\lambda}_2 = 1.13...$$

and hence, using $[G(3/2)]^4/\pi = 0.4160...$ we find that in the large $N$ limit

$$\lambda_0 = 1.430\sqrt{N},$$
$$\lambda_1 = 0.61\sqrt{N},$$
$$\lambda_2 = 0.47\sqrt{N}.$$  

The results (112) and (113) are to be compared with the numerical fits (100) and (101) for $\lambda_0$ and $\lambda_1$. The agreement is remarkable.

The limiting scaled natural orbitals are also of interest. FIGS. 6, 7, 8 show $\varphi_j(X)$, together with $(\sqrt{2N})^{1/4}\varphi_j(x)$ computed from (88) with $N = 25$, for $k = 0, 1, 2$. It is clear that already by $N = 25$ the eigenfunctions of the large $N$ equation (106) provide a good approximation to the finite $N$ results, only really differing outside the support. The cause of the sharp decrease as $X \to \pm 1$ can be understood by noting that (109) implies that $\varphi_j(X)$ vanishes like $(1 - X^2)^{1/8}$ in this limit.

We remark that $\varphi_j(X)$ is an even (odd) function when $j$ is even (odd). For reference, we list the computed values of the central maxima and the area under the curve for $\varphi_0(X)$ and $\varphi_2(X)$. Whilst the area under $\varphi_2(X)$ is certainly smaller than that under $\varphi_0(X)$, it is not so much smaller as to be negligible.

$$\varphi_0(0) = 0.853... \quad \lambda_0(0) = 1.20...$$

$$\int_{-1}^{1} dX \varphi_0(X) = 1.38... \quad \int_{-1}^{1} dX \varphi_2(x) = 0.21...$$

FIG. 7: Comparison of the limiting large $N$ natural orbital $\varphi_1(X)$, denoted by the dashed line, with the scaled natural orbital $\sqrt{2N}\varphi_1(x)$ for $N = 25$.

FIG. 8: Comparison of the limiting large $N$ natural orbital $\varphi_2(X)$, denoted by the dashed line, with the scaled natural orbital $\sqrt{2N}\varphi_2(x)$ for $N = 25$.

IV. CONCLUSION

We have given an exhaustive study of the particle occupation numbers for the 1d impenetrable boson systems. Our feature results are presented in Section III for the harmonically trapped systems. These results are of such strikingly similarity to those for the untrapped boson systems presented in Section II as to make all the results collectively invaluable.

We commend the challenge to the experimentalists of measuring these signature quantities.

Acknowledgments

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APPENDIX A: SUMMARY OF GROUND STATE ENERGIES OF SYSTEMS SUBJECT TO VARIOUS BOUNDARY CONDITIONS

We list here for ease of reference the ground state energies per particle, $U_0/N$, and the Fermi energies, $\epsilon_F$, for finite one dimensional systems of impenetrable bosons of mass $m$ subject to periodic, Dirichlet, and Neumann boundary conditions and the analogous results in the thermodynamic limit, as well as for impenetrable bosons confined by a harmonic well. These results are identical to the analogous noninteracting Fermi results.

| System          | $U_0/N$                  | $\epsilon_F$       |
|-----------------|--------------------------|---------------------|
| Circle          | $(N^2 - 1)\pi^2\hbar^2/6mL^2$ | $(N - 1)\pi^2\hbar^2/2mL^2$ |
| Dirichlet       | $(N + 1)(N + 1/2)\pi^2\hbar^2/6mL^2$ | $N^2\pi^2\hbar^2/2mL^2$ |
| Neumann         | $(N - 1)(N + 1/2)\pi^2\hbar^2/6mL^2$ | $(N - 1)\pi^2\hbar^2/2mL^2$ |
| Thermodynamic limit | $N^2\pi^2\hbar^2/6mL^2$ | $N^2\pi^2\hbar^2/2mL^2$ |
| Harmonic well, $V(z) = m\omega^2z^2/2$ | $N\hbar\omega_z/2$ | $(N - 1/2)\hbar\omega_z$ |

TABLE III: Summary of ground state energies per particle and Fermi energies for a systems of impenetrable bosons subject to periodic, Dirichlet and Neumann boundary conditions, and a harmonic well.

APPENDIX B: TRIAL SERIES SOLUTION FOR $\bar{\lambda}_0$

We demonstrate here that it is possible to learn a good deal about $\bar{\lambda}_0$ by suitably approximating the integrand of (109). To begin with, simply taking $Y = 0$ in (109) yields the following bound for $\bar{\lambda}_0$

$$\bar{\lambda}_0 = \int_{-1}^{1} \frac{\varphi_0(X)(1 - x^2)^{1/8}}{\varphi_0(0) |x|^{1/2}} dx$$

$$\bar{\lambda}_0 < 2 \int_{0}^{1} \frac{(1 - x^2)^{1/8}}{|x|^{1/2}} dx = B(1/4, 9/8) = 3.84108... (B1)$$

A very good approximation to the value of $\bar{\lambda}_0$ can be obtained by inserting the formal Maclaurin expansion for $\varphi_0(X)$,

$$\varphi_0(X) = \varphi_0(0)(1 - AX^2 - BX^4 - ...) (B2)$$

into (109) and equating coefficients of powers of $Y$ to obtain the unknown coefficients and $\bar{\lambda}_0$. Keeping only terms to order $Y^2$ and $X^2$ in the expansion of the integrand we thus obtain

$$\int_{0}^{1+Y} \frac{dt}{\sqrt{t}}[1 - (A + \frac{1}{8})(t - Y)^2]$$

$$+ \int_{0}^{1-Y} \frac{dt}{\sqrt{t}}[1 - (A + \frac{1}{8})(t + Y)^2] = \bar{\lambda}_0[1 - (A - \frac{1}{8})Y^2] (B3)$$

which then yields, upon equating coefficients

$$\bar{\lambda}_0 = 4 - \frac{4}{5} A + \frac{1}{8},$$

$$\bar{\lambda}_0 \left[ A - \frac{1}{8} \right] = \frac{1}{2} + \frac{3}{2} \left[ A + \frac{1}{8} \right],$$

and the solution of these two simultaneous equations gives

$$A = 0.57627... \quad \bar{\lambda}_0 = 3.43899... (B6)$$

Carrying out this procedure again now keeping terms to fourth order we find that $A$ and $\bar{\lambda}_0$ shift only slightly

$$A = 0.57682... \quad B = 0.01914... (B7)$$

$$\bar{\lambda}_0 = 3.4378... (B8)$$
which shows that the procedure is quite stable. This value of $\lambda_0$ is in excellent agreement with our numerical solution of (109) given in (111).