Universal contact for a strongly interacting 1D Bose gas

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Universality

- *Universal properties*: do not depend on microscopic details (eg in proximity of a phase transition)
- *In quantum gases:* possibility to tune the interactions to very large values (eg with Feschbach resonances)

  s-wave scattering amplitude $f_k = \frac{-1}{a_s^{-1} + ik - k^2 r_e/2}$

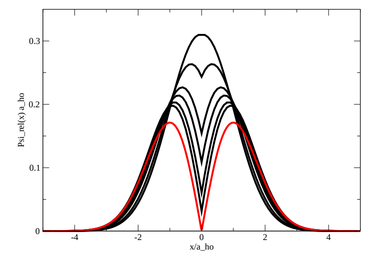
  if $a_s \to \infty$, $r_e \ll a_s, n^{-1/3} \Rightarrow$ spatial scale invariance, no length scale associated to interactions
- *A largely studied case:* 2-component Fermi gas in the unitary limit $1/k_F a_s = 0$
- *In this work:* universal aspects of a 1D Bose gas with strong repulsive interactions

Plan

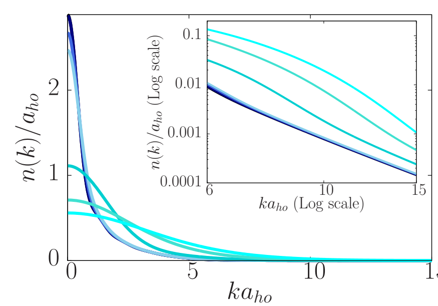
exact solutions for strongly interacting 1D gases:

external confinement and effects of temperature

- *Overview on 1D gases*
  theoretical approaches: Luttinger liquid, Bethe Ansatz, Tonks-Girardeau



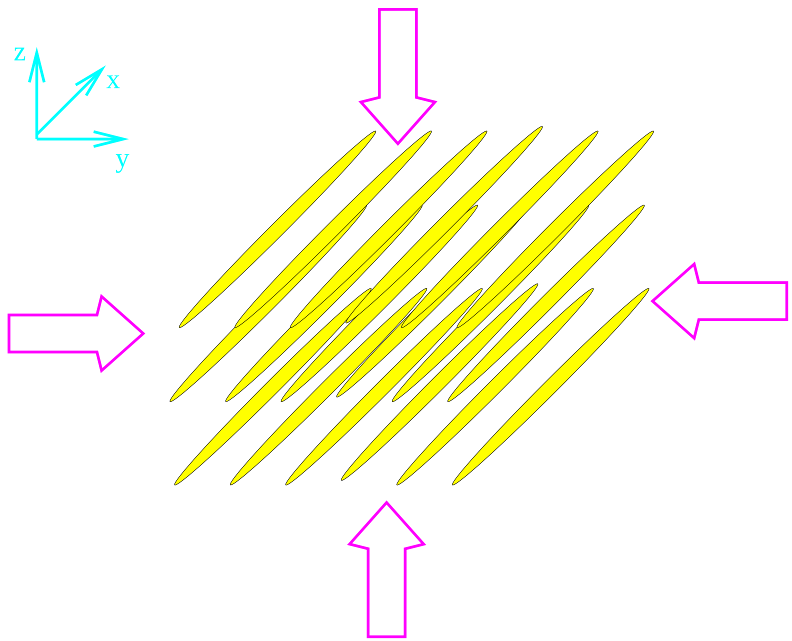
- *One-body coherences for a TG gas at finite temperature:*
  momentum distribution
  large momentum tails



Many-body properties of strongly interacting 1D Bose fluids

1D quantum gases

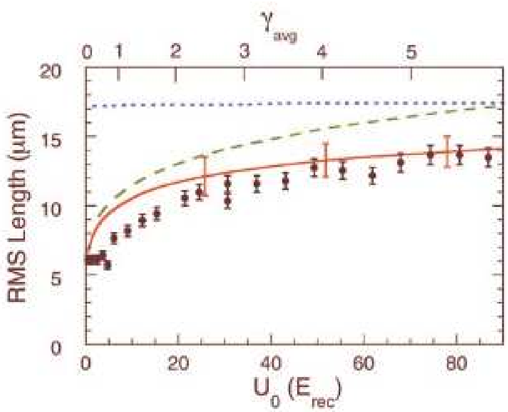
- Quasi-1D geometry:
  ultracold atoms in tight transverse confinement
  $$\mu, k_B T \ll \hbar\omega_\perp$$
  2D deep optical lattices, chip traps



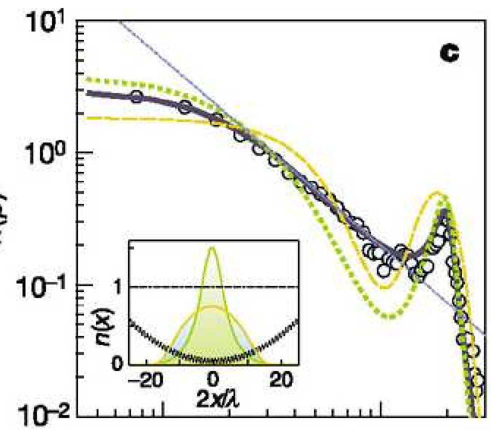
Some experimental results

1D bosons in the strongly interacting regime

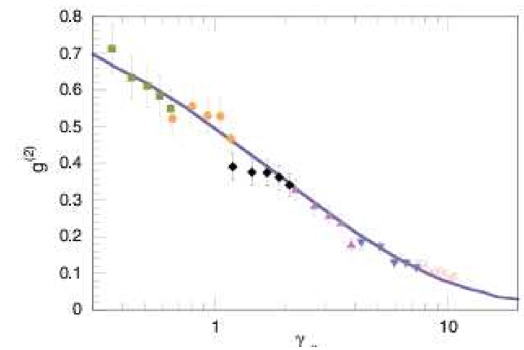
density profiles, momentum distribution, correlation functions, collective modes, transport, number fluctuations...



[T Kinoshita et al (2004)]



[B. Paredes et al, (2004)]



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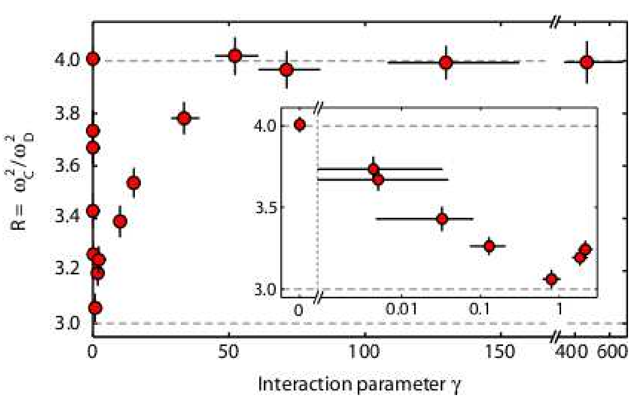
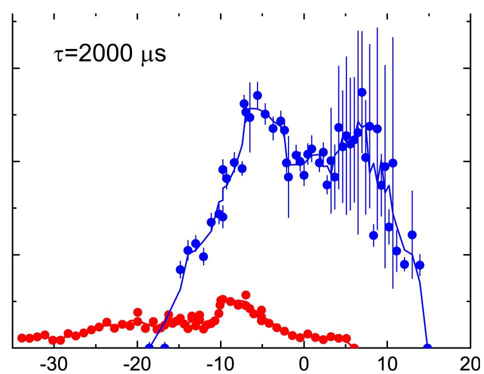
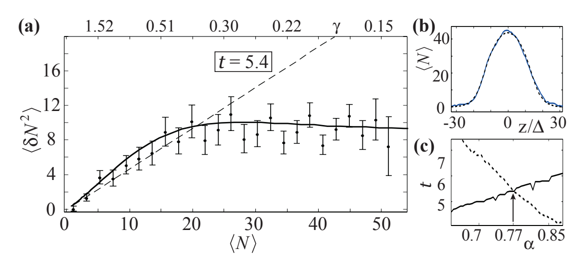


[E Haller et al, (2009)]



[S. Palzer et al, (2009)]



[T. Jacqmin et al, (2011)]

The model

- ultracold dilute bosonic gases in 3D: binary interactions through s-wave scattering length a_s
- for atoms in a tight waveguide *[Olshanii, 1998]*

$$v(x) = g\delta(x) \text{ with } g = 2a_s\hbar\omega_\perp(1 - 0.4602\, a_s/a_\perp)^{-1}$$

- model Hamiltonian *[Lieb and Liniger, 1963]*

$$\mathcal{H} = \sum_i -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x_i^2} + V(x_i) + g\sum_{i<j}\delta(x_i - x_j)$$

Lieb-Liniger model with external potential

coupling strength:

$$\gamma = gn/(\hbar^2 n^2/m)$$

note: *strong* coupling at *weak* densities

Peculiar properties in 1D

- No BEC for a homogeneous 1D Bose gas
  - ideal gas:

$$n = \int dk \, \frac{1}{\exp[\beta(\varepsilon_k - \mu)] - 1} = \frac{1}{\lambda_{dB}} g_{1/2}(e^{\beta\mu})$$

    always invertible, no macroscopic occupation of $n_{k=0}$
  - interacting gas:

    Bogoliubov-Hohenberg-Mermin inequality at $T > 0$

$$n_k \geq \frac{m k_B T}{\hbar^2 k^2 n} n_0 - \frac{1}{2}$$

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  - interacting gas:

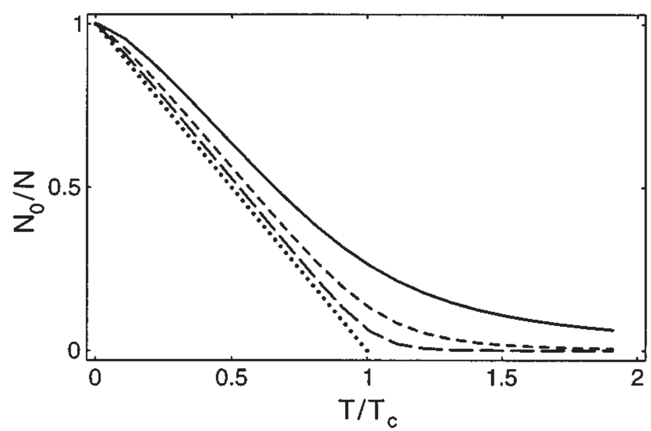
Pitaevskii-Stringari inequality at $T = 0$ $S(k)$: structure factor

$$n_k \geq \frac{n_0}{4nS(k)} - \frac{1}{2}$$

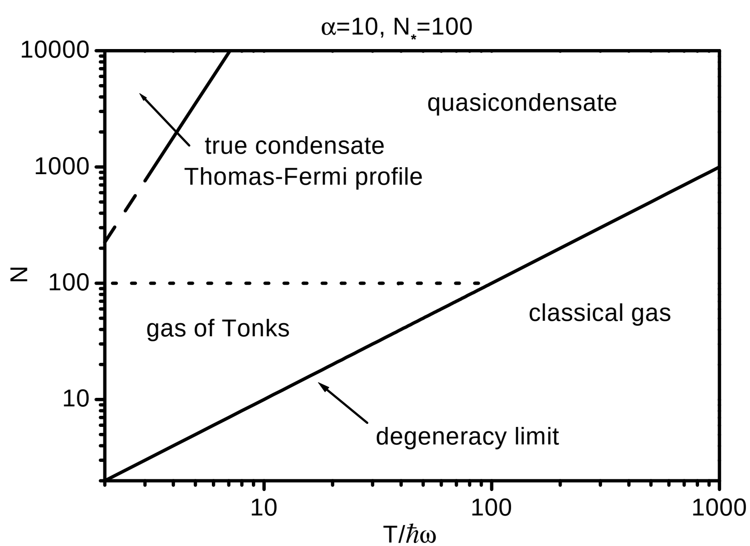
$\Rightarrow$ from $n = \int dk \, n_k$ then $n_0 = 0$

1D gases in harmonic trap

- BEC possible at weak interactions and low temperature; destroyed by thermal and quantum fluctuations



[Ketterle and Van Druten, 1996]



[Petrov and Shlyapnikov, 2000]

From quasicondensate to TG

- Bose-Einstein condensation in 3D: off-diagonal long range order for $|\mathbf{x}-\mathbf{x}'| \to \infty$ *[Penrose and Onsager, 1965]*

$$\langle \Psi^\dagger(\mathbf{x})\Psi(\mathbf{x}')\rangle \to n_0$$

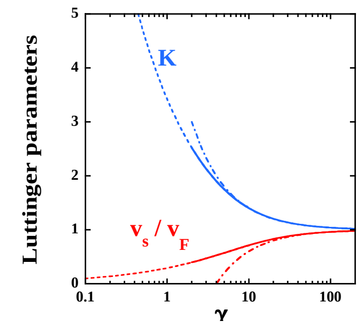
From quasicondensate to TG

quantum fluctuations: important in one-dimension

- in 1D *quasi*-long range order for $|x - x'| \to \infty$ *[Haldane, 1981]*

$$\langle \Psi^\dagger(x)\Psi(x')\rangle \to \frac{1}{|x - x'|^{1/2K}}$$

K: Luttinger parameter
depends on interactions



- Regimes of quantum degeneracy at $T = 0$:

  $\gamma \ll 1$ "quasicondensate"
  condensate with fluctuating phase, $K \gg 1$
  $\gamma \gg 1$ "Tonks-Girardeau" gas
  impenetrable-boson limit, $K = 1$

Several theory approaches

in addition to powerful numerical methods

- homogeneus system, arbitrary interaction strengths: exact solution with the Bethe Ansatz
- (mainly) homogeneous system, arbitrary interactions, low energy: the Luttinger-liquid approach
- inhomogeneous system, infinite interactions: the Tonks-Girardeau exact solution

The Bethe-Ansatz solution

[E Lieb and W Liniger, Phys Rev 130, 1605 (1963)]

- Many-body wavefunction

$$\Psi(x_1, ...x_N) = \sum_P a(P) e^{i \sum_j k_{P(j)} x_j}$$

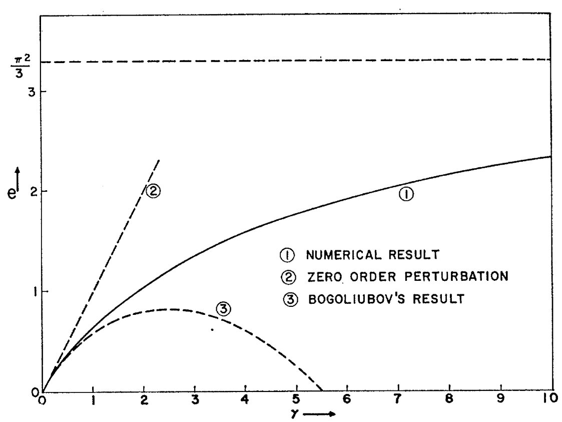
with $a(P)$ amplitudes connecting different permutation sectors, k_j momentum rapidities defined from

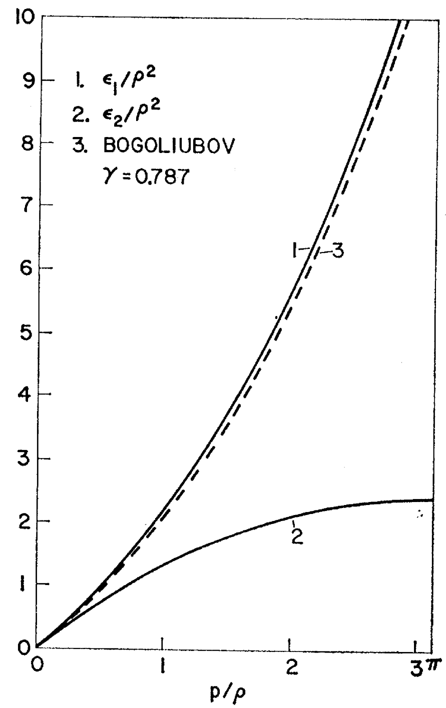
$$k_j L + \sum_\ell 2 \arctan[(k_j - k_\ell)/c] = 2\pi I_j$$

with $c = mg/\hbar^2$, and I_j given integers (half integers) for N odd (even), a set of quantum numbers

The Bethe-Ansatz solution

- Ground state energy $E = \sum_j k_j^2$ and excitation spectrum





Two excitation branches: the "Lieb-I" and "Lieb-II" modes

- Several recent advances to compute *correlation functions*: J.S. Caux, J.M. Maillet, ...

The Luttinger liquid method

- A quantum hydrodynamic approach (hyp: linear sound dispersion)

$$\mathcal{H}_{LL} = \hbar v_s \int \frac{\mathrm{d}x}{2\pi} \left[K \left(\nabla\phi(x)\right)^2 + \frac{1}{K} \left(\nabla\theta(x)\right)^2\right]$$

  K: Luttinger parameter

  $\theta(x)$ and $\phi(x)$: fields for density and phase

- Calculation of correlation functions: use the bosonic field operator

$$\Psi^\dagger(x) = \mathcal{A} \left[\rho_0 + \partial_x\theta(x)/\pi\right]^{1/2} \sum_{m=-\infty}^{+\infty} \mathrm{e}^{2mi\theta(x)+2mi\pi\rho_0 x} \mathrm{e}^{-i\phi(x)}$$

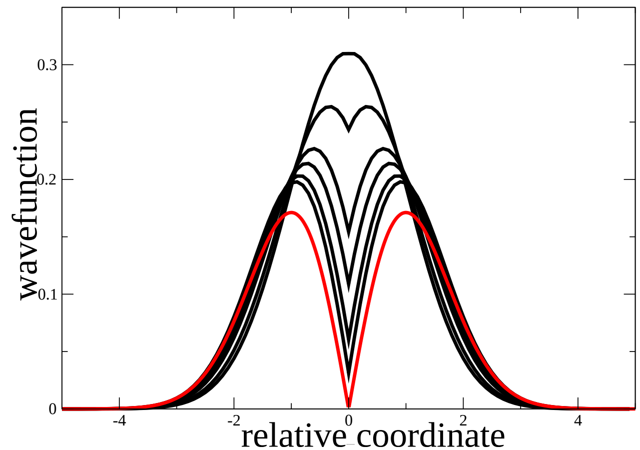
  and the mode expansion ($\mathcal{H}_{LL} = \hbar v_s \sum_{j\neq 0} k_j b_j^\dagger b_j$)

$$\phi(x) = \sqrt{\frac{\pi}{2KL}} \sum_{j\neq 0} \frac{\mathrm{sign}(k_j)\mathrm{e}^{-a|k_j|/2}}{\sqrt{|k_j|}} \left(\mathrm{e}^{ik_j x} b_j + \mathrm{e}^{-ik_j x} b_j^\dagger\right) + \phi_0 + \frac{\pi x}{L} J$$

$$\theta(x) = \sqrt{\frac{\pi K}{2L}} \sum_{j\neq 0} \frac{\mathrm{e}^{-a|k_j|/2}}{\sqrt{|k_j|}} \left(\mathrm{e}^{ik_j x} b_j + \mathrm{e}^{-ik_j x} b_j^\dagger\right) + \theta_0 + \frac{\pi x}{L} (\hat{N} - N)$$

Impenetrable boson limit

- Example: solution of the Schroedinger equation for two particles in harmonic oscillator at increasing γ



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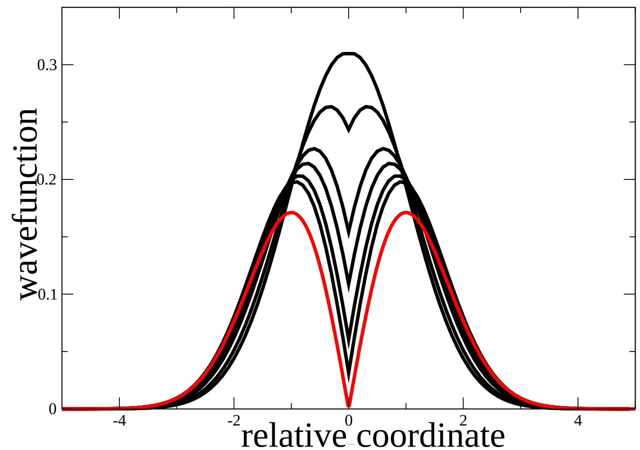

- For $\gamma \to \infty$ the many-body wavefunction vanishes at contact

$$\Psi(...x_j = x_\ell...) = 0$$

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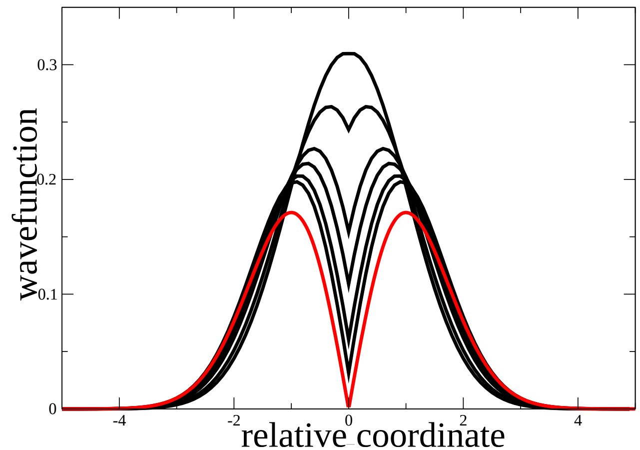

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$$\Psi(...x_j = x_\ell...) = 0$$

- "Fermionization": interactions play the role of the Pauli exclusion principle: the many-body wavefunction can be constructed exactly

Girardeau exact solution

- Interactions are turned onto a cusp condition
- Exact solution by mapping onto noninteracting fermions

  [MD Girardeau, 1960]

$$\Psi(x_1...x_N) = \Pi_{1\leq j<\ell\leq N}\mathrm{sign}(x_j - x_\ell)\frac{1}{\sqrt{N!}}\det[u_l(x_k)]$$

with $u_l(x)$ single particle orbitals

satisfies the many-body Schroedinger equation and the boundary conditions in each coordinate sector

valid for arbitrary external potential, also time dependent

- Further progress in harmonic potential with $u_l(x) \propto H_l(x)e^{-x^2/2}$:

$$\Psi(x_1...x_N) = \Pi_{1\leq j<\ell\leq N}|x_j - x_\ell|e^{-\sum_j x_j^2/2}$$

Fermionic aspects of the TG gas

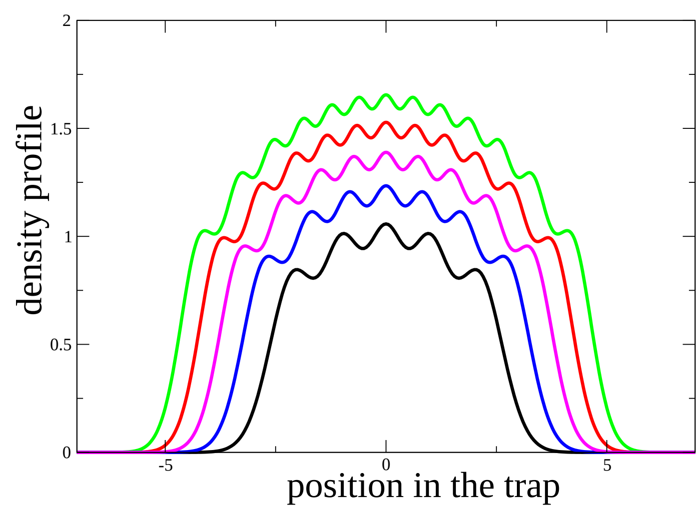
observables that do not depend on the sign of $\Psi(x_1 ... x_N)$

- Density profiles of a TG gas in harmonic trap:

$$n(x) = \int dx_2 ... dx_N |\Psi(x, x_2 ... x_N)|^2 = \sum_{j=1}^{N} |u_j(x)|^2$$

Green's function method for large N

[P Vignolo, AM, MP Tosi, (2000)]



the density profile coincides with the one of a Fermi gas

First-order coherences: the one-body density matrix and momentum distribution of a strongly interacting 1D Bose gas

One-body density matrix

important for bosonic systems

- A measure of first-order coherence and quasi long-range order

$$\rho_1(x,y) = \langle \Psi^\dagger(x)\Psi(y)\rangle$$

- associated to the momentum distribution

$$n(k) = \int dxdy\, e^{ik(x-y)}\rho_1(x,y)$$

a truly bosonic observable: very different from the one of the mapped Fermi gas

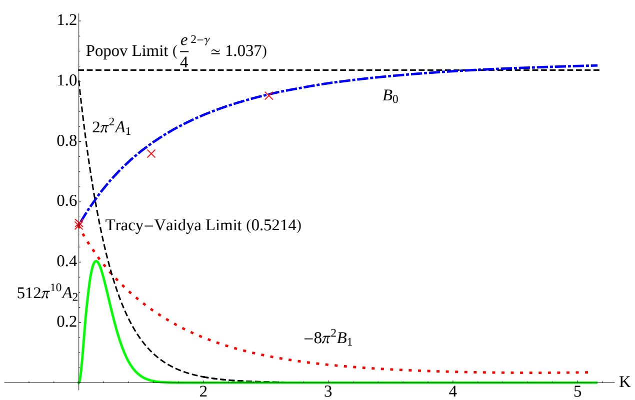
One-body density matrix

from Luttinger liquid approach

- Large-distance behaviour from regularized LL model: general structure at arbitrary interactions *[N Didier, AM, F Hekking, (2009)]*, additional terms wrt *[D Haldane, 1981]*

$$\rho_1(x) \sim \frac{1}{|x|^{1/2K}} \left[1 + \sum_{n=1}^{\infty} \frac{a'_n}{x^{2n}} + \sum_{m=1}^{\infty} b_m \frac{\cos(2mx)}{x^{2m^2K}} \left(\sum_{n=0}^{\infty} \frac{b'_n}{x^{2n}} \right) + \sum_{m=1}^{\infty} c_m \frac{\sin(2mx)}{x^{2m^2K+1}} \left(\sum_{n=0}^{\infty} \frac{c'_n}{x^{2n}} \right) \right],$$

- the coefficients a'_n, b_m, b'_n, c_m and c'_n are nonuniversal; calculated by Bethe Ansatz *[A Shashi et al, (2011)]*



One-body density matrix

of a Tonks-Girardeau gas, homogeneous case

- in the TG limit: evaluation of a (N-1) dimensional integral
  $\rho_1(x,y) = N\int dx_2..dx_N \Psi_{TG}(x,x_2..,x_N)\Psi^*_{TG}(y,x_2,..,x_N)$
- large-distance behaviour at large N: a mathematical challenge *[Lenard, Vadya and Tracy, Gangardt,..]*
  $$\rho_1^{\mathrm{TG}}(z) = \frac{\rho_\infty}{|z|^{1/2}}\left[1 - \frac{1}{32}\frac{1}{z^2} - \frac{1}{8}\frac{\cos(2z)}{z^2} - \frac{3}{16}\frac{\sin(2z)}{z^3} + ..\right],$$
  with $z = k_F(x-y)$
- at short distance: cusp behaviour originating from the effect of the interactions *[Forrester et al (2003)]*
  $$\rho_1(z)/\rho(0) = 1 - \frac{z^2}{6} + \frac{|z|^3}{9\pi}$$
- Lenard's important simplification: reduction to the calculation of the determinant of single-variable integrals!

One-body density matrix

in harmonic trap, not translationally invariant

- *[Forrester et al, 2003]* generalization of the Lenard's trick: $\rho_1(x,y)$ again reduced to the determinant of single-variable integrals

$$\rho_1(x,y) \propto e^{-(x^2+y^2)/2} \det[b_{jk}(x,y)]$$

with an analytic expression for $b_{j,k} = \int dt e^{-t^2} |x-t||y-t| t^{j+k-2}$

$\Rightarrow$ cusp $|x-y|^3$ at short distances

- Absence of Bose-Einstein condensation: from natural orbitals $\phi_j(x)$

$$\int dy \rho_1(x,y)\phi_j(y) = \lambda_j \phi_j(x)$$

eigenvalue of the lowest natural orbital $\lambda_1 \propto \sqrt{N}$

Momentum distribution

results at arbitrary interactions

- uniform case, at small k, $n(k) \propto k^{1/2K-1}$
- large-momentum tails *[AM, P Vignolo, MP Tosi (2002), M Olshanii, V Dunjko (2003)]*

$$n(k) = \mathcal{C} k^{-4} \qquad \text{for large } k$$

from a theorem on Fourier transforms,

$$\int dz e^{-ik(z-z_0)}|z-z_0|^{\alpha-1}F(z) \to \frac{2}{|k|^\alpha}F(z_0)\cos(\pi\alpha/2)\Gamma(\alpha)$$

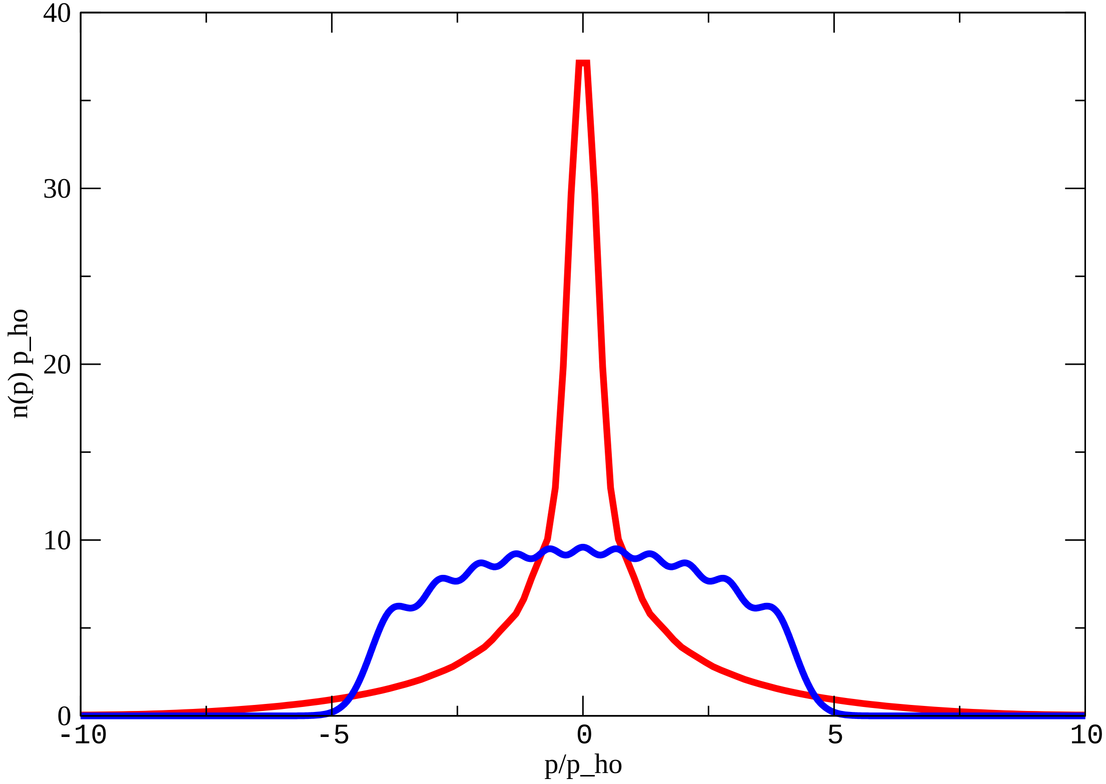
- tails fixed by the Tan's contact *[S Tan, (2008), M Barth, W Zwerger, (2011)]*

$$\mathcal{C} = \frac{4}{a_{1D}^2}\langle\Psi^\dagger(x)\Psi^\dagger(x)\Psi(x)\Psi(x)\rangle$$

measuring two-body correlations

Momentum distribution

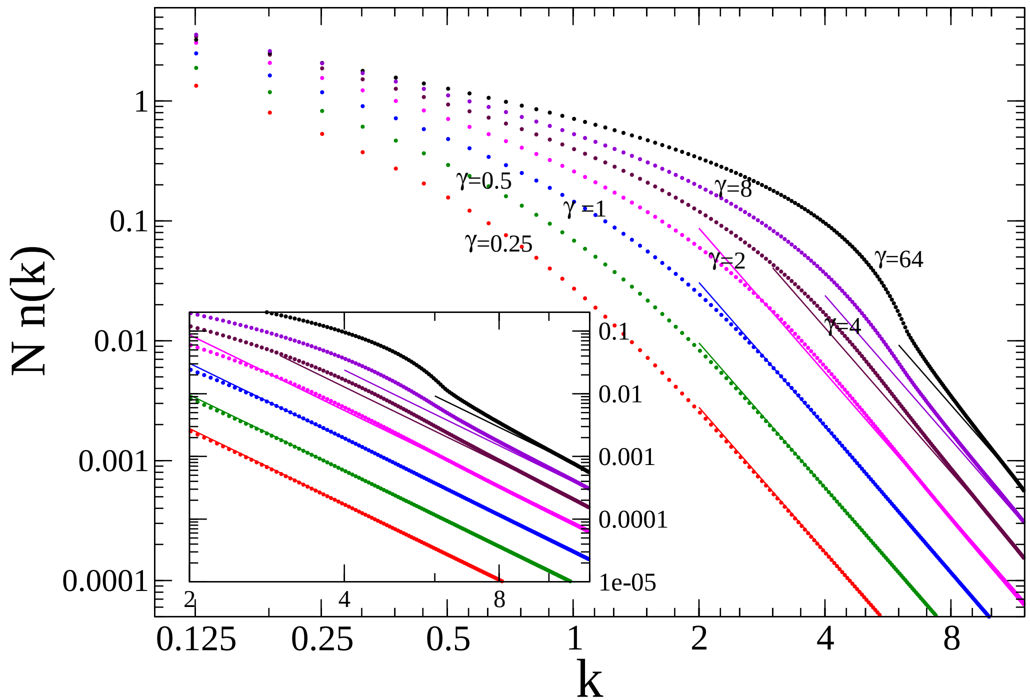
of a TG gas in harmonic trap at zero temperature



bosonic vs fermionic case

Momentum distribution tails

of a homogeneous Bose gas at zero temperature: Bethe Ansatz result



[JS Caux, P Calabrese, NA Slavnov (2007)]

the weight of the tails increases at increasing interaction strength γ : focus on the Tonks-Girardeau limit

Finite temperature effects

description of a thermal Tonks-Girardeau gas

- The Bose-Fermi mapping holds at finite temperature *[M Girardeau and K Das, (2002)]*: for any N-particle excited state with quantum numbers $\alpha = \{\nu_1, ...\nu_N\}$

$$|\Psi^B_{N,\alpha}\rangle = \hat{A}|\Psi^F_{N,\alpha}\rangle$$

with $\hat{A}$ mapping operator

- Statistical average of an observable $\hat{O}$:

$$\langle\hat{O}\rangle = \sum_{N,\alpha} P_{N,\alpha}\langle\Psi^F_{N,\alpha}|\hat{A}^{-1}\hat{O}\hat{A}|\Psi^F_{N,\alpha}\rangle$$

in the grand-canonical ensemble $P_{N,\alpha} = e^{-\beta(E_N-\mu N)}/Z$, $E_N = \sum_{j=1}^N \varepsilon_{\nu_j}$

One-body density matrix

for a thermal Tonks-Girardeau gas

- The fermionic observables are easy, eg density profile

$$n(x) = \sum_{j=1}^{N} f_{\nu_j} |u_{\nu_j}(x)|^2$$

where $f_{\nu_j} = \frac{1}{e^{\beta(\varepsilon_{\nu_j} - \mu)} - 1}$

- Thermal one-body density matrix:

$$\rho_1(x, y) =$$
$$\sum_{N,\alpha} P_{N,\alpha} \int dx_2, ...dx_N \Psi_{N\alpha}(x, x_2.., x_N) \Psi^*_{N\alpha}(y, x_2, .., x_N)$$

...a formidable complexity?!

... how to sum on all the quantum states α and the particle numbers N?

Lenard's trick

(another one! *[A. Lenard, J Math Phys 7, 1268 (1966)]*)

- The *bosonic* one body density matrix as a *series of fermionic* $j-$*body* density matrices

$$\rho_{1B}(x,y) = \sum_{j=0}^{\infty} \frac{(-2)^j}{j!} (\mathrm{sign}(x-y))^j \times \int_x^y dx_2 ... dx_{j+1} \rho_{j+1,F}(x, x_2, ... x_{j+1}; y, x_2, ... x_{j+1})$$

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- Factorization of the fermionic density matrices

$$\rho_{1F}(x_1, x_2, ... x_n; x'_1, x'_2, ... x'_n) = \det[\rho_{1F}(x_i, x'_\ell)]_{i,\ell=1,n}$$

with fermionic one-body density matrix $\rho_{1F}(x,y) = \sum_{j=1}^{N} f_{\nu_j} u_{\nu_j}(x) u^*_{\nu_j}(y)$

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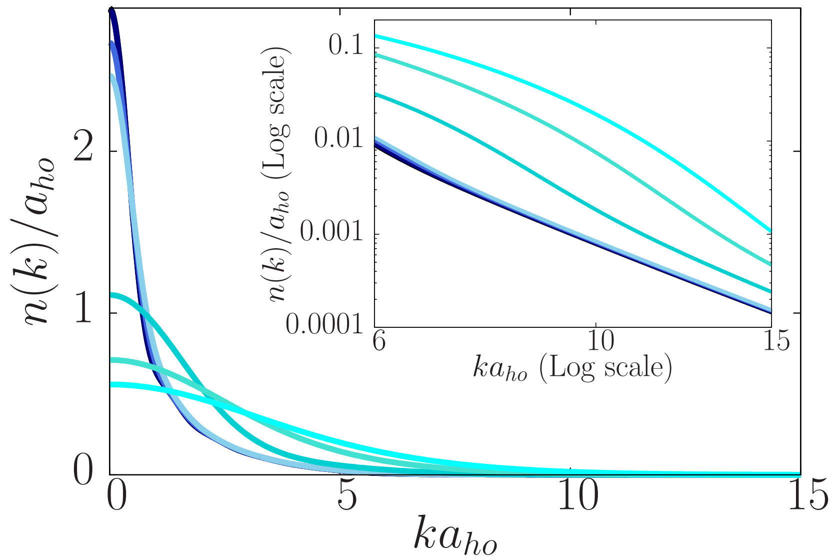
with fermionic one-body density matrix $\rho_{1F}(x,y) = \sum_{j=1}^{N} f_{\nu_j} u_{\nu_j}(x) u^*_{\nu_j}(y)$

- The j-variables integration can be reduced as combination of single-particle integrals

$$\rho^j_{1B}(x,y) = \sum_{\nu_1 .. \nu_{j+1}} f_{\nu_1} ... f_{\nu_{j+1}} \sum_{k=1}^{j+1} u_{\nu_1}(x) A_{\nu_1 \nu_k}(x,y) u^*_{\nu_k}(y)$$

Thermal momentum distribution

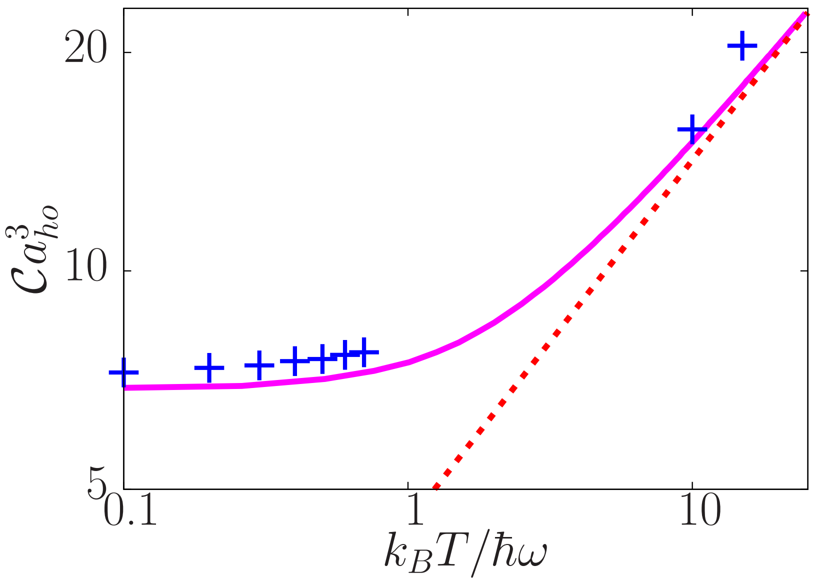


Zoom on the tails: they increase with temperature !

- $n(k) \sim \mathcal{C}/k^4$ from the $j = 1$ term (only) of the one-body density matrix

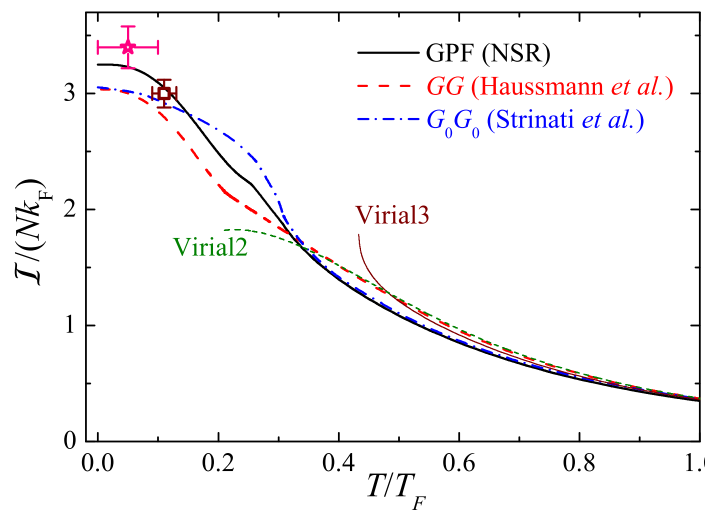
$$\rho_{1b}^{j=1} \sim |x - y|^3 F((x + y)/2) \qquad \mathcal{C} = \frac{3}{\pi} \int dR\, F(R)$$

Finite temperature contact



the weight of the momentum distribution tails increases with temperature

different from a unitary Fermi gas: *[Hui Hu et al, 2011]*



High-temperature contact

- We use Tan's sweep theorem (from Hellman-Feynman relation)

$$\frac{dE}{da_{1D}} = \langle \frac{\partial \mathcal{H}}{\partial a_{1D}} \rangle = \frac{\hbar^2}{2m}\mathcal{C}$$

with $a_{1D} = -2\hbar^2/mg$

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with $a_{1D} = -2\hbar^2/mg$

- in its thermodynamic form *[Hui Hu et al, (2011)]*, with Ω the grandthermodynamic potential

$$\left.\frac{d\Omega}{da_{1D}}\right|_{\mu,T} = \frac{\hbar^2}{2m}\mathcal{C}$$

(by changing the interactions changes only the internal energy)

Virial approach

to understand high temperature behaviour of the contact

- Virial expansion :

$$\Omega = -k_B T Q_1 (z + b_2 z^2 + b_3 z^3 + ...)$$

with $z = e^{\beta\mu}$,
$b_2 = \frac{Q_2}{Q_1} - \frac{Q_1}{2}$, $Q_2 = Q_1 \sum_\nu e^{-\beta\epsilon_\nu^{\mathrm{rel}}}$
and $Q_n = \mathrm{Tr} e^{-\beta\mathcal{H}_n}$, n-body cluster

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- High-temperature virial expansion for Tan's contact

$$\mathcal{C} = \frac{2m}{\hbar^2 \lambda_{dB}} k_B T Q_1 (z^2 c_2 + z^3 c_3 + ...)$$

with $c_n = -\frac{\partial b_n}{\partial (a_{1D}/\lambda_{dB})}$

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- in the TG limit, consequence of scale invariance: universality! c_n=constant (ie independent on temperature) as (a_{1D}/λ_{dB}) vanishes

Universal contact coefficient

- we need the eigenvalues $\epsilon_\nu^{\mathrm{rel}}$ solution of the interacting two-body problem and $\partial\epsilon_\nu^{\mathrm{rel}}/\partial a_{1D}$

  in harmonic trap $\epsilon_\nu^{\mathrm{rel}} = \hbar\omega(\nu + 1/2)$

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- analytic expression for the universal coefficient c_2 in the TG limit, $\nu = 2n + 1$:

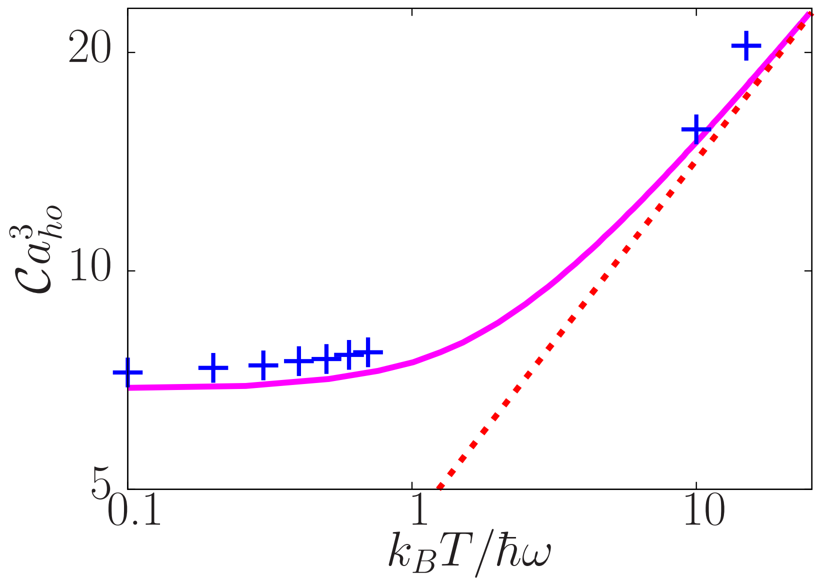
  $c_2 = \frac{2\beta\hbar\omega\lambda_{dB}}{\pi} \sum_n \frac{\Gamma(n+3/2)}{n!} e^{-\beta\hbar\omega(2n+3/2)}$

  evaluating the sum, taking the large temperature limit

$$c_2 = \frac{1}{\sqrt{2}}$$

universal contact coefficient for the Tonks-Girardeau gas

Finite temperature contact



$\mathcal{C} = \frac{2m}{\hbar^2\lambda_{dB}} k_B T Q_1 (z^2 c_2 + z^3 c_3 + ...)$

high-temperature leading behaviour

$$\mathcal{C} = \frac{N^2}{\pi^{3/2}} \sqrt{\frac{k_B T}{\hbar\omega}}$$

using $Q_1 = k_B T/\hbar\omega$, $z = N\hbar\Omega/k_B T$, $\lambda_{dB} = \sqrt{\frac{2\pi\hbar^2}{m k_B T}}$

Conclusions

Unievrsal properties of a Tonks-Girardeau gas

- *Coherences at finite temperature:* tails of the momentum distribution and high-temperature contact coefficients