The Density Matrix for the Ground State of 1-d Impenetrable Bosons in a Harmonic Trap

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1-d Impenetrable Bosons

Hamiltonian $N$ bosons $x_j \in (-\infty, \infty)$

$$H = -\sum_{i=1}^{N} \frac{\partial^2}{\partial x_i^2} + \sum_{j=1}^{N} x_j^2 + 2c \sum_{1 \leq i < j \leq N} \delta(x_i - x_j), \quad c > 0$$

Ground State eigenfunction $\Psi_0(x_1, \ldots, x_N)$ satisfies

$$H \Psi_0 = E_0 \Psi_0$$

subject to boundary conditions

1. $\Psi_0|_{x_i=x_j+0} = \Psi_0|_{x_i=x_j-0}$

2. $$\left( \frac{\partial \Psi_0}{\partial x_i} - \frac{\partial \Psi_0}{\partial x_j} \right)|_{x_i=x_j+0} - \left( \frac{\partial \Psi_0}{\partial x_i} - \frac{\partial \Psi_0}{\partial x_j} \right)|_{x_i=x_j-0} = 2c \, \Psi_0|_{x_i=x_j \pm 0}$$

Bethe Ansatz solution without harmonic trap [Lieb+Liniger 1963]

Impenetrable Bose wavefunction $c \to \infty$ [Girardeau 1960].

The wave function for impenetrable bosons must vanish at coincident coordinates,

$$\Psi_0(x_1, \ldots, x_i, \ldots, x_j, \ldots, x_N) = 0 \text{ for } x_i = x_j, (i \neq j),$$

This means that for any fixed ordering of the particles $x_1 < x_2 < \ldots < x_N$ there is no distinction between impenetrable bosons and free fermions.
Schrödinger Operator

\[ H_R = - \sum_{j=1}^{N} \frac{\partial^2}{\partial x_j^2} + \sum_{j=1}^{N} x_j^2 \]

Normalised single particle eigenstates \( \{ \phi_k(x) \}_{k=0,1,...} \)

\[ \phi_k(x) = \frac{2^{-k}}{c_k} e^{-x^2/2} H_k(x), \quad (c_k)^2 = \pi^{1/2} 2^{-k} k! \]

\( H_k(x) \) denotes the Hermite polynomial of degree \( k \).

Ground state wave function \( \Psi_0 \) as a Slater determinant of distinct single-particle states

\[ \Psi_0(x_1, \ldots, x_N) = \frac{1}{(N!)^{1/2}} \left| \det[\phi_k(x_j)]_{j=1,\ldots,N \atop k=0,\ldots,N-1} \right| \]

where the factor of \( (N!)^{-1/2} \) is included so that

\[ \int_{-\infty}^{\infty} dx_1 \cdots \int_{-\infty}^{\infty} dx_N |\Psi_0(x_1, \ldots, x_N)|^2 = 1. \]
Density Matrix

Density Matrix is defined as

$$\rho_N(x; y) \equiv N \int_{\mathbb{R}} dx_2 \ldots \int_{\mathbb{R}} dx_N \Psi_0(x, x_2, \ldots, x_N) \Psi_0(y, x_2, \ldots, x_N),$$

so that

$$\int_{\mathbb{R}} dx \rho_N(x; x) = N$$

Using this one must solve the eigenvalue problem

$$\int_{\mathbb{R}} \rho_N(x; y) \psi_k(y) dy = \lambda_k \psi_k(x), \quad k \in \mathbb{Z}_{\geq 0}.$$

Note

$$\lambda_0 > \lambda_1 > \ldots > \lambda_{N-1} > 0, \quad \sum_{j=0}^{N-1} \lambda_j = N.$$
GUE Averages

Recall
\[ \rho_N(x; y) = N \int_{\mathbb{R}} dx_2 \ldots \int_{\mathbb{R}} dx_N \Psi_0(x, x_2, \ldots, x_N) \Psi_0(y, x_2, \ldots, x_N) \]

Vandermonde determinant formula with \( p_j(x) \) a monic polynomial of degree \( j \),
\[ \det[p_{j-1}(x_k)]_{j,k=1,\ldots,N} = \det[x_k^{j-1}]_{j,k=1,\ldots,N} = \prod_{1 \leq j < k \leq N} (x_k - x_j) \]

Product formula for \( \Psi_0 \)
\[ \Psi_0(x_1, \ldots, x_N) = \frac{1}{C_N} \prod_{j=1}^{N} e^{-x_j^2/2} \prod_{1 \leq j < k \leq N} |x_k - x_j|, \quad (C_N)^2 = N! \prod_{l=0}^{N-1} (c_l)^2. \]

This coincides precisely with the multivariate probability distribution function (p.d.f.) for a particular class of random matrices
\[ |\Psi_0|^2 = \mathbb{E}_{GUE_N} \]

namely, GUE\(_N\), the Gaussian unitary ensemble of \( N \times N \) complex Hermitian matrices,
Density matrix \( \rho_{N+1}(x; y) \) can be written as an average over this eigenvalue p.d.f
\[ \rho_{N+1}(x; y) = \frac{1}{c_N^2} e^{-x^2/2-y^2/2} \mathbb{E}_{GUE_N} \left( \prod_{l=1}^{N} |x - x_l||y - x_l| \right) \]
Criteria for Bose-Einstein condensation (BEC) are -

- Onsager-Penrose 1956 criteria for BEC

\[
\frac{\lambda_0(N)}{N} = \begin{cases} 
  e^{\mathcal{O}(1)} & \text{BEC} \\
  \mathcal{o}(1) & \text{no BEC}
\end{cases} \quad \text{as } N \to \infty
\]

- Off Diagonal Long Range Order criteria of Yang 1962

\[
\rho_\infty(x) \xrightarrow{|x| \to \infty} C > 0
\]

NB: already in thermodynamic limit \( N \to \infty \)
[Jimbo Miwa Mori Sato 1980] Density Matrix $\rho_\infty(x; 0)$ is now identified with a $\tau$-function of the fifth Painlevé system

$$
\rho_\infty(x; 0) = \rho_0 \exp \left( \int_0^{\pi \rho_0 x} \sigma_V(t) \frac{dt}{t} \right),
$$

where $\rho_0$ denotes the bulk density. $\sigma_V$ satisfies the non-linear equation

$$(x\sigma'_V)^2 + 4(x\sigma'_V - \sigma_V - 1)(x\sigma'_V - \sigma_V + (\sigma'_V)^2) = 0$$

subject to the $x \to 0$ boundary condition

$$\sigma_V(x) \sim \frac{x^2}{3} + \frac{x^3}{3\pi} + O(x^4).$$

[Lenard 1972] Eigenvalues of the density matrix are Fourier coefficients

$$
\lambda_k = \int_0^L \rho_N(x; 0)e^{2\pi i k x/L} dx.
$$

The $N \to \infty$ asymptotic expansion

$$
\rho_N(x; 0) \sim \rho_0 A \left( \frac{\pi}{N \sin(\pi \rho_0 x/N)} \right)^{1/2}, \quad A = \frac{G^4(3/2)}{\sqrt{2\pi}}
$$

where $G(x)$ denotes the Barnes’ G-function, valid for $x/N$ fixed. Therefore

$$
\lambda_0 \sim c \sqrt{N}
$$

a specific $c$ computable from the above.
[FFGW 2003] Finite system of $N + 1$ particles on a ring of circumference $L$, $x \in [0, L]$.

Wavefunction

$$\Psi_0(x_1, \ldots, x_N) = \frac{1}{L^{N/2} (N!)^{1/2}} \prod_{1 \leq j < k \leq N} 2 \left| \sin \frac{\pi (x_k - x_j)}{L} \right|$$

Density Matrix $\rho_{N+1}(x; 0)$

$$\rho_{N+1}(x; 0) = \frac{1}{L} \mathbb{E}_{U(N)} \left( \prod_{l=1}^{N} \left| 2 \sin \left( \frac{\pi x}{L} - \frac{\theta_l}{2} \right) \right| \left| 2 \sin \left( \frac{\theta_l}{2} \right) \right| \right)$$

Density Matrix can be identified with a member of a $\tau$-function sequence in the sixth Painlevé system with Okamoto parameters

$$b = \left( \frac{1}{2} N, 1 + \frac{1}{2} N, \frac{1}{2} N, -1 - \frac{1}{2} N \right).$$

Thermodynamic limit made by substituting $x = e^{2it/N}$ and taking $N \to \infty$ with $N/L$ fixed.
Determinants

The general Heine identity

\[ N! \det \left[ \int_{\mathbb{R}} dx \ w(x)x^{j+k-2} \right]_{j,k=1,\ldots,N} = \int_{\mathbb{R}} dx_1 \cdots \int_{\mathbb{R}} dx_N \prod_{l=1}^{N} w(x_l) \prod_{1\leq j<k\leq N} |x_j - x_k|^2 \]

Determinant formula

\[ \rho_{N+1}(x; y) = \frac{1}{c_N^2} e^{-x^2/2-y^2/2} \det[a_{j,k}(x; y)]_{j,k=1,\ldots,N} \]

with matrix elements

\[ a_{j,k}(x; y) = \frac{2^{-j-k+2}}{c_{j-1}c_{k-1}} \int_{-\infty}^{\infty} dt |x-t||y-t|H_{j-1}(t)H_{k-1}(t)e^{-t^2} \]

To simplify further, we note

\[ |x-t||y-t| = \begin{cases} (x-t)(y-t), & t \notin [x, y] \\ -(x-t)(y-t), & t \in [x, y] \end{cases} \]
Orthogonal Polynomial System (OPS)

Orthogonal polynomial system \( \{p_n(t)\}_{n=0}^{\infty} \) defined by the orthogonality relations

\[
\int_{\mathbb{R}} dt \ w(t)p_n(t)t^m = \begin{cases} 0 & 0 \leq m < n \\ h_n & m = n \end{cases}
\]

A consequence of the orthogonality relation is the three term recurrence relation

\[
a_{n+1}p_{n+1}(t) = (t - b_n)p_n(t) - a_np_{n-1}(t), \quad n \geq 1
\]

Central objects in our probabilistic model are the Hankel determinants

\[
\Delta_n := \det[\mu_{j+k-2}]_{j,k=1,...,n}, \quad n \geq 1, \quad \Delta_0 := 1,
\]

in terms of the moments of the weight \( \{\mu_n\}_{n=0,1,...,\infty} \)

\[
\mu_n := \int_{\mathbb{R}} dt \ w(t)t^n
\]

Alternatively

\[
\Delta_n = \frac{1}{n!} \int_{\mathbb{R}} dt_1 \ldots \int_{\mathbb{R}} dt_n \prod_{l=1}^{n} w(t_l) \prod_{1 \leq j < k \leq n} (t_k - t_j)^2, \quad n \geq 1
\]

result in orthogonal polynomial theory

\[
a_n^2 = \frac{\Delta_{n+1}\Delta_{n-1}}{\Delta_n^2}, \quad n \geq 1,
\]
[Bauldry 1990, Bonan and Clark 1990]

Orthogonal polynomials satisfy a system of coupled first order linear differential equations with respect to $t$ ($' ≡ d/dt$)

$$Wp'_n = (\Omega_n - V)p_n - a_n\Theta_n p_{n-1}, \quad n ≥ 1,$$

with the coefficient functions $V(t), W(t), \Theta_n(t), \Omega_n(t)$.

Compatibility Condition → Coefficient functions satisfy the recurrence relations

$$\Omega_{n+1} + \Omega_n = (t - b_n)\Theta_n, \quad n ≥ 0,$$

$$(\Omega_{n+1} - \Omega_n)(t - b_n) = W + a^2_{n+1}\Theta_{n+1} - a^2_n\Theta_{n-1}, \quad n ≥ 0.$$
Semi-Classical weights defined by

\[
\frac{1}{w(t)} \frac{d}{dt} w(t) = \frac{2V(t)}{W(t)}
\]

with \(V(t)\) and \(W(t)\) irreducible polynomials in \(t\).

**Deformed Hermite Orthogonal Polynomials** with weight

\[
w(t; x, y) = |t - x||t - y|e^{-t^2}, \quad t \in \mathbb{R},
\]

\[
= [1 - 2\chi_{(x,y)}(t)](t - x)(t - y)e^{-t^2}
\]

where

\[
\chi_{I}(t) = \begin{cases} 
1 & \text{if } t \in I \\
0 & \text{otherwise}
\end{cases}
\]
[Magnus 1995, ...]
Numerator and denominator polynomials

\[ W(t) = (t - x)(t - y), \quad 2V(t) = -2t^3 + 2(x + y)t^2 + 2t(1 - xy) - x - y \]

N.B. we have finite singularities at \( t = x, y \).
Coefficient functions are

\[ \Theta_n(t) = -2t^2 + 2(x + y - b_n)t \]
\[ \quad + 2n + 1 + 2(x + y)b_n + 2(1 - xy) - 2[a_{n+1}^2 + a_n^2 + b_n^2], \quad n \geq 0 \]

and

\[ \Omega_n(t) = -t^3 + (x + y)t^2 + (n + 1 - xy - 2a_n^2)t \]
\[ \quad + \sum_{i=0}^{n-1} b_i + (x + y)(2a_n^2 - n - \frac{1}{2}) - 2a_n^2(b_n + b_{n-1}), \quad n \geq 1 \]
Proposition

Density matrix is given by

\[ \rho_{N+1}(x; y) = \frac{(N + 1)!}{C_{N+1}^2} e^{-x^2/2-y^2/2} \Delta_N, \]

and

\[ \Delta_{N+1} = a_N^2 \frac{\Delta_N^2}{\Delta_{N-1}}, \]

subject to \( \Delta_0 = 1, \Delta_1 = \mu_0 \). Coupled recurrences for the polynomial coefficients are

\[
\sum_{i=0}^{n} b_i + (n + 1 - xy)b_n - b_n^3 + (x + y)[b_n^2 - n - 1] \\
+ a_{n+1}^2[x + y - 2b_n - b_{n+1}] - a_n^2[x + y - 2b_n - b_{n-1}] = 0
\]

and

\[
a_{n+1}^2[2n + 5 - 2xy + 2(x + y)(b_{n+1} + b_n) - 2(a_{n+2}^2 + a_{n+1}^2 + b_{n+1}^2 + b_n^2 + b_{n+1}b_n)] \\
- a_n^2[2n + 1 - 2xy + 2(x + y)(b_n + b_{n-1}) - 2(a_n^2 + a_{n-1}^2 + b_n^2 + b_{n-1}^2 + b_nb_{n-1})] \\
+ (b_n - x)(b_n - y) = 0
\]
Initial Data and Moments

The initial data for $b_n$ and $a_n^2$ are given by

$$b_{-1} = 0, \quad b_0 = \frac{\mu_1}{\mu_0}, \quad a_0^2 = 0, \quad a_1^2 = \frac{\mu_0 \mu_2 - \mu_1^2}{\mu_0^2}$$

where for $x < y$

$$\mu_0 = \sqrt{\pi} \left( \frac{1}{2} + xy \right) \left[ 1 + \text{erf}(x) - \text{erf}(y) \right] + ye^{-x^2} - xe^{-y^2}$$

$$\mu_1 = -\frac{1}{2} \sqrt{\pi} \left( x + y \right) \left[ 1 + \text{erf}(x) - \text{erf}(y) \right] - e^{-x^2} + e^{-y^2}$$

$$\mu_2 = \sqrt{\pi} \left( \frac{3}{4} + \frac{1}{2} xy \right) \left[ 1 + \text{erf}(x) - \text{erf}(y) \right] + \left( y - \frac{1}{2} x \right) e^{-x^2} - \left( x - \frac{1}{2} y \right) e^{-y^2}$$
Deformed Hermite Orthogonal Polynomials with weight

\[ w(t; x, y) = (t - x)^\mu (t - y)^\nu e^{-t^2}, \quad t \in \Gamma \]

where \( \partial \Gamma \in \{-\infty, x, y, \infty\} \).

Numerator and denominator polynomials

\[ W(t) = (t - x)(t - y), \quad 2V(t) = -2(t - x)(t - y) + \nu(t - x) + \mu(t - y) \]

Coefficient functions are

\[ \Theta_n(t) = -2(t - x)(t - y) - 2b_n(t - x - y) + \theta_n, \quad n \geq 0 \]

and

\[ \Omega_n(t) = -t(t - x)(t - y) - (2a_n^2 - n)(t - x - y) + \frac{1}{2} \nu(t - x) + \frac{1}{2} \mu(t - y) + \omega_n, \quad n \geq 1 \]
Proposition

Coupled first order recurrences $n \mapsto n + 1$ for system $\{a_n^2, b_n, \theta_n, \omega_n\}$

\[
\theta_n + 2b_n x = \frac{[\omega_n + (2a_n^2 - n)x][\omega_n + (2a_n^2 - n)x - \nu(x - y)]}{a_n^2(\theta_{n-1} + 2b_{n-1}x)}
\]

\[
\theta_n + 2b_n y = \frac{[\omega_n + (2a_n^2 - n)y][\omega_n + (2a_n^2 - n)y + \mu(x - y)]}{a_n^2(\theta_{n-1} + 2b_{n-1}y)}
\]

\[
a_{n+1}^2 + a_n^2 = -b_n^2 + \frac{1}{2}(2n + 1 + \mu + \nu - \theta_n)
\]

\[
\omega_{n+1} + \omega_n = (x + y)\theta_n + b_n(2xy - \theta_n) - \mu x - \nu y
\]
2 × 2 matrix system

\[ Y_n(t; x, y) = \begin{pmatrix} p_n & \epsilon_n/w \\ p_{n-1} & \epsilon_{n-1}/w \end{pmatrix} \]

where the associated functions are

\[ \epsilon_n(s; x, y) = \int_{\Gamma} dt \, w(t) \frac{p_n(t)}{s - t}, \quad s \notin \Gamma \]

**Proposition**

Assume \( \text{Re}\mu > 0, \text{Re}\nu > 0 \) and \( x \neq y \). The spectral derivatives satisfy

\[ \frac{\partial}{\partial t} Y_n = \left\{ 2t \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} + 2a_n \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} + \frac{A_x}{t - x} + \frac{A_y}{t - y} \right\} Y_n \equiv AY_n \]

where the residue matrices are

\[ A_x(t; x, y; \mu, \nu) \equiv \begin{pmatrix} \omega_n + (2a_n^2 - n)y \quad -a_n(\theta_n + 2b_n y) \\ a_n(\theta_n-1 + 2b_n-1 y) \quad -\omega_n + (2a_n^2 - n)y - \mu \end{pmatrix}, \quad (1) \]

and \( A_y = A_x |_{x \leftrightarrow y, \mu \leftrightarrow \nu} \).

Properties: \( \text{Tr}A_x = -\mu, \det A_x = 0 \)
Two-variable Garnier Systems

\[ L(1, 1, 1, 1; 2) \quad \kappa_0, \kappa_1, \kappa_\infty, \theta_1, \theta_2 \]

\[ L(1, 1, 1, 2; 2) \quad \kappa_0, \kappa_1, \kappa_\infty, \theta_2 \]

\[ L(1, 1, 3; 2) \quad \kappa_0, \kappa_1, \kappa_\infty \quad \text{and} \quad L(1, 2; 2) \quad \kappa_0, \kappa_1, \kappa_\infty \]

\[ L(1, 4; 2) \quad \kappa_0, \kappa_\infty \quad \text{and} \quad L(2, 3; 2) \quad \kappa_0, \kappa_\infty \]

\[ L(5; 2) \quad \alpha \]

\[ L(\frac{9}{2}; 2) \]
Proposition

Assume $\text{Re}\mu > 0, \text{Re}\nu > 0$ and $x \neq y$. The deformation derivatives with respect to $x$ or $y$ satisfy

\[
\frac{\partial}{\partial x} Y_n = \left\{ \frac{1}{2} \frac{1}{x - y} \begin{pmatrix} -\theta_n - 2b_n y & 0 \\ 0 & \theta_{n-1} + 2b_{n-1} y \end{pmatrix} - \frac{A_x}{t - x} \right\} Y_n \equiv B_x Y_n
\]

\[
\frac{\partial}{\partial y} Y_n = \left\{ \frac{1}{2} \frac{1}{x - y} \begin{pmatrix} \theta_n + 2b_n x & 0 \\ 0 & -\theta_{n-1} - 2b_{n-1} x \end{pmatrix} - \frac{A_y}{t - y} \right\} Y_n \equiv B_y Y_n
\]
Special diagonal case: $x = y = 0$ yields

$$b_n = 0$$

and

$$a_{n+1}^2 \left[ 2n + 5 - 2a_{n+2}^2 - 2a_{n+1}^2 \right] = a_n^2 \left[ 2n + 1 - 2a_n^2 - 2a_{n-1}^2 \right]$$

with

$$a_0^2 = 0, \quad a_1^2 = \frac{3}{2}$$

Solution?
Special diagonal case: $x = y = 0$ yields

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and

$$a_{n+1}^2 \left[ 2n + 5 - 2a_{n+2}^2 - 2a_{n+1}^2 \right] = a_n^2 \left[ 2n + 1 - 2a_n^2 - 2a_{n-1}^2 \right]$$

with

$$a_0^2 = 0, \quad a_1^2 = \frac{3}{2}$$

Solution?

$$a_n^2 = \frac{n + 1}{2} - \frac{1}{2}(-1)^n$$
Special diagonal case: \( x = y = 0 \) yields

\[
   b_n = 0
\]

and

\[
   a_{n+1}^2 \left[ 2n + 5 - 2a_{n+2}^2 - 2a_{n+1}^2 \right] = a_n^2 \left[ 2n + 1 - 2a_n^2 - 2a_{n-1}^2 \right]
\]

with

\[
   a_0^2 = 0, \quad a_1^2 = \frac{3}{2}
\]

Solution?

\[
   a_n^2 = \frac{n + 1}{2} - \frac{1}{2}(-1)^n
\]

or for general \( y = x \neq 0 \)
N → ∞ Asymptotics

Special diagonal case: $x = y = 0$ yields

$$b_n = 0$$

and

$$a^2_{n+1} \left[ 2n + 5 - 2a^2_{n+2} - 2a^2_{n+1} \right] = a^2_n \left[ 2n + 1 - 2a^2_n - 2a^2_{n-1} \right]$$

with

$$a^2_0 = 0, \quad a^2_1 = \frac{3}{2}$$

Solution?

$$a^2_n = \frac{n + 1}{2} - \frac{1}{2} (-1)^n$$

or for general $y = x \neq 0$

$$a^2_n = \frac{n}{2} \frac{(n + 2)H^2_{n+1} - (n + 1)H_{n+2}H_n}{(n + 1)H^2_n - nH_{n+1}H_{n-1}} \left[ nH^2_{n-1} - (n - 1)H_nH_{n-2} \right]$$
Where to from here?

- Can the density matrix eigenvalues (or just the lowest one) be accessed directly and analytically using these ideas?
- the theory is easily generalisable to calculate other quantities, higher correlations etc,
- take the thermodynamic limit,
- finite temperature extensions may be possible within the structures,
- the situation for finite interparticle repulsion $c < \infty$ is more challenging,
- certainly other non-integrable potentials can be handled with a little more effort with the resulting difference and differential systems being non-integrable
- extensions to 2 dimensions would require a major task at the level of the basic mathematical theory


