Transition from a BEC to a Tonks-Girardeau Gas

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Outline

1 Introduction
- System
- Girardeau’s Theory
- Gross-Pitaevskii Theory
- Experiments

2 Method
- Exact Diagonalization
- Conserved Quantities
- $\delta$-Approximation

3 Results And Discussion
- Density
- Various Energies
- Mean Occupation
- Momentum Distribution
- Correlation Functions

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Considered System

- Spinless bosons (e.g. $^{87}\text{Rb}$ atoms with frozen spin degrees of freedom)

- 3D harmonic potential ($\omega_x \ll \omega_\perp$)

$$V_{\text{ext}}(\vec{r}) = \frac{1}{2} m \omega_x^2 x^2 + \frac{1}{2} m \omega_\perp^2 (y^2 + z^2)$$

- Extremely short ranged repulsive interaction

$$V_{\text{int}}(|\vec{r} - \vec{r}'|) = \frac{4\pi \hbar^2 a_s}{m} \delta(\vec{r} - \vec{r}')$$

- We are interested in ground state properties
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Girardeau’s Theory ($a_s = \infty$)

- $a_s = \infty \Rightarrow$ additional boundary condition

$$\Psi(x_1, ..., x_N) = 0 \quad \text{if} \quad x_i = x_j$$

- Schrödinger equation exactly solvable:

$$\Psi_B(x_1, ..., x_N) = \prod_{1 \leq i < j \leq N} \text{sgn}(x_i - x_j)\Psi_F(x_1, ..., x_N)$$

- $\Psi_F$ solves Schrödinger eq. in $x_i \neq x_j$
- $\Psi_F = 0$ if $x_i = x_j$
- Product of sgn-functions makes wave function symmetric

- Ground state

$$\Psi_{TG}(x_1, ..., x_N) = |\det[\phi_i(x_j)]| \quad i, j = 1, 2, ..., N$$
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**Similarities**

- Many similarities between \( N \) infinitely strong \( \delta \)-interacting bosons and \( N \) non-interacting fermions
- All quantities which can be calculated with the absolute square of the real space wave function are equal: e.g. density \( \rho(x) \), correlation function \( g^{(2)}(x, x') \), all energies \( (E_{tot}, E_{kin}, ...) \)
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**Girardeau’s Theory** \( (a_s = \infty) \)

### Differences 1

- **Tonks-Girardeau wave function has kinks at** \( x_i = x_j \):
  - 2 non-interacting fermions in a 1D harmonic oscillator
    \[
    \Psi_F(x_1, x_2) \propto (x_1 - x_2) e^{-\frac{x_1^2 + x_2^2}{2}}
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  - Tonks-Girardeau wave function of 2 bosons
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  - Generalization to \( N \) bosons
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Differences 2
- We need fast oscillating functions to represent the kink
  - Mean occupation \( \langle N_i \rangle \) of single particle states is different
  - Momentum distribution \( \rho(p_x) \) is different
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Gross-Pitaevskii Theory ($a_s \gtrapprox 0$)

- Ansatz for many-particle wave function

$$\Psi_B(x_1, \ldots, x_N) \propto \prod_{i=1}^{N} \phi(x_i)$$

- All bosons occupy same single-particle wave function
- The optimal shape of $\phi(x)$ minimizes the total energy of $\Psi_B(x_1, \ldots, x_N)$
- $\phi(x)$ solves Gross-Pitaevskii (GP) eq.

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_{\text{ext}}(x) + N \frac{4\pi \hbar^2 a_s}{m} |\phi(x)|^2 \right] \phi(x) = \mu \phi(x)$$
Gross-Pitaevskii Theory ($a_s \approx 0$)

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Motivation for Exact Diagonalization Studies

- Comparison with other approximations: local density approximation, mean-field calculations with modified energy functionals

First experimental realization 2004

- Experimentally produced gases consisted of ≈ 50 atoms
  ⇒ Accurate predictions with exact diagonalization method possible?
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Basis

- **Single-particle basis**: eigenfunctions of 3D harmonic oscillator

\[
\phi_{(n_x, n_y, n_z)}(\vec{r}) = \phi_{n_x}(x) \phi_{n_y}(y) \phi_{n_z}(z)
\]

with

\[
\phi_{n_\xi}(\xi) \propto \frac{1}{\sqrt{l_\xi}} H_{n_\xi} \left( \frac{\xi}{l_\xi} \right) e^{-\frac{1}{2} \left( \frac{\xi}{l_\xi} \right)^2}
\]

\[
l_\xi = \sqrt{\frac{\hbar}{m_\omega_\xi}}: \text{oscillator length of } \xi\text{-direction}
\]

- **Many-particle basis**: Fock states with lowest potential and kinetic energy

\[
| 1 \rangle = | N_g : (0, 0, 0) \rangle,
\]

\[
| 2 \rangle = | (N_g - 1) : (0, 0, 0); 1 : (1, 0, 0) \rangle, \ldots
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External potential: 3D harmonic potential \( (\omega_x \ll \omega_\perp) \)

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Internal potential: \( \delta \)-interaction

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V_{\text{int}}(|\vec{r} - \vec{r}'|) = \frac{4\pi \hbar^2 a_s}{m} \delta(\vec{r} - \vec{r}')
\]

Coupling strength \( U_{3D} \)

\[
U_{3D} l_x l_y l_z = \frac{4\pi \hbar^2 a_s}{m}
\]

\( \hbar \omega_x < U_{3D} \ll \hbar \omega_\perp \)
**Potentials**

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Second Quantized Hamiltonian

\[ H = \sum_{ij} a_i^{\dagger} a_j \int d^3 r \phi_i(\vec{r}) \left[ -\frac{\hbar^2}{2m} \Delta + V_{\text{ext}}(\vec{r}) \right] \phi_j(\vec{r}) \]
\[ + \frac{1}{2} U_{3D} l_x l_y l_z \sum_{ijkl} a_i^{\dagger} a_j^{\dagger} a_k a_l \int d^3 r \phi_i(\vec{r}) \phi_j(\vec{r}) \phi_k(\vec{r}) \phi_l(\vec{r}) \]

with \( i = (n_{xi}, n_{yi}, n_{zi}) \)

- Interaction integrals have dimension \( \frac{1}{l_x l_y l_z} \)
- We want to study ground state properties in the regime \( \hbar \omega_x < U_{3D} \ll \hbar \omega_\perp \)
  \Rightarrow Transverse motion restricted to zero-point oscillations:
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Matrix Elements of Hamiltonian

- System is quasi 1D: \( i \rightarrow n_{xi} = 0, 1, 2, \ldots, \) \( U_{3D} \rightarrow U_{1D} = \frac{U_{3D}}{2\pi} \)

\[
\langle N|H|N' \rangle = \delta_{NN'} \left[ N_g \hbar \omega_\perp + \hbar \omega_x \sum_i N_i \left( i + \frac{1}{2} \right) \right] + \frac{1}{2} U_{1D} \sum_{ijkl} \tilde{I}_{ijkl} \langle N|a_i^{\dagger}a_j^{\dagger}a_l a_k|N' \rangle
\]

- \( \tilde{I}_{ijkl} \): dimensionless interaction integrals of x-direction
- \( N_g \hbar \omega_\perp \): Zero-point energy of transverse motion. Constant offset of diagonal elements of \( H \Rightarrow \) does not effect eigenstates of system
- \( U_{1D} = 2\sqrt{m\hbar \omega_x a_s \omega_\perp} \Rightarrow U_{1D} \propto \omega_\perp \)
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+ \frac{1}{2} U_{1D} \sum_{ijkl} \tilde{I}_{ijkl} \langle N | a_i^\dagger a_j^\dagger a_l a_k | N' \rangle
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- \( \tilde{I}_{ijkl} \): dimensionless interaction integrals of x-direction
- \( N_g \hbar \omega_{\perp} \): Zero-point energy of transverse motion. Constant offset of diagonal elements of \( H \Rightarrow \) does not effect eigenstates of system
- \( U_{1D} = 2\sqrt{m\hbar \omega_x a_s \omega_{\perp}} \Rightarrow U_{1D} \propto \omega_{\perp} \)
Matrix Elements of Hamiltonian

- System is quasi 1D: $i \rightarrow n_{xi} = 0, 1, 2, \ldots$, $U_{3D} \rightarrow U_{1D} = \frac{U_{3D}}{2\pi}$

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Conservation of Parity

- Eigenfunctions of 1D harmonic oscillator $\phi_i(x)$ have even or odd parity $\mathbb{P}$
  \[ \mathbb{P}[\phi_i] = (-1)^i \]

- Interaction integrals $I_{ijkl} = \int dx \phi_i \phi_j \phi_k \phi_l$ are only non-zero if integrand has even parity
  \[ I_{ijkl} \neq 0 \iff i + j + k + l = 0 \mod 2 \]
  \[ \Rightarrow i + j = k + l \mod 2 \]

- Parity $\mathbb{P}$ is conserved during collision of two particles
- Define parity $\mathbb{P}$ of Fock state $|N\rangle$
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We want to calculate interaction integrals. Switch to center of mass and relative motion coordinates

\[ I_{ijkl} = \int dX dx \phi_i(X + \frac{x}{2}) \phi_j(X + \frac{x}{2}) v_{int}(x) \phi_k(X + \frac{x}{2}) \phi_l(X + \frac{x}{2}) \]

Make Taylor expansion of wave functions

\[ \phi_i \phi_j \phi_k \phi_l(X, x) = \phi_i \phi_j \phi_k \phi_l(X, 0) + x \frac{\partial}{\partial x} \phi_i \phi_j \phi_k \phi_l(X, 0) + ... \]

\[ \Rightarrow I_{ijkl} = \int dx v_{int}(x) \int dX \phi_i(X) \phi_j(X) \phi_k(X) \phi_l(X) + ... \]

Neglect all higher order terms if product of wave functions changes slowly within range of \( v_{int} \)
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Neglect all higher order terms if product of wave functions changes slowly within range of \( v_{\text{int}} \)
\[ \Rightarrow I_{ijkl} \approx C \int dx_1 dx_2 \phi_i(x_1) \phi_j(x_2) \delta(x_1 - x_2) \phi_k(x_2) \phi_l(x_1) \]

with \( C = \int dx v_{int}(x) \)

- Use effective \( \delta \)-potential
  - to calculate low energy properties
  - if low energy single-particle wave functions change slowly within range of interaction potential

\[ v_{int} \rightarrow v_{int}^{\text{eff}} = C \delta(x_1 - x_2) \]
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\[ v_{int} \rightarrow v_{int}^{\text{eff}} = C \delta(x_1 - x_2) \]
Density

\[ \rho(x) \]

\[ x [l_x] \]

\[ U = 0.25 \hbar \omega_x \]
\[ U = 1 \hbar \omega_x \]
\[ U = 3 \hbar \omega_x \]
\[ U = 5 \hbar \omega_x \]
\[ U = 8 \hbar \omega_x \]
\[ U = 20 \hbar \omega_x \]
Density: Discussion

- $U \lesssim 3 \hbar \omega_x$: mean-field wave function $\phi(x)$ flattens $\Rightarrow$ density $\rho(x) = |\sqrt{N}\phi(x)|^2$ becomes lower
- $U \gtrsim 5 \hbar \omega_x$: five density maxima form
- Girardeau: "infinitely strong $\delta$-interacting bosons in 1D behave like non-interacting fermions"
- No visible difference between density of five non-interacting fermions

$$\rho(x) \propto \sum_{i=0}^{4} |\phi_i(x)|^2$$

and density of five bosons at $U = 20 \hbar \omega_x$
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Results And Discussion

Energies

\[ E_{\text{int}} \]
\[ E_{\text{kin},x} \]
\[ E_{\text{pot},x} \]
\[ E_{\text{tot},x} \]
\[ E_{T\Gamma} \]

\[ \hbar \omega_x \] vs. \[ U \ [\hbar \omega_x] \]
Results And Discussion

Energies: Discussion

- **Limit:** $U = 0$

  \[
  E_{\text{tot}} = 5 \cdot \frac{1}{2} \hbar \omega_x = 2.5 \hbar \omega_x
  \]

  \[
  E_{\text{kin}} = E_{\text{pot}} = \frac{E_{\text{tot}}}{2} = 1.25 \hbar \omega_x
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- **Limit:** $U = \infty$

  \[
  E_{\text{tot}} = \sum_{i=0}^{4} \left( i + \frac{1}{2} \right) \hbar \omega_x = \frac{5^2}{2} \hbar \omega_x = 12.5 \hbar \omega_x
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- $E_{\text{int}} = 0$ in both limiting cases
Energies: Discussion

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Mean-field kinetic energy at low coupling strength $U$:

$$E_{kin}^{MF} = \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \left( \frac{d\sqrt{\rho(x)}}{dx} \right)^2$$
Comparison of mean-field and exact kinetic energy. $E_{\text{kin}}^{MF}$ was calculated from the exact density $\rho(x)$. 
Kinetic Energy: Discussion

- Mean-field kinetic energy at low coupling strength $U$:

$$E_{kin}^{MF} = \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} dx \left( \frac{d \sqrt{\rho(x)}}{dx} \right)^2$$

- $\rho(x)$ flatter $\Rightarrow E_{kin}^{MF}$ smaller

- Good agreement for $0 \leq U \lesssim 0.5 \hbar \omega_x$

- But we cannot explain the increase at higher coupling strengths $U$

- Look closer at exact many-particle wave function ...
Results And Discussion

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Kinetic Energy: Discussion

- Wave function of $N$ non-interacting bosons

$$\Psi_{U=0}(x_1, ..., x_N) \propto \prod_{i=1}^{N} e^{-\frac{x_i^2}{2l_x^2}}$$

- Wave function of $N$ infinitely strong $\delta$-interacting bosons

$$\Psi_{U\to\infty}(x_1, ..., x_N) \propto \prod_{1\leq i<j\leq N} |x_i-x_j| \prod_{k=1}^{N} e^{-\frac{x_k^2}{2l_x^2}}$$

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- $\delta$-interaction causes formation of notches
Wave function of 2 bosons at different $U$. δ-interaction forces formation of a notch at $x_1 = x_2 = 0$
Kinetic Energy: Discussion

\[ U = 20 \hbar \omega_x, \text{x-coordinate of first boson varies} \]
Kinetic Energy: Discussion

- Exact many-particle kinetic energy
  
  \[ E_{\text{kin}} = \frac{\hbar^2}{2m} \sum_{i=1}^{N} \int dx_1 \ldots dx_N \left[ \frac{\partial}{\partial x_i} \psi(x_1, \ldots x_N) \right]^2 \]

- Increase of $U$ has two counteracting effects:
  - Total height of wave function decreases $\Rightarrow$ $E_{\text{kin}}$ becomes smaller
  - Notches form $\Rightarrow$ $E_{\text{kin}}$ becomes larger

- $U \lesssim 0.5 \hbar \omega_x$: Total height decreases faster than notch forms $\Rightarrow$ $E_{\text{kin}}$ becomes smaller

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Summary: Kinetic Energy

- Low $U$: mean-field wave function $\phi(x)$ becomes flatter $\Rightarrow E_{kin}$ decreases
- High $U$: formation of notches rapidly lowers probability of finding 2 bosons at same place $\Rightarrow E_{kin}$ becomes larger
- Mean-field region smaller than $U \approx 0.5 \hbar \omega_x$
Results And Discussion

Kinetic Energy: Discussion

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Average local correlation function $G^{(2)}$: probability of finding two bosons at same place - averaged over entire $x$-range

$$G^{(2)} = \frac{1}{2} \int dx \langle \hat{\Psi}^\dagger(x) \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \hat{\Psi}(x) \rangle$$

($\hat{\Psi}(x), \hat{\Psi}^\dagger(x)$: Field operators)
Average local correlation function $\overline{G^{(2)}}(U)$. Initial value: $\overline{G^{(2)}}(U = 0) = 0.63 \frac{1}{l_x l_y l_z}$. Rapid decrease to zero with $U$. 
Average local correlation function \( G^{(2)} \): probability of finding two bosons at same place - averaged over entire x-range

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G^{(2)} = \frac{1}{2} \int dx \langle \hat{\Psi}^\dagger(x) \hat{\Psi}^\dagger(x) \hat{\Psi}(x) \hat{\Psi}(x) \rangle
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\((\hat{\Psi}(x), \hat{\Psi}^\dagger(x): \text{Field operators})\)

\( E_{\text{int}} \propto U \cdot G^{(2)} \)

\( E_{\text{int}} \) increases linearly at low \( U \) and decreases to zero at \( U \gtrsim 3 \hbar \omega_x \)

\( E_{\text{pot}} \) increases monotonously because wave function spreads out with increasing \( U \)
Average local correlation function $\overline{G^{(2)}}$: probability of finding two bosons at same place - averaged over entire $x$-range

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Interaction and Potential Energy: Discussion

- Average local correlation function $G^{(2)}$: probability of finding two bosons at same place - averaged over entire $x$-range

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Results And Discussion

Mean Occupation

\[ U = 1 \hbar \omega_x \]

\[ U = 3 \hbar \omega_x \]

\[ U = 6 \hbar \omega_x \]

\[ U = 20 \hbar \omega_x \]
Mean Occupation: Discussion

- **$U = \infty$:** Not one boson in each of the five lowest single-particle states
- **$U$ increases:** Particles leave ground state and occupy excited states
- **$U = 20\hbar\omega_x$:** More than two bosons still occupy ground state
- Comparatively high occupation of states with even parity
- Mean-field: $\phi_{MF}$ is superposition of single-particle states $\phi_0$, $\phi_2$, $\phi_4$, ... $\Rightarrow$ occupation of $\phi_1$, $\phi_3$, ... is zero
- Parity conservation favors states with even parity
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Momentum Distribution

$U = 0$

$U = 3\,\hbar\omega_x$

$U = 20\,\hbar\omega_x$

five fermions
Momentum Distribution: Discussion

- Momentum distribution of many-particle states

\[
\langle \rho(p) \rangle = \left\langle \int dx \hat{\Psi}^\dagger(x) e^{\frac{i}{\hbar}px} \int dx \hat{\Psi}(x) e^{-\frac{i}{\hbar}px} \right\rangle
\]

(\(\hat{\Psi}(x), \hat{\Psi}^\dagger(x)\): Field operators)

- Fourier transform of 1D harmonic oscillator eigenfunctions

\[
\mathcal{F}[\phi_n(x)] = (-i)^n \phi_n(p)
\]

- Density of five non-interacting bosons is Gaussian

- Density of five non-interacting fermions has same form as in real space
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Momentum distributions of infinitely strong $\delta$-interacting bosons and non-interacting fermions look completely different.

- Momentum distribution is peaked and has long tails: "condensation in momentum space"
- $U \approx 3 \hbar \omega_x$: Momentum distribution has maximum height
- $U = 20 \hbar \omega_x$: Shoulders at $p = \pm 1 \frac{\hbar}{l_x}$
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![Graph showing momentum distribution with peak and tails for different values of $U$.](image-url)
Results And Discussion

Correlation Functions of five bosons

First particle at $x_1 = 0$. Scale of y-axis is different in each line.
Results And Discussion

Correlation Functions of five bosons 2

First particle at $x_1 = 0$. Scale of $y$-axis is different in each line.
$U = 20 \hbar \omega_x$. Position of first particle varies. Scale of y-axis is different in each line.
Exact diagonalization method allows detailed study of transition from BEC to Tonks-Girardeau regime

Transition from BEC to Tonks-Girardeau like density at $U \approx 5 \hbar \omega_x$

Formation of notches explains behavior of kinetic and interaction energy at all coupling strengths $U$

Behavior of kinetic energy gives upper bound of Gross-Pitaevskii mean-field region: $U \lesssim 0.5 \hbar \omega_x$

Parity conservation favors occupation of single-particle states with even parity at all coupling strengths $U$

Maximum condensation in momentum space at $U \approx 3 \hbar \omega_x$

Formation of Tonks-Girardeau gas almost completely finished at $U = 20 \hbar \omega_x$
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